

Numerical PDEs

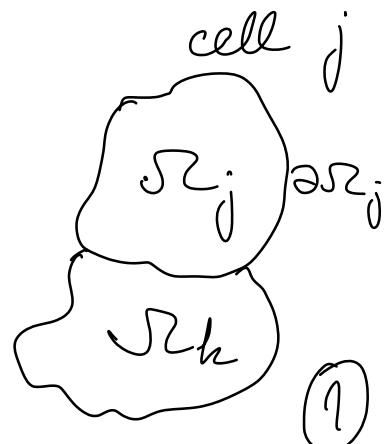
A. DONEV, Fall 2021

Finite Volume Methods

The bible on this topic is
book "FVM for hyperbolic problems"
R. LeVeque
— freely available as PDF to you

Key idea: Break up domain into
a grid of cells, and use
as variables the average
of n over each cell

$$\bar{u}_j = \frac{1}{|\Sigma_j|} \int_{\Sigma_j} u \, d\sigma$$



Conservation law

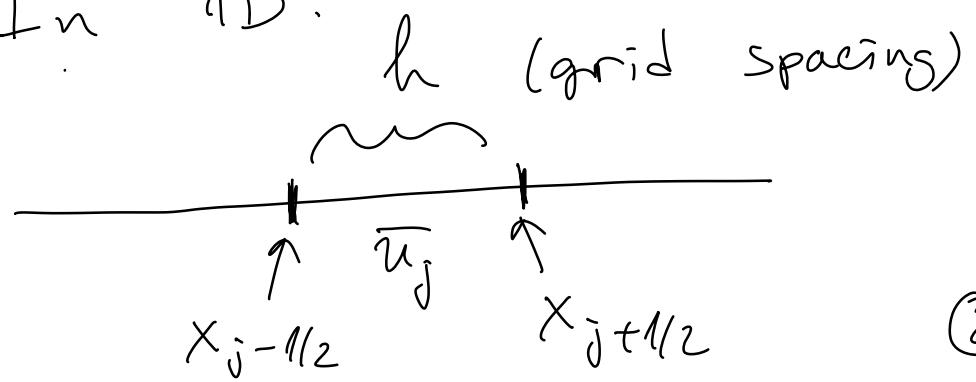
$$\int_{\Sigma_j} \frac{\partial u}{\partial t} dr = - \int (\nabla \cdot \vec{f}) dr$$

$$|\Sigma_j| \frac{d \bar{u}_j}{dt} = - \int_{\partial \Sigma_j} \vec{f} \cdot \vec{n} dA$$

$$\frac{d \bar{u}_j}{dt} = - \frac{1}{|\Sigma_j|} \int_{\partial \Sigma_j} \vec{f} \cdot \vec{n} dA$$

which is a system of ODEs

In 1D:



②

In 1D advection:

$$h \cdot \frac{d}{dt} \bar{u}_j = - \left(f_{j+1/2} - f_{j-1/2} \right) =$$

$$- \left[a(x_{j+1/2}) u(x_{j+1/2}) - a(x_{j-1/2}) u(x_{j-1/2}) \right] \\ + \left[d(x_{j+1/2}) u_x(x_{j+1/2}) - d(x_{j-1/2}) u_x(x_{j-1/2}) \right]$$

This is a **weak form of PDE**
and not (yet) a discretization,
i.e., it is exact.

To make it into a scheme we
need to figure out the
fluxes in terms of the
cell averages.

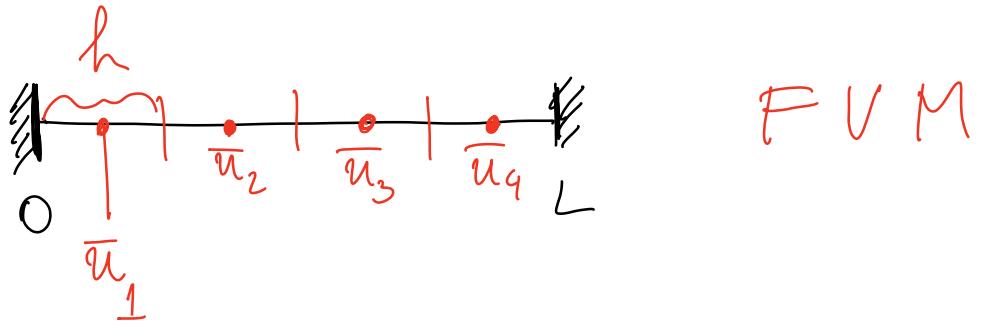
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Note that for low-order (1st or 2nd) schemes there is really not that much difference between finite difference & finite volume - it is more of a matter of mental picture.

Key to FVM is to write fluxes not divergence of fluxes.

Another difference is with boundary conditions:

Physical boundaries should overlap with cell boundaries for FVM schemes.



We know the cell averages,
not a function $u(x)$.

Constructing an approximation $u(x)$ from \bar{u} 's is called reconstruction in FVM.

As with finite difference (FD) methods, there are two main approaches:

- MOL (method of lines): write ODEs for \bar{u}_j and solve
- Space time schemes: write $(\bar{u}_j^{n+1} - \bar{u}_j^n)/\Delta t$

⑤

For space time:

$$\frac{\bar{u}_j^{n+1} - \bar{u}_j^n}{\Delta t} = \frac{1}{h} \int_{j-\frac{1}{2}}^{j+\frac{1}{2}} \int_{n\Delta t}^{(n+1)\Delta t} (f(t) - f(\tau)) dt$$

So we need a way to approximate the total or average flux over a time step.

