Finite Difference Methods for Hyperbolic PDEs

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The "right way" to solve hyperbolic conservation laws such as the advection equation or the wave eq. is to use finite volume methods.

However, for periodic domains, and up to only 2^{nd} order in space/time, there is no practical difference between FD and FV, so we proceed

We will focus on the advection eq:

$$u_t + (a(x)\,u)_x = 0,$$

written in conservation form as:

$$u_t = -\frac{\partial}{\partial x} f(u, x, t)$$

flux

where the advective flux

$$f = a u$$

gives the amount of conserved quantity transported through the point/plane at x per unit time

②

The advective velocity $a(x)$ has units of length / time.

<u>**Conservation**</u>:

$$\frac{d}{dt}\left[\int_{x-h/2}^{x+h/2} d\tilde{x}\;\; u(\tilde{x},t)\right] =$$

$$\int_{x-h/2}^{x+h/2} d\tilde{x}\;\; \partial_t u(\tilde{x},t) = -\int_{x-h/2}^{x+h/2} d\tilde{x}\;\; \frac{\partial f}{\partial x}(\tilde{x},t)$$

$$= -f\left(u(x+\tfrac{h}{2}), x+\tfrac{h}{2}, t\right)$$
$$+ f\left(u(x-h/2), x-h/2, t\right)$$

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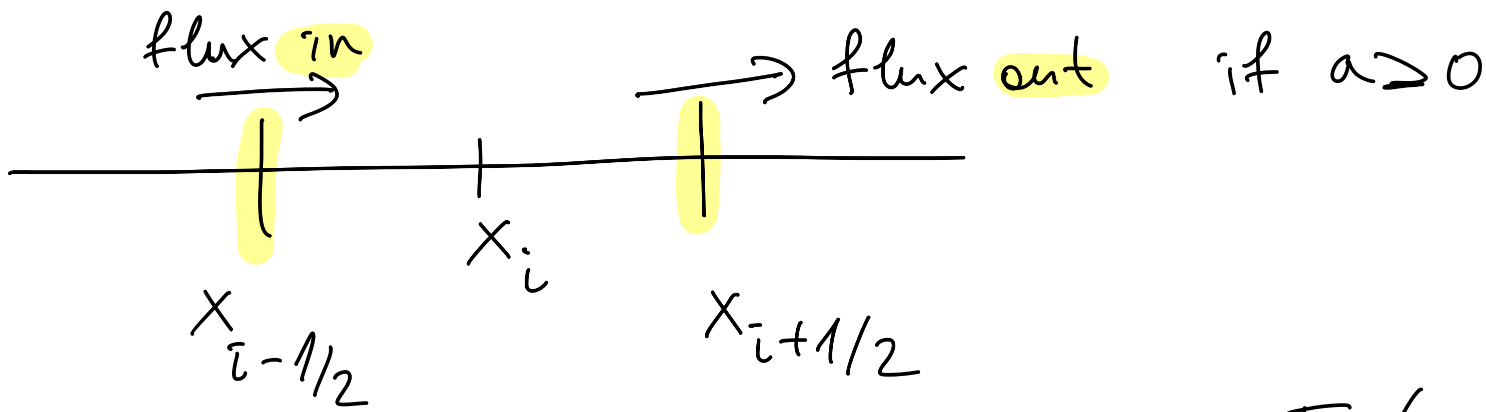

This is the basis of the FV method but we will not cover it. Nevertheless, understanding the concept of <u>advective flux</u> is crucial to understanding hyperbolic laws & solving them.
The other key concept (see PDE class) are space-time characteristics.

These notes only cover 1D periodic (ring) domains. But, important for future — see class Computational Methods for PDEs, Fall 2023, A. Donev (FV) & G. Stadler (FE) — are

