

Numerical PDEs

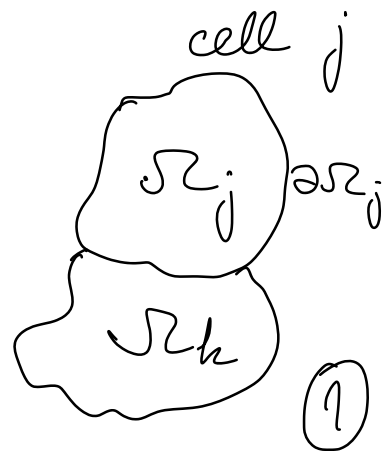
A. DONEV, Fall 2021

Finite Volume Methods

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

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

$$\bar{u}_j = \frac{1}{|\Omega_j|} \int_{\Omega_j} u \, dr$$



Conservation law

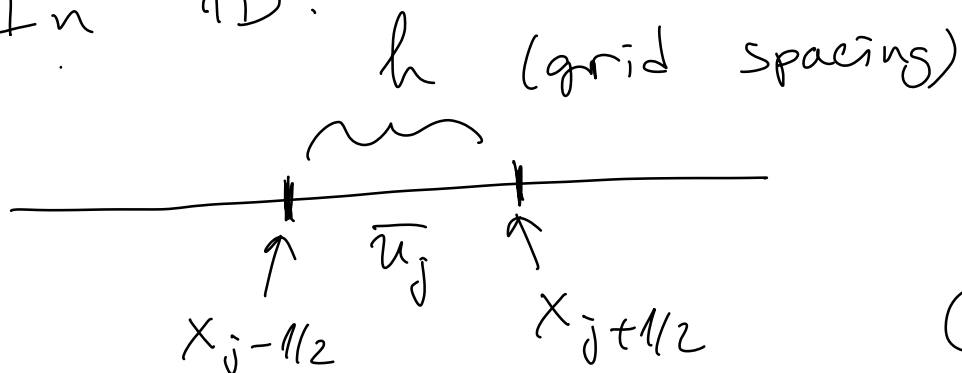
$$\int_{\Omega_j} \frac{\partial u}{\partial t} dr = - \int_{\Omega_j} (\nabla \cdot \vec{f}) dr$$

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

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

which is a system of ODEs

In 1D:



In 1D adv-diff:

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

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.

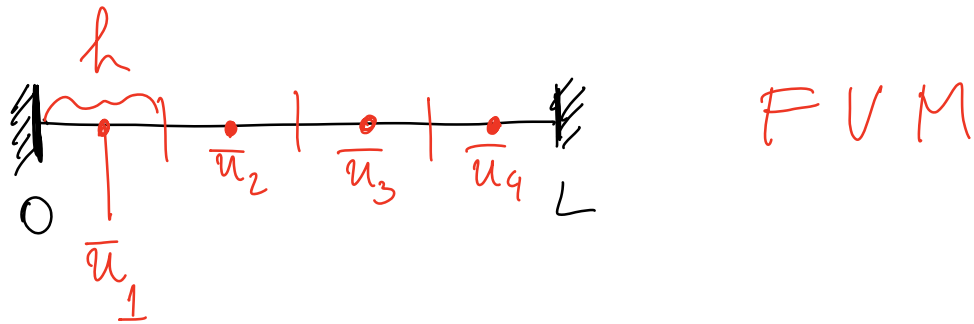
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Note that for low-order (1st or 2nd) schemes there is really not that much difference between finite difference & finite volume - it is more of a matter of mental picture.

