Notes for HW 1:

1) Re-read part in red at the beginning & absorb the message (it is an important one)

2) Read & apply Appendix E.6 in FD LeVeque book to HW & resubmit

3) Explain / justify every decision made. E.g. "I set $h = ?$ and $\tau = ?$" Why? Did you try other (larger) values

4) Are you sure your results converge to the true PDE solution? Why? This is code validation

5) If your method is unconditionally unstable, how do you set τ?

$\tau = O(h)$ is NOT enough

$\tau = Ch$ and what is C?

This will help us answer a question later:

Why don't we do advection implicitly, most of the time.

6) For any method, answer:

- What is its order of acc.
- What is approximately the stability condition
- Can you handle $d=0$?

Numerical PDEs

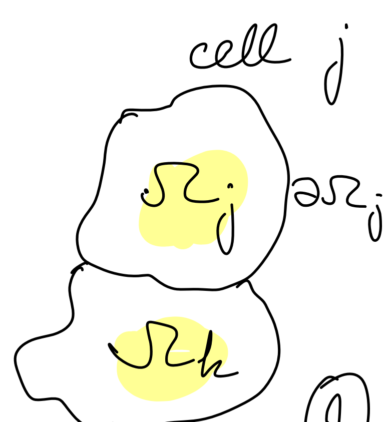
A. Donev, Fall 2021

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 u over each cell

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



Conservation law

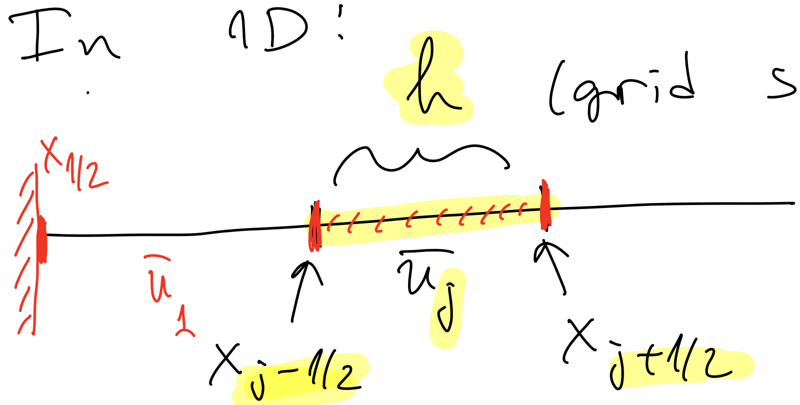
$$\int_{\Omega_j} \frac{\partial u}{\partial t}\, dr = -\int_{\Omega_j} (\nabla \cdot \vec{f})\, dr$$

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

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

which is a system of ODEs

In 1D:



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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.

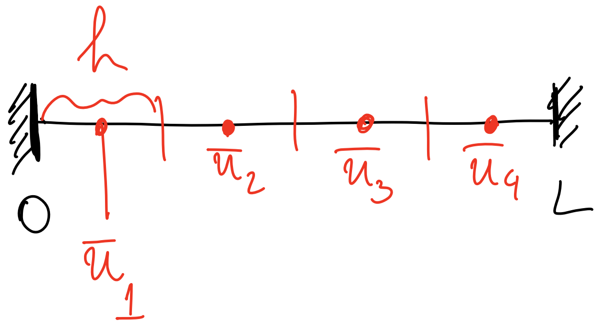
To make it into a scheme we need to figure out the fluxes in terms of the cell averages.

Note that for low-order (1^{st} or 2^{nd}) 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 <ins>not</ins> divergence of fluxes.

Another difference is with boundary conditions:

<ins>Physical boundaries should overlap</ins> with cell boundaries for FVM schemes.



FVM

We know the cell averages, <u>not</u> 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 $(\bar{u}_j^{n+1} - \bar{u}_j^{n})/\Delta t \approx u_t$

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For space time:

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

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

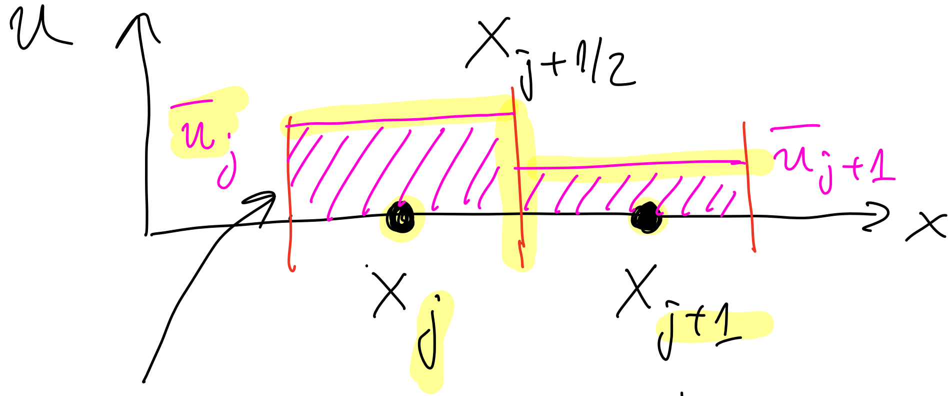
For MOL, we need to estimate:

