(4) However, MOL is not the only approach. Also, it can be misleading to consider space and time as disjoint dimensions, and it is better to analyze the spatio-temporal error.

Let us first consider an example of a non-MOL scheme, the famous Lax-Wendroff scheme.

Although not originally developed this way, this is our first example of a semi-Lagrangian scheme.

5 So far we have considered Eulerian schemes: the grid is fixed and the fluid moves relative to the grid.

But for pure advection it is much more natural to ~~xxxx~~ follow the characteristics of the equation, which is a Lagrangian method:

$$u_t + \underline{a} \cdot \nabla u = 0 \quad , \quad \underline{a}(r,t) \text{ known}$$

Define a Lagrangian tracer:

$$\frac{d\xi(t)}{dt} = \underline{a}\left[\xi(t), t\right]$$

$$\Rightarrow \frac{du}{dt}\left[\xi(t), t\right] = 0 \Rightarrow u\left[\xi(t), t\right] = \text{const}$$

(6) So we can ~~~~ solve the pure advection equation by following the characteristics $\xi(t)$ along a collection of Lagrangian points

$$\boxed{u[\xi(t), t] = u[\xi(0), 0]}$$

This has many practical issues (discuss on board).

An alternative is to combine Eulerian and Lagrangian approaches. In <u>semi-Lagrangian</u> approaches we read the values of $u(r,t)$ on a fixed

(7) Eulerian grid, but we do this by following the characteristics backward in time to find the value from the past:

$$\begin{cases} u(x_j, t_{n+1}) = u(\xi(t_n), t_n) \\ \dfrac{d\xi}{dt} = a(\xi, t) \quad \text{(Backward from } t_{n+1} \to t_n) \\ \xi(t_{n+1}) = x_j \end{cases}$$

How do we now discretize this?
Let's focus on Lax-Wendroff

(8) $u_t + a u_x = 0$

$\Rightarrow u(x_j, t_{n+1}) = u(x_j - \tau a, t_n)$

Denote $\boxed{\nu = \frac{\tau a}{h}}$ $\rightarrow$ advective Courant or CFL number

$\Rightarrow \tau a = \nu h$

Lax-Wendroff can be obtained by using quadratic interpolation to get $u(x_j - \tau a, t_n)$:

Assume $\boxed{-1 \leq \nu \leq 1}$ CFL condition interpolate

$$u(x_j - \nu h) \approx \frac{1}{2}\nu(\nu+1)\, u(x_{j-1}) + (1-\nu^2)\, u(x_j) + \frac{1}{2}\nu(\nu-1)\, u(x_{j+1})$$

$a \geq 0$ <u>or</u> $a \leq 0$

This leads to the scheme: Lax-Wendroff

$$\boxed{w_j^{n+1} = w_j^n + \frac{a\tau}{2h}\underbrace{\left(w_{j-1}^n - w_{j+1}^n\right)}_{\text{forward Euler for centered advection}} + \frac{1}{2}\left(\frac{a\tau}{h}\right)^2 \underbrace{\left[w_{j-1}^n - 2w_j^n + w_{j+1}^n\right]}_{\text{second-order diffusive correction}}}$$

Lax-Wendroff (the usual one) solves (8)

$$u_t = A u$$

$$u^{n+1} = \{ I + \underbrace{A \Delta t}_{\substack{\text{centered}\\ \text{difference}}} + \underbrace{\tfrac{1}{2} A^2 \Delta t^2}_{\substack{\text{centered diffusion}\\ \neq (\text{centered diff})^2}} \} u^n$$

$$\left(\frac{A^2}{2} u^n\right)_i = \frac{a^2}{2} \frac{1}{2\Delta x} \left[\left(\frac{u_{i+1+1} - u_{i+1-1}}{2\Delta x} \right) - \left(\frac{u_{i-1+1} - u_{i-1-1}}{2\Delta x} \right) \right]$$

$$= \frac{a^2}{8\Delta x^2} \left[u_{i+2} - 2u_i + u_{i-2} \right]$$

$$\neq \frac{a^2}{2\Delta x^2} \left[u_{i+1} - 2u_i + u_{i-1} \right]$$

So what Lax-Wendroff is doing (9)
is really

$$u^{n+1} = \left\{ I + A\,\Delta t + \frac{1}{2}\tilde{A}^2 \Delta t^2 \right\} u^n$$

where $\tilde{A}^2 \approx A^2$ but not equal

This is why it is $\underline{\underline{\text{NOT}}}$ an MOL scheme - MOL would only have one A!