- wave equation

$$u_{tt} = c^2(x)\, u_{xx}$$

- 2D / 3D advection:

$$u_t = -\vec{\nabla} \cdot \left(\vec{f}\,(u, \vec{x}, t) \right) = -\vec{\nabla} \cdot \left(\vec{a}\, u \right)$$

where $a(\vec{x}, t)$ is a velocity field

Aside: Wave equation as 1^{st} order system:

density of air

velocity

speed of sound

$$\begin{cases} \partial_t(\rho \vec{v}) = -\nabla(\underbrace{\rho c^2}_{\text{pressure}}) & \leftarrow \text{momentum conservation} \\ \underbrace{\partial_t \rho = -\nabla\cdot(\rho\vec{v})}_{\text{mass conservation}} & \end{cases}$$

$$\partial_{tt}\rho = -\nabla\cdot\partial_t(\rho\vec{v}) = -\nabla\cdot\nabla(\rho c^2) \Rightarrow$$

$$\partial_{tt}\rho = -\nabla^2\left[\rho\,(c(\rho,x,t))^2\right]$$

is a more general wave equation for acoustic waves/sound in air

Second aside: Light waves

Maxwell equations in empty vacuum:

$$\begin{cases} \nabla\cdot E = 0 & \text{(electric field)} \\ \nabla\cdot B = 0 & \text{(magnetic field)} \\ \nabla\times E = -\dfrac{\partial B}{\partial t} \\ \nabla\times B = \dfrac{1}{c^2}\dfrac{\partial E}{\partial t} \end{cases}$$

speed of light

$$\Rightarrow \nabla\times\frac{\partial B}{\partial t} = \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} = -\nabla\times(\nabla\times E)$$

$$= -\Big(\nabla\underbrace{(\nabla\cdot E)}_{\text{zero}} - \nabla^2 E\Big) = \nabla^2 E \Rightarrow$$

$$\boxed{\partial_{tt} E = c^2\nabla^2 E}$$

← wave equation

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For now focus on seemingly (!) trivial equation

$$\begin{cases} u_t + a u_x = 0 \\ u(x,0) = \eta(x) \end{cases} \qquad x \in [0, L) \text{ periodic domain}$$

Aside: In higher dimensions, if $\nabla \cdot \vec{a} = 0$ (incompressible velocity field), then $u_t + \vec{a} \cdot \vec{\nabla} u = 0$

Solution $u(x,t) = \eta(x - at)$ simply translates with speed a to the right if $a > 0$, or to the left if $a < 0$.

Surprisingly, very few numerical methods can obtain the exact solution. And those that do, do not work for non-constant $\vec{a}$!

So we should not try to rely on the fact a is constant in our numerical methods at all.

Why is advection harder than diffusion for numerical methods

[class discussion of properties of heat vs. advection eq.]

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Go to Fourier space:

$$\hat{u}_t = -iak\hat{u}$$

$\Rightarrow$ eigenvalues $\lambda_k = -iak$ of PDE are purely imaginary: No dissipation (smoothing), only transport. Shocks can form for nonlinear PDEs.

$$\|u\|_2 = \|\hat{u}\|_2 = \text{const}$$

But numerical methods will have a hard time with that

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physical constraint, especially for non-smooth solutions.

Numerical methods introduce artificial

- dissipation: $\mathrm{Re}(\lambda_k) < 0$ for most k
- dispersion: $|\lambda_k| \not\sim |k|$, i.e., different frequencies/wavelengths travel at different speeds - solution is distorted

This is covered in detail in Comp. methods for PDE class. Here we will do a demo in Matlab in class...

$$u_t = -a u_x$$

Let's try Method-of-Lines (MOL)
Finite-Difference (FD):

$$\frac{d}{dt} u_j = -\underbrace{\frac{a}{2h}\left(u_{j+1} - u_{j-1}\right)}_{\text{centered difference}}$$

$$\frac{d\vec{u}}{dt} = \overleftrightarrow{A}\,\vec{u} \quad \text{(linear ODEs)}$$

$$\vec{u}(t) = \exp\left(\overleftrightarrow{A}\,t\right)\vec{u}(0)$$

$$A = -\frac{a}{2h}\begin{bmatrix} 0 & 1 & & & -1 \\ -1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ 1 & & & -1 & 0 \end{bmatrix}$$

In Fourier space (DFT):

$$\frac{d}{dt}\hat{u}_k = -a\left(\frac{e^{+ikh} - e^{-ikh}}{2h}\right)\hat{u}_k$$

$$\frac{d}{dt}\underline{\hat{u}} = \hat{A}\,\underline{\hat{u}} \quad \text{where}$$

$$\hat{A} = \mathrm{Diag}\left\{ -\frac{ia}{h} \sin\left(\frac{2\pi}{L} k h\right) \right\}$$

k = wave index

$$\lambda_k = -\frac{ia}{h} \sin(kh) = -iak + O(h^2)$$

purely imaginary

second order

This means we cannot use explicit RK1 (Euler) or RK2,

need at least RK3 for centered advection (explicit) if we want <u>strong</u> stability.