a) Advective flux

$$f^{(a)}_{j+1/2} = \underset{\uparrow}{a}(x_{j+1/2})\, u(x_{j+1/2})$$

"easy" (evaluate $a(x)$)

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



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?

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

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

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

Upwind flux

For diffusive flux, "obviously":

$$f^d_{j+1/2} = d(x_{j+1/2})\, u_x(x_{j+1/2})$$

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

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

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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

wavenumber, wave frequency

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

where k is the wave number

$\omega(k)$

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.

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

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

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

Special case is simple advection:

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

"non-dispersive"

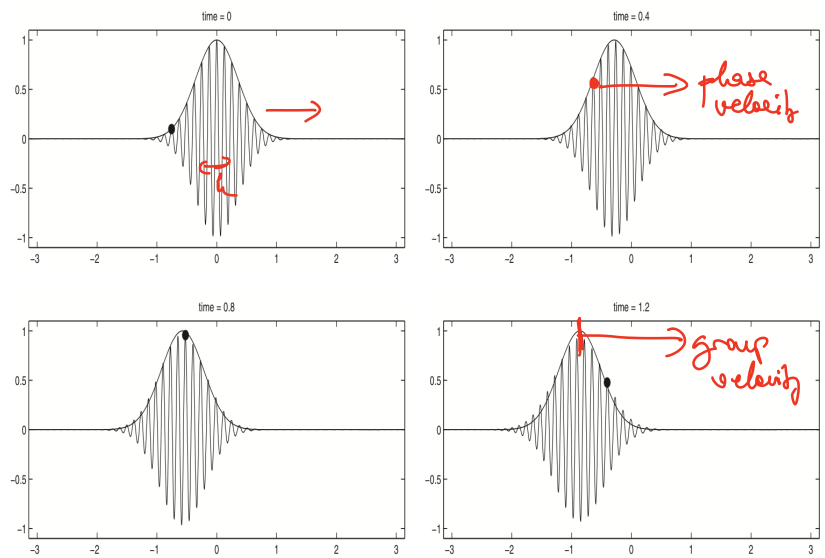

Figure E.2. *The oscillatory wave packet satisfies the dispersive equation $u_t + au_x + bu_{xxx} = 0$. Also shown is a black dot attached to one wave crest, translating at the phase velocity $c_p(\xi_0)$, and a Gaussian that is translating at the group velocity $c_g(\xi_0)$. Shown for a case in which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

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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 $a_2 = a_4 = 0$,

$$c_p(k) = a_1 - \underline{a_3} k^2$$

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

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

For a numerical method, find numerical dispersion relation by plugging into method wave:

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

An alternative, which gives us intuition quickly but is <u>not</u> rigorous, is to look at

modified equations: find a PDE that the method solves to <u>higher</u> order than it does the PDE we want to solve.

We can do this to a MOL scheme <u>separately</u> 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.

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

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

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

Since

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

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

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

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

Another way to see this:

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

$$+\underbrace{\frac{ah/2}{h^2}\left(\bar{u}_{j+1}-2\bar{u}_j+\bar{u}_{j-1}\right)}_{\text{artificial diffusion}}$$

What's better?

If we used

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

(centered scheme)

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

which is now second-order accurate in space, then we would get the modified equation

$$\tilde{u}_t + a\tilde{u}_x = \underbrace{-\frac{a h^2}{6}\tilde{u}_{xxx}}_{\text{artificial dispersion}}$$

$O(h^2)$

which has phase velocity

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

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 <u>all</u> of Ch. 10 in Finite Difference book of Le Veque.

