MAT228B - Lecture 1 - 1/9/17

Recall in 228A - studied Poisson eqn $\Delta u = f$
& used this to learn
- how to discretize (mostly finite difference)
- how to solve discretized eqns (algebraic)
- how to talk about accuracy, convergence

In this course (228B) - time-dependent problems

Heat/Diffusion eqn: $u_t = D u_{xx}$
Advection eqn: $u_t + a u_x = 0$
(standard model problems for this course)

Wave eqn: $u_{tt} = c^2 u_{xx}$ (equivalent to 2 advection eqns)

Mixed eqns: $u_t + a u_x = D u_{xx} + R(u)$ advection-diffusion-reaction eqns.

Burger's eqn: $u_t + u \cdot u_x = D u_{xx}$

Inviscid burger's $D=0 \Rightarrow$ soln develops shocks!

All leads up to background for Incompressible Navier-Stokes

$$\rho(\underline{u}_t + \underline{u} \cdot \nabla \underline{u}) = -\nabla p + \mu \Delta u$$
$$\nabla \cdot \underline{u} = 0$$

Conservation Laws: $u_t + (f(u))_x = 0$ in 1D

$u_t + \nabla \cdot (\underline{F}(u)) = 0$ in higher D

Let $\rho(x,t)$ be a density, e.g. mass/length (in 1D volume)
Let $f(\rho)$ be a flux function = rate of stuff thru surface

e.g. in 1D, have $\frac{\text{mass}}{\text{time}}$ moving through a point
in 3D, $\frac{\text{mass}}{\text{time} \cdot \text{area}}$ thru surface

Let A be the amt. of stuff in $[x_1, x_2]$

$$A(t) = \int_{x_1}^{x_2} \rho(x,t)\,dx$$

$$\Rightarrow \frac{dA}{dT} = \frac{d}{dt}\int_{x_1}^{x_2} \rho(x,t)\,dx = -f(\rho(x_2,t)) + f(\rho(x_1,t)) = -\int_{x_1}^{x_2} (f(\rho))_x\,dx$$

nice enough $\Rightarrow \int_{x_1}^{x_2} \rho_t + (f(\rho))_x\,dx = 0$ integral form of conservation law

ρ nice, $[x_1, x_2]$ arbitrary $\Rightarrow$ integrand 0.

& we get $\rho_t + (f(\rho))_x = 0$ differential form

Let u be a chemical concentration (mols/vol)

u transported by a velocity a $\Rightarrow$ flux fn. $f(u) = \underset{\frac{\text{length}}{\text{time}}}{a}\,\underset{\text{amt./length}}{u} = \left[\frac{\text{amt.}}{\text{time}}\right]$ (in 1D)

advective flux.

Conservation law $\Rightarrow$ $u_t + (au)_x = 0$ ~~← advection eqn if a is constant.~~

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u transported by diffusion: diffusive flux fn. $f(u) = -Du_x$.

Conservation law $\Rightarrow$ $u_t + (-Du_x)_x = 0$ ← diffusion eqn. if D is constant

Example system of nonlinear conservation laws: Euler eqns (gasdynamics)

- → conservation of mass $\rho_t + (v\rho)_x = 0$
- → conservation of momentum $(\rho v)_t + (\rho v^2 + p)_x = 0$
- → conservation of energy $\mathcal{E}_t + (v(\mathcal{E}+p))_x = 0$

Diffusion eqn is model parabolic eqn.
Advection eqn is model hyperbolic eqn.
] behave way differently! need diff. numerical schemes

MATL 248 - Lecture 2 - 1/11/17

Appendix E MATERIAL: **Model Problems:**

- $u_t = D u_{xx}$ (parabolic eqn) $\quad u_t + a u_x = 0$ (hyperbolic eqn) $\Big]$ solns have very diff. behavior!

Def: $u_t = Lu$, where L is a diff. op., is parabolic if L is elliptic.

Def: The linear second order operator $L = \sum_{ij} a_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_i b_i \frac{\partial}{\partial x_i} + c$ is elliptic if $[A]_{ij} = a_{ij}$ is positive or negative definite.

Ex: If $A = I$, then L is the Laplacian.

Def: The linear first order system $\underline{u}_t + A \underline{u}_x = 0$ is hyperbolic if A has real eigenvalues & is diagonalizable.
(can rewrite as set of advection eqns. on the eigendirections)

Thm: The Wave Eqn $u_{tt} = c^2 u_{xx}$ is hyperbolic.

Pf: $u_{tt} = c^2 u_{xx}$

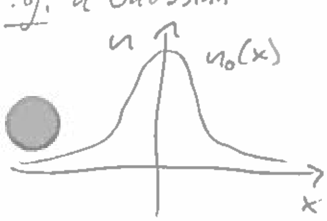
Consider $q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}$ w/ $q_1 = u_t$, $q_2 = -u_x$

Then $\partial_t q_1 = u_{tt} = c^2 u_{xx} = -c^2 \partial_x q_2$
& $\partial_t q_2 = -u_{xt} = -\partial_x (u_t) = -\partial_x q_1$ $\quad \Rightarrow \quad \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}_t = \begin{pmatrix} 0 & -c^2 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}_x$

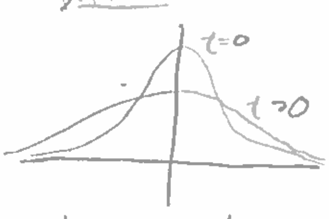
Hence $u_{tt} = c^2 u_{xx}$ is equiv. to $q_t + \underbrace{\begin{pmatrix} 0 & c^2 \\ 1 & 0 \end{pmatrix}}_{\text{eig. vals are } \pm c \,\leftarrow\, \text{wavespeeds!}} q_x = 0$
which is hyperbolic. $\square$

To solve either model problem, need an initial condition $u(x,0) = u_0(x)$.

e.g. a Gaussian:

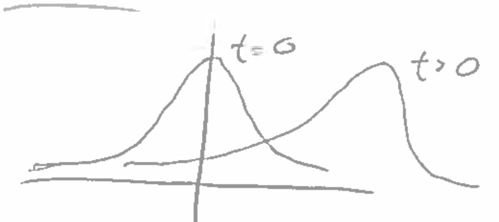


Diffusion:



soln spreads out

Advection



for $a > 0$, moves $u_0(x)$ to the right.
Soln: $u(x,t) = u_0(x - at)$

Consider initial condition $u_0(x) = e^{i\xi x}$

Look for solns of the form: $u(x,t) = G(t)e^{i\xi x}$

Then $u_t = g'e^{i\xi x}$, $u_x = i\xi g e^{i\xi x}$, $u_{xx} = -\xi^2 g e^{i\xi x}$

~~Advection eqn: $u_t + a u_x = 0$~~

$$g'e^{i\xi x} + ai\xi g e^{i\xi x} = 0, \quad g(0) = 1.$$

$$\Rightarrow g' = -ai\xi g \Rightarrow g(t) = e^{-ai\xi t}$$

Hence $u(x,t) = e^{i\xi(x-at)} = u_0(x-at)$.

change of phase

& $|u(x,t)| = 1 = |u_0(x)|$.

Transports initial data

☆ hard on discrete grid

Diffusion eqn: $u_t = Du_{xx} \Rightarrow g'e^{i\xi x} = -D\xi^2 g e^{i\xi x}$

$$\Rightarrow \begin{cases} g' = -D\xi^2 g \\ g(0) = 1 \end{cases}$$

$$\Rightarrow g(t) = e^{-D\xi^2 t} \Rightarrow u(x,t) = e^{-D\xi^2 t} e^{i\xi x}.$$

change of amplitude

& $|u(x,t)| = e^{-D\xi^2 t} \to 0$ as $t \to \infty$.

smooths initial data

☆ easy numerics

☆ Speed of decay depends on D and freq. ξ.

For diffusion eqn, if the initial data is discont's (or worse), it is instantly smoothed out
i.e. the soln is C^∞ for $t > 0$.

Fourier Transforms: $u(x) \in L^2(\mathbb{R})$ has Fourier transform

$$\hat{u}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} u(x) e^{-i\xi x} dx \in L^2(\mathbb{R})$$

& has inverse transform $u(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{u}(\xi) e^{i\xi x} d\xi$.

Parseval's Relation: $\|u\|_2 = \|\hat{u}\|_2$.

We'll use a discrete version of this to analyze numerical schemes

Fourier transform of Derivative. $u(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{u}(\xi) e^{i\xi x} d\xi$

$$u_x(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} i\xi \hat{u}(\xi) e^{i\xi x} d\xi$$

$$\Rightarrow \widehat{u_x}(\xi) = i\xi \hat{u}(\xi), \quad \widehat{u_{xx}}(\xi) = -\xi^2 \hat{u}(\xi).$$

$\begin{cases} u_t = Du_{xx} \\ u(x,0) = u_0(x) \end{cases}$ Apply FT

$\begin{cases} \hat{u}_t = -D\xi^2 \hat{u} \\ \hat{u}(\xi,0) = \hat{u}_0(\xi) \end{cases}$ ODE!

MAT228B - Lecture 3 - 1/13/17

Forward-time centered-space discretization of diffusion & advection

Problem:
$$\begin{cases} u_t = D u_{xx} & \text{on } (0,1)\times[0,\infty) \\ u(0,t) = 0 \\ u(1,t) = 0 \\ u(x,0) = g(x) \end{cases}$$

Start by discretizing space

$j=0$, $j=1$, ..., $j=N$, $j=N+1$; from 0 to 1 $\qquad \Delta x = \frac{1}{N+1}$

$x_j = j\Delta x$

$u_j(t) \approx u(x_j,t)$

Use standard 3-pt. diff operator to approx u_{xx}:

$$u_{xx}(x_j,t) \approx \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2}(t)$$

set of ODEs $\Rightarrow$
$$\begin{cases} \frac{du_j}{dt}(t) = D\frac{(u_{j-1} - 2u_j + u_{j+1})}{\Delta x^2}(t) & \text{for } j=1,\dots,N \\ u_j(0) = g(x_j) \end{cases}$$

$$\Rightarrow \begin{cases} \frac{d\underline{u}}{dt} = DL\underline{u} \\ \bar{u}(0) = \bar{g} \end{cases}$$

$\leftarrow$ can use ODE solvers on this eqn.
called the Method of Lines
be careful w/ choice of solver!
Often will find that a method designed for the PDE is more efficient

Simplest ODE Solver - Forward Euler: Divide time into equal spaced pts Δt apart.

Then discrete time $t_n = n\Delta t$. $\quad \frac{dy}{dt} = f(y)$ is our ODE to solve.

If $y^n \approx y(t_n)$, then $\frac{y^{n+1} - y^n}{\Delta t} \doteq f(y^n) \Rightarrow y^{n+1} \doteq y^n + \Delta t f(y^n)$.

For diffusion, $u_j^n \approx u(x_j,t_n)$, so $\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{D}{\Delta x^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n)$

$$\Rightarrow u_j^{n+1} = u_j^n + \frac{D\Delta t}{\Delta x^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n)$$

? will always work for small enough Δt. $\leftarrow$ blows up?!? sometimes depends on time step size & spatial scale.

What about Advection eqn: $\begin{cases} u_t + a u_x = 0 & \text{on } (0,1) \text{ periodic} \times [0,\infty) \\ u(x,0) = g(x) \end{cases}$

Discretize space, use standard 2-pt 2nd order centered difference operator for $\frac{d}{dx}$, & then forward-Euler for time:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) = 0$$

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

Solns grow slowly from initial data (BAD) & get slight lag

↳ seems to always happen despite tiny Δt.