But for purposes of $\underline{\underline{\text{error}}}$ analysis (second-order accuracy) we can treat Lax-Wendroff as doing $\tilde{A}^2 = A^2$

(10) The Lax-Wendroff scheme is not a MOL scheme in the usual sense. Note that it can be generalized to non-constant coefficients and higher dimensions (more to follow)

In either case (MOL or space-time), linear one-step difference schemes for linear PDEs look like

$$\boxed{B_0 w_{n+1} = B_1 w_n + G_h(t_n, t_{n+1})}$$

$\mathbb{R}^{m \times m}$ matrices

implicit part

explicit

(11) <u>Global error</u> $\varepsilon_n = u_h(t_n) - w_n$
(space-time)

<u>Truncation error</u> ρ_n:

$$B_0 u_h(t_{n+1}) = B_1 u_h(t_n) + G(t_n, t_{n+1}) + \underline{\underline{\tau \rho_n}}$$

$$\Rightarrow \quad B_0 \varepsilon_{n+1} = B_1 \varepsilon_n + \tau \rho_n$$

$$\Rightarrow \quad \boxed{\varepsilon_{n+1} = B_0^{-1} B_1 \varepsilon_n + \delta_n}$$ error growth

$$\boxed{\delta_n = \tau B_0^{-1} \rho_n}$$ $\rightarrow$ <u>Local error</u>
(space-time)

If $B_0 = I \Rightarrow \delta_n = \rho_n$

(12)

$$\begin{cases} \varepsilon_{n+1} = B\,\varepsilon_n + \delta_n \\ B = B_0^{-1} B_1 \end{cases}$$

Consistency: $\|\rho_n\| \to 0$ as $(\tau, h) \to 0$

Stability: $\begin{cases} \|B^n\| \le K_n, \; n \ge 0, \; n \le \frac{T}{\tau} \\ K_n \text{ independent of } \tau, h \end{cases}$

If we assume the natural

$$\|B_0^{-1}\| \le C \Rightarrow$$

independent of h, τ

$$\|\delta_n\| \le C\tau \|\rho_n\| \quad \text{so}$$

so consistency bounds the local error

$$\boxed{\text{consistency} + \text{stability} \Longleftrightarrow \text{convergence}}$$

(Lax Equivalence theorem)

$$\|\varepsilon_n\| \leq K\|\varepsilon_0\| + K\sum_{k=0}^{n-1}\|\delta_k\|$$

$$\boxed{\|\varepsilon_n\| \leq K\|\varepsilon_0\| + KC\,t_n \max_{0\leq k\leq n-1}\|\delta_k\|}$$

error estimate / bound

The Lax-Wendroff scheme is consistent and stable if $\boxed{|\nu| \leq 1}$, which is a typical stability condition for advection.

Space – Time METHODS

FOR ADVECTION – DIFFUSION

CFD FALL 2014

A. DONEV

(some notes & comments)

Recall that Lax-Wendroff is NOT an MOL (method-of-lines) scheme, it is a space-time scheme.

It's local truncation error is:

$$\tau = -\frac{1}{6} a \Delta x^2 (1-\nu^2) u_{xxx} + O(\Delta t^3)$$

where $\nu = \frac{a \Delta t}{\Delta x}$ is CFL number

$$\rho = -\frac{1}{6} u_{xxx} \left(\Delta x^2 - a^2 \Delta t^2 \right)$$

which is a sum of a spatial and a temporal error just like MOL schemes. But this is NOT always the case.