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

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

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

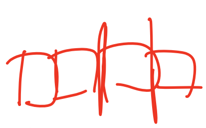
3rd-order upwind biased

which gives for $a = $ const:

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

stencil

if $a > 0$



stencil

<u>more</u> information from upwind

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

How to show this:

$$u_t + (au)_x = u_t + u a_x + a u_x = 0$$

If 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 $(*)$

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

If Finite Volume:

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

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

and $\bar{u}_j = \frac{1}{h}\int_{\mathcal{V}_j} u(x,t)\,dx$

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

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

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:

$$\tilde{u}_t + a\tilde{u}_x = \underbrace{-\frac{|a|}{12} h^3 \tilde{u}_{xxxx}}_{\text{stabilizing artificial dissipation (good!)}} \xleftarrow{} O(h^3)$$

which is higher-order & less dissipation than upwind

Temporal for 3rd order upwind biased

(0) Explicit schemes

(1) 3rd order $\tau = O(h)$

(2) $\tau \leq c \frac{h}{a}$ (stability condition)

(3) 3rd order in space-time

Options:

$\rightarrow$ RK3 $\frac{du}{dt} = Au$

stage 1: $u^{n+1,*} = u^n + \tau A u^n$

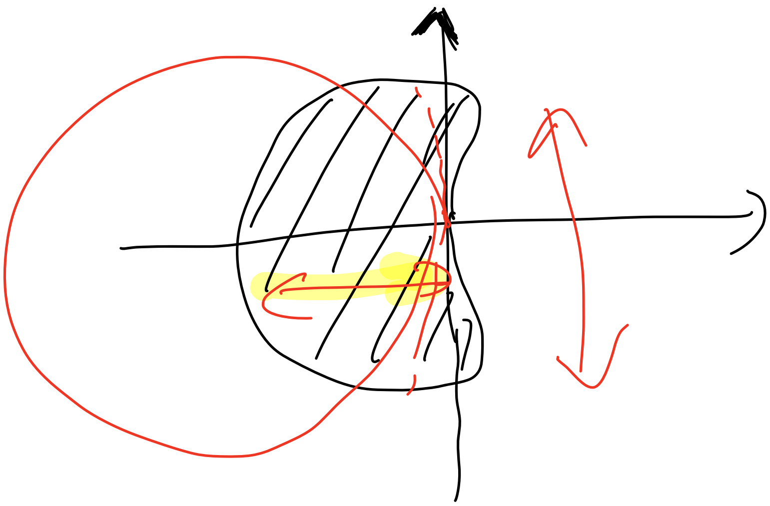
stage 2: $u^{n+1} = u^n + \frac{\tau A}{2}(u^n + u^{n+1,*})$

$= u^n + \tau A u^n + \frac{\tau A^2}{2} u^n$

$= I + \tau A + \tau^2 A^2/2\, u^n$

RK3:

$$u^{n+1} = \left(I + \tau A + \frac{\tau^2 A^2}{2} + \frac{\tau^3 A^3}{6}\right) u^n$$



AB3

Diffusion easy to add
but also works for $d = 0$!

IMEX RK methods
(implicit diffusion, explicit advection)

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

To get an actual 3^{rd} 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*:

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

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

$$\begin{cases} \theta = 0 : & \text{forward Euler} \\ \theta = 1/2 : & \text{Implicit midpoint} \\ & (2^{nd} \text{ order}) \\ \theta = 1 : & \text{Backward Euler (implicit)} \end{cases}$$

Local truncation error:

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

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

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

Therefore, the modified equation is

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

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

midpoint

$$\begin{cases} \text{FE } (\theta = 0): & \tilde{A} \simeq A - \dfrac{\tau A^2}{2} \\ \text{BE } (\theta = 1): & \tilde{A} \simeq A + \dfrac{\tau A^2}{2} \\ \text{Mid } (\theta = 1/2): & \tilde{A} \simeq A - \dfrac{\tau^2}{12} A^3 \end{cases}$$

For advection

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

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

So we get :

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

artificial dispersion

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

Consider the simplest FD/FV 1st order upwind :

$$\bar{u}_j^{n+1} = \bar{u}_j^n - \frac{a\tau}{h}\left(\bar{u}_j^n - \bar{u}_{j-1}^n\right)$$

(or add bars for FV)

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

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

$0 \le \nu \le 1$ 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

$$u_j^{n+1} = u_{j-1}^n \quad (a > 0)$$

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

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

this uses FD interpretation but also OK to 2^{nd} order for FV and is simpler so we use it

Now do Taylor series $\Rightarrow$

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

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

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

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

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HW 1 discussion

$$u_j^{n+1} = u_{j-1}^n$$

1. Why is upwinding so good for

$$\tau = \frac{h}{a} \Rightarrow \nu = \frac{a\tau}{h} = 1$$

2. Empirical order of accuracy

a) method

b) plots

c) asymptotic regime (small p)