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:

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

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

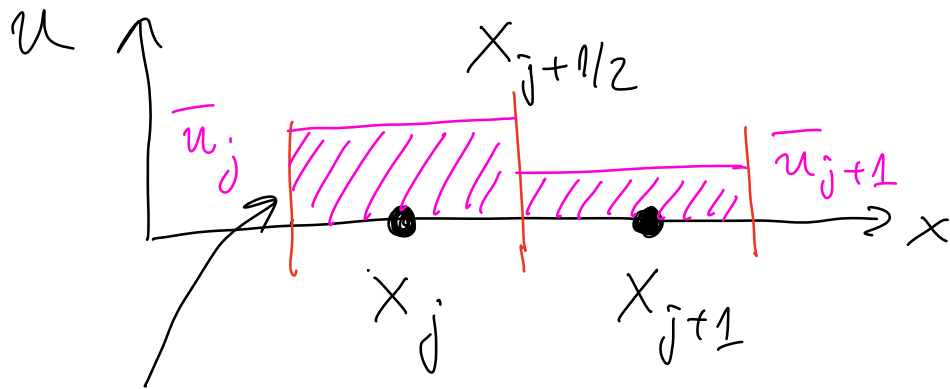
For MOL, we need to estimate:

a) Advective flux

$$f_{j+\frac{1}{2}}^{(a)} = \underset{\substack{\uparrow \\ \text{"easy" (evaluate } a(x))}}{a(x_{j+\frac{1}{2}})} u(x_{j+\frac{1}{2}})$$

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":

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

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

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

⑧

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.

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

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

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"

(10)

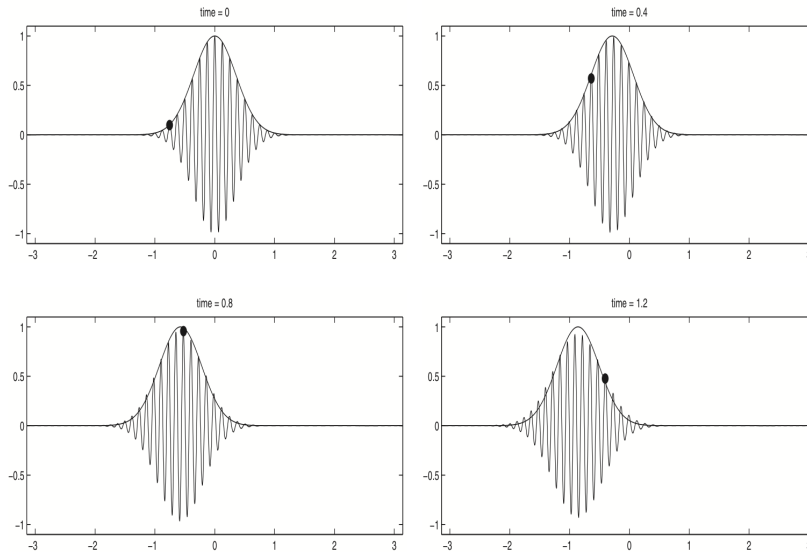


Figure E.2. The oscillatory wave packet satisfies the dispersive equation $u_t + au_x + bu_{xxx} = 0$. Also shown is a black dot attached to one wave crest, translating at the phase velocity $c_p(\xi_0)$, and a Gaussian that is translating at the group velocity $c_g(\xi_0)$. Shown for a case in which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

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

E.g. $u_t + a_1 u_x + a_2 u_{xx} + a_3 u_{xxx} + a_4 u_{xxxx} = 0 \Rightarrow$

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

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

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:

$$\bar{u}_j^n = e^{-i\omega n \Delta t} e^{ikjh}$$

(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.

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

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

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

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:

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

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

Another way to see this:

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

artificial diffusion

What's better?