Consider the Lax-Friedrichs method

$$u_i^{n+1} = \underbrace{\frac{1}{2} \left(u_{i-1}^n + u_{i+1}^n \right)}_{\substack{\text{stabilization} \\ \text{(not MOL)}}} - \underbrace{(\Delta t) a \frac{u_{i+1}^n - u_{i-1}^n}{2 \Delta x}}_{\substack{\text{Centered difference} \\ \text{+ Euler (UNSTABLE)}}}$$

Stable if $CFL \leq 1$

Doing Taylor series on (3)

$$\frac{1}{2}\left(u_{i-1}^n + u_{i+1}^n\right) = u_i^n + \frac{1}{2}\Delta x^2 u_{xx}$$

we see that the <u>modified equation</u> is

$$u_t = -a u_x + \underbrace{\frac{1}{2}\frac{\Delta x^2}{\Delta t} u_{xx}}_{\text{Numerical (artificial) dissipation}}$$

The Lax-Friedrichs method is <u>not</u> even <u>consistent</u> if $\Delta t \to 0$ keeping Δx fixed: One must refine both space <u>and</u> time together for space-time schemes

The error for Lax-Friedrichs is

$$\varepsilon = \frac{1}{2} a \Delta x \left(\nu^{-1} - \nu \right) u_{xx} + O(\Delta t^2)$$

so it must be run with $\nu \simeq 1$

When talking about non-MOL schemes we are looking at space-time error

$$\boxed{\nu = \text{const} \Rightarrow \Delta t = O(\Delta x) \quad \text{(for advection problems)}}$$

Note that for explicit (conditionally stable) methods we can never refine in space only due to $\nu \leq 1$ limit

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High-Resolution Advection

A. Donev, CFD, Fall 2014

Recall the Lax-Wendroff scheme for

$$u_t + a u_x = 0$$

$$u_i^{n+1} = b_{-1} u_{i-1}^n + b_0 u_i^n + b_1 u_{i+1}^n$$

$$\begin{cases} b_{-1} = \frac{1}{2} c(1+c) \\ b_0 = 1 - c^2 \\ b_1 = -\frac{1}{2} c(1-c) \end{cases} \quad \text{where } c = \frac{a \Delta t}{\Delta x}$$

which we derived as a semi-Lagrangian scheme by tracing characteristics backward

(2) Note that the coefficients b_{-1}, b_0, b_1 can easily be derived by performing truncation error (in both space and time) analysis to obtain the 2nd order accuracy conditions:

$$\begin{cases} b_{-1} + b_0 + b_1 = 1 \\ b_{-1} + b_1 = c^2 \\ b_{-1} - b_1 = -c \end{cases}$$

But here our focus will be on alternative derivations that could be generalized to other equations

3 ANOTHER WAY TO DERIVE LAX-WENDROFF:

$$u_t + a u_x = 0 \Rightarrow$$

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

$$= + a^2 (u_x)_x = a^2 u_{xx}$$

$$u(\Delta t) = u(0) + \Delta t\, u_t + \frac{\Delta t^2}{2} u_{tt} =$$

$$= u(0) \underbrace{- \Delta t\, u_x}_{\text{Use centered advection}} + \underbrace{\frac{\Delta t^2 a^2}{2} u_{xx}}_{\text{Use centered diffusion}}$$

This kind of game swapping time for space derivatives is common!

(13) We can also try a <u>midpoint</u> scheme where we try to <u>extrapolate</u> state to the faces at the midpoint:

$$\left(f_{i+1/2}^{\downarrow}\right)^{n} \simeq a\, u_{i+1/2}^{n+1/2}$$

$$\simeq a\, u\left(x_i + \frac{\Delta x}{2},\ t^n + \frac{\Delta t}{2}\right)$$

Use Taylor series and the PDE

$$u_t = -f_x = -a u_x$$

$$u_{i+1/2}^{n+1/2} \simeq u_i^n + \frac{\Delta t}{2}(u_t)_i^n + \frac{\Delta x}{2}(u_x)_i^n$$

$$= u_i^n - \frac{a\Delta t}{2}(u_x)_i^n + \frac{\Delta x}{2}(u_x)_i^n$$

(14)

$$u_{i+1/2}^{n+1/2} \approx u_i^n + \frac{1}{2}(\Delta x - a\Delta t)(u_x)_i^n$$

New we need to approximate the slope by finite differences

Use centered approximation

$$(u_x)_i^n \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

$$f_{i+1/2}^n = a u_i + \frac{a(1-c)}{4}(u_{i+1} - u_{i-1})$$

which is the same as <u>Fromm's method</u> but derived from a different perspective