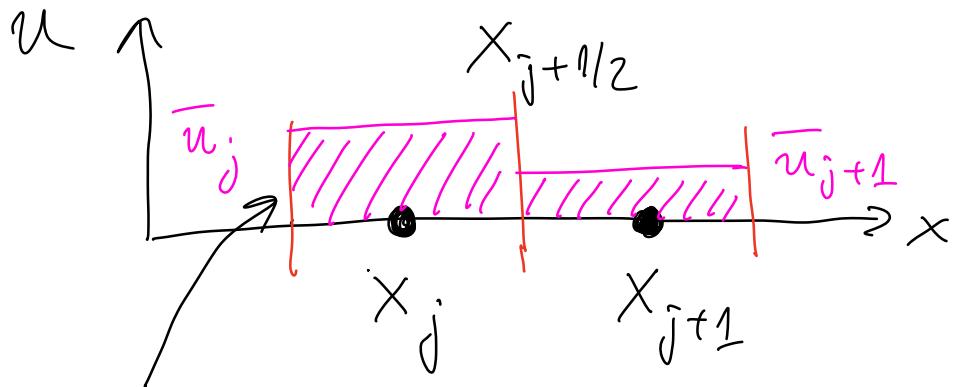
For MOL, we need to estimate:

a) Advection flux

$$f_j^{(a)} = a(x_{j+\frac{1}{2}}) u(x_{j+\frac{1}{2}})$$

↑
"easy" (evaluate $a(x)$)

But how do we get $u(x_{j+\frac{1}{2}})$ from \bar{u} 's? This is the key complexity for advection:
 extrapolate from cell centers to faces. ⑥



Piecewise constant reconstruction

$$u(x_{j-1/2} < x < x_{j+1/2}) = \bar{u}_j + O(h^2)$$

This is discontinuous at

$x_{j+1/2}$: Do we set?

$$f_{j+1/2} = \begin{cases} a_{j+1/2} \bar{u}_j & \text{or} \\ a_{j+1/2} \bar{u}_{j+1} \end{cases}$$

If $a_{j+1/2} > 0$ then we know solution moves to the right, i.e., information comes from the left: upwind! (7)

$$f_{j+1/2} = \begin{cases} a_{j+1/2} \bar{u}_j & \text{if } a_{j+1/2} > 0 \\ a_{j+1/2} \bar{u}_{j+1} & \text{otherwise} \end{cases}$$

Upwind flux

For diffusive flux,

"obviously" :

$$f_j^d = d(x_{j+1/2}) u_x(x_{j+1/2})$$

$$\approx d(x_{j+1/2}) \left(\frac{\bar{u}_{j+1} - \bar{u}_j}{h} \right)$$

to $O(h^2)$, and this is what is most often used in CFD codes.

The real challenge in CFD is handling advection, i.e., handling hyperbolic conservation laws more generally. The physical reason for this is:

Advection is non-dissipative & simple advection is "non-dispersive". Dissipation stabilizes numerical methods, but we don't want it.

For dispersion, read appendix E.3.9 in FD book of LeVeque (it is excellent!)

Basic idea: In Fourier space

$$\hat{u}(k, t) = e^{-i\omega(k)t} \hat{u}(0, t)$$

where k is the wave number

(9)

The equation relating ω to k
is called the **dispersion relation**.

It can be found by putting

$$u(x, t) = e^{-i\omega t} e^{ikx}$$

into the PDE for simple
constant-coefficient equations.

$$c_p(k) = \frac{\omega(k)}{k} \quad \text{is phase velocity}$$

$$c_g(k) = \frac{d\omega(k)}{dk} \quad \text{is group velocity}$$

If $\omega(k)$ is real then the
PDE is non-dissipative.

Special case is simple advection:

$$c_p = c_g = a = \text{const.}$$

"non-dispersive"

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Appendix E. Partial Differential Equations

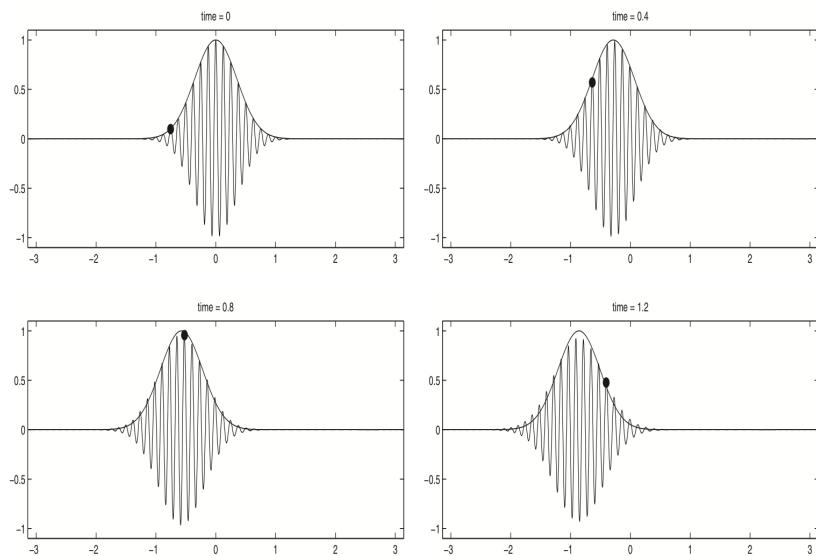


Figure E.2. The oscillatory wave packet satisfies the dispersive equation $u_t + au_x + bu_{xxx} = 0$. Also shown is a black dot attached to one wave crest, translating at the phase velocity $c_p(\xi_0)$, and a Gaussian that is translating at the group velocity $c_g(\xi_0)$. Shown for a case in which $c_g(\xi_0) < 0 < c_p(\xi_0)$.

c_g determines the speed of propagation of the envelope of the wave packet, while c_p of an individual peak / crest.

$$\text{E.g. } u_t + a_1 u_x + a_2 u_{xx} + a_3 u_{xxx} +$$

$$a_4 u_{xxxx} = 0 \Rightarrow$$

$$\omega(k) = a_1 k + i a_2 k^2 - a_3 k^3 - i a_4 k^4$$

(11)

$$\hat{u}(k, t) = e^{(a_2 k^2 - a_4 k^4)t} e^{i(a_1 k - a_3 k^3)t} \hat{u}(k, 0)$$

Dissipative
for $a_2 < 0, a_4 > 0$

For $a_2 = a_4 = 0$,

$$c_p(k) = a_1 - a_3 k^2$$

$$c_g(k) = a_1 - 3a_3 k^2$$

$$u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(k, 0) e^{ik(x - c_p(k)t)} dk$$