If we used

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

(centered scheme)

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

which is now second-order accurate in space,

then we would get the modified equation

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

artificial dispersion

which has phase velocity

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

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:

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

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

3rd-order upwind biased

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

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

if $a > 0$
more information from upwind

(17)

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:

$$u_t + (au)_x = u_t + ua_x + au_x = 0$$

∴ Finite Difference:

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

Compare this to Taylor series of r.h.s. of (*) (18)

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

If Finite Volume:

$$\frac{d\bar{u}_j}{dt} = \frac{1}{h} \int_{x_j - h/2}^{x_j + h/2} u_t(x, t) dx$$

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

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

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

$$\frac{d\bar{u}_j}{dt} + \frac{1}{h} \left((au)(x_{j+1/2}) - (au)(x_{j-1/2}) \right) = O(h^3)$$

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:

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

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:

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

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

$\theta = 0$: forward Euler

$\theta = 1/2$: Implicit midpoint
(2nd order)

$\theta = 1$: Backward Euler (implicit)

Local truncation error:

$$S_n = \left(\frac{u(t_{n+1}) - u(t_n)}{\bar{\tau}} \right) - \left(\frac{u^{n+1} - u^n}{\bar{\tau}} \right)$$

$$= \left(\frac{1}{2} - \theta \right) \bar{\tau} u''(t_n) + \left(\frac{1}{6} - \frac{\theta}{2} \right) \bar{\tau}^2 u'''(t_n)$$

(21)

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

Therefore, the modified equation is

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

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

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

For advection

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

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

So we get:

$$\tilde{u}_t + a \tilde{u}_x = \begin{cases} -\frac{\bar{a}^2}{2} \tilde{u}_{xx} & \text{FE (anti-diffusion)} \\ \frac{\bar{a}^2}{2} \tilde{u}_{xx} & \text{BE artificial dissipation} \\ -\frac{\bar{a}^3}{12} \tilde{u}_{xxx} & \text{implicit midpoint artificial dispersion} \end{cases}$$

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

Consider the simplest FD/FV
1st order upwind:

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

(or add bars for FV)

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

Define CFL number $\nu = \frac{a \bar{t}}{h}$

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

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

Observe that for $a = \text{const}$
and $\nu = 1$ 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 so 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

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

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

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

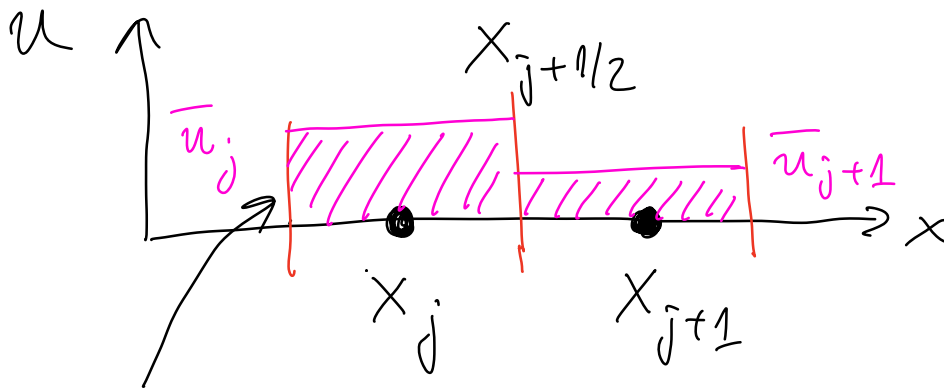
as derived already

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.