If we only want Lax-Richtmyer stability, for forward Euler

$$\frac{\vec{u}^{\,n+1} - \vec{u}^{\,n}}{\tau} = \overleftrightarrow{A}\,\vec{u}^{\,n}$$

$$\| \overleftrightarrow{I} + \tau \overleftrightarrow{A} \|_2 \leq 1 + \alpha \tau$$

for all $h < h_0$

$$\Rightarrow \quad |1 + \tau \lambda_{max}|^2 \leq 1 + \tau^2 |\lambda_{max}|^2$$

$$= 1 + \alpha \tau$$

$$|\lambda_{max}| = \left|\frac{ia}{h}\right| = \frac{|a|}{h}$$

$$\Rightarrow \quad 1 + \tau^2 \frac{|a|^2}{h^2} = 1 + \alpha\tau$$

$$\tau = \alpha \frac{h^2}{|a|} \Rightarrow \tau = O(h^2) \text{ for Euler}$$

This does <u>not</u> make physical sense at <u>all</u> for advection, even by physical units $\left(\text{time} = \frac{\text{length}}{\text{speed}}\right)$

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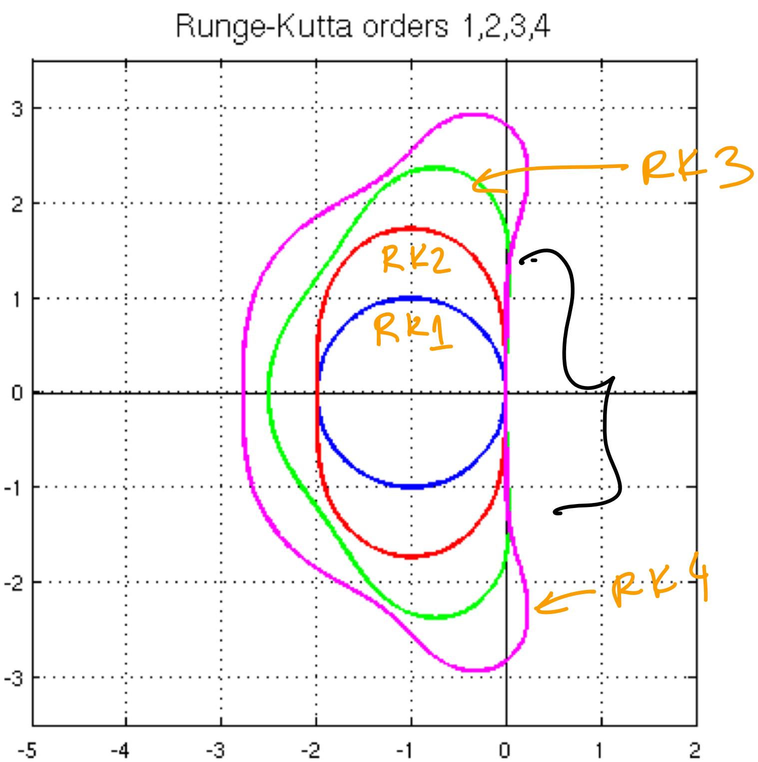
Instead, if we use RK3+



absolute stability region includes

$[-ic, +ic]$

then we get <u>strong</u> stability if

$$\boxed{\tau \le c\,\frac{h}{|a|}} \equiv$$ Advective CFL / courant condition

$c = O(1)$

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$$\nu = \frac{\tau |a|}{h} \leq C \leftarrow$$ Courant advective number

Now this makes sense physically in terms of domain of dependence of PDE (see 10.7 in LeVeque), and units make sense too

$$\text{time} = \frac{\text{length}}{\text{space}}$$

Information must not propagate by further than (about) one grid cell per time step

But, RK3 is expensive!

Temporal error $= O(\tau^3) = O(h^3)$

but spatial error $= O(h^2)$,

and recall we want

spatial error $\simeq$ temporal error $\simeq O(h^2)$

How can we accomplish that?

RK2 is not absolutely stable for imaginary eigs. $\Rightarrow$

We MUST switch to a non-MOL scheme to do 1^{st} or 2^{nd} order!