Now consider using Lax-Wendroff with diffusion (5)

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

First, figure out what the correct second-order Taylor series is:

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

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

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

$$\Rightarrow u^{n+1} = u^n + (-a u_x + d u_{xx})\Delta t + \frac{\Delta t^2}{2}(a^2 u_{xx} - 2ad\, u_{xxx} + d^2 u_{xxxx}) + \dots$$

It is NOT a good idea to now proceed to discretize everything using centered differences. Instead, use Lax-Wendroff only for advection and Crank-Nicolson (implicit midpoint) for diffusion. How?

First, let us consider a more general splitting framework:

$$u_t = A\,u + B\,u$$

linear operators

$$\begin{cases} A \equiv -a\,\partial_x \\ B = d\,u_{xx} \end{cases}$$ in our case

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

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

In our case $A^2 = a^2 \partial_{xx}$,

$B^2 = d^2 u_{xxxx}$, $AB = -ad\, u_{xxx} = BA$

Note, however, that generally $AB \neq BA$ (non-constant coefficients, boundary conditions) so we should not assume this if we want a general approach.

So what Lax-Wendroff is doing is really 9

$$u^{n+1} = \left\{ I + A\,\Delta t + \frac{1}{2}\tilde{A}^2 \Delta t^2 \right\} u^n$$

where $\tilde{A}^2 \approx A^2$ but not equal

This is why it is <u>NOT</u> an MOL scheme - MOL would only have one A!

But for purposes of <u>error</u> analysis (second-order accuracy) we can treat Lax-Wendroff as doing $\tilde{A}^2 = A^2$

First try:

$$\frac{u^{n+1} - u^{n}}{\Delta t} = \text{Lax-Wendroff for advection} + d\left(\frac{u_{xx}^{n+1} + u_{xx}^{n}}{2}\right)$$

Crank-Nicolson

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

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

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

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Expand

$$\left(I - \frac{B\Delta t}{2}\right)^{-1} = I + \frac{B\Delta t}{2} + \frac{B^2\Delta t^2}{4}$$

to get

$$u^{n+1} = \left(I + \frac{B\Delta t}{2} + \frac{B^2\Delta t^2}{4}\right)$$

$$\left(I + \frac{B\Delta t}{2} + A\Delta t + \frac{A^2\Delta t^2}{2}\right) u^n$$

$$= \Big(I + B\Delta t + A\Delta t + \frac{A^2}{2}\Delta t^2$$

$$+ \frac{B^2\Delta t^2}{2} + \frac{BA}{2}\Delta t^2 + O(\Delta t^3)\Big) u^n$$

We are <u>missing</u> $\frac{AB}{2}\Delta t^2$! NOT SECOND ORDER

How to fix this?

There are many ways up to second order:

- Time splitting (e.g. Strang)
- Predictor-corrector schemes

They are expensive because they require either two CN-solves or two Lax-Wendr. steps per time step.

Instead:

(1) Solve $u_t^{(LW)} = Au + Bu^n$ ← source term

(2) Solve $u_t = Bu + u_t^{(LW)}$

where the approximation of the Lax-Wendr. is now a source term.