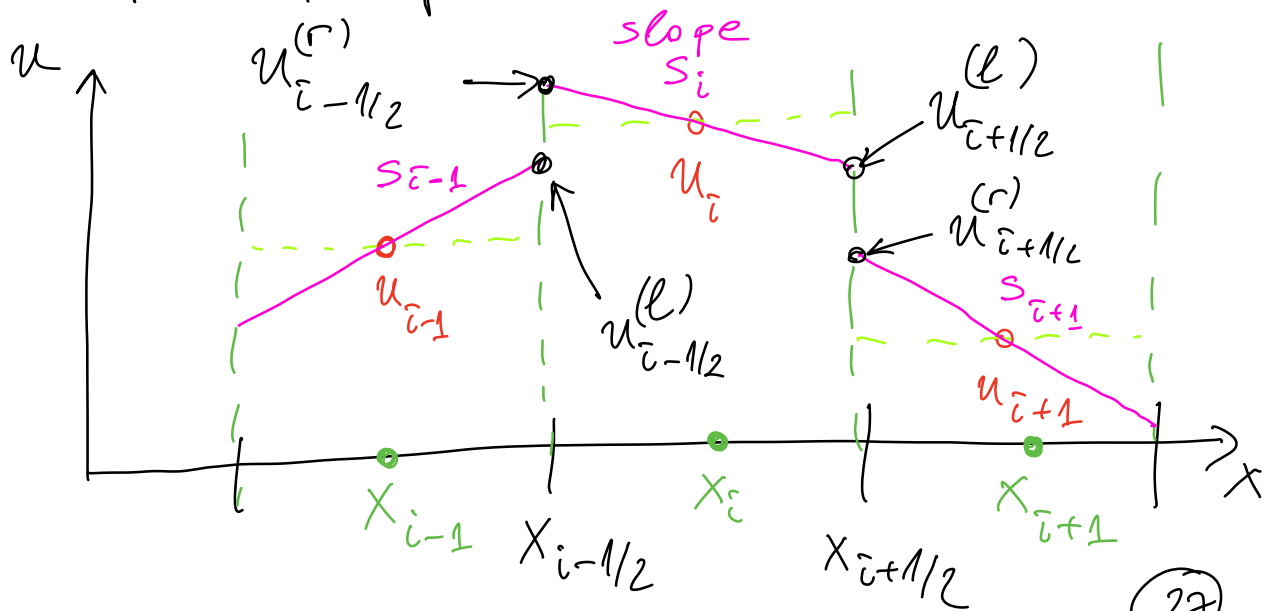
For upwind we used a



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:



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

$$u(x_{i-1/2} < x < x_{i+1/2}) = u_i \leftarrow \text{conservation}$$

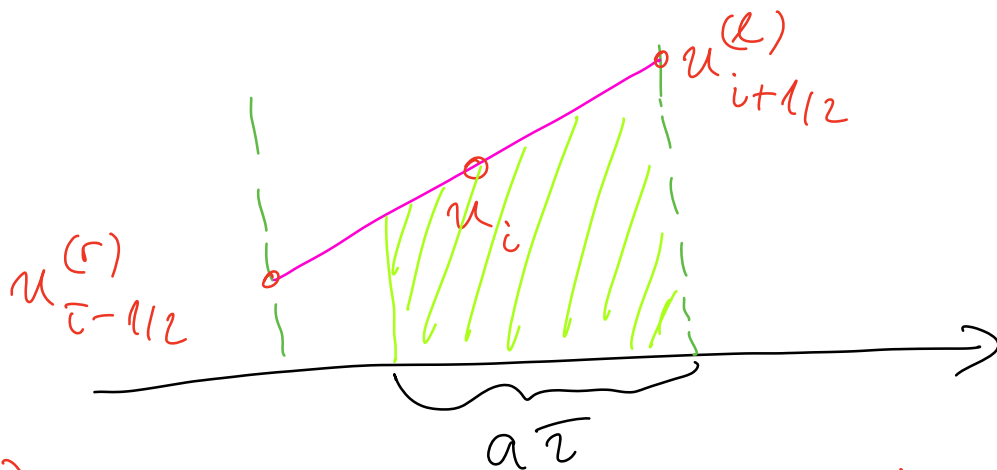
$$+ s_i (x - x_i) \quad \underbrace{+ O(h^2)}_{\text{still same order}}$$

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 $u_{i+1/2}^{(l)}$ and one from the right $u_{i+1/2}^{(r)}$

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 :



(*) Assume $a = \text{const}$ for now

Upwind average flux :

$$f_{i+1/2}^{(t)} = \frac{\text{(shaded area)}}{\bar{\tau}} = f_{i+1/2}$$

if $a > 0$

(29)