For a numerical method, find

numerical dispersion relation

by plugging into method wave:

$$\bar{u}_j^n = e^{-iwnst} e^{ikjh}$$

(12)

An alternative, which gives us intuition quickly but is not rigorous, is to look at modified equations: find a PDE that the method solves to higher order than it does the PDE we want to solve. We can do this to a MOL scheme separately for the spatial discretization (the rhs of the system of ODEs), separately for the temporal discretization, or, as we have to for space-time schemes, combine the spatial & temporal errors.

$$u_t + a u_x = 0 \quad , \quad a > 0$$

$$\frac{d\bar{u}_j}{dt} = \frac{a}{h} (\bar{u}_{j-1} - \bar{u}_j) \quad \begin{matrix} \text{upwind} \\ \text{spatial} \end{matrix}$$

$$\bar{u}_j = u(x_j) + O(h^2)$$

Since

$$\frac{1}{h} (u(x-h) - u(x)) = -u_x(x) + \frac{h}{2} u_{xx}(x) + O(h^2)$$

the upwind difference gives a 2nd order approximation to the modified equation:

$$\tilde{u}_t + a \tilde{u}_x = \underbrace{\frac{ah}{2} u_{xx}}_{O(h)} \quad (\text{upwind})$$

$$\tilde{u}_t + a \tilde{u}_x = \underbrace{\frac{ah}{2} u_{xx}}_{\text{artificial dissipation}}$$

This spurious dissipation makes upwinding the most robust but also least accurate scheme (14)

Another way to see this:

$$\frac{a}{h} (\bar{u}_{j-1} - \bar{u}_j) = \frac{a}{2h} (\bar{u}_{j-1} - \bar{u}_{j+1}) + \frac{ah/2}{h^2} (\bar{u}_{j+1} - 2\bar{u}_j + \bar{u}_{j-1})$$

$\underbrace{\qquad\qquad\qquad}_{\text{artificial diffusion}}$

What's better?

If we used

$$u_{j+1/2} = \frac{\bar{u}_j + \bar{u}_{j+1}}{2}$$

(centered scheme)

$$\Rightarrow \frac{\bar{u}_j}{\Delta t} = -a \left(\frac{\bar{u}_{j+1} - \bar{u}_{j-1}}{2h} \right)$$

which is now second-order accurate in space,

(15)

then we would get the modified equation

$$\tilde{u}_t + a \tilde{u}_x = -\frac{ah^2}{6} \tilde{u}_{xxx}$$

artificial dispersion

$O(h^2)$

which has phase velocity

$$c_p = a \left(1 - O((kh)^2) \right)$$

So higher frequency (wavenumber) modes lag behind and cause unphysical oscillations in the solution.

Central dilemma is CFD :

Trade-off between (higher order) accuracy & robustness : what is the minimal artificial dissipation we need ?

If needed, go through all of Ch. 10 in Finite Difference book of LeVeque.

What is a better MOL scheme?
We will "derive" this soon:

$$\bar{u}_{j+1/2} = \frac{1}{6h} \left[-\bar{u}_{j-1} + 5\bar{u}_j + 2\bar{u}_{j+1} \right]$$

if $a_{j+1/2} > 0$

3rd-order upwind biased

which gives for $a = \text{const}$:

(*)

$$\frac{\partial \bar{u}_j}{\partial t} = \frac{a}{h} \left[-\frac{1}{6} \bar{u}_{j-2} + \bar{u}_{j-1} - \frac{\bar{u}_j}{2} - \frac{\bar{u}_{j+1}}{3} \right]$$

if $a > 0$
more information from upwind

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For $a = \text{const}$, this upwind biased spatial discretization is 3rd order either as a FD or FV scheme. But, only 3rd order for non-constant advection as finite volume. (see Maple worksheet on webpage!)

How to show this:

$$u_t + (au)_x = u_t + u_{xx} + a u_x = 0$$

If Finite Difference:

$$\frac{du}{dt}_j = u_t(x_j, t) = -u(x_j) a_x(x_j) - a(x_j) u_x(x_j)$$

Compare this to Taylor series of r.h.s. of (*)

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and you will see a mismatch
of $O(h^2)$ if $a(x) \neq \text{const.}$

If Finite Volume:

$$\frac{\bar{u}_j}{\Delta t} = \frac{1}{h} \int_t^{x_j + h/2} u(x, t) dx$$

$$= -\frac{1}{h} \int_{x_j}^{x_j + h/2} (au)_x dx = -\frac{1}{h} (au) \Big|_{x_j - h/2}^{x_j + h/2}$$

and $\bar{n}_j = \frac{1}{h} \int_{x_j}^{x_j + h/2} n(x, t) dx$

So now do Taylor series with
these integrals (see symbolic
algebra Maple code) to see

$$\frac{\bar{u}_j}{\Delta t} + \frac{1}{h} ((au)(x_j + h/2) - (au)(x_j - h/2)) = O(h^3)$$

This shows that for higher than 2nd order there is a difference FD vs. FV
interpretation (scheme is the same, it's how we interpret the output (input))

For $a = \text{const}$, modified equation for 3rd order upwind biased

Spatial discretization is:

$$\tilde{u}_t + a \tilde{u}_x = - \frac{|a|}{12} h^3 \underbrace{\tilde{u}_{xxxx}}_{O(h^3)}$$

stabilizing artificial dissipation (good!)

which is higher-order & less dissipation than upwind

This was so far just MOL & focused on Spatial discretization.

To get an actual 3rd order upwind biased method, we need a temporal integrator. Which one to use? Discuss in class

The temporal integrator in MOL schemes will itself add some artificial dispersion / dissipation.

We can analyze this formally by considering a "perfect" spatial discretization. Let's do this for linear equations (we will consider implicit methods in homework).