↳ Will always grow! Bad numerical scheme, always fails.

What about Runge-Kutta(2) for time? No slippage, still small growth & then blows up.

- Still get phase lag!

↳ Always bound to fail eventually.

Runge-Kutta(4) for time? Norm shrinks, phase lag, soln-form gets awful

↳ works decently for smooth initial data.

☆ Will design schemes for advection eqn.

MAT 228B - Lecture 4 - 1/18/17

Given an ODE: $\begin{cases} y' = f(y) \\ y(0) = y_0 \end{cases}$ - an ODE method returns a sequence $y^n \approx y(n\Delta t)$ w/ $y^0 = y(0)$

Apply this method to $y' = \lambda y$ for $\lambda \in \mathbb{C}$. Let $z = \lambda \Delta t$.

Def: z is in the region of absolute stability of the method if

$$y^n \to 0 \quad \text{as} \quad n \to \infty. \quad \text{(limit of sequence, i.e. } n^{th} \text{ term goes to } 0\text{)}.$$

Region of absolute stability for Forward Euler:

$$\frac{y^{n+1} - y^n}{\Delta t} = \lambda y^n \quad \Rightarrow \quad y^{n+1} = y^n + \lambda \Delta t \, y^n = (1+z) y^n$$

Solve: $y^n = (1+z)^n y^0$ hence $y^n \to 0$ if $|1+z| < 1$

So z is in the region of absolute stability if $|1+z| < 1$.

For z real, this is $-1 < 1+z < 1 \Rightarrow -2 < z < 0$

$\Rightarrow -2 < \lambda \Delta t < 0$ for decaying solns, λ is negative $\Rightarrow \Delta t < \frac{\lambda}{2}$.

Max Time step prescribed!

For z complex, $|1+z| < 1$ is a disc of rad. 1 centered about $z = -1$

if λ neg. real part, expect decaying oscillations, ensure z in region for correct behavior!

Forward Euler for diffusion: $\begin{cases} u_t = D u_{xx} \\ u(0,t) = u(1,t) = 0 \\ u(x,0) = f(x) \end{cases}$

Discretize space & time:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{D}{\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) \quad \text{or} \quad \frac{\underline{u}^{n+1} - \underline{u}^n}{\Delta t} = L \underline{u}^n$$

So require $|1 + \lambda \Delta t| < 1$ for all λ eigvals of L

Eigvals of L are $\lambda_k = \frac{2D}{\Delta x^2}(\cos(k\pi \Delta x) - 1) = \frac{-4D}{\Delta x^2} \sin^2\left(\frac{k\pi \Delta x}{2}\right)$

$/ k = 1, \ldots, N$

w/ $\Delta x = \frac{1}{N+1}$. All real & negative, largest magnitude is $\lambda_N \approx -\frac{4D}{\Delta x^2}$.

Require that $-1 < 1 + \lambda_N \Delta t < 1 \Rightarrow -2 < -\frac{4D}{\Delta x^2}\Delta t < 0 \Rightarrow \boxed{0 < \Delta t < \frac{\Delta x^2}{2D}}$

for forward-Euler to be stable for the diffusion eqn.

Forward-Euler for advection (w/ centered difference):

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\,\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = 0$$

$$\frac{\underline{u}^{n+1} - \underline{u}^n}{\Delta t} = A\underline{u}^n$$

$\uparrow$ compute eig. values of cent. diff. op.

Eigvals of centered diff. op. on periodic domain:

Eigfns are $v_j^k = e^{\pi i k x_j}$ ← k^{th} eig. fn at j^{th} grid point.

Plugged into cent. diff. op:
$$\frac{e^{i\pi k x_{j+1}} - e^{i\pi k x_{j-1}}}{2\Delta x} = \frac{e^{i\pi k(x_j+\Delta x)} - e^{i\pi k(x_j-\Delta x)}}{2\Delta x}$$

$$(D_0\,\underline{v}^k)_j = \underbrace{\left(\frac{e^{i\pi k\Delta x} - e^{-i\pi k\Delta x}}{2\Delta x}\right)}_{\lambda} e^{i\pi k x_j}$$

Eigvals of cent. diff. op: $\lambda_k = \dfrac{i\sin(\pi k\Delta x)}{\Delta x}$

Region of absolute stability:

← eigvals on Im axis!
No way to fit all in region, always outside region!

The Diffusion eqn is numerically stiff.

↳ Negative real part eigenvalues w/ a large ratio
(some negative eigvals, & some really big negative eigvals)

$$\frac{d}{dt}y = \lambda y \implies \lambda \text{ neg. real is a decay rate}$$

For diffusion, $\lambda_k = -\dfrac{2D}{\Delta x^2}\left(\cos(k\pi\Delta x) - 1\right)$

Smallest eigvals are $O(1)$, largest eigvals are $O(1/\Delta x^2)$

Extreme scale separation in time.

MAT228B - Lecture 5 - 1/20/17

1D Diffusion eqn w/ Forward Euler, method of lines

$$\frac{u^{n+1} - u^n}{\Delta t} = L u^n$$ w/ eigvals of L: $\lambda_k = \frac{2D}{\Delta x^2}(\cos(k\pi\Delta x) - 1$

$k = 1, \ldots N$ = # grid pts

& eig fns. $(v_k)_j = \sin(k\pi x_j)$.

small $k \to \lambda_k = O(1)$ smooth eigfns. low freq. $\to$ timescale $O(1)$

large $k \to \lambda_k = O(\Delta x^{-2})$, high freq. eigfns. $\to$ timescale $O(\Delta x^2)$

Generically, physical timescale is $O(1)$, underresolved if timescale is $O(x^2)$.

Don't want to time step on the fastest timescales!

For stiff eqns, there are methods which perform well.

↳ Backward Euler: $y' = f(t, y)$ — Example of an implicit time method

$$\frac{y^{n+1} - y^n}{\Delta t} = f(t_{n+1}, y^{n+1})$$

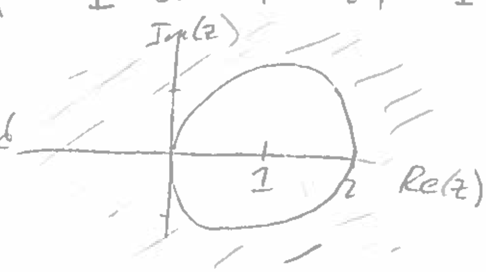
Backward Euler is a good stiff solver, show by calculating region of abs. stability:

$$\frac{y^{n+1} - y^n}{\Delta t} = \lambda y^{n+1} \Rightarrow y^{n+1} - y^n = \Delta t \lambda y^{n+1} = z y^{n+1}$$

$$\Rightarrow y^{n+1} = \frac{1}{1-z} y^n \Rightarrow \text{Region is } \left|\frac{1}{1-z}\right| < 1 \text{ or } |1-z| > 1$$

$\Rightarrow$ entire negative real plane is in Region of absolute stability!

everything outside the unit disc centered at 1.



BE for diffusion is unconditionally stable (stable for any Δt since all λ's on neg. real axis)

BE is an example of an A-stable method - a method where the entire left half plane of $\mathbb{C}$ is in the region of absolute stability.

↳ a soln which should decay, will decay in discrete time.

- to BE! Have to solve for the implicitly defined y^{n+1} (big linear/nonlin. system).

Both FE & BE are first-order accurate in time.

Accuracy: BE + FE 1st order accurate in time.

Let $u(x,t)$ be the soln. to $u_t = Du_{xx}$ + b.c + ic.

Local truncation error (amount by which analytic soln to PDE fails to satisfy the difference eqns.)

Forward-Euler diffusion has difference eqns: $\dfrac{u_j^{n+1} - u_j^n}{\Delta t} = \dfrac{D}{\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right)$

LTE is $$\tau_j^n = \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} - \frac{D}{\Delta x^2}\left(u(x_{j-1}, t_n) - 2u(x_j, t_n) + u(x_{j+1}, t_n)\right)$$

Expand about $x = x_j$, $t = t_n$ as $\Delta x, \Delta t \to 0$ w/ TS and cancel stuff out!

$$\tau_j^n = u_t + \frac{\Delta t}{2}u_{tt} + O(\Delta t^2) - D\left(u_{xx} + \frac{\Delta x^2}{12}u_{xxxx} + O(\Delta x^4)\right)\Big|_{\substack{x = x_j \\ t = t_n}}$$

$$\Rightarrow \quad \tau = \frac{\Delta t}{2}u_{tt} - \frac{D}{12}\Delta x^2 u_{xxxx} + \text{h.o.t.}$$

Also, · Don't forget to utilize the PDE: $u_t = Du_{xx}$

$$u_{tt} = D(u_t)_{xx} = D^2 u_{xxxx}$$

$$\Rightarrow \quad \tau = \left(\frac{\Delta t}{2}D^2 - \frac{D}{12}\Delta x^2\right)u_{xxxx} + \text{h.o.t.}$$

Same analysis for Backward-Euler gives

$$\tau = -\left(\frac{\Delta t}{2}D^2 + \frac{D}{12}\Delta x^2\right)u_{xxxx} + \text{h.o.t.}$$

How do we get higher order accuracy? 2nd order accuracy in time?

utilize symmetry of τ! Average forward & backward Euler!

Trap. rule $\dfrac{y^{n+1} - y^n}{\Delta t} = \dfrac{1}{2}\left(f(y^n) + f(y^{n+1})\right)$ ← A-stable method

Midpt rule $\dfrac{y^{n+1} - y^{n-1}}{2\Delta t} = f(y^n)$ < just use 2nd order approx of $\frac{d}{dt}$
terrible stability restrictions.

BDF2 - one sided backwards diff. in time ← use 3pt, 2nd order approx of time & keep A-stability

$$\frac{3y^{n+1} - 4y^n + y^{n-1}}{2\Delta t} = f(y^{n+1})$$

All 2nd order acc. in time, only trap + BDF2 are A-stable.

MAT228 B – Lecture 6 – 1/23/17

Trapezoidal rule: $\dfrac{y^{n+1}-y^n}{\Delta t} = \frac{1}{2}\left(f(y^{n+1})+f(y^n)\right) = f(y^{n+1/2}) + O(\Delta t^2)$

↑ centered diff. about $t^{n+1/2}$
clearly 2nd order accurate in time

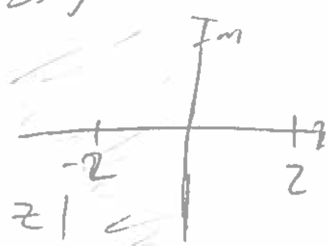
BDF-2: $\dfrac{3y^{n+1}-4y^n+y^{n-1}}{2\Delta t} = f(y^{n+1})$ ← 3 pt. approx ⇒ 2nd order acc. in time.

Both these methods are A-stable.

Region of absolute stability for Trapezoid rule:

$$\frac{y^{n+1}-y^n}{\Delta t} = \frac{\lambda}{2}(y^n+y^{n+1}) \Rightarrow \left(1-\frac{z}{2}\right)y^{n+1} = \left(1+\frac{z}{2}\right)y^n$$

$$\Rightarrow y^{n+1} = \left(\frac{2+z}{2-z}\right)y^n \quad \rightarrow \text{Region } \left|\frac{2+z}{2-z}\right| < 1$$



points z closer to −2 than to 2 ⟵ $|2+z| < |2-z|$

↳ left half-plane

Trap. rule in time for diffusion w/ 3-pt. 2nd order spatial discretization is called Crank–Nicolson.