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Sidenote: We could use RK4 with a 4^{th} order centered discretization of the first derivative:

$$u_j'(t) = -a \cdot \left[\frac{u_{j-2}(t) - 8u_{j-1}(t) + 8u_{j+1}(t) - u_{j+2}(t)}{12h} \right]$$

no $u_j(t)$!

How good is this? DEMO in class

We could also use RK3 with a 3^{rd} order left-biased difference

$$u_j' = -a \cdot \left[\frac{u_{j-2} - 6u_{j-1} + 3u_j + 2u_{j+1}}{6h} \right] \ldots (*)$$

Is this good? We will see ☺

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For the 4^{th} order centered, in Fourier space (von-Neumann analysis)

$$\hat{u}_k' = -ik a\left(1 - \frac{1}{30}(kh)^4 + O(kh)^5\right)$$

purely imaginary

For the 3^{rd} order left-biased,

$$\hat{u}_k' = -iak\left(\underbrace{1 - \frac{1}{30}(kh)^4 + O(kh)^5}_{4^{th}\text{ order}}\right) \underbrace{- a\left(\frac{k^4 h^3}{12} + O(h^5)\right)}_{3^{rd}\text{ order}}$$

if $a>0$ then real part ≤ 0 for $|k| \leq \frac{\pi}{h}$

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Upwind Method

Let's consider first-order methods to begin. Consider the upwind scheme:

$$u_j^{n+1} = u_j^n - a\frac{\tau}{h}\left(u_j^n - u_{j-1}^n\right)$$

This uses one-sided difference for first derivative in space, and forward Euler in time.

Is it stable?

Do von Neumann stability analysis:

$$\hat{u}_k^{n+1} = g_k(\tau)\, \hat{u}_k^{n}$$

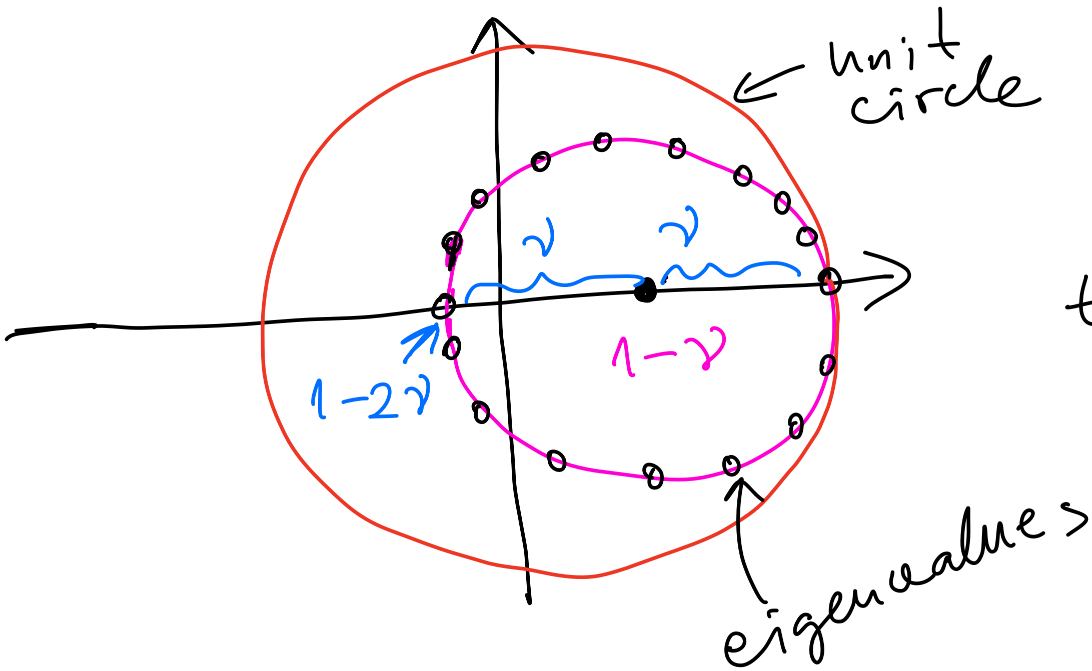
$$g_k(\tau) = 1 - \frac{a\tau}{h}\left(e^{0} - e^{-ikh}\right)$$