(from book on "Advection-Diffusion-Reaction" by Hundsdorfer / Verwer)

Since we have linear systems of ODEs, consider generically:

$$u' = \frac{du}{dt} = Au, \quad A \text{ matrix}$$

$$u^{n+1} = u^n + (1-\theta) \bar{\tau} Au^n + \theta \bar{\tau} Au^{n+1}$$

$\left\{ \begin{array}{l} \theta = 0: \text{forward Euler} \\ \theta = 1/2: \text{Implicit midpoint} \\ \quad (2^{\text{nd}} \text{ order}) \\ \theta = 1: \text{Backward Euler (implicit)} \end{array} \right.$

Local truncation error:

$$\begin{aligned} S_n &= \left(\frac{u(t_{n+1}) - u(t_n)}{\bar{\tau}} \right) - \left(\frac{u^{n+1} - u^n}{\bar{\tau}} \right) \\ &= \left(\frac{1}{2} - \theta \right) \bar{\tau} u''(t_n) + \left(\frac{1}{6} - \frac{\theta}{2} \right) \bar{\tau}^2 u'''(t_n) \end{aligned} \quad (21)$$

$$S_n = \left[\left(\frac{1}{2} - \theta \right) \bar{\epsilon} A^2 + \left(\frac{1}{6} - \frac{\theta}{2} \right) \bar{\epsilon} A^3 \right] u(t_n)$$

Therefore, the modified equation is

$$\tilde{u}' = \tilde{A} \tilde{n}$$

$$\tilde{A} = A + \left(\theta - \frac{1}{2} \right) \bar{\epsilon} A^2 + \left(\frac{\theta}{2} - \frac{1}{6} \right) \bar{\epsilon} A^3$$

$$\left\{ \begin{array}{l} \text{FE } (\theta=0) : \tilde{A} \approx A - \frac{\bar{\epsilon} A^2}{2} \\ \text{BE } (\theta=1) : \tilde{A} \approx A + \frac{\bar{\epsilon} A^2}{2} \\ \text{Mid } (\theta=1/2) : \tilde{A} \approx A - \frac{\bar{\epsilon}^2}{12} A^3 \end{array} \right.$$

For advection

$$A = -a \partial_x \Rightarrow$$

$$A^2 = a^2 \partial_{xx} \quad A^3 = -a^3 \partial_{xxx}$$

So we get :

$$\tilde{u}_t + a \tilde{u}_x = \left\{ \begin{array}{l} -\frac{\bar{c}a^2}{2} \tilde{u}_{xx} \quad \text{FE (anti-diffusion)} \\ \frac{\bar{c}a^2}{2} \tilde{u}_{xx} \quad \text{BE artificial dissipation} \\ -\frac{\bar{c}^2}{12} a^3 \tilde{u}_{xxx} \quad \text{implicit midpoint} \\ \text{artificial dispersion} \end{array} \right.$$

This artificial dispersion / dissip. adds with the one from the spatial discretization.

Consider the simplest FD/FV
1st order upwind:

$$u_j^{n+1} = u_j^n - \frac{a\bar{c}}{h} (u_j^n - u_{j-1}^n)$$

(or add bars for FV)

$$\tilde{u}_t + a \tilde{u}_x = \underbrace{\frac{ah}{2} \tilde{u}_{xx}}_{\text{spatial}} - \underbrace{\frac{a^2 \tau}{2} \tilde{u}_{xx}}_{\text{temporal}}$$

artificial Johnson

Define CFL number $\gamma = \frac{a \tau}{h}$

$0 \leq \gamma \leq 1$ for stability
(from Num. Meth. II)

$$\tilde{u}_t + a \tilde{u}_x = \underbrace{\frac{ah}{2} (1-\gamma) \tilde{u}_{xx}}_{\text{artificial dissipation}}$$

Observe that for $a = \text{const}$
and $\gamma = 1$ the scheme is an
exact $u_j^{n+1} = u_{j-1}^n$ ($a > 0$)

In 10.4 in FD book of leVeque,
this is derived directly :

$$\tilde{u}(x, t+\bar{\tau}) - \tilde{u}(x, t) = -\frac{a\bar{\tau}}{h} (\tilde{u}(x, t) - \tilde{u}(x-h, t))$$

This uses FD interpretation but
also OK to 2nd order for FV
and is simpler \Rightarrow we use it

Now do Taylor series \Rightarrow

$$\tilde{u}_t + a \tilde{u}_x = \frac{ah}{2} \tilde{u}_{xx} - \frac{\bar{\tau}}{2} \tilde{u}_{tt}$$

Since $\tilde{u} \approx u$ and

$$u_{tt} = -(au_x)_t = -a(u_t)_x = a^2 u_{xx}$$

$$u_{tt} = a^2 u_{xx} \quad \text{- will be used multiple times later}$$

$$\Rightarrow \tilde{u}_t + \tilde{a}\tilde{u}_x = \frac{\alpha h}{2} \left(1 - \frac{\alpha^2}{h}\right) \tilde{u}_{xx}$$

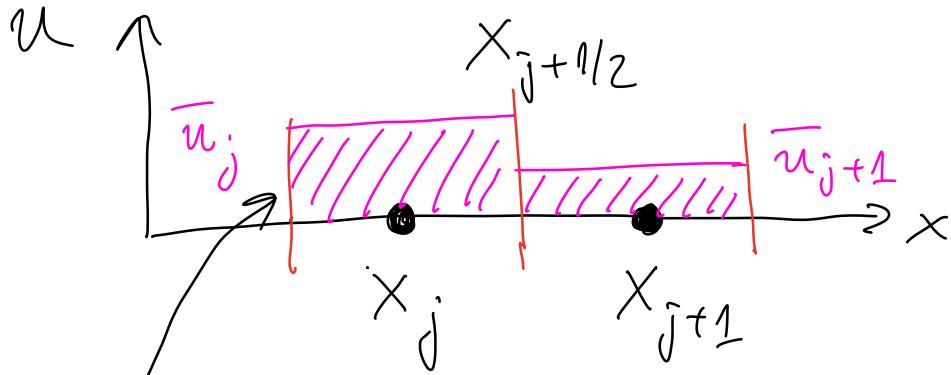
as derived already

Second-order FV in 1D

How can we construct other (better) methods for advection-diffusion that are at least 2nd order accurate?

The book of LeVeque does this in chapter 10 very nicely from an FD perspective. The same works for FV also to second order. But here I will focus on other approaches that generalize to more cases & fit FV interpretation better.