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

where advective CFL number

$$\nu = \frac{a \bar{v}}{h}$$

Recall we assumed $a = \text{const}$
(see end of lecture for $a \neq \text{const}$)

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:

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

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

centered advection

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

centered diffusive correction
to dissipate

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

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

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

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

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

which directly leads to LW
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:

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

$$\epsilon = O(\bar{v}^3, h^3)$$

$$- \underbrace{\epsilon}_{\text{dissipation}} \tilde{u}_{xxxx}$$

Centered slopes

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

with linear reconstruction gives the time-averaged upwind flux:

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

Which leads to Fromm's method

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

upwind

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

upwinded 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 \sim (to $O(h^2)$)

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

So for Fromm:

$$u(x, t + \bar{\tau}) \approx u - a \bar{\tau} u_x + \frac{ah\bar{\tau}}{2} u_{xx}$$

upwind piece

$$- \frac{\gamma h^2}{2} u_{xx} + \frac{(\gamma h)^2}{2} u_{xx} + O(h^3)$$

which is the correct Taylor Series just like LW, so Fromm is also second order in space-time.

Another way to get Fromm as a FV is to estimate fluxes at midpoint of time step to get 2nd order in time:

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

Works for non-constant advection

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.

Take $a = \text{const}$ for now:
 If $a > 0$, use a Taylor series in the upwind cell:

$$\begin{aligned}
 u_{i+1/2}^{n+1/2} &= u_i^n + \frac{\tau}{2} (u_t)_i^n + \frac{h}{2} (u_x)_i^n \\
 &= u_i^n - \frac{a\tau}{2} (u_x)_i^n + \frac{h}{2} (u_x)_i^n \\
 &= \bar{u}_i^n + \frac{h}{2} (1-\nu) S_i^n \leftarrow \text{slope}
 \end{aligned}$$

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:

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

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:
works for $a \neq \text{const}$

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

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

(3P)

Advection - 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:

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

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

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

← PDE →

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

hard part

(40)

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:

$$\begin{aligned} & - (a(x)u(x))_x + (d(x)u_x)_x = \\ & - a_x u - a u_x + d_x u_x + d u_{xx} \end{aligned}$$

Discuss why in class

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

splitting advection & diffusion

$$u_t = \underbrace{A} u + \underbrace{B} u$$

e.g. advection e.g. diffusion

I imagine we already have a second-order method for solving

$$u_t = Au \quad \& \quad u_t = Bu$$

How do we combine them.

the classical approach is

Strang splitting

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

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

Here is a better space-time approach.

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

$$u^{n+1} = u^n + \bar{\tau} (A+B)u^n + \frac{\bar{\tau}^2}{2} (A^2 + B^2 + AB + BA)u^n + O(\bar{\tau}^3)$$

Note that for $A = -a \partial_x$ and $B = d \partial_{xx}$

$$A^2 = a^2 \partial_{xx}, \quad B^2 = d^2 \partial_{xxxx}$$

$$\& \quad AB = BA = -ad u_{xxx}$$

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,

$$\frac{u^{n+1} - u^n}{\tau} = \text{Lax-Wendroff or Froumer etc.}$$

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

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

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

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

$$\begin{aligned}
&= \left(I + B \frac{\bar{\tau}}{2} + \frac{B^2 \bar{\tau}^2}{4} + O(\bar{\tau}^3) \right) \\
&\left[I + B \frac{\bar{\tau}}{2} + A \bar{\tau} + \frac{A^2 \bar{\tau}^2}{2} \right] u^n \\
&= \left(I + B \bar{\tau} + A \bar{\tau} + \frac{A^2 \bar{\tau}^2}{2} + \frac{B^2 \bar{\tau}^2}{2} \right. \\
&\quad \left. + \frac{BA}{2} \bar{\tau}^2 + O(\bar{\tau}^3) \right) u^n
\end{aligned}$$

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

How do we get it?