Lax-Wendroff with spatial source term (13)

$$u_t + a u_x = S(x)$$

$\nwarrow$ NOT a function of time

$$u_{tt} = -a(u_t)_x = -a(-a u_x + S)_x$$

$$= a^2 u_{xx} - a S_x$$

So

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

(for example)

In our case

$$S \equiv B u^n = d\, u_{xx}^n$$

$$S_i^n = d \left(\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \right)$$

Algebraically, what we have done is

$$u^{n+1} = \left(I + A\Delta t + B\Delta t + \frac{\tilde{A}^2}{2} \Delta t^2 + \frac{AB}{2} \Delta t^2 \right) u^n$$

which is <u>almost</u> second-order accurate (now missing $\frac{BA}{2} \Delta t^2$ term)

But it would not be A-stable because diffusion is treated explicitly

Instead, do Crank-Nicolson for diffusion but treat the Lax-Wendroff update as a source term:

$$\frac{u^{n+1}-u^{n}}{\Delta t} = \frac{B}{2}\left(u^{n+1}+u^{n}\right) + \left(A\,\Delta t + \frac{\tilde{A}^2\Delta t^2}{2} + \frac{AB}{2}\Delta t^2\right)u^n$$

centered advection

centered diffusion

Lax-Wendroff

source-term second correction

So now

$$u^{n+1} = \left(I + \frac{B\Delta t}{2} + \frac{B^2\Delta t^2}{4}\right) + O(\Delta t^3) \leftarrow \text{SECOND ORDER !}$$

$$\times\left(I + \frac{B\Delta t}{2} + A\,\Delta t + \frac{\tilde{A}^2}{2}\Delta t^2 + \frac{AB}{2}\Delta t^2\right)u^n$$

$$= \left[I + (A+B)\Delta t + \tfrac{1}{2}\left(\tilde{A}^2 + B^2 + AB + BA\right)\Delta t^2\right]u^n$$

How about stability? Is the only limitation now $\frac{a\Delta t}{\Delta x} \leq C \simeq 1$?

It turns out no, to get true stability for any diffusive CFL number we need some upwinding.

So, instead of Lax-Wendroff consider

Fromm's scheme (with diffusion)

We need source term:

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

to Fromm's method

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Extrapolate state to faces at midpoint as we did before: (17)

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

$$= u^n_j + \frac{\Delta x}{2}(u^n_x)_j + \frac{\Delta t}{2}\left(-a(u^n_x)_j + S_j\right)$$

$$= \left.u^n_j + \frac{1}{2}(\Delta x - a\Delta t)(u^n_x)_j \right\} \text{as before}$$

$$\left. + \frac{\Delta t}{2} S^n_j \right\} \text{new term}$$

And here $S \equiv d\, u_{xx}$ so

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

Note that this is <u>upwinded</u> since the extrapolation is done from the cell to the left!

Now

$$u_j^{n+1} = u_j^n - \Delta t\, a \left(\frac{u_{j+1/2}^{n+1/2} - u_{j-1/2}^{n+1/2}}{\Delta x} \right) + S_j^n \cdot \Delta t$$

is Fromm's scheme with a source.

The extra term added in $u_{j+1/2}^{n+1/2} - u_{j-1/2}^{n+1/2}$:

$$-\frac{a\, d\, \Delta t^2}{2\Delta x^3} \left[(u_{j+1} - 2u_j + u_{j-1}) - (u_j - 2u_{j-1} + u_{j-2}) \right]$$

$$= -\frac{a\, d\, \Delta t^2}{2\Delta x^3} \left[u_{j+1} - 3u_j + 3u_{j-1} - u_{j-2} \right]$$

$$\rightarrow -\frac{ad}{2} (u_{xxx})_j\, \Delta t^2$$

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Talyor series shows this is a discretization of $A\frac{B\Delta t^2}{2} \equiv -\frac{ad}{2}(u_{xxx})_j \Delta t^2$

but here u_{xxx} is <u>upwind biased</u>.

Compare this to what Lax-Wendroff does, giving $AB\Delta t^2/2$ in the form

$$-\frac{a\,d\,\Delta t^2}{2\Delta x^3}\left[(u_{j+2}-2u_{j+1}+u_j)-(u_j-2u_{j-1}+u_{j-2})\right]$$

$$=-\frac{a\,d\,\Delta t^2}{2\Delta x^3}\left[u_{j+2}-2u_{j+1}+2u_{j-1}-u_{j-2}\right]$$

$$\rightarrow -\frac{ad}{2}(u_{xxx})_j\,\Delta t^2$$

but this is centered now.