3. Validation

a) Conservation

b) Term-by-term

c) Exact solution

d) Manufactured solution

Method of manufactured solution

$$u_t + (au)_x = (du_x)_x + s(x,t)$$

Choose $\quad u = \sin^{100}(\pi(x-at))$

$$(\underbrace{du_x}_{\text{flux}})_x = \underline{d_x u_x + d u_{xx}},$$

$$(au)_x = a_x u + a u_x$$

$$DU$$

$-\,SPD \qquad d \geq 0$

$$(du_x)_x = (\underbrace{\partial_x \, d \, \partial_x}) U$$

$$\partial_x^* = -\partial_x$$

$$-\hat{A} B A^T \qquad = -(\partial_x^* \underline{d} \, \partial_x) U$$

$$\mathrm{Diff} = -D^T d D$$

$$(Du)_{j+1/2} = \frac{u_{j+1} - u_j}{h}$$

$$(D^T f)_j = \frac{f_{j+1/2} - f_{j-1/2}}{h}$$

$$\tau \sim h$$

$$\tau = h/a$$

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

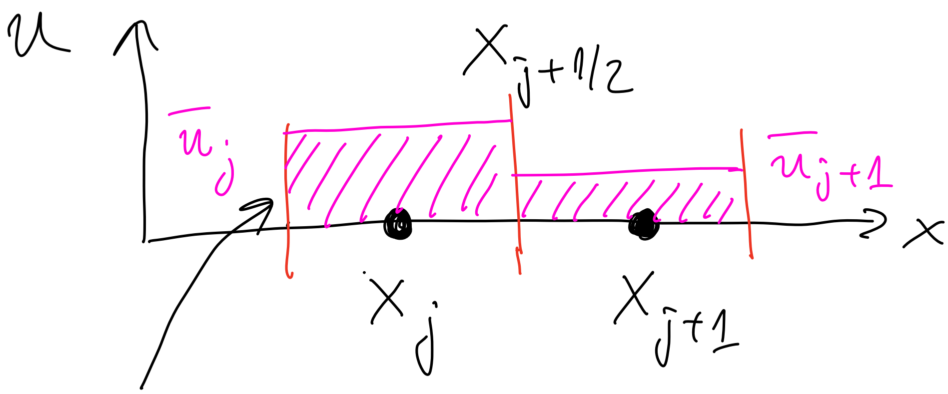
as derived already

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 Le Veque 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.

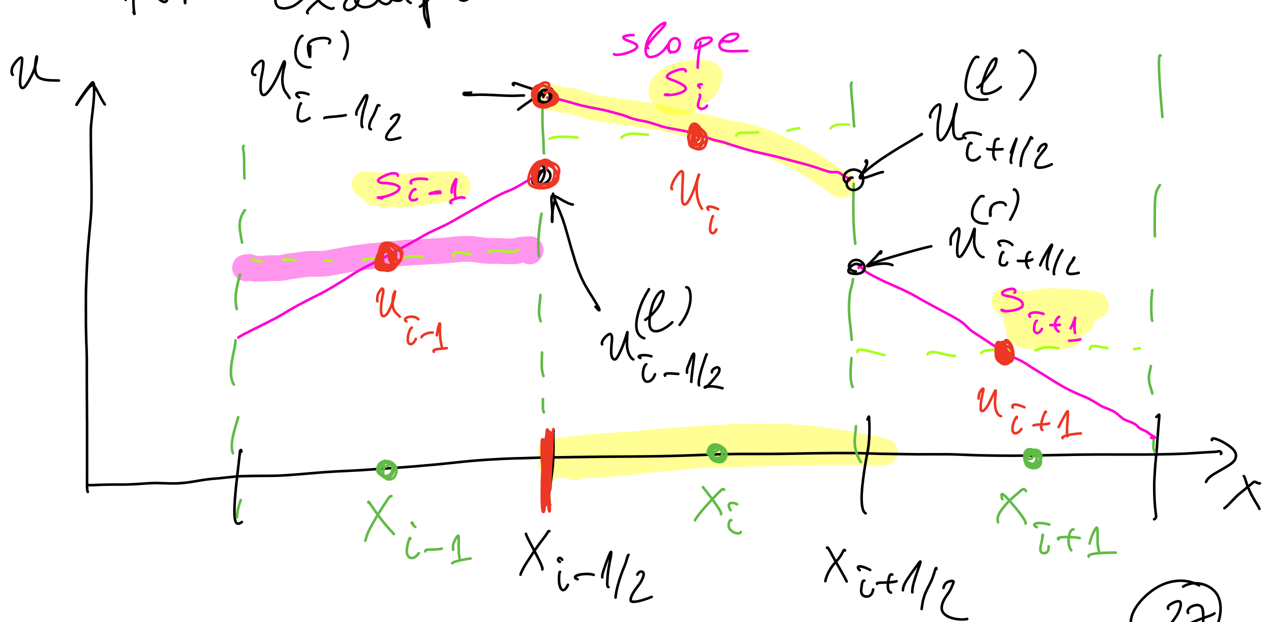
For upwind we used a



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 <u>slopes</u> s_i of the linear reconstruction.