① Solve $u_t = A u + \underbrace{B u}_{\substack{\text{constant} \\ \text{source term}}}$ over one step using a 2nd order space-time scheme (LW or Fromm) to compute diffusive-corrected advective fluxes F_{adv}

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

Why does this work?

① $u_t = A u + B u^n \leftarrow \text{constant source term}_n$

$\Rightarrow u^{n+1,*} = I + \tau A \left(I + \frac{\tau}{2} A + \frac{\tau}{2} B \right) u^n + \tau B u^n + O(\tau^3)$

$\tau(\nabla \cdot F^{\text{adv}})$ for us!
 - this has the missing term $(\tau/2) A B u^n$!

② Now we solve

$u_t = B u + A \left(I + \frac{\tau}{2} A + \frac{\tau}{2} B \right) u^n$

constant source term

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

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

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

as required for second-order accuracy in time!

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

$$\begin{cases}
u_t = A u + s \leftarrow \text{constant} \\
u_t = B u + s \leftarrow \text{source term}
\end{cases}$$

(47)

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-Bashforth + source

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

is 2nd order in time for ODE:

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

(48)

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

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

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

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

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

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

$g(y^{n+1/2, *}) \leftarrow$ source term

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?

$$u_t + a u_x = \underbrace{S(x)}_{\text{cell-centered}}$$

function of space
only not time

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

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

$$\Rightarrow u(t+\bar{v}) = u(t) - \bar{v} a u_x + \bar{v} s$$

$$+ \frac{\bar{v}^2}{2} (a^2 u_{xx} - a s_x)$$

Discretizing, for example, using centered differences, gives LW with source:

$$u_i^{n+1} = u_i^n - \frac{a\bar{v}}{2h} (u_{i+1}^n - u_{i-1}^n) + S_i \Delta t$$

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

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

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

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 advective 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 😊

Note that the highlighted term

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

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

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

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

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

centered difference for $(u_{xxx})_j$ does not involve u . \rightarrow instability

A Memorandum: Fromm method with
 source & non-constant advection
 A. DONEV

$$u_t = -(a(x)u)_x + g(x)$$

(↑
constant in time)

We will follow the approach
 of extrapolating state to
 faces at midpoint in time:

$$u_{j+1/2}^{n+1/2} = \bar{u}_j^n + \frac{\Delta x}{2} (u_x^n)_j + \frac{\Delta t}{2} (u_t^n)_j$$

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

And here we will use chain
 rule + PDE to estimate u_t^n :

$$u_t = -\underbrace{a u_x}_{\text{use } a \text{ at face}} - \underbrace{u a_x}_{\text{easy to get at cell centers}} + g$$

one can also use
 a_j or $(a_{j-1/2} + a_{j+1/2})/2$ (1)

$$\left(u_t^n\right)_j = -a_{j+1/2}^{n+1/2} S_j - u_j \left(\frac{a_{j+1/2}^{n+1/2} - a_{j-1/2}^{n+1/2}}{h} \right) + g_j$$

centered slopes
 $S_j = \frac{u_{j+1} - u_{j-1}}{2h}$
 for Fromm

Advection flux estimate:

$$F_{j+1/2}^{adv} = a_{j+1/2}^{n+1/2} u_{j+1/2}^{n+1/2}$$

← has to be $n+1/2$

Homework: Implement method and confirm second-order in space-time.

Remember that for advection-diff.