For upwind we used a



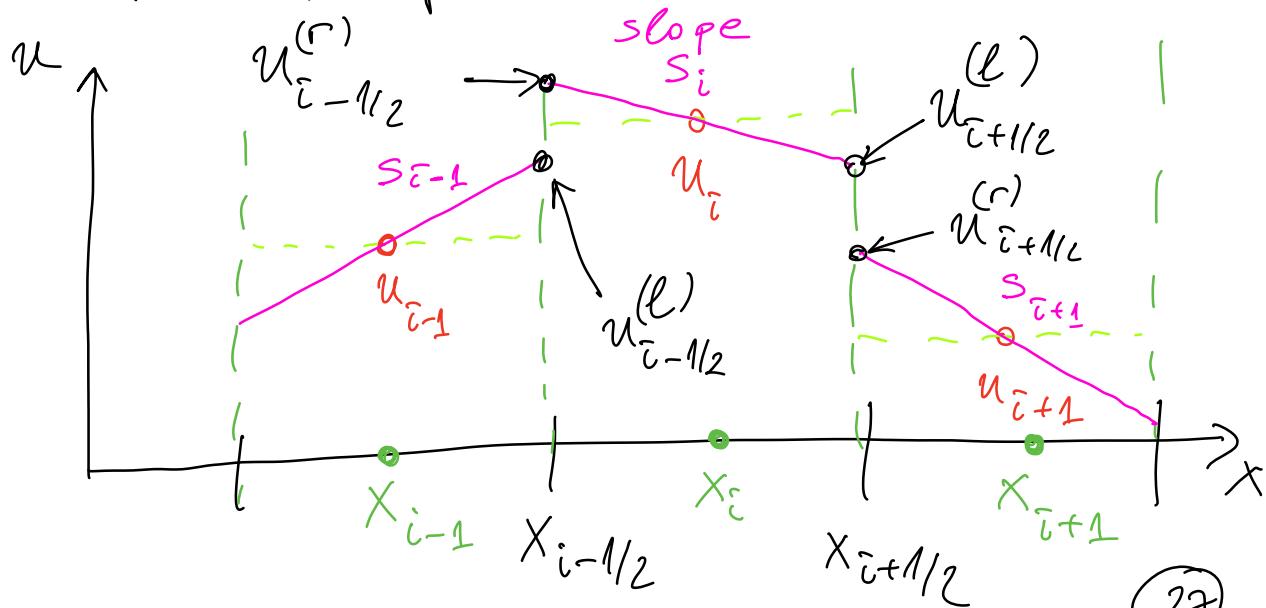
Piecewise constant reconstruction

$$u(x_{j-1/2} < x < x_{j+1/2}) = \bar{u}_j + O(h^2)$$

We can do better by using a

higher-order reconstruction,

for example linear:



(27)

In each cell, we first need to estimate slopes s_i of the linear reconstruction.

$$u(x_{i-1/2} < x < x_{i+1/2}) = \bar{u}_i \leftarrow \begin{array}{l} \text{conservation} \\ + s_i (x - x_i) \end{array} + O(h^2)$$

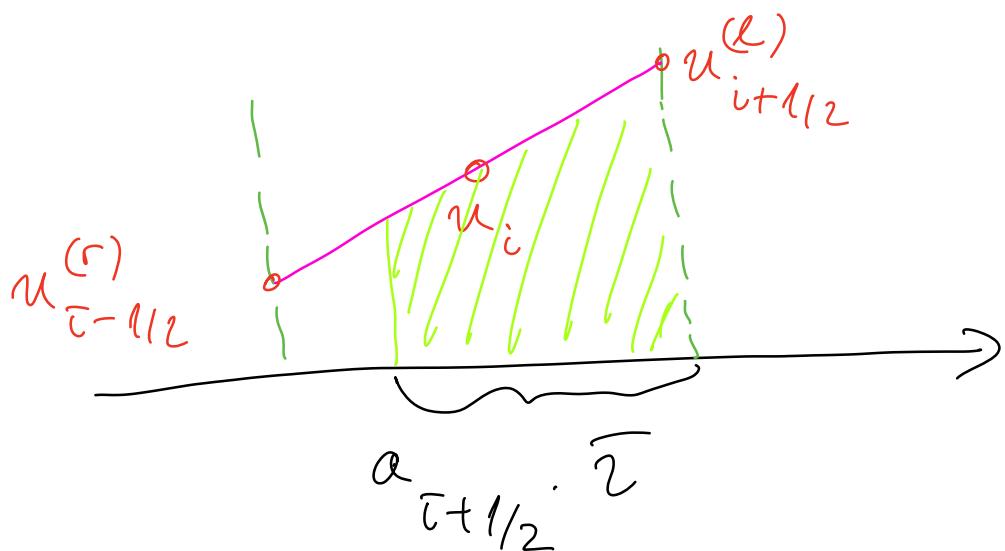
still same
order

Note $\int_{x_{i-1/2}}^{x_{i+1/2}} u(x) dx = \bar{u}_i \cdot h$ as it must in FV

This reconstruction is still only piecewise smooth, and at every face $i+1/2$ we still have two different states, one from the left $\bar{u}_{i+1/2}^{(L)}$ and one from the right $\bar{u}_{i+1/2}^{(R)}$

Now we need to decide if we want a MOL scheme (instantaneous fluxes) or a space-time scheme (time-average fluxes).

Let's start with Space-Time:



Upwind average flux:

$$f_{i+1/2}^{(l)} = \frac{\text{(shaded area)}}{h} \cdot a_{i+1/2} = f_{i+1/2}$$

if $a_{i+1/2} > 0$

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$$f_{i+1/2} = a_{i+1/2} \left(\bar{u}_i + \frac{h}{2} s_i (1-\gamma) \right)$$

where advection CFL number

$$\gamma_{i+1/2} = \frac{a_{i+1/2} \bar{c}}{h}$$

Now let's assume $a = \text{const}$
for simplicity.

To complete the scheme we
need to choose the slopes.