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

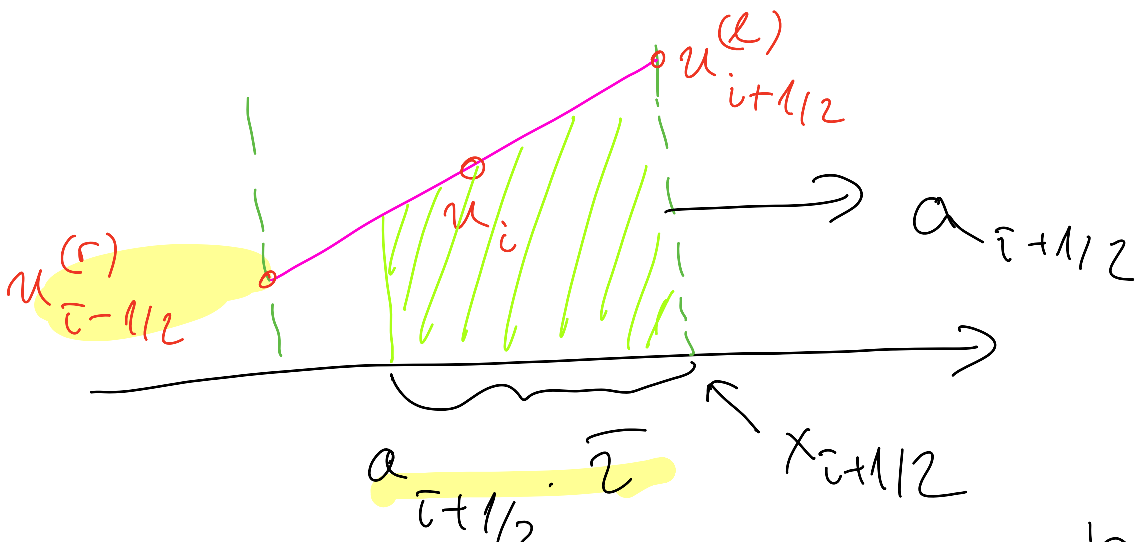
$$+ s_i (x - x_i) \quad \underbrace{+ O(h^2)}_{\text{still same order}}$$

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

Now we need to decide if we want a MOL scheme (instantaneous fluxes) or a space-time scheme (time-average fluxes). NOTE! STUFF BELOW ONLY CORRECT FOR $a = \text{const}$

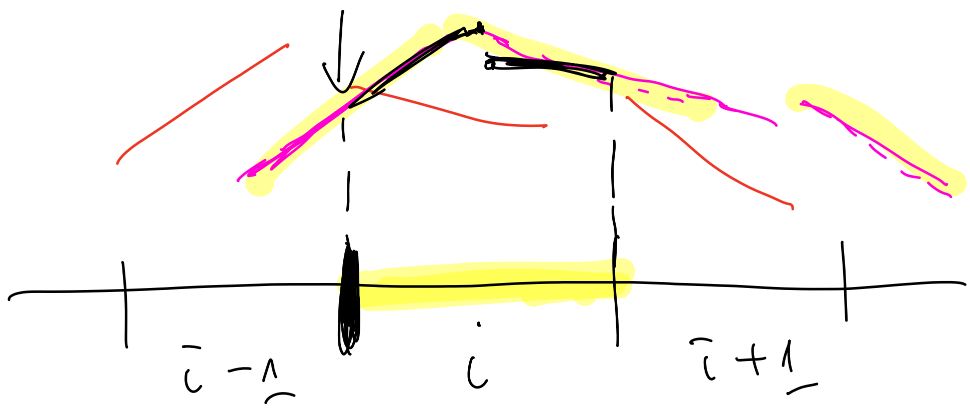
Let's start with Space-Time:



Upwind average flux:

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

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



reconstruct → advect by Δt

→ average to cells

$$f_{i+1/2} = a_{i+1/2}\Big(\overbrace{\bar{u}_i + \frac{h}{2}\, s_i \,(1-\nu_{i+1/2})}^{\text{area of trapezoid}}\Big)$$

where advective CFL number

$$\nu_{i+1/2} = \frac{a_{i+1/2}\,\bar{\tau}}{h}, \quad 0 < \nu_{i+1/2} < 1$$

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

To complete the scheme we need to choose the slopes.