Crank-Nicolson is 2nd order in space & time & is unconditionally stable.

Generalizations of Forward Euler → Runge-Kutta vs. Multistep Methods

Runge-Kutta methods

(Single-step but multistage – only data from current time)

2-stage method

$$y^* = y^n + \Delta t f(y^n) \quad \leftarrow \text{Improved FE}$$

$$y^{n+1} = y^n + \frac{\Delta t}{2}\left(f(y^n)+f(y^*)\right) \quad \text{2nd order acc.}$$

General r-stage Runge-Kutta method for $y' = f(y,t)$

$$y_i^* = y^n + \Delta t \sum_{j=1}^{r} A_{ij} f(t_n + c_j\Delta t, y_j^*) \quad i=1,\dots,r$$

$$y^{n+1} = y^n + \Delta t \sum_{j=1}^{r} b_j f(t_n + c_j \Delta t, y_j^*)$$

⇒ A_{ij}, b_j, c_j define RK class – A_{ij} – RK matrix, b_j – RK weights, c_j – RK nodes] – Butcher tables

Linear Multistep Methods

(uses more than 1 past time level)

- Adams-Bashforth 2 (AB2):

$$\frac{y^{n+1}-y^n}{\Delta t} = \frac{1}{2}\left(3f(y^n) - f(y^{n-1})\right)$$

- BDF2 (implicit time)

Example Butcher table for RK:

$$\begin{array}{c|c} \underline{c} & A \\ \hline & \underline{b}^T \end{array}$$

Butcher table for 2-stage RK:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

$y_1^* = y^n$

$y_2^* = y^n + \Delta t f(t_n, y_1^*)$

$y_{n+1} = y^n + \frac{\Delta t}{2}\left(f(t_n, y_1^*) + f(t_n + \Delta t, y_2^*)\right)$

Classical RK-4:

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$

last class of multistep:

BDF - backwards-difference formula

$$\sum_{j=0}^{r} \alpha_j y^{n+j} = \Delta t \beta_r f(y^{n+r})$$

really good for stiff equations

BE = BDF1

saw BDF2

Higher $r \to$ better accuracy but loses stability.

If A is strictly lower-triangular, the RK method is explicit time

Implicit time method has full $A \to$ have to do a full solve on all stages at once expensive

Diagonally implicit (DIRK) methods - lower triangular

Ex: TR-BDF2 method:

$$y^* = y^n + \frac{\Delta t}{4}\left(f(y^n) + f(y^*)\right)$$

$$y^{n+1} = \frac{1}{3}\left(4y^* - y^n + \Delta t f(y^{n+1})\right)$$

(trap rule followed by BDF-2)

butcher table:

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/4 & 1/4 & 0 \\ 1 & 1/3 & 1/3 & 1/3 \\ \hline & 1/3 & 1/3 & 1/3 \end{array}$$

Linear Multistep method:

General r-step method:

$$\sum_{j=0}^{r} \alpha_j y^{n+j} = \Delta t \sum_{j=0}^{r} \beta_j f(y^{n+j})$$

Adams methods: $$\frac{y^{n+r} - y^{n+r-1}}{\Delta t} = \sum_{j=0}^{r} \beta_j f(y^{n+j})$$

If $\beta_r = 0$, Adams-Bashforth: $\frac{y^{n+1} - y^n}{\Delta t} = f(y^n)$ (Forward Euler)

AB 2 $\quad \frac{y^{n+1} - y^n}{\Delta t} = \frac{1}{2}\left(3f(y^n) - f(y^{n-1})\right)$

If $\beta_r \neq 0$, Adams-Moulton method (implicit time) - e.g. Trap. rule

MAT228B - Lecture 7 - 1/25/17

Consistency, stability, & convergence:

Def: A numerical method is convergent if for $(x^*, t^*) \in$ domain
$$\| u_j^n - u(x_j, t_n) \| \to 0 \text{ as } \Delta x, \Delta t \to 0 \;\&\; x_j \to x^*,\; t_n \to t^*.$$
(u_j^n: discrete soln; $u(x_j,t_n)$: analytic soln.)

Notes:
- Sometimes, have to constrain $\Delta x, \Delta t$ as $\to 0$
  e.g. FE for diffusion requires $\Delta t \le \Delta x^2/2D$ as $\Delta t, \Delta x \to 0$.
- Def. requires specifying a norm (discrete 2-norm, 1-norm, inf. norm, etc)
  ↳ will see examples of problems which converge in a norm but not others.

Local Truncation/Discretization Error error of the difference scheme
how well differences approx. derivatives.

Def: A scheme is consistent if the local truncation error $\to 0$ as $\Delta x, \Delta t \to 0$.

Ex: FE for Diffusion: $\dfrac{u_j^{n+1} - u_j^n}{\Delta t} = \dfrac{D}{\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right)$

Let $u(x,t)$ solve $u_t = D u_{xx}$.
Let τ_j^n be the LTE at x_j, t_n. Then
$$\tau_j^n = \frac{u(x_j, t_n + \Delta t) - u(x_j, t_n)}{\Delta t} - \frac{D}{\Delta x^2}\left(u(x_j - \Delta x, t_n) - 2u(x_j, t_n) + u(x_j + \Delta x, t_n)\right)$$
$$\tau_j^n = \frac{\Delta t}{2} u_{tt}(x_j, t_n) - \frac{D}{12}\Delta x^2 u_{xxxx}(x_j, t_n) + \text{h.o.t.}$$
$= O(\Delta t) + O(\Delta x^2) \to 0$ as $\Delta x, \Delta t \to 0$ so FE for diffusion is consistent.

We would like some relationship between LTE & convergence
Relate thru stability!

Thm (Lax-Equivalence): (Fundamental thm. of finite differences)

A linear, consistent difference scheme to a well-posed linear PDE is convergent if & only if it is stable.

☆ stability + consistency $\Rightarrow$ convergence ☆

Consider the linear update $u^{n+1} = Bu^n + b^n$

Let u^n & v^n be two different solns. to the difference scheme.

Def: The method is stable if for each $T>0$, $\exists$ constant K_T s.t.

$$\|u^n - v^n\| \leq K_T \|u^0 - v^0\| \text{ independent of } u^0, v^0, \ \forall n\Delta t \leq T$$

Def: The scheme is Lax-Richtmeyer stable if for each time T, $\exists$ constant $C_T > 0$ independent of Δt s.t.

$$\|B^n\| \leq C_T \quad \forall n\Delta t \leq T.$$

MAT 228B - Lecture 8 - 1/27/17

Show: Consistent + Stable $\Rightarrow$ Convergent

Scheme: $u^{n+1} = Bu^n + b^n \quad (1)$

Let u_{sol}^n be the soln of the PDE sampled on the mesh at time level t_n.

Want: $e^n = u^n - u_{sol}^n \to 0$ as $\Delta x, \Delta t \to 0$.

More about scheme: Ex: Forward Euler $\dfrac{u^{n+1} - u^n}{\Delta t} = Lu^n + f^n$

Local trunc. error

(using def. of LTE) Plug in $u_{sol}^n \to \dfrac{u_{sol}^{n+1} - u_{sol}^n}{\Delta t} = Lu_{sol}^n + f^n + \tau^n$

$$\Rightarrow u_{sol}^{n+1} = (I + \Delta t L)u_{sol}^n + \Delta t f^n + \Delta t \tau^n$$

Plug in u_{sol}^n into generic scheme:

$$u_{sol}^{n+1} = Bu_{sol}^n + b^n + \Delta t \tau^n. \quad (2)$$

Subtract eq. (2) from eq. (1):

$$e^{n+1} = Be^n - \Delta t \tau^n$$

Assume initial condition correct: $e^0 = 0$ (no initial error)

$\Rightarrow \lVert e^n \rVert = \Delta t \left\lVert \sum_{k=0}^{n-1} B^{n-k-1} \tau^k \right\rVert$	$e^1 = -\Delta t \tau^0$
$\leq \Delta t \sum_{k=0}^{n-1} \lVert B^{n-k-1} \tau^k \rVert$	$e^2 = -\Delta t B \tau^0 - \Delta t \tau^1$
	$e^3 = -\Delta t (B^2 \tau^0 + B \tau^1 + \tau^2)$
	$\vdots$
$\Rightarrow \lVert e^n \rVert \leq \Delta t \sum_{k=0}^{n-1} \lVert B^{n-k-1} \rVert \, \lVert \tau^k \rVert.$	$e^n = -\Delta t \sum_{k=0}^{n-1} B^{n-k-1} \tau^k$

[...]n stability, $\lVert B^{n-k-1} \rVert \leq C_T$ since $n-k-1 < n$ $\Rightarrow \lVert e^n \rVert \leq \Delta t C_T \sum_{k=0}^{n-1} \lVert \tau^k \rVert$

and $\lVert \tau^k \rVert \leq \max_k \lVert \tau^k \rVert$ $\Rightarrow \lVert e^n \rVert \leq n \Delta t C_T \max_k \lVert \tau^k \rVert = T C_T \max_k \lVert \tau^k \rVert \to 0$

as $\Delta x, \Delta t \to 0$ b/c scheme is consistent ... $\square$

Stability Analysis of Crank-Nicolson for Diffusion:

$$\frac{u^{n+1}-u^n}{\Delta t} = \frac{1}{2}\left(Lu^n + Lu^{n+1}\right) + \underbrace{f^{n+1/2}}_{\frac{1}{2}(f^n+f^{n+1})}$$

$$\Rightarrow \left(I - \frac{\Delta t}{2}L\right)u^{n+1} = \left(I + \frac{\Delta t}{2}L\right)u^n + \Delta t f^{n+1/2}$$ ← more efficient calc!

$$u^{n+1} = \underbrace{\left(I - \frac{\Delta t}{2}L\right)^{-1}}\left(I + \frac{\Delta t}{2}L\right)u^n + \Delta t\left(I - \frac{\Delta t}{2}L\right)^{-1} f^{n+1/2}$$

inverse exists since eigvals of L are ≤ 0
so eigvals. of $I - \frac{\Delta t}{2}L$ are bounded away from 0!

For analysis, $B = \left(I - \frac{\Delta t}{2}L\right)^{-1}\left(I + \frac{\Delta t}{2}L\right)$

Note: L is symmetric $\Rightarrow$ each ( ) is symmetric
& these matrices commute (same eigvectors $\Rightarrow$ simultaneously diagonalizable)

$\Rightarrow B$ is symmetric $\rightarrow$ 2-norm = spectral radius of B $\|B^n\|_2 \leq \|B\|_2^n$.

Let λ_k be an eigval of L. Then eigvals of B are $\mu_k = \dfrac{1+\frac{\Delta t}{2}\lambda_k}{1-\frac{\Delta t}{2}\lambda_k}$

Then $\|B\|_2 = \max_k \left|\dfrac{1+\frac{\Delta t}{2}\lambda_k}{1-\frac{\Delta t}{2}\lambda_k}\right| \leq 1$ (since $\lambda_k \leq 0$)

Hence $\|B^n\|_2 \leq 1$. Thus Crank-Nicolson is stable!