Downwind slope: $s_i = \frac{\bar{u}_{i+1} - \bar{u}_i}{h}$

leads to the Lax-Wendroff
scheme:

$$f_{i+1/2} = \frac{a}{2} \left[(1+\gamma) \bar{u}_i + (1-\gamma) \bar{u}_{i+1} \right]$$

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$$\bar{u}_i^{n+1} = \bar{u}_i^n - \gamma h \underbrace{\left(\frac{\bar{u}_{i-1} - \bar{u}_{i+1}}{2h} \right)}_{\text{centered advection}}$$

$$+ \frac{(\gamma h)^2}{2} \underbrace{\left(\frac{\bar{u}_{i-1} - 2\bar{u}_i + \bar{u}_{i+1/2}}{h^2} \right)}_{\text{centered diffusive correction to dissipate}}$$

You may have encountered LW before and derived it from the second-order Taylor series in time :

$$u(t+\Delta t) = u(t) + \bar{i} \frac{\partial u}{\partial t}(t)$$

$$+ \frac{\bar{i}^2}{2} \frac{\partial^2 u}{\partial t^2} + O(\bar{i}^3)$$

Now from $u_t = -au_x$ we
already got using the PDE

$$u_{tt} = a^2 u_{xx}$$

Giving

$$u(t+\Delta t) \approx u(t) - \sqrt{h} u_x(t) + \frac{(\sqrt{h})^2}{2} u_{xx}(t)$$

which directly leads to LWR
if we use 2nd order FD for
all spatial derivatives, thus
ensuring that the overall scheme
is 2nd order in space-time.

But this approach obscures the
FV nature of the method &
is hard to generalize to other
hyperbolic equations

Note LW is not a MOL scheme - why? [Discuss in class]

The modified equation for LW is:

$$\tilde{u}_t + a \tilde{u}_x + \underbrace{\frac{a^2}{6} (1-\nu^2) \tilde{u}_{xxx}}_{\text{dispersion}} = \underbrace{\varepsilon \tilde{u}_{xxxx}}_{\text{dissipation}}$$

$$\varepsilon = O(\bar{i}^3, h^3)$$

Centered slopes

$$S_i = \frac{\bar{u}_{i+1} - \bar{u}_i}{2h}$$

with linear reconstruction gives the time-averaged upwind flux:

$$f_{\bar{i}+1/2} = a \left(\bar{u}_i + \frac{(1-\nu)}{4} (\bar{u}_{i+1} - \bar{u}_{i-1}) \right)$$

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Which leads to Froum's method

$$\bar{u}_i^{n+1} = \bar{u}_i^n - (\gamma h) \left(\frac{\bar{u}_i - \bar{u}_{i-1}}{h} \right)$$

$\underbrace{\phantom{\bar{u}_i - \bar{u}_{i-1}}}_{\text{upwind}}$

$$- \frac{\gamma(1-\gamma)h^2}{2} \left(\frac{\bar{u}_{i+1} - \bar{u}_i - \bar{u}_{i-1} + \bar{u}_{i-2}}{h^2} \right)$$

$\underbrace{\phantom{\bar{u}_{i+1} - \bar{u}_i - \bar{u}_{i-1} + \bar{u}_{i-2}}}_{\text{upwind difference } \approx u_{xx}}$

This method is superior to Lax-Wendroff in practice.

Is it second order?

We know that upwinding has a modified equation (to $O(h^2)$)

$$\tilde{u}_t + a \tilde{u}_x = \frac{ah}{2} \tilde{u}_{xx}$$

So for Froum:

$$u(x, t+\Delta t) \approx u - a\bar{u}_x + \underbrace{\frac{ah^2}{2} \bar{u}_{xx}}_{\text{upwind piece}}$$
$$- \frac{\gamma h^2}{2} \bar{u}_{xx} + \frac{(\gamma h)^2}{2} u_{xx} + O(h^2)$$

which is the correct Taylor series just like LW, so Froum is also second order in space - true.

Another way to get Froum as a FV is to estimate fluxes at mid point of time step to get 2nd order in time:

$$f_{\bar{t}+1/2}^n \approx a u_{\bar{t}+1/2}^{n+1/2} \approx a u\left(x_i + \frac{h}{2}, t + \frac{\bar{t}}{2}\right)$$

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This is still not a MOL scheme since we are not applying a midpoint temporal integrator to an ODE, but is similar & often simpler than computing time-averaged fluxes.

If $\alpha > 0$, use a Taylor series in the upwind cell:

$$\begin{aligned} u_{i+1/2}^{n+1/2} &= u_i^n + \frac{\gamma}{2} (u_t)_i^n + \frac{h}{2} (u_x)_i^n \\ &= u_i^n - \frac{\alpha \gamma}{2} (u_x)_i^n + \frac{h}{2} (u_x)_i^n \\ &= \bar{u}_i^n + \frac{h}{2} (1-\gamma) s_i^n \quad s_i \leftarrow \text{slope} \end{aligned}$$

which leads to Fromm once we use centered slopes
 (it is not hard to see this is identical to linear reconstruction + time averaged upwind)

Now let's consider higher-order reconstruction with MOL schemes

To get a 3rd order MOL scheme, we need a **quadratic** reconstruction

$$u_i(x) = c_0 + c_1 x + c_2 x^2$$

With FV conditions:

$$\left\{ \begin{array}{l} \int_{x_{i-1/2}}^{x_{i+1/2}} u_i(x) dx = \bar{u}_i \cdot h \\ \int_{x_{i-1/2}}^{x_{i-1/2}} u_i(x) dx = \bar{u}_{i-1} \cdot h \\ \int_{x_{i-3/2}}^{x_{i+3/2}} u_i(x) dx = \bar{u}_{i+1} \cdot h \end{array} \right.$$

Solving for c_1, c_2 & c_0 gives:

$$u_i(x; \bar{u}) = \bar{u}_i + \left(\frac{\bar{u}_{i+1} - \bar{u}_{i-1}}{2h} \right) (x - x_i)$$

$$+ \frac{1}{2} \left(\frac{\bar{u}_{i+1} - 2\bar{u}_i + \bar{u}_{i-1}}{h^2} \right) \left[(x - x_i)^2 - \frac{h^2}{12} \right]$$

If it were FD third-order we wouldn't have this piece!