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

leads to the Lax-Wendroff scheme:

$$\rightarrow f_{i+1/2} = \frac{a_{i+1/2}}{2}\Big[(1+\nu_{i+1/2})\,\bar{u}_i + (1-\nu_{i-1/2})\,\bar{u}_{i+1}\Big]$$

assume $a = \text{const}$

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

A

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

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

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

LW is $\underline{\underline{\text{not}}}$ MOL

$$\bar{u}_t = A\bar{u}$$

$$\bar{u}(t+\tau) = \bar{u}(t) + A\bar{u}\tau + \left(\frac{A^2}{2}\right)_{LW}\tau^2\,\bar{u} + h.o.t.$$

$$\frac{A^2\tau^2}{2}\bar{u} =$$

centered

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

wide stencil

$\underline{\underline{\text{NOT}}}$ a good stencil

odd & even points decouple

has zero eigenvalues

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

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

Giving

$$u(t+\Delta t) \simeq u(t) - \nu h\, u_x(t) + \frac{(\nu h)^2}{2} u_{xx}(t)$$

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 obsures the FV nature of the method & is hard to generalize to other hyperbolic equations

Note LW is <u>not</u> a MOL scheme – why?

$\boxed{\text{Discuss in class}}$

The modified equation for LW is:

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

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

Centered slopes

$$\Rightarrow \quad s_i = \frac{\bar{u}_{i+1} - \bar{u}_{i-1}}{2h}$$

with linear reconstruction gives the time-averaged upwind flux:

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

assume $a = \text{const}$.

Which leads to Fromm's method (*much* better than LW)

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

not second order

$$- \frac{\nu(1-\nu)h^2}{2}\underbrace{\left(\frac{\bar{u}_{i+1} - \bar{u}_i - \bar{u}_{i-1} + \bar{u}_{i-2}}{h^2}\right)}_{\text{upwinded difference } \sim\, u_{xx}}$$

not second order

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 Fromm:

$$\Rightarrow u(x, t+\tau) \simeq \underbrace{u - a\tau u_x + \cancel{\frac{ah\tau}{2}} u_{xx}}_{\text{upwind piece}}$$

$$- \cancel{\frac{\nu h^2}{2}} u_{xx} + \frac{(\nu h)^2}{2} u_{xx} + O(h^2)$$

which is the correct Taylor series just like LW, so Fromm is also <u>second order</u> in space-time.

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

$$\Rightarrow f^n_{i+1/2} \simeq a\, u^{n+1/2}_{i+1/2} \simeq a\, u_{i+1/2}\left(x_i + \frac{h}{2},\, t^n + \frac{\tau}{2}\right)$$

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 $a>0$, use a Taylor series in the <u>upwind</u> cell:

$$u_{i+1/2}^{n+1/2} = u_i^n + \frac{\tau}{2}(u_t)_i^n + \frac{h}{2}(u_x)_i^n$$

$\downarrow$ PDE const. coeff.:

$$\xrightarrow{a_{i+1/2}} \quad = u_i^n - \frac{a\tau}{2}(u_x)_i^n + \frac{h}{2}(u_x)_i^n$$

$i \quad i+1/2$

$$= \bar{u}_i^n + \frac{h}{2}(1-\nu)\, S_i^n \Leftarrow \text{slope}$$

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 3^{rd} order MOL scheme, we need a quadratic reconstruction

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

With FV conditions:

$$\begin{cases} \displaystyle\int_{x_{i-1/2}}^{x_{i+1/2}} u_i(x)\,dx = \bar{u}_i \cdot h \\ \displaystyle\int_{x_{i-3/2}}^{x_{i-1/2}} u_i(x)\,dx = \bar{u}_{i-1} \cdot h \\ \displaystyle\int_{x_{i+1/2}}^{x_{i+3/2}} u_i(x)\,dx = \bar{u}_{i+1} \cdot h \end{cases}$$

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:

upwind cell

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

leads to the 3^rd order upwind-biased scheme:

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

if $a>0$

that I mentioned before

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.