Denote the advective Courant/CFL number $\nu = a\tau/h$ $\Rightarrow$

$$g_k(\tau) = \underbrace{(1-\nu)}_{\text{center of circle}} + \underbrace{\nu}_{\text{radius of circle}} e^{-ikh}, \quad |k| \le \frac{\pi}{h}$$

We want $|g_k(\tau)| \leq 1 \quad \forall k$

The points $g_k \in \mathbb{C}$ lie on a circle at $1-\nu$ of radius ν:



We want the magenta circle to be inside the red unit circle.

$$\Rightarrow \begin{cases} 1-2\nu \geq -1 \\ 1-\nu < 1 \end{cases}$$

$$\boxed{0 \le \nu \le 1}$$ — Advective Courant / CFL condition

$\Rightarrow$ $a \geq 0$ is required

We conclude that a stable first-order upwind scheme is:

$$\frac{u_j^{n+1} - u_j^n}{\tau} = -\frac{a}{h} \begin{cases} u_j^n - u_{j-1}^n & \text{if } a \geq 0 \\ u_{j+1}^n - u_j^n & \text{if } a \leq 0 \end{cases}$$

Always use points "upwind" from you and not "downwind"

This is a general rule for all hyperbolic equations:

Use information along the characteristic line from the past to update solution now (causality)

Note: If we followed the characteristic backward in time to $t = -\tau$ and interpolated the value of u at that point at time $t = -\tau$, we would get the value of u at the current point in space & time (semi-Lagrangian advection)

$$0 \leq \nu = O(1) \leq 1 \implies$$

$$\tau \sim h \longrightarrow \text{first-order convergence}$$

$$\begin{cases} \text{spatial error} = O(h) \\ \text{temporal error} = O(h) \end{cases}$$

<u>Observation</u> (demo in class):

First-order upwind is way too dissipative — it smears the solution out very quickly via artificial dissipation (see Comp PDE class)

Can we do 2^{nd} order?

Key idea: Use 2^{nd} order Taylor series in time:

$$u(t+\tau) = u(t) + \underbrace{u_t}\,\tau + \frac{1}{2} u_{tt}\,\tau^2 + \dots$$

$$\begin{cases} u_t = -a u_x \\ u_{tt} = -a(u_t)_x = a^2 u_{xx} \end{cases}$$

$$u(t+\tau) \simeq u(t) - a u_x \tau + \underbrace{\frac{a^2\tau^2}{2}} u_{xx}$$

positive = artificial diffusion

If we were solving

$$u_t = -a u_x + d u_{xx}$$

with Forward Euler:

$$u(t+\tau) = u(t) - a u_x \tau + d\tau u_{xx}$$

$\Rightarrow$ "effective" diffusion coefficient $\boxed{d = \dfrac{a^2 \tau}{2}}$

Since diffusion is a nice smoothing process, this sounds like a good thing for numerical methods

Now let's discretize in space:

$$u_j^{n+1} = u_j^n - \frac{a\tau}{2h}\left(u_{j+1}^n - u_{j-1}^n\right) + \frac{a^2\tau^2}{2h^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)$$

centered difference (2nd order in space)

this is clearly 2nd order in both space and time

2nd order Lax-Wendroff scheme

$\underbrace{\text{Lax-Wendroff}}_{\text{Courant Institute}}$

Is it strongly stable?

Go back to von Neumann stability analysis assuming a periodic domain:

$$\hat{u}_k^{n+1} = g_k \hat{u}_k^n$$

$$g_k = 1 - \frac{\nu}{2}\left(e^{ikh} - e^{-ikh}\right) + \frac{\nu^2}{2}\left(e^{ikh} - 2 + e^{-ikh}\right)$$