∞-norm stability for Forward Euler for diffusion:

Scheme: $\dfrac{u^{n+1}-u^n}{\Delta t} = Lu^n + f^n \rightarrow u^{n+1} = \overbrace{(I + \Delta t L)}^{B}u^n + \Delta t f^n$

$\|B^n\|_\infty \leq \|B\|_\infty^n$. $\|B\|_\infty$ = max row sum

j^{th} row of B

$$u_j^{n+1} = \left(\frac{D\Delta t}{\Delta x^2}u_{j-1}^n + \left(1 - \frac{2D\Delta t}{\Delta x^2}\right)u_j^n + \frac{D\Delta t}{\Delta x^2}u_{j+1}^n\right) + \Delta t f_j^n$$

$\Rightarrow \|B\|_\infty = \left|\dfrac{D\Delta t}{\Delta x^2}\right| + \left|1 - \dfrac{2D\Delta t}{\Delta x^2}\right| + \left|\dfrac{D\Delta t}{\Delta x^2}\right|$ ← same as condition from random-walk derivation for diffusion

If $1 - \dfrac{2D\Delta t}{\Delta x^2} \geq 0$, then drop $|\cdot|$ & $\|B\|_\infty = 1$.

$\Rightarrow \|B\|_\infty = 1$ if $\underline{\Delta t \leq \dfrac{\Delta x^2}{2D}}$ (same restriction seen earlier)

stuff moves left ← stuff stays put.

$\Rightarrow \|B^n\|_\infty \leq 1 \Rightarrow$ stable if.

MAT228B - Lecture 9 - 1/30

Last time: (*) $u^{n+1} = Bu^n + b^n$ stable if $\|B^n\| \le C_T$ ← ind. of Δt

Examples last time we showed $\|B\| \le 1 \Rightarrow \|B^n\| \le \|B\|^n \le 1$.

What if the solution is supposed to grow in time?

Cor: If there is a constant $\alpha \ge 0$ independent of Δt (for small enough Δt) s.t. $\|B\| \le 1 + \alpha\Delta t$, then scheme (*) is Lax-Richmeyer stable

Pf: Supp. $\|B\| \le 1+\alpha\Delta t$, show $\|B^n\| \le C_T$.

$$\|B^n\| \le \|B\|^n \le (\underbrace{1+\alpha\Delta t}_{\text{first 2 terms of TE of } e^{\alpha\Delta t}})^n \le e^{\alpha n\Delta t} = e^{\alpha T}. \quad \square$$

$$e^{\alpha\Delta t} = 1+\alpha\Delta t + \underbrace{\frac{(\alpha\Delta t)^2}{2} + \frac{(\alpha\Delta t)^3}{3!} + \ldots}_{\text{all positive terms}}$$

Consider $u_t = u_{xx} + ku$ (reaction-diffusion)

Consider Forward-Euler stability in the ∞-norm

$$u^{n+1} = \underbrace{(I + \Delta t L + k\Delta t I)}_{B} u^n$$

$$\|B\|_\infty = \left|\frac{\Delta t}{\Delta x^2}\right| + \left|1 - \frac{2\Delta t}{\Delta x^2} + k\Delta t\right| + \left|\frac{\Delta t}{\Delta x^2}\right|$$

$$\le \frac{2\Delta t}{\Delta x^2} + \left|1 - \frac{2\Delta t}{\Delta x^2}\right| + |k|\Delta t$$

Require $1 - \frac{2\Delta t}{\Delta x^2} \ge 0 \Rightarrow \boxed{\Delta t \le \Delta x^2/2}$

$$\le 1 + \underbrace{|k|}_{\alpha}\Delta t.$$ So by Cor, scheme is Lax-Richmeyer stable w/ the restriction on Δt

Technically stable as $\Delta t \to 0$ for $k>0$, but should be more careful! When $k<0$, expect soln to PDE to decay, so use a tighter Δt restriction.

Want $\|B\|_\infty \le 1$.

Use restriction $1 - \frac{2\Delta t}{\Delta x^2} + k\Delta t \ge 0 \Rightarrow \boxed{\Delta t \le \Delta x^2/(2-k\Delta x^2)}$.

Then $\|B\|_\infty = 1 + k\Delta t \le 1$ for $\Delta t \le -1/k$. ← restriction covers other!

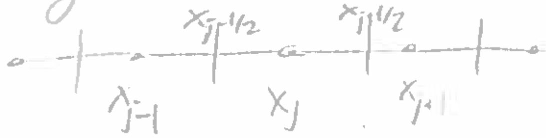
& scheme is definitely stable & decaying.

Variable-Coefficient Diffusion: $u_t = (a(x)u_x)_x$ ← conservative form $u_t = -\nabla\cdot J$ w/ $J = -a(x)\nabla$

better numerically to discretize conservative form than to manipulate to $u_t = a(x)u_{xx} + a_x(x)u_x$ & discretize.

$\boxed{\text{RESPECT THE PDE! RESPDE!}}$

Discretizing the conservative form.



Approx flux w/ intermed. mesh pts:

$$J = -a(x)u_x$$

$$J_{j-1/2} = -a(x_{j-1/2})\frac{u_j - u_{j-1}}{\Delta x}$$

flux at edges

Now $u_t = -J_x$

Approx J_x by diff. across point: $\frac{d}{dt}u(x_j) = -\left(\frac{J_{j+1/2} - J_{j-1/2}}{\Delta x}\right)$

All-together

$$\Rightarrow \left[(a(x)u_x)_x\right]_j = -\left(\frac{J_{j+1/2} - J_{j-1/2}}{\Delta x}\right) = \frac{a_{j+1/2}(u_{j+1}-u_j) - a_{j-1/2}(u_j - u_{j-1})}{\Delta x^2}$$

$$= \frac{1}{\Delta x^2}\left[a_{j-1/2}u_{j-1} - (a_{j-1/2} + a_{j+1/2})u_j + a_{j+1/2}u_{j+1}\right]$$

(Note this matches w/ original when $a(x) = D$ constant)

Stability of Forward Euler in ∞-norm:

using constant-coefficient problem, $\Delta t \le \Delta x^2 / (2\max_x(a(x)))$

FE: $u^{n+1} = (I + \Delta t A)u^n = Bu^n$

$$\|B\|_\infty = \max_j\left(\left|\frac{a_{j-1/2}\Delta t}{\Delta x^2}\right| + \left|1 - (a_{j-1/2} + a_{j+1/2})\frac{\Delta t}{\Delta x^2}\right| + \left|\frac{a_{j+1/2}\Delta t}{\Delta x^2}\right|\right)$$

Choose Δt s.t. $\forall j$, $1 - (a_{j-1/2} + a_{j+1/2})\frac{\Delta t}{\Delta x^2} \ge 0$

$$\Rightarrow \Delta t \le \Delta x^2 / (a_{j-1/2} + a_{j+1/2}) \quad \forall j$$

& $\|B\|_\infty \le 1$ hence stability.

These are effectively the same restrictions on Δt.

MAT228B - Lecture 10 - 2/1/17

Von Neumann Analysis - stability analysis of difference schemes using Fourier analysis:

$$u_t = D u_{xx} \xrightarrow{\text{Fourier transform}} \hat{u}_t(\xi,t) = -D\xi^2 \hat{u}(\xi,t)$$ inf set of ODEs parametrized by ξ

Von Neumann analysis is used to analyze constant coefficient, linear problems on the whole real line or periodic domain

Say applying difference scheme to infinite lattice:

Use fact that complex exponentials $v_j = e^{i\xi x_j}$ are eigenfns of difference operators.

$$(D_+ v)_j = \frac{v_{j+1} - v_j}{\Delta x} = e^{i\xi x_j}\left(\frac{e^{i\xi\Delta x} - 1}{\Delta x}\right) = \lambda(\xi) v_j.$$

$$(D^2 v)_j = \frac{v_{j-1} - 2v_j + v_{j+1}}{\Delta x^2} = e^{i\xi x_j}\left(\frac{e^{-i\xi\Delta x} - 2 + e^{i\xi\Delta x}}{\Delta x^2}\right) = v_j\left(\frac{2}{\Delta x^2}(\cos\xi\Delta x - 1)\right) = \lambda(\xi) v_j$$

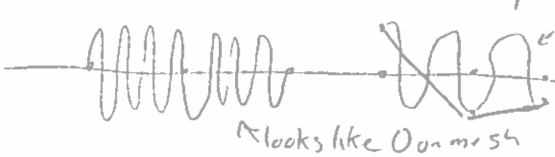
$$= v_j\left(-\frac{4}{\Delta x^2}\left(\sin^2\left(\frac{\xi\Delta x}{2}\right)\right)\right)$$

Fourier Transform of discrete fn:

Let v_j be discrete fn. on $x_j = j\Delta x$, $j \in \mathbb{Z}$.

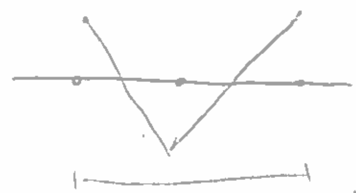
FT of v_j is: $$\hat{v}(\xi) = \frac{\Delta x}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} v_j e^{-i\xi x_j}$$ ← projection of discrete fn onto eigenfns.

ξ is cont's, but bounded. Can't represent high frequencies on a discrete mesh.



Highest possible: $\frac{2\pi}{\xi} = 2\Delta x$

$\Rightarrow \xi = \frac{\pi}{\Delta x}$



Range for ξ: $-\frac{\pi}{\Delta x} \le \xi \le \frac{\pi}{\Delta x}$

Inverse transform: $$v_j = \frac{1}{\sqrt{2\pi}} \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{v}(\xi) e^{i\xi x_j} \, d\xi.$$

Real space, cont's bounded interval $x \in [0, 2\pi]$ ⟷ Fourier space, discrete variable

Real space discrete ⟷ Fourier space cont's & bounded $-\frac{\pi}{\Delta x} \le \xi \le \pi/\Delta x$.

Parseval's Relation: $\|\hat{v}(\xi)\|_2 = \|v(j)\|_h \equiv \left(\Delta x \sum |v_j|^2\right)^{1/2}$

Use Parseval's relation for stability analysis

Scheme $\to u^{n+1} = B u^n$ $\leftarrow$ Want $\|B\|_2 \le 1 + \alpha \Delta t$ for stability.

What if we showed $\|u^{n+1}\| \le (1+\alpha\Delta t)\|u^n\|_2$? $\leftarrow$ Claim gives stability.

Pf: $\frac{\|u^{n+1}\|_2}{\|u^n\|_2} = \frac{\|Bu^n\|_2}{\|u^n\|_2} \le 1+\alpha\Delta t \quad \Rightarrow \|B\|_2 \le 1+\alpha\Delta t$

$\nwarrow$ doesn't dep. on choice of u^n, true for all u. Stable. ∎

Now, if we can show that $\|\hat{u}^{n+1}\|_2 \le (1+\alpha\Delta t)\|\hat{u}^n\|_2$, then scheme is stable!

Ex: Forward Euler for Diffusion

$$u_j^{n+1} = u_j^n + \frac{\Delta t}{\Delta x^2} D\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right)$$

Use $u_j^n = \frac{1}{\sqrt{2\pi}} \int_{-\pi/\Delta x}^{\pi/\Delta x} \hat{u}^n(\xi) e^{i\xi x_j} d\xi$ on RHS:

$$u_j^{n+1} = \frac{1}{\sqrt{2\pi}} \int_{-\pi/\Delta x}^{\pi/\Delta x} \left[1 + \frac{\Delta t}{\Delta x^2} D\left(e^{-i\xi\Delta x} - 2 + e^{i\xi\Delta x}\right)\right] \hat{u}^n(\xi) e^{i\xi x_j}\, d\xi$$

projection onto $e^{i\xi x_j}$!