Upwind instantaneous flux :

$$f_{i+1/2}(\bar{u}(t)) = a_{i+1/2} u_i(x_{i+1/2}; \bar{u}(t))$$

leads to the 3rd order upwind-biased scheme

$$\frac{d\bar{u}_j}{dt} = \frac{a}{h} \left[-\frac{1}{6} \bar{u}_{j-2} + \bar{u}_{j-1} - \frac{\bar{u}_j}{2} - \frac{\bar{u}_{j+1}}{3} \right]$$

that I mentioned before

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A dvection - Diffusion

How do we add diffusion to this? Up to second order, the standard spatial discretization is obvious & good. The harder part is temporal integration.

If we use an MOL scheme, it is easy, diffusion is just one more term added to the r.h.s. of the system of ODEs.

Diffusion adds dissipation (negative real part to the Jacobian eigenvalues), so it only helps stability.

[Discuss some options in class]

How about space-time
methods of 2nd order for
advection-diffusion?

Do you know of any? Discuss

One option is to follow one
of the routes to Lax-Wendroff
& use a second-order in time

Taylor series:

$$u(t + \bar{\tau}) \approx u(t) + u_t \bar{\tau} + \frac{1}{2} u_{tt} \bar{\tau}^2$$

$$u_{tt} = (-au_x + d u_{xx})_t$$

$$= -a(u_t)_x + d(u_t)_{xx} =$$

$\underbrace{}_{\text{PDE}}$

$$= a^2 u_{xx} - 2ad u_{xxx} + d^2 u_{xxxx}$$

$\underbrace{-2ad u_{xxx}}_{\text{hard part}}$

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To turn this into a scheme we would need to choose a finite-difference spatial discretization of

u_{xxx} and u_{xxxx} .

This approach is not great - why?

Discuss pros and cons in class

This is related to how it is NOT a good idea to use chain rule to expand:

$$-(a(x)u(x))_x + (d(x)u_x)_x = \\ -a_x u - au_x + d_x u_x + du_{xx}$$

Discuss why in class

Let's go to higher-level thinking & think about splitting advection & diffusion

$$u_t = \underbrace{A u}_\text{e.g. advection} + \underbrace{B u}_\text{e.g. diffusion}$$

Imagine we already have a second-order method for solving

$$u_t = A u \quad \& \quad u_t = B u$$

How do we combine them.

The classical approach is

Strang splitting

$$u^{n+1} = \underbrace{A\left(\frac{\Delta t}{2}\right)}_\text{e.g. advect for half a step} \underbrace{B(\Delta t)}_\text{diffuse for one step} \underbrace{A\left(\frac{\Delta t}{2}\right)u^n}_\text{advect for half a step}$$

While this is a good method for ODEs, it has problems for PDEs. [Discuss in class issues]

Here is a better space-time approach.

$$u_t = (A+B) u \Rightarrow$$

$$\begin{aligned} u^{n+1} &= u^n + \bar{\epsilon} (A+B) u^n + \\ &\quad \frac{1}{2} (A^2 + B^2 + AB + BA) \bar{\epsilon}^2 \\ &\quad + O(\bar{\epsilon}^3) \end{aligned}$$

Note that for
 $A = -\alpha \partial_x$ & $B = \beta \partial_{xx}$

$$A^2 = \alpha^2 \partial_{xx}, \quad B^2 = \beta^2 \partial_{xxxx}$$

$$\text{&} \quad AB = BA = -\alpha \beta u_{xxx}$$

BUT in general (BCs, higher dimensions, non-constant coefficients)

$AB \neq BA$ do not commute
 and we should not assume
 that.

If we just tried, for example,

$$\frac{u^{n+1} - u^n}{\bar{\tau}} = \text{Lax-Wendroff}$$

or
Froumer etc.

$$+ d \left(\frac{u_{xx}^{n+1} + u_{xx}^n}{2} \right) \leftarrow \text{Crank-Nicolson}$$

We would get to $O(\bar{\tau}^3)$

$$\frac{u^{n+1} - u^n}{\bar{\tau}} = \left(A + \frac{A^2}{2} \bar{\tau} \right) u^n$$

$$+ \frac{B}{2} (u^n + u^{n+1}) \Rightarrow$$

$$u^{n+1} = \left(I - \frac{B \bar{\tau}}{2} \right)^{-1} \left[\left(A + \frac{A^2 \bar{\tau}}{2} \right) \right.$$

$$\left. + \left(I + \frac{B \bar{\tau}}{2} \right) \right] u^n$$

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$$= \left[I + \frac{B\bar{z}}{2} + \frac{B^2}{4}\bar{z}^2 + O(\bar{z}^3) \right].$$

$$\left[I + \frac{B\bar{z}}{2} + A\bar{z} + \frac{A^2}{2}\bar{z}^2 \right] u^n$$

$$= \left(I + B\bar{z} + A\bar{z} + \frac{A^2}{2}\bar{z}^2 + \frac{B^2}{2}\bar{z}^2 + \frac{BA}{2}\bar{z}^2 + O(\bar{z}^3) \right) u^n$$

We are missing $\frac{AB}{2}\bar{z}^2$

How do we get it?

- ① Solve $u_t = Au + Bu^n$
- over one step
using a 2nd order
space-time scheme (LW or Froum)
to compute diffusion-corrected
advection fluxes F^{adv}

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② Solve $u_t = Bu + \underbrace{\nabla \cdot F}_{\text{constant source term}}^{\text{adv}}$
 with any 2nd order scheme to compute
 $u^{n+1} \approx u(t+\tau)$

Why does this work?

$$\begin{aligned} ① \quad u_t &= Au + Bu^n \leftarrow \text{constant source term}_n \\ \Rightarrow u^{n+1,*} &= I + \bar{i}A \left(I + \frac{\bar{i}}{2}A + \frac{\bar{i}}{2}B \right) u \\ &\quad + \bar{i}Bu^n + O(\bar{i}^3) \end{aligned}$$

$\bar{i}(\nabla \cdot F \text{ (adv)})$ for us!
 - this has the missing term $(\bar{i}/2)ABu^n$!