$\boxed{\text{Discuss some options in class}}$

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:

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

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

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

PDE

$$= a^2 u_{xx} \underbrace{-2ad\, u_{xxx}}_{\text{hard part}} + d^2 u_{xxxx}$$

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:

$$-\left(a(x)u(x)\right)_x + \left(d(x)u_x\right)_x =$$

$$-a_x u - a u_x + d_x u_x + d u_{xx}$$

Discuss why in class

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

$$\boxed{u_t = \underbrace{Au}_{\text{e.g. advection}}} + \underbrace{Bu}_{\text{e.g. diffusion}}$$

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

$$\Rightarrow u^{n+1} = \underbrace{A\left(\tfrac{\tau}{2}\right)}_{\text{advect for half a step}} \underbrace{B(\tau)}_{\text{Diffuse for one step}} \underbrace{A\left(\tfrac{\tau}{2}\right)}_{\text{advect for half a step}} u^n$$

e.g. advect for half a step, Diffuse for one step, advect for half a step

While this is a good method for ODEs, it has problems for PDEs. $\boxed{\text{Discuss in class issues}}$

BCs hard to implement & expensive

Here is a better space-time approach.

$$u_t = \overbrace{(A+B)}^{C} u \implies$$

$$u(t+\tau) = u(t) + C\tau\, u(t) + \frac{C^2\tau^2}{2} u(t)$$

$$u^{n+1} = u^n + \tau (A+B) u^n +$$

$$\implies \frac{\tau^2}{2}\left(A^2 + B^2 + AB + BA\right) u^n + O(\tau^3)$$

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

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

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

<u>**BUT**</u> in general (BCs, higher dimensions, non-constant coefficients) $AB \neq BA$ do <u>not</u> commute and we should <u>not</u> assume that.

If we just tried, for example,

$$\frac{u^{n+1} - u^n}{\tau} = \text{Lax-Wendroff or Frommer etc.} + d\left(\frac{u_{xx}^{n+1} + u_{xx}^n}{2}\right) \leftarrow \text{Crank-Nicolson}$$

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

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

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

$$= \left(I + \frac{B\tau}{2} + \frac{B^2\tau^2}{4} + O(\tau^3)\right] \cdot$$

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

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

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

How do we get it?

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

constant source term

② Solve $u_t = Bu + \underbrace{\nabla \cdot F^{adv}}_{\text{constant source term}}$

with any 2nd order scheme to compute $u^{n+1} \simeq u(t+\tau)$

Why does this work?

① $u_t = Au + Bu^n$ ← constant source term

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

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

② Now we solve

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

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

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

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

$$+ \frac{\tau^2}{2} B \left[A\left(I + \underbrace{\cancel{\frac{\tau}{2}A + \frac{\tau}{2}B}}_{O(\tau^3)}\right)u^n \right]$$

$$= \left[\left(I + \tau A + \frac{\tau^2}{2}A^2\right) + \left(I + \tau B + \frac{\tau^2}{2}B^2\right) + \frac{\tau^2}{2}\left(\underline{AB + BA}\right) + O(\tau^3) \right] u^n$$

as required for second-order accuracy in time!

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

$$\begin{cases} u_t = Au + s & \leftarrow \text{constant} \\ u_t = Bu + s & \leftarrow \text{source term} \end{cases}$$

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 excercise that this 2-step Adams-Bashforth + source

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

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

is 2^{nd} order in time for ODE:

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

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

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

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

<u>Aside</u>: Later, in immersed-boundary methods, we will solve:

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

using:

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

Lax-Wendroff with source term

Back to solving

(1) $u_t = Au + S$

(2) $u_t = Bu + S$

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

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

How do we add source term for advection?

cell-centered

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

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

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

$$\Rightarrow \quad u(t+\tau) = u(t) - \tau a u_x + \tau s + \frac{\tau^2}{2}\left(a^2 u_{xx} - a s_x\right)$$

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

$$u_i^{n+1} = u_i^n - \frac{a\tau}{2h}\left(u_{i+1}^n - u_{i-1}^n\right) + s_i \cancel{\Delta t} + \frac{a\tau^2}{2h^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right) - \frac{a\tau^2}{4h}\left(s_{i+1} - s_{i-1}\right)$$

?

All terms on rhs involving $\boxed{a}$ 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 advective Courant (CFL) number but not diffusive CFL, i.e., we want

$$\frac{a\,\Delta t}{\Delta x} \le C \simeq 1$$

$$\frac{d\tau}{h^2} \le \frac{1}{2} \quad = 10$$

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 Fromm

TO BE FINISHED....

Note that the highlighted term

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

$S = Bu^n$

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

$$S_j = \frac{d}{h^2}\left(u^n_{j+1} - 2u^n_j + u^n_{j-1}\right)$$

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

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

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

Addendum: 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:

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

$$u^{n+1/2}_{j+1/2} = \bar{u}^n_j + \frac{\Delta x}{2}\underbrace{(u^n_x)_j}_{=S_j} + \frac{\Delta t}{2}\left(u^n_t\right)_j$$

PDE

space der

And here we will use chain rule + PDE to estimate u^n_t:

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

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

centered slopes

$$S_j = \frac{u_{j+1} - u_{j-1}}{2h}$$

for Fromm

Advective flux estimate:

has to be $n+1/2$

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

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

Remember that for advection-diff.