Transform both sides:

$$\hat{u}^{n+1}(\xi) = \left[1 + \frac{\Delta t D}{\Delta x^2} 2\left(\cos(\xi\Delta x) - 1\right)\right] \hat{u}^n(\xi)$$

of the form $\hat{u}^{n+1}(\xi) = g(\xi)\,\hat{u}^n(\xi)$. $g(\xi)$ is the amplification factor

Have now: $\|\hat{u}^{n+1}\|_2 = \|g(\xi)\hat{u}^n\|_2 \le \|g(\xi)\|_\infty \|\hat{u}^n\|_2$

If $\max_\xi |g(\xi)| \le 1+\alpha\Delta t$, then the scheme is stable.

$$g(\xi) = 1 - \frac{4D\Delta t}{\Delta x^2}\sin^2\left(\frac{\xi\Delta x}{2}\right) \overset{\text{want}}{\Rightarrow} |g(\xi)| \le 1 \ \forall \xi$$

$$\Rightarrow -1 \le 1 - \frac{4D\Delta t}{\Delta x^2}\sin^2\left(\frac{\xi\Delta x}{2}\right) \le 1 \Rightarrow 0 \le \frac{4D\Delta t}{\Delta x^2}\sin^2\left(\frac{\xi\Delta x}{2}\right) \le 2$$

max this over ξ

Ineq. holds $\forall \xi$ if $\Delta t \le \Delta x^2/2D$.

MAT 228B - Lecture 12 - 2/6/17

von Neumann analysis

- 1-step method - Assume $u_j^n = e^{i\xi x_j}$, then $u_j^{n+1} = g(\xi) e^{i\xi x_j}$
(involves only u^n & u^{n+1}) Want $|g(\xi)| \le 1 + \alpha\Delta t \;\; \forall \xi$.

FE: $u_j^{n+1} = u_j^n + \frac{\Delta t D}{\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right)$

$$u_j^{n+1} = e^{i\xi x_j} + \frac{\Delta t D}{\Delta x^2}\left(e^{i\xi(x_j-\Delta x)} - 2e^{i\xi x_j} + e^{i\xi(x_j+\Delta x)}\right)$$

don't need to do whole discrete Fourier transform

$$= \left(1 + \frac{\Delta t D}{\Delta x^2}\left(e^{-i\xi\Delta x} - 2 + e^{i\xi\Delta x}\right)\right) e^{i\xi x_j}$$

Show leapfrog scheme in unstable for diffusion ← could write as single step, 2-variable system

$$\frac{u_j^{n+1} - u_j^{n}}{2\Delta t} = \frac{D}{\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right)$$

Assume $u_j^n = g^n e^{i\xi x_j}$ — 2 eigenvalues

$$\frac{g^{n+1} - g^{n-1}}{2\Delta t} = \frac{D}{\Delta x^2} g^n\left(-4\sin^2\left(\frac{\xi\Delta x}{2}\right)\right)$$ divide by g^{n-1}

- $$g^2 - 1 = \underbrace{-\frac{8D\Delta t}{\Delta x^2}\left(\sin^2\left(\frac{\xi\Delta x}{2}\right)\right)}_{0 \le \beta(\xi)\ \forall \xi} g$$

2 amplification factors! Need both $\le 1 + \alpha\Delta t$

$$g^2 + \beta(\xi) g - 1 = 0$$

$g_1 g_2 = -1$ → one bigger than 1, one less than 1, $\boxed{\text{unstable!}}$

can show g_1, g_2 real ⇗ or $g_{+/-} = \frac{1}{2}\left(-\beta \pm (\beta^2+4)^{1/2}\right)$

$\Rightarrow |g_-| \ge 1$ for $\beta \ne 0$ $\quad g_- = \frac{1}{2}\left(-\beta - (\beta^2+4)^{1/2}\right) \ge -1$ UNSTABLE

Computation: Implicit vs. Explicit in Time:

Forced diffusion: $u_t = b u_{xx} + f$

FE presents time step restriction
1D: $\Delta t \le \Delta x^2/2b$ ← ∞-norm analysis, from diagonal term $1 - \frac{2b\Delta t}{\Delta x^2} \ge 0$
2D: $\Delta t \le \Delta x^2/4b$ ← diag. term $1 - \frac{4b\Delta t}{\Delta x^2} \ge 0$
3D: $\Delta t \le \Delta x^2/6b$ ← diag. term $1 - \frac{6b\Delta t}{\Delta x^2} \ge 0$

- In practice, we generally use an implicit time method to avoid these restrictions.

Let L be the discrete Laplacian $\quad \frac{u^{n+1} - u^n}{\Delta t} = \frac{b}{2}\left(Lu^n + Lu^{n+1}\right) + f^{n+1/2}$

Solve lin. system at each timestep — $\left(I - \frac{b\Delta t}{2}L\right)u^{n+1} = \left(I + \frac{b\Delta t}{2}L\right)u^n + \Delta t f^{n+1/2}$

For implicit-time methods, we need to solve a linear system at each time step

Is it worth it? $\quad (I - \frac{b\Delta t}{2}L)u^{n+1} = (I + \frac{b\Delta t}{2}L)u^{n} + f^{n+1/2}$

$\Delta x \sim \frac{1}{N}$. Assume Δt is proportional to Δx in implicit method

Choose N. How much work does it take to solve as fn of N? Up to time $T = 1/\Delta t$.

~~Take $O(1/\Delta x) = O(N)$ time steps~~

0 $\qquad\qquad$ T

Cost per time step (in 1-D): With tridiagonal solver, $O(N)$ solve per step

Total work $= \underline{O(N^2)}$ ← cost of implicit method

Vs. Forward Euler: $\Delta t \le \frac{\Delta x^2}{2b} \Rightarrow$ # time steps $\sim \frac{T}{\Delta t} = O(1/\Delta x^2) = O(N^2)$.

work per time step $O(N)$

Total work $= O(N^3)$.

Asymptotically, FE is more computationally expensive than implicit-time methods.

Consider $u_t = -k u_{xxxx}$ ← bending structures in viscous fluid

For Forward Euler, need $\Delta t \le C\Delta x^4$ for stability

$\Rightarrow O(N^5)$ work

Still only $O(N^2)$ work for implicit-time methods! Penta vs. tridiagonal matrices still $O(N)$ work to solve.

MAT228B - Lecture 13 - 2/8/17

Implicit-time methods multiD $u_t = b\Delta u$

CN $(I - \frac{b\Delta t}{2}L)u^{n+1} = (I + \frac{\Delta t b}{2}L)u^n$

BE $(I - \Delta t b L)u^{n+1} = u^n$

BDF2 $\frac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t} = bLu^{n+1}$

$(I - \frac{2}{3}b\Delta t L)u^{n+1} = \text{stuff}$

Solve $(I - \beta\Delta t L)u^{n+1} = f$ every time step for all these

use SOR, MG, PCG, specialized direct methods - block cyclic reduction

FFT method - requires structure & constant coefficient.

How well do the iterative methods work?

Condition # of L is $O(1/\Delta x^2)$

$A = I - \beta\Delta t L$, $K(A) = O(\frac{\Delta t}{\Delta x^2})$

If $\Delta t = O(\Delta x)$, then $K(A) = O(1/\Delta x)$ ← better conditioned already!

Actual convergence rate depends on size of $\beta\Delta t/\Delta x^2$.

Two extreme cases on BE:

$\frac{\beta\Delta t}{\Delta x^2} \to 0$ ← $\Delta t \to 0$, dumb $\frac{\beta\Delta t}{\Delta x^2} \to \infty$ ← refining mesh w/ $\Delta t = O(\Delta x)$

$(I - \Delta t b L)u^{n+1} = u^n + \Delta t f^{n+1}$ ← if f contains BCs, then $f = O(1/\Delta x^2)$

$\frac{\beta\Delta t}{\Delta x^2} \to 0$, $A \to I$, iterative methods converge rapidly. (but explicit would be better here since timestep tiny)

$\frac{\beta\Delta t}{\Delta x^2} \to \infty$, get $-\Delta t b L u^{n+1} = \Delta t f^{n+1}$ ← Poisson eqn.

Worst we can do is as well as solving the Poisson eqn.

Expect iterative methods to converge faster than for Poisson eqn.

(look at HW3 from 228A)

MG on 64^2 periodic domain had convergence factor for Poisson eqn $\rho \simeq 0.16$

$\Rightarrow$ # iterations per digit of accuracy $= -\frac{1}{\log_{10}\rho} \simeq 1.26$.

$\Delta t = \Delta x$ here

$(I - \Delta t \beta L)$ - same MG on 64^2 periodic domain — compared to Poisson eqn solve

$\beta = 1 \quad \rho = 0.11 \rightarrow -\frac{1}{\log_{10}\rho} \simeq 1.04 \leftarrow$ 20% fewer iterations

$\beta = 10^{-1} \quad \rho \simeq 0.05 \rightarrow -\frac{1}{\log_{10}\rho} \simeq 0.77 \leftarrow$ 40% fewer iterations

might do better than this since

How big? $\frac{\beta \Delta t}{\Delta x^2} = \beta/\Delta x = \beta/2^{-6} \rightarrow 64,\ 6.4$

Initial guess for iterative methods is last time step! $\leftarrow$

$(u^{n+1})^0 = u^n$ compared to Poisson eqn where initial guess was $u=0$.

There is another way to solve that was not available for Poisson eqn.

Exploit the time dependence explicitly.

ADI - alternating direction implicit

LOD - locally one-dimensional scheme

] can be good preconditioners for PCG.

In 2D, $\Delta u = u_{xx} + u_{yy}$ What if we diffuse in each dimension sequentially?

$L = L_x + L_y$

Compare w/ CN: $(I - \frac{b\Delta t}{2} L_x - \frac{b\Delta t}{2} L_y) u^{n+1} = (I + \frac{b\Delta t}{2} L_x + \frac{b\Delta t}{2} L_y) u^n$

Solve sequentially: 1-D CN

$$(I - \tfrac{b\Delta t}{2} L_x) u^* = (I + \tfrac{b\Delta t}{2} L_x) u^n$$
$$(I - \tfrac{b\Delta t}{2} L_y) u^{n+1} = (I + \tfrac{b\Delta t}{2} L_y) u^*$$

] LOD scheme

looks like a fractional stepping method: $\frac{du}{dt} = bL_x u + bL_y u$

Evolve $\frac{du}{dt} = bL_x u$, then follow by $\frac{du}{dt} = bL_y u$.

Is this stable, consistent?

MAT228B - Lecture 15 - 2/13/17

ADI schemes (continued)

Recall - 2 step scheme: Peaceman-Rashford

$$\left(I - \frac{\Delta t}{2} b L_x\right) u^* = \left(I + \frac{\Delta t b}{2} L_y\right) u^n$$

$$\left(I - \frac{\Delta t}{2} b L_y\right) u^{n+1} = \left(I + \frac{\Delta t b}{2} L_x\right) u^*$$

Showed this is a stable, consistent, 2^{nd} order accurate scheme.