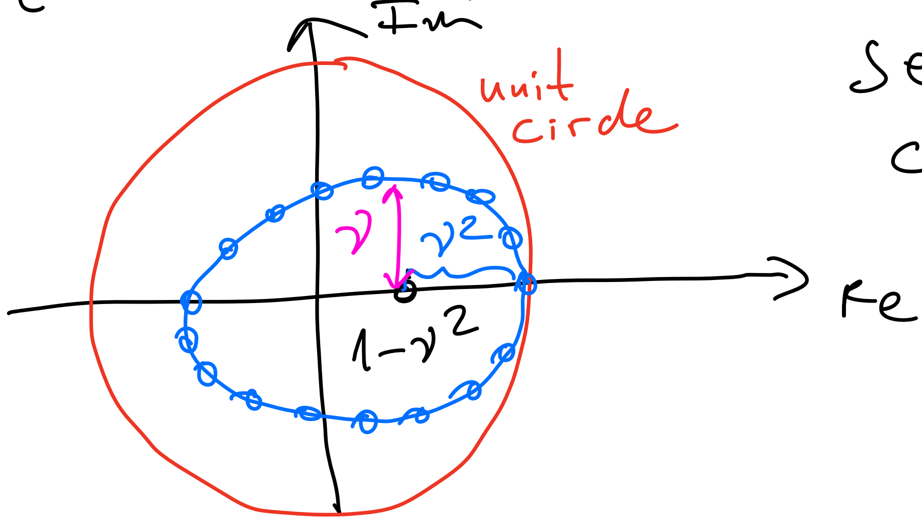
(do algebra, see 10.3 in LeVeque)

$$g_k = \left(1 - \nu^2(1-\cos\theta)\right) - i\nu\sin\theta$$

$$-\pi \leq \theta = kh \leq \pi$$

$$g_k = (1-\nu^2) + \nu(\nu\cos\theta - i\sin\theta)$$

The points g_k lie on an <u>ellipse</u> in the complex plane:



semiaxes: $|\nu|$ & ν^2
centered at
$z = 1-\nu^2$

It is easy to see that for $|\nu| = 1$ the blue ellipse overlaps the unit circle, and for any $|\nu| < 1$ the ellipse is entirely contained inside the circle:

LW is stable if $|\nu| \leq 1$

which is the same as upwind scheme but now a can be of either sign <u>without</u> changing the spatial FD stencil!

Imagine if instead of

$\frac{a^2 \bar{z}^2}{2h^2}$ as in LW, we used $\alpha \frac{a^2 \bar{z}^2}{2h^2}$.

then we would have

$$g_k = (1 - \alpha \nu^2) + \nu(\alpha \nu \cos\theta - i \sin\theta)$$

Semiaxis $= \alpha \nu^2$ and $|\nu|$

$\Rightarrow$ radius of curvature of ellipse at $z = 1$ is

$\frac{\nu^2}{\alpha \nu^2} = \frac{1}{\alpha}$. If $\alpha < 1$, then ellipse sticks out of unit circle

Conclusion:

Lax-Wendroff adds the minimal amount of diffusion to stabilize Forward Euler. Plus it is 2^{nd} order!

Observe that we can rewrite the upwind scheme as $(a>0)$:

$$u_j^{n+1} = u_j^n - \frac{a\tau}{2h}\left(u_{j+1}^n - u_{j-1}^n\right) + \frac{a\tau}{2h}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)$$

$\alpha = \nu^{-1} \geq 1$, $d = O(\tau) \Rightarrow$ much more artificial dissipation

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There are many other LW-like schemes, e.g., the beam-warming scheme:

$$u_j^{n+1} = u_j^n - \frac{a\tau}{2h}\left(3u_j^n - 4u_{j-1}^n + u_{j-2}^n\right) + \frac{a^2\tau^2}{2h^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right)$$

which is also second order but in practice better than LW (see in-class demo) but it is hard to justify why or how with analysis...

Both LW & Beam Warming are NOT MOL schemes !

They are instead space-time schemes. For them, we talk about convergence of spatio-temporal error as we simultaneously refine $h \sim \tau \to 0$ (spatio-temporal refinement). Error is not spatial + temporal any more

This is a big difference between parabolic & hyperbolic PDEs

Why is LW not MOL ?

Imagine we first discretized in space :

$$\frac{du_j}{dt} = -a\left(\frac{u_{j+1} - u_{j-1}}{2h}\right)$$ 2^{nd} order in space

$$\frac{d\vec{U}}{dt} = -a\overleftrightarrow{D}_0\vec{U}$$

RK2 : $\vec{U}^{n+1} = \vec{U}^n - a\overleftrightarrow{D}_0\vec{U}^n\tau + \frac{1}{2}a\tau^2 \cdot \overleftrightarrow{D}_0^2\vec{U}^n$

(DIY) Is this stable ?

But LW uses $\overleftrightarrow{D}^2$ not $\overleftrightarrow{D}_0^2$!