② Now we solve

$$u_t = Bu + \underbrace{A(I + \frac{\bar{i}}{2}A + \frac{\bar{i}}{2}B)u^n}_{\text{constant source term}}$$

to get u^{n+1} , to get

$$\begin{aligned}
u^{n+1} &= \left(I + \bar{i}B + \frac{\bar{i}^2}{2}B^2 \right) u^n + O(\bar{i}^3) \\
&\quad + \bar{i} \left[A \left(I + \frac{\bar{i}}{2}A + \frac{\bar{i}}{2}B \right) u^n \right] \\
&\quad + \frac{\bar{i}^2}{2} B \left[A \left(I + \cancel{\frac{\bar{i}}{2}A} + \cancel{\frac{\bar{i}}{2}B} \right) u^n \right] \\
&\quad \qquad \qquad \qquad O(\bar{i}^3) \\
&= \left[\left(I + \bar{i}A + \frac{\bar{i}^2}{2}A^2 \right) + \left(I + \bar{i}B + \frac{\bar{i}^2}{2}B^2 \right) \right. \\
&\quad \left. + \frac{\bar{i}^2}{2} (AB + BA) + O(\bar{i}^3) \right] u^n
\end{aligned}$$

as required for second-order accuracy in time!

To implement this we need to know how to solve to second-order:

$$\begin{cases} u_t = Au + s \leftarrow \text{constant} \\ u_t = Bu + s \leftarrow \text{source term} \end{cases}$$
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Note: This trick would be much harder to get to work for third order accuracy - use MOL + RK for high order accuracy.

To second order, it is often not hard to construct specialized schemes (we will do this multiple times in this class).

For example, prove as an **exercise** that this 2-step

Adams-Basforth + source

$$u^{n+1} = u^n + \frac{3}{2} f(u^n) - \frac{1}{2} f(u^{n-1}) + \frac{B}{2} (u^m + u^{m+1})$$

is 2nd order in time for ODE:

$$u_t = f(u) + Bu$$

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You can just use $f(u) = Au$ for simplicity if you'd like, and you should get something like:

$$u^{n+1} = \left(I + \frac{\bar{I}}{2} B + \frac{\bar{I}^2}{4} B^2 + O(\bar{I}^3) \right)$$

$$\left(I + A\bar{I} + \frac{B\bar{I}}{2} + \frac{\bar{I}^2}{2} A(A+B)\bar{I}^2 + O(\bar{I}^3) \right)^n$$

which is correct to $O(\bar{I}^3)$

Aside: Later, in immersed-boundary methods, we will solve:

$$\begin{cases} x_t = f(x) + g(y) \\ y_t = h(x, y) \end{cases} \text{ using:}$$

$$\begin{cases} y^{n+1/2,*} = y^n + \frac{\bar{I}}{2} h(x^n, y^n) \\ \frac{x^{n+1} - x^n}{\bar{I}} = \frac{1}{2} (f(x^n) + f(x^{n+1})) + g(y^{n+1/2,*}) \end{cases}$$

g(y^{n+1/2,}) ↪ source term*

$$y^{n+1} = h\left(\frac{x^n + x^{n+1}}{2}, y^{n+1/2,*}\right)$$

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Lax-Wendroff with source term

Back to solving

$$\textcircled{1} \quad u_t = Au + S$$

$$\textcircled{2} \quad u_t = Bu + S$$

For diffusion, we can simply use Crank-Nicolson with source:

$$\textcircled{2} \quad \frac{u^{n+1} - u^n}{\tau} = B \left(\frac{u^n + u^{n+1}}{2} \right) + S$$

How do we add source term for advection?

$$u_t + a u_x = \underbrace{S(x)}_{\substack{\text{function of space} \\ \text{only } \underline{\text{not time}}}}$$

Following one of the routes to derive LW (but do the same as an exercise for Fromm):

$$u_{tt} = -\alpha (u_t)_x = \alpha^2 u_{xx} - \alpha s_x$$

$$\Rightarrow u(t+\bar{\tau}) = u(t) - \bar{\tau} \alpha u_x + \bar{\tau} s$$

$$+ \frac{\bar{\tau}^2}{2} (\alpha^2 u_{xx} - \alpha s_x)$$

Discretizing, for example, using centered differences, gives LW

with source:

$$u_i^{n+1} = u_i^n - \frac{\alpha \bar{\tau}}{2h} (u_{i+1}^n - u_{i-1}^n) + s_i \Delta t$$

$$+ \frac{\alpha \bar{\tau}^2}{2h^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

$$- \frac{\alpha \bar{\tau}^2}{4h} (s_{i+1} - s_{i-1})$$

All terms on rhs involving $\frac{1}{\alpha}$
get put as source term for
diffusion solve $\equiv \nabla \cdot F^{(adv)}$

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The only question to answer now is what the stability of the new second-order space time scheme for advection-diffusion is.

What we want is to only limit advection Courant (CFL) number but not diffusive CFL, i.e., we want

$$\frac{a \Delta t}{\Delta x} \leq c \approx 1$$

to be sufficient for stability.

This is subject of homework and there is reading on the course home page.

You may find that LW is not as good of a choice as Froum 

TO BE FINISHED ...

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Note that the highlighted term

$$\frac{\bar{z}^2}{2} AB = - \frac{a \bar{z}^2}{4 h} (S_{i+1} - S_{i-1}),$$

which is the diffusion correction to the advective fluxes, represents $\frac{\bar{z}^2}{2} AB u^n$ in the Taylor series, and for LW writes as:

$$S_j = \frac{d}{h^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

$$\Rightarrow \left(\frac{\bar{z}^2 AB}{2} u \right)_j = - \frac{a d \bar{z}^2}{2 h^3} (S_{j+1} - S_j)$$

$$= - \frac{a d \bar{z}^2}{2} \underbrace{\left(\frac{u_{j+2} - 2u_{j+1} + 2u_{j-1} - u_{j-2}}{h^3} \right)}_{\text{centered difference for } (u_{xxx})_j}$$

centered difference for $(u_{xxx})_j$ does not involve $u_j \rightarrow \text{instability}$ (53)