Showed effectively equivalent to a perturbation of CN by $O(\Delta t^2)$.

rewrite as: $\left(I - \frac{\Delta t b}{2} L_x\right)\left(I - \frac{\Delta t}{2} b L_y\right) u^{n+1} = \underbrace{\left(I + \frac{\Delta t b}{2} L_x\right)\left(I + \frac{\Delta t}{2} b L_y\right)}_{} u^n$

vs. Crank-Nicolson

$$\left(I - \frac{\Delta t b}{2} L_x - \frac{\Delta t b}{2} L_y\right) u^{n+1} = \underbrace{\left(I + \frac{\Delta t}{2} b L_x + \frac{\Delta t b}{2} L_y\right)}_{} u^n$$

approximate factorization of this operator

What about a 3D ADI scheme?

Naive: $\left(I - \frac{\Delta t b}{2} L_x\right)\left(I - \frac{\Delta t b}{2} L_y\right)\left(I - \frac{\Delta t b}{2} L_z\right) u^{n+1} = \left(I + \frac{\Delta t b}{2} L_x\right)\left(I + \frac{\Delta t b}{2} L_y\right) \cdot \left(I + \frac{\Delta t b}{2} L_z\right) u^n$

Von Neumann analysis -> unconditionally stable

Add terms to balance high order stuff?

BE-like 2D ADI scheme?

BE: $(I - \Delta t b L_x - \Delta t b L_y) u^{n+1} = u^n$

ADI scheme: $(I - \Delta t b L_x)(I - \Delta t b L_y) u^{n+1} = u^n + \Delta t^2 b^2 L_x L_y u^n$

Fractional Step Methods. good for mixed PDEs, e.g. reaction-diffusion

$$u_t = b \Delta u + f(u) \qquad \text{e.g. } f(u) = Ku(1-u)$$

How to solve?

- Can try method of lines (implicit time, e.g. CN)
- Can try IMEX - some terms implicit, some explicit
- Fractional step - separate solvers for diff terms.

Let's try Trap. rule discretization + method of lines

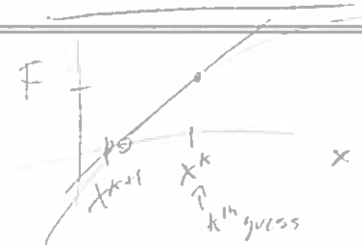
$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{b}{2}\left(Lu^n + Lu^{n+1}\right) + \frac{1}{2}\left(f(u^n) + f(u^{n+1})\right)$$

$$\Rightarrow \quad u^{n+1} - \frac{b\Delta t}{2} L u^{n+1} - \frac{\Delta t}{2} f(u^{n+1}) = u^n + \frac{b\Delta t}{2} L u^n + \frac{\Delta t}{2} f(u^n)$$

If f is nonlinear, have to do a nonlinear solve every time step — can be expensive!

Say we use a Newton-like method to solve

Newton's method for scalar eqn: Finds x s.t. $F(x) = 0$, where F is nonlinear



Take a guess x^k, approx. $F(x^k)$ by a 1st order Taylor poly & find zero.

$$F'(x^k)\cdot(x^{k+1} - x^k) = 0 - F(x^k)$$

$$x^{k+1} = x^k - F(x^k)/F'(x^k)$$

Newton's method for vector eqn: $F: \mathbb{R}^n \to \mathbb{R}^n$ nonlinear. solve $F(u) = 0$

$$J(u^k)\,(u^{k+1} - u^k) = -F(u^k)$$

Jacobian operator eval. at u^k, matrix of partials.

Step 1: Solve for δ in $J\delta = -F(u^k)$, step 2: $u^{k+1} = u^k + \delta$.

Fractional Step idea: $u_t = b\Delta u + f(u)$

discretize space: $\frac{d\underline{u}}{dt} = L\underline{u} + \underline{f}(\underline{u})$

Have u^n. Evolve $\frac{d\underline{u}}{dt} = L\underline{u}$ w/ initial condition $\underline{u}(t_n) = \underline{u}^n$] solve this for time length Δt to get $\underline{u}^*$.

Then solve $\frac{d\underline{u}}{dt} = \underline{f}(\underline{u})$, $\underline{u}(t_n) = u^*$ for time length Δt & get u^{n+1}.] can do nonlinear solve way faster than in coupled method

MAT 228B - Lecture 16 - 2/15/17

Fractional stepping $u_t = A(u) + B(u)$

Have u^n (1) Solve $u_t = A(u)$ starting at u^n for time length Δt to get u^*

(2) Solve $u_t = B(u)$ starting at u^* for time length Δt to get u^{n+1}.

Analyze independent of schemes for steps 1 & 2.

Consider linear problem: $\frac{du}{dt} = A\underline{u} + B\underline{u}$

Have $u^n = u(t_n)$, solution $u(t_{n+1}) = e^{(A+B)\Delta t} \cdot u(t_n)$

Fractional stepping: Solve $u_t = Au \Rightarrow u^* = e^{A\Delta t} u^n$

Then solve $u_t = Bu \Rightarrow u^{n+1} = e^{B\Delta t} u^* = e^{B\Delta t} e^{A\Delta t} u^n$ — may not commute

Single step error of fractional step:

$$u(t_{n+1}) - u^{n+1} = \left(e^{(A+B)\Delta t} - e^{B\Delta t} e^{A\Delta t}\right) u^n$$

$$e^{(A+B)\Delta t} = I + \Delta t(A+B) + \frac{\Delta t^2}{2}\underbrace{(A+B)^2}_{A^2+AB+BA+B^2} + O(\Delta t^3)$$

$$e^{B\Delta t} e^{A\Delta t} = \left(I + \Delta t B + \frac{\Delta t^2}{2}B^2 + O(\Delta t^3)\right)\left(I + \Delta t A + \frac{\Delta t^2}{2}A^2 + O(\Delta t^3)\right)$$

$$= I + \Delta t(A+B) + \frac{\Delta t^2}{2}(A^2 + B^2 + 2BA) + O(\Delta t^3)$$

not equal unless A, B commute

$\Rightarrow \|u(t_{n+1}) - u^{n+1}\| = O(\Delta t^2)$ ← single step error

But take $O(\Delta t^{-1})$ time steps $\Rightarrow$ Error of fractional stepping overall is $O(\Delta t)$

How to get 2nd order in time?

Strang Splitting - 3 steps per time step: 1. Solve $u_t = A(u)$ start at u^n for time length $\Delta t/2$ get u^*

2. Solve $u_t = B(u)$ start at u^*, for Δt, get u^{**}.

3. Solve $u_t = A(u)$ start at u^{**}, for $\Delta t/2$, get u^{n+1}. 2nd order in time! why?

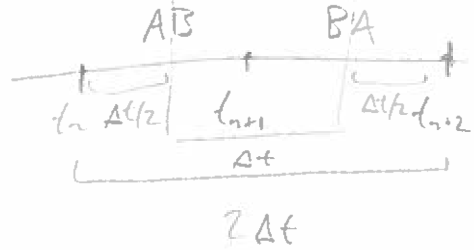
$$e^{\Delta t/2 A} e^{\Delta t B} e^{\Delta t/2 A} = I + \Delta t(A+B) + \Delta t^2/2\,(A^2 + AB + BA + B^2) + O(\Delta t^3) = e^{(A+B)\Delta t} + O(\Delta t^3)$$

single step $O(\Delta t^3) \to O(\Delta t^{-1})$ steps $\Rightarrow O(\Delta t^2)$ accurate!

Another way to get 2^{nd} order — Strang Splitting over 2 timesteps.

- odd time step: 1. $u_t = A(u)$
  2. $u_t = B(u)$
- even time step: 1. $u_t = B(u)$
  2. $u_t = A(u)$

$\Big\} \; 2\Delta t$



IMEX methods

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

Assume A operator is stiff (use implicit solve), B is not (explicit solve)

Ex: Navier-Stokes $\quad \underline{u}_t + \underbrace{\underline{u}\cdot\nabla\underline{u}}_{\text{not stiff}} = \underbrace{\nu\Delta\underline{u}}_{\text{stiff}} - \nabla p + \underline{f}$

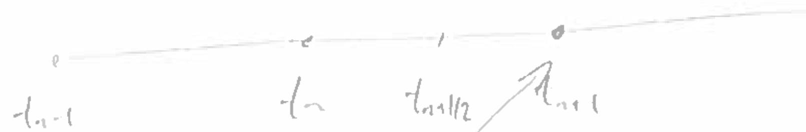
Common scheme: CN/ABF2 $\quad \dfrac{u^{n+1}-u^n}{\Delta t} = \frac{1}{2}\left(A(u^n)+A(u^{n+1})\right) + \frac{3}{2}B(u^n) - \frac{1}{2}B(u^{n-1})$

2^{nd} order acc. w/ time restriction.

Swap in BDF-2 for CN? $\quad \dfrac{3u^{n+1}-4u^n+u^{n-1}}{2\Delta t} = A(u^{n+1}) + \;?$

can't just use this, drops to 1^{st} order accuracy

$2B(u^n) - B(u^{n-1})$



CN does a centered diff in time here

ABF2 approxs. B at $t_{n+1/2}$ from an extrapolation from 2 prev. time pts.

$$\frac{3}{2}B(u^n) - \frac{1}{2}B(u^{n-1}) = B(u^{n+1/2}) + O(\Delta t^2)$$

BDF-2 uses 3pts to approx. $A(u^{n+1})$ to 2^{nd} order.

Should extrapolate B to t_{n+1}! $\quad B(u^{n+1}) + O(\Delta t^2) = 2B(u^n) - B(u^{n-1})$

MAT 228B - Lecture 18 - 2/22/17

Hyperbolic Eqns.

$$\underline{u}_t + A\underline{u}_x = 0$$

Linear: is hyperbolic if A has real λ's & is diagonalizable.

Nonlinear: $\underline{u}_t + (\underline{f}(\underline{u}))_x = 0$

is hyperbolic if Jacobian of f has real λ's & is diagonalizable.

Start w/ advection eqn: $\begin{cases} u_t + a u_x = 0 \\ u(x,0) = u_0(x) \end{cases}$

Soln: $u(x,t) = u_0(x-at)$. ← hard to do transport/translation numerically

Forward-time, centered space: $\dfrac{u_j^{n+1} - u_j^n}{\Delta t} + a\dfrac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = 0$ is unstable.

Von Neumann Analysis: $u_j^{n+1} = u_j^n - \dfrac{a\Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n)$ Let $r = \dfrac{a\Delta t}{\Delta x}$, the Courant #.

a has dims length/time so r is dimless.

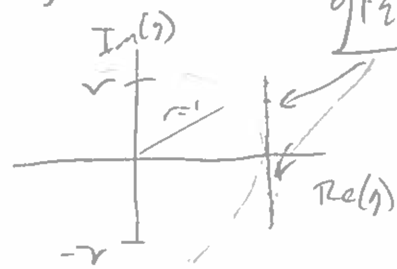
$a\Delta t$ is distance translated per timestep

$u_j^n = e^{i\xi x_j}$

$u_j^{n+1} = g e^{i\xi x_j}$

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

$g(\xi) = 1 - ir\sin(\xi\Delta x)$



$\Rightarrow |g(\xi)| \geq 1 \;\; \forall \xi$.

Unstable

$|g|^2 = 1 + \dfrac{\Delta t^2 a^2}{\Delta x^2}\sin^2(\xi\Delta x)$. What if I pick $\Delta t = C\Delta x^2$?