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

comes from diffusion. For constant

$$a(x) = a = \text{const}$$

(2)

this approach gives an extra term:

$$u_j^{n+1} = u_j^n - \bar{v} a \left(u_{j+1/2}^{n+1/2} - u_{j-1/2}^{n+1/2} \right)$$

= usual Fromm scheme

$$- \frac{a d \bar{v}^2}{2} \left(\frac{u_{j+1} - 3u_j + 3u_{j-1} - u_{j-2}}{h^3} \right)$$

Upwind difference for $(u_{xxx})_j$

to be compared to Lax-Wendroff scheme:

$$- \frac{a d \bar{v}^2}{2} \left(\frac{u_{j+2} - 2u_{j+1} + 2u_{j-1} - u_{j-2}}{h^3} \right)$$

which is centered (no u_j !) and leads to spurious stability limit (3)

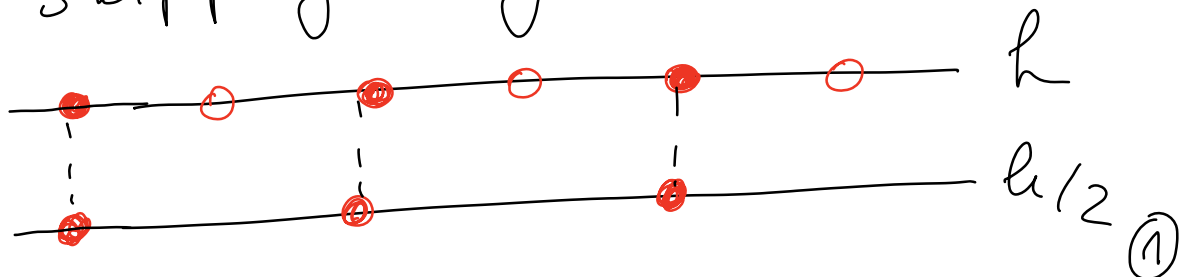
Addendum: Empirical error for FVM

In order to estimate the error via successive refinement

$$\tilde{E}(x, h) = u_h(x) - u_{h/2}(x)$$

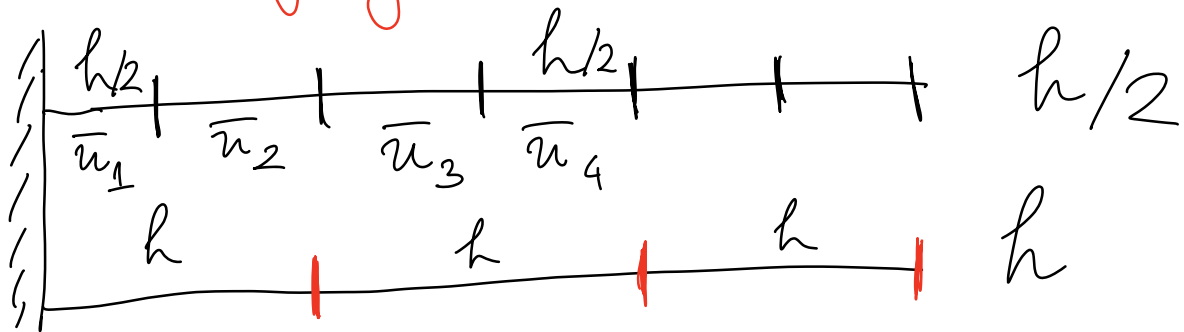
we need to be able to compare u_h & $u_{h/2}$ on the same grid.

For FD methods, this is easily done by just skipping every other point:



But for FV methods remember we know \bar{u}_k not u_k , so we coarsen the grid by

averaging :



$$\bar{u}_2(h) = \frac{1}{2} \left(\bar{u}_3^{(h/2)} + \bar{u}_4^{(h/2)} \right)$$

Note that this coarsening is exact, just like in the FD case, i.e., no additional error is introduced here (no need for interpolation etc.)

(2)

Importantly, however, for method of manufactured solution, you must set

$$u_j(t) = \frac{1}{h} \int_{x_j - h/2}^{x_j + h/2} u_{\text{manuf.}}(x, t) dx$$

where the integral is evaluated to sufficient order of accuracy.

For 2nd order schemes,

$$u_j(t) = u_{\text{manuf.}}(x_j, t)$$

is ok, but not for third order \rightarrow do integral analytically
OR 3pt Gaussian quadrature

(3)