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

comes from diffusion. For constant

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

this approach gives an extra term:

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

$$= \text{usual Fromm scheme}$$

$$- \frac{a d \tau^2}{2} \underbrace{\left(\frac{u_{j+1} - 3u_j + 3u_{j-1} - u_{j-2}}{h^3} \right)}_{\text{Upwind difference for } (u_{xxx})_j}$$

to be compared to Lax-Wendroff scheme:

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

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

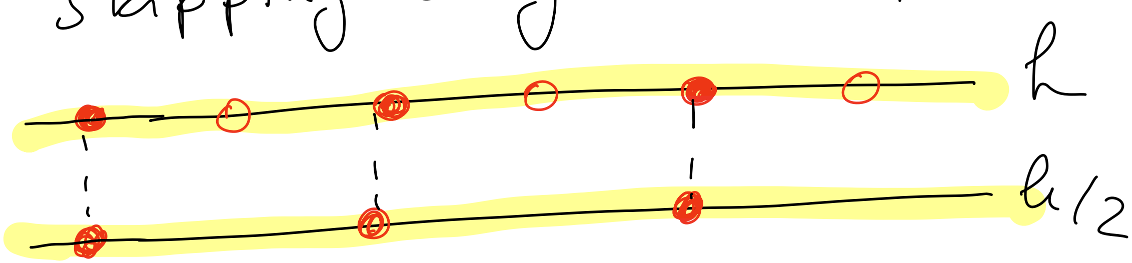
Addendum: Empirical error for FVM

In order to estimate the error via successive refinement

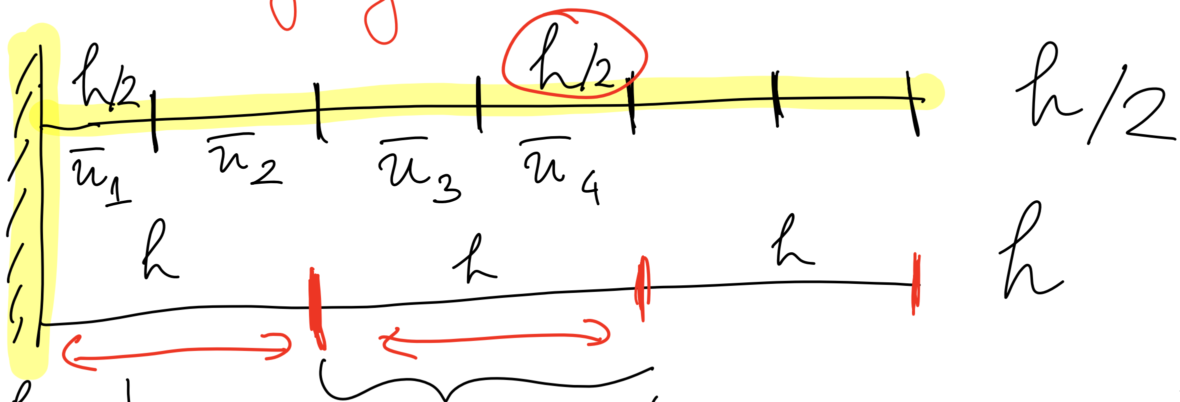
$$\tilde{E}(x,h) = u_h(x) - u_{h/2}(x)$$

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:

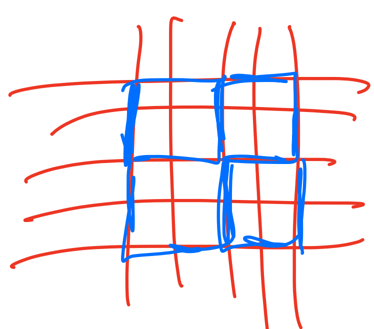


But for FV methods remember we know $\overline{u}_k$ not u_k, so we coarsen the grid by averaging:



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

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.)



$$u_t = Au + Bu$$

$$u_t + (au)_x = (d u_x)_x$$

$$\frac{u^{n+1} - u^n}{\Delta t} + \underbrace{\left[(au)_x \right]^{n+1/2}}_{\text{Fromm}} = \frac{(d u_x)_x^{n+1} + (d u_x)_x^n}{2}$$

$$\int_{x_j - \frac{h}{2}}^{x_j + h/2} u_{exact}(x, t)\, dx$$