Then $|g|^2 = 1 + C\Delta t a^2 \sin^2(\xi\Delta x) \Rightarrow |g| \leq 1 + \alpha\Delta t + \ldots$ α ind of Δt.

Technically stable, allows growth so not useful. Very tight timestep restriction.

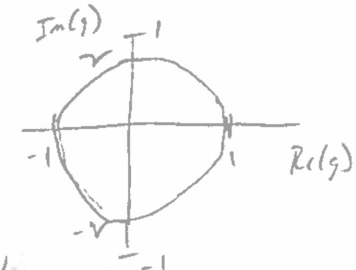
In general, for hyperbolic problems we can take $\Delta t = \mathcal{O}(\Delta x)$.

Slight modification to above scheme to get Lax-Friedrichs scheme:

$$u_j^{n+1} = \frac{u_{j-1}^n + u_{j+1}^n}{2} - \frac{a\Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n)$$

Von Neumann analysis for Lax-Friedrich's: $g(\xi) = \cos(\xi\Delta x) - i\nu\sin(\xi\Delta x)$

Then $|g(\xi)| \le 1$ iff $|\nu| \le 1$.



For stability of LF, require $\Delta t \le \dfrac{\Delta x}{|a|}$

~~Makes sense, $|a\Delta t|$ is amount translated in one time step~~

require this translation be less than 1 grid spacing Δx.

Is this scheme consistent? Just a 2nd order perturbation of previous consistent scheme...

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

(subtracted u_j^n from both sides of scheme & div. by Δt)

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

$$u_t + a u_x = O(\Delta t) + O(\Delta x^4/\Delta t) + O(\Delta x^2/\Delta t) + O(\Delta x^2)$$

Consistent provided $\Delta x^2/\Delta t \to 0$

W/ stability restriction of ν, this will be consistent $\Rightarrow$ LF converges.

This analysis suggests why LF is stable but FTCS is not.

$$\text{LF:} \quad \frac{u_j^{n+1} - u_j^n}{\Delta t} = -\frac{a}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right) + \underbrace{\varepsilon\left(\frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{\Delta x^2}\right)}_{\text{added numerically diffusive term to fight the unstable growth}}, \quad \varepsilon = \frac{\Delta x^2}{2\Delta t}$$

From HW2, $\nu = \dfrac{a\Delta t}{\Delta x}$, $\mu = \Delta t/\Delta x^2\, \varepsilon$

Showed above advection-diffusion scheme stable iff $\nu^2 \le 2\mu \le 1$

Here, $\mu = \dfrac{\Delta t}{\Delta x^2} \cdot \dfrac{\Delta x^2}{2\Delta t} = \dfrac{1}{2}$ for LF $\Rightarrow \nu^2 \le 1$. ← drops diffusive term from inequality

This ε is the smallest "diffusion" coeff. to avoid further restricting time step thru ν

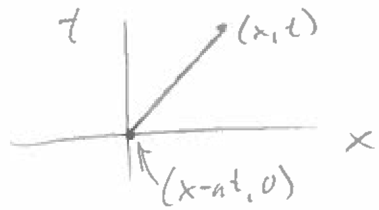
gives $\nu^2 \le 1 \Rightarrow \Delta t \le \Delta x/|a|$.

Lecture 18 cont'd – 2/22/17

CFL condition (Courant-Friedrichs-Lewy)

In hyperbolic eqns, there is a finite speed of propagation. Should consider this in designing numerical schemes.

Def the domain of dependence of the point (x,t) is the set of all points on which the soln depends at (x,t).



easy for advection eqn
soln propagates on curves $x-at=x_0$
So domain of dep. of (x,t) is just the singleton $(x-at,0)$.

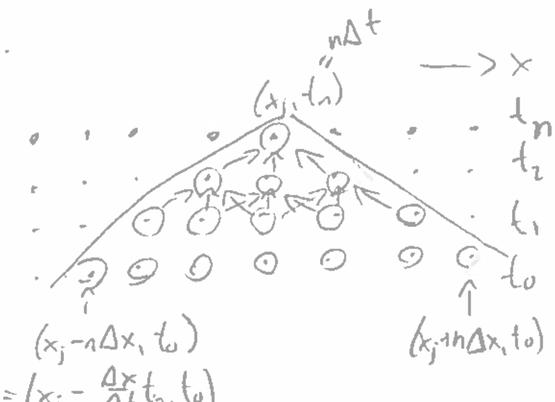
What if eqn is $u_t + au_x = f(t)$? Need whole characteristic line from $(x-at,0)$ to (x,t).

There will also be a numerical domain of dep. it must contain DoD for convergence

Lecture 19 – 2/24/17

CFL condition: the analytic domain of dependence is contained within the numerical dom. of dep.

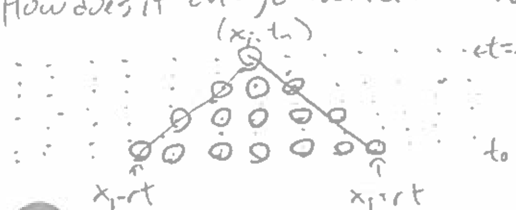
↳ CFL cond'n is necessary cond'n for convergence.



Numerical D.o.D for explicit/3-pt centered scheme

Define the mesh w/ Δx & Δt proportional $\frac{\Delta x}{\Delta t} = \text{const.}$

How does it change numerical DoD?



$t = n\Delta t$ Get more pts. in DoD but same region of space-time

$\frac{\Delta x}{\Delta t} = r \Rightarrow$ cover $(x_j - rt, x_j + rt)$ at initial time level.

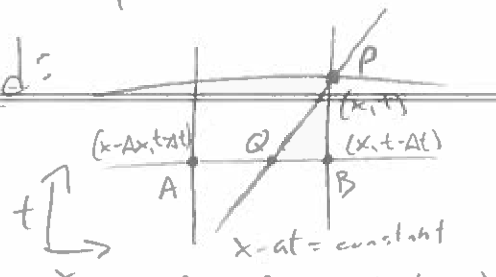
CFL for advection eqn requires $x - rt \le x - at \le x + rt$

$\Rightarrow \gamma = \frac{|a|\Delta t}{\Delta x} \le 1$ ← Forward time-centered space doesn't converge even w/ this cond'n though.

$$u_t + a u_x = 0$$

Suppose $a > 0$. Why do we need to include information from right? Only need info from past time on the Left. Why centered scheme?

Upwind Method:



$(Q = (x - a\Delta t, t - \Delta t))$

$u(P) = u(Q)$ ← to approx $u(Q)$ use weighted average of $u(A)$ & $u(B)$

$$|QA| = \Delta x - a\Delta t = \Delta x(1-r)$$
$$|QB| = a\Delta t = \Delta x \cdot r$$

$$u(Q) \approx \frac{\Delta x(1-r)\,u(B) + \Delta x\, r\, u(A)}{\Delta x(1-r) + \Delta x\, r} = (1-r)u(B) + r u(A)$$

Upwind for $a > 0$

$$u_j^{n+1} = (1-r)u_j^n + r u_{j-1}^n$$
$$u_j^{n+1} = u_j^n - r(u_j^n - u_{j-1}^n)$$
$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\left(\frac{u_j^n - u_{j-1}^n}{\Delta x}\right) = 0$$

← forward-time backward-space discret. of advec. equ.

first-order in time & space & consistent

☆ upwind method has a nice maximum principle

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

$m^n = \max_j |u_j^n|$, $m^{n+1} \le (1-r)m^n + r m^n = m^n$

☆ max value of numeric soln is nonincreasing

If $a < 0$, use forward-space difference.

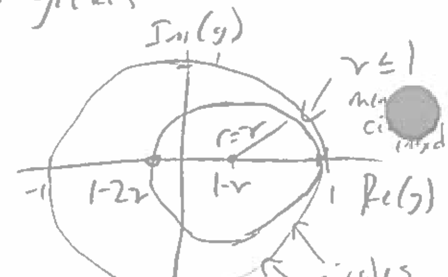
General: $u_j^{n+1} = \begin{cases} u_j - \frac{a\Delta t}{\Delta x}(u_j^n - u_{j-1}^n), & a > 0 \\ u_j - \frac{a\Delta t}{\Delta x}(u_{j+1}^n - u_j^n), & a \le 0 \end{cases}$ ← probably not how we'd deal with actual variable coefficient advection

This is a scheme for $u_t + a u_x = 0$.

Different: $u_t + (a(x)u)_x = 0$ ← use finite volume methods

Stability of upwind: Let $a > 0$. Von Neumann analysis yields

$$g(\xi) = 1 - r(1 - e^{-i\xi\Delta x}) = (1-r) + r e^{-i\xi\Delta x}$$

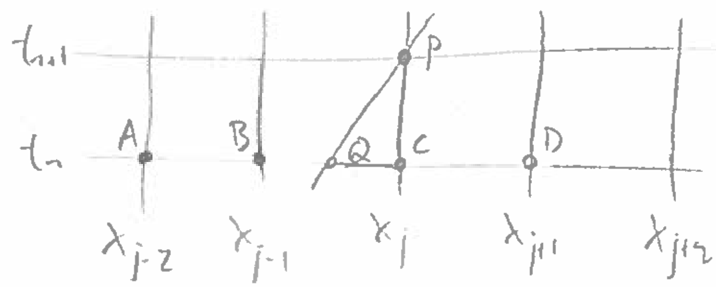


$r \le 1$ by CFL cond'n; makes upwind stable.

MAT228B - Lecture 20 - 2/27/17

2 working schemes for Advection eqn - Lax-Friedrichs & Upwinding
but these are only first-order in time & space - want better!

2nd order Methods:



assume $a>0$, $\nu \le 1$

quadratic interpolation for $u(Q)$ to get second-order accuracy. Need 3pts.

Could use points B, C, D to get Lax-Wendroff scheme
Could use points A, B, C to get Beam-Warming (2nd order Upwind / 1-sided LW)

Derive LW/BW from Taylor Expansion:

$$u(x,t+\Delta t) = u(x,t) + \Delta t\, u_t + \frac{\Delta t^2}{2} u_{tt} + O(\Delta t^3)$$

Use PDE to express time derivatives as space derivatives: $u_t = -a u_x$, $u_{tt} = -a u_{tx} = a^2 u_{xx}$

$$u(x,t+\Delta t) = u(x,t) - a\Delta t\, u_x + \frac{a^2\Delta t^2}{2} u_{xx} + O(\Delta t^3)$$

Use finite differences to approx. spatial derivatives

If we use centered 2nd-order diffs, get Lax-Wendroff method:

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

If we use (upwind) one-sided 2nd order diffs, get Beam-Warming method (for $a>0$):

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

Truncation Error for LW:

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

$$u_t + \frac{\Delta t}{2}u_{tt} + O(\Delta t^2) + a u_x + O(\Delta x^2) = \frac{a^2\Delta t}{2}u_{xx} + O(\Delta t\Delta x^2) \quad \leftarrow \text{but } u_{tt} = a^2 u_{xx} \text{ by PDE!}$$

$$u_t + a u_x = \underbrace{O(\Delta t^2) + O(\Delta x^2)}_{LTE} \qquad \text{2nd order in space \& time!}$$

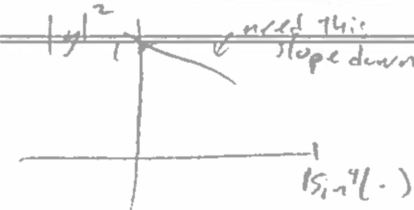
Truncation Error for Beam-Warming: $u_t + \frac{\Delta t}{2} u_{tt} + \mathcal{O}(\Delta t^2) + a u_x + \mathcal{O}(\Delta x^2)$

$$= \frac{a^2 \Delta t}{2} u_{xx} + \mathcal{O}(\Delta t \Delta x)$$

LTE: $\mathcal{O}(\Delta t \Delta x) + \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2)$

2^{nd}-order accurate scheme for $\Delta t \propto \Delta x$.

Stability of LW: $|g(\xi)|^2 = 1 - 4\nu^2(1-\nu^2)\sin^4\left(\frac{\xi \Delta x}{2}\right)$



Require $4\nu^2(1-\nu^2) \geq 0$

$\Rightarrow \nu^2 \leq 1 \Rightarrow \frac{\Delta t |a|}{\Delta x} \leq 1$ ← don't need to worry about sign of a!

Stability of B-W, $a > 0 \Rightarrow \frac{\Delta t a}{\Delta x} \leq 2$. ← get slightly larger time step!

Demos: Smooth Initial Data

1^{st} order methods: Lax-Friedrichs: · diffuses out bumps
· not good, no phase error

Upwinding: · diffuses out bumps less than LF
· not good, better than LF, no phase

2^{nd} order methods - Lax-Wendroff: better than Upwinding at diffusion
· doesn't diffuse bumps!
· phase error

Refining mesh helps a lot w/ diffusion error, helps some w/ phase error

Discont's Initial Data

LF - "looks like shit" - diffuses step

Upwinding - diffuses step a lot, not as bad as LF

LW - less diffusive, getting lots of wiggles

Refining mesh - Upwinding still diffuses, holds shape better, LW still has wiggles
↳ Gibbs phenomenon

Why does Upwinding smear, why does LW wiggle?
Can we do better? High resolution methods

MAT 228B - Lecture 21 - 3/1/17

Modified Eqns

PDE $\xrightarrow{\text{discretized}}$ Difference eqns

observed behavior in difference eqns not present in soln to PDE.
e.g. wiggles, phase lags, smearing/damping

find PDE to understand the difference eqns!
⇒ Modified eqns.

Upwinding for $a>0$: $u_j^{n+1} = u_j^n - \frac{a\Delta t}{\Delta x}(u_j^n - u_{j-1}^n)$

rearrange like advection: $\frac{u_j^{n+1}-u_j^n}{\Delta t} + \frac{a}{\Delta x}(u_j^n - u_{j-1}^n) = 0$

Let $v(x,t)$ be a smooth fn which satisfies the difference eqn.

$$\frac{v(x,t+\Delta t)-v(x,t)}{\Delta t} + a\left(\frac{v(x,t)-v(x-\Delta x,t)}{\Delta x}\right) = 0$$

V is smooth, so expand for small $\Delta x, \Delta t$:

$$v_t + \frac{1}{2}\Delta t\, v_{tt} + \frac{1}{6}\Delta t^2 v_{ttt} + O(\Delta t^3) + a\left(v_x - \frac{\Delta x}{2}v_{xx} + \frac{\Delta x^2}{6}v_{xxx} + O(\Delta x^3)\right) = 0$$

suppose $\Delta t = O(\Delta x)$:

$$v_t + a v_x + \left(\frac{\Delta t}{2}v_{tt} - a\frac{\Delta x}{2}v_{xx}\right) + \left(\frac{\Delta t^2}{6}v_{ttt} + \frac{\Delta x^2}{6}v_{xxx}\right) + O(\Delta x^3) + O(\Delta t^3) = 0$$

Truncate to first-order: Upwinding gives a first order approx to $u_t + a u_x = 0$

$$v_t + a v_x = -\frac{1}{2}(\Delta t\, v_{tt} - a\Delta x\, v_{xx})$$

← but a second order approx to this PDE

Take ∂_t:

$$v_{tt} = -a v_{tx} + O(\Delta t)$$

Take ∂_x:

$$v_{tx} = -a v_{xx} + O(\Delta t) \Rightarrow v_{tt} = a^2 v_{xx} + O(\Delta t)$$

$$\Rightarrow v_t + a v_x = \frac{1}{2}(a\Delta x - a^2\Delta t)v_{xx} + \cancel{O(\Delta t^2)} \text{ ignore}$$

$$v_t + a v_x = \frac{a\Delta x}{2}(1-\nu)v_{xx}$$

← Upwinding approx. this modified eqn to $O(\Delta t^2) + O(\Delta x^2)$.

← Advection - Diffusion

Upwinding better approxes. an Advection-Diffusion eqn than the advection eqn

↳ explains the damping + smearing we saw in the simulation.

2^{nd} order approx to $v_t + a v_x = \underbrace{\frac{a\Delta x}{2}(1-\nu)}_{D_{up}} v_{xx}$. 1^{st} order approx to $u_t + a u_x = 0$

~~As $\Delta t, \Delta x \to 0$, $D_{up} = \frac{a\Delta x}{2}(1-\nu) \to 0 \Rightarrow$ better approx to~~

when $\nu = 1$, Upwinding gives exact soln (just tracing along characteristics)

Problem: $\nu = \frac{\Delta t a}{\Delta x}$, so decreasing just Δt alone increases D_{up} & increases the diffusion/smearing from Upwinding.

Modified Eqn for Lax-Friedrichs: $v_t + a v_x = \underbrace{\frac{\Delta x^2}{2\Delta t}(1-\nu^2)}_{D_{LF}} v_{xx}$ ← 2^{nd} order approx.

This also has numerical diffusion, we saw in simulation that $D_{LF} >> D_{up}$, let's check!

$$\frac{D_{LF}}{D_{up}} = \frac{\frac{\Delta x^2}{2\Delta t}(1-\nu^2)}{\frac{a\Delta x}{2}(1-\nu)} = \frac{\Delta x}{a\Delta t}(1+\nu) = \frac{1}{\nu}(1+\nu) = 1 + \frac{1}{\nu} > 1$$

For ν close to 1, $D_{LF} \gtrsim 2 \cdot D_{up}$. For tiny ν, $D_{LF} >>> D_{up}$.

Modified Eqn for Lax-Wendroff: Note Lax-Wendroff gives 2^{nd} order approx to $u_t + a u_x = 0$

& a 3^{rd} order approx to $v_t + a v_x = \frac{a\Delta x^2}{6}(\nu^2 - 1) v_{xxx}$.

This PDE is weird: $v_t + a v_x = \mu v_{xxx}$ ← dispersive eqn.

Solve on whole real line using FT:

$\hat{v}_t + a i \xi \hat{v} = -\mu i \xi^3 \hat{v} \to \hat{v}_t = -(a i \xi + \mu i \xi^3)\hat{v}$ ← inf # of ODEs param. by ξ.

$\Rightarrow \hat{v}(\xi, t) = \hat{v}(\xi, 0) e^{-(a i \xi + \mu i \xi^3)t}$ FT back to real space

$$v(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{v}(\xi,t) e^{i\xi x} d\xi = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{v}(\xi,0) e^{i\xi x - (a i \xi + \mu i \xi^3)t} d\xi$$

$$= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{v}(\xi,0) e^{i\xi(x - c(\xi)t)} d\xi \quad w/\ c(\xi) = a + \xi^2 \mu$$ ← $\mu > 0$ for LW

This is translation w/ variable speed depending on freq. ξ.

Each freq oscillation ξ translates by speed $a + \xi^2 \mu$

small ξ → long wavelengths, smooth has $c \approx a$, correct speed. For large ξ, expect incorrect slower speed ...

MAT228B - Lecture 22 - 3/3/17

Modified eqn for Lax-Wendroff. $v_t + a v_x = \mu v_{xxx}$

Lax-Wendroff is 3rd order approx of ↗ $\mu = \frac{a\Delta x^2}{6}(\nu^2 - 1)$

Solution: $v(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} v(x,0)\, e^{-i\xi(a - c(\xi)t)}\, d\xi$, $c(\xi) = a + \mu \xi^2$

$c(\xi)$ is the phase velocity - depends on wave # ξ.

Low wave #, small freq $\xi \Rightarrow c \approx a$. Big wave #, high freq $\xi \Rightarrow |c-a| \gg c$

This behavior is called dispersion

Why does dispersion happen so much worse for discont's initial data?

For u piecewise-smooth w/ jump discontinuities,

$\hat{u}(\xi)$ scales like $1/|\xi|$ for large ξ.

u is C^∞, then $\hat{u}(\xi) = O(1/|\xi|^p)$ for all p.

E.g., C^∞ + some condition $\Rightarrow \hat{u}(\xi)$ decays like $e^{-a|\xi|}$.

Contribution of high freq. much larger (noticeable in discont's $u(x,0)$) ☆

We could include more terms & get a better modified eqn:

-W: $v_t + a v_x = \mu v_{xxx} - \varepsilon v_{xxxx}$ LW gives 4th order soln to this

$\mu = \frac{a\Delta x^2}{6}(\nu^2-1)$, $\varepsilon = O(\Delta x^3)$

v_{xxxx} term dampens high freq. faster than diffusion, low freqs. slower than diffusion

↳ Dissipation term, smooths!

Convergence Analysis of Upwinding on Discont's Initial Data using a Modified Eqn.

Advection: $u_t + a u_x = 0$ on $\mathbb{R}$

$$u(x,0) = u_0(x) = \begin{cases} 1, & x \le 0 \\ 0, & x > 0 \end{cases}$$

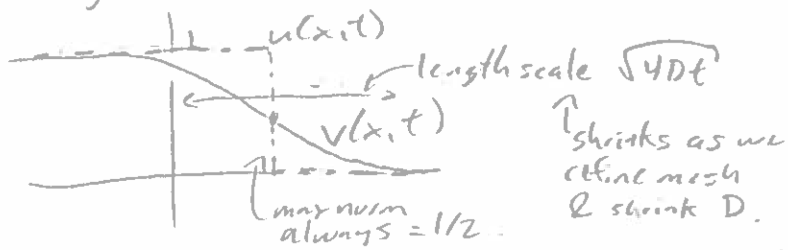
~~Analytic soln: $u(x,t) = u_0(x-at)$~~

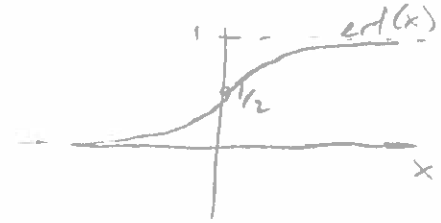
Modified Eqn:

$$\left.\begin{aligned} v_t + a v_x &= D v_{xx} \\ v(x,0) &= u_0(x) \end{aligned}\right\} \text{ Upwinding gives } 2^{\text{nd}} \text{ order accurate approx soln.}$$

Analytic soln: $v(x,t) = 1 - \mathrm{erf}\left(\frac{x-at}{\sqrt{4Dt}}\right)$, w/ $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_{-\infty}^{x} e^{-z^2}\,dz$

Sketch analytic solns for $a>0$:





Upwinding does not converge in ∞-norm for discontinuous problem

Convergence in 1-norm:

$$\|u-v\|_1 = \int_{\mathbb{R}} |u(x,t) - v(x,t)|\,dx = \int_{\mathbb{R}} \left|u_0(x-at) - \left(1 - \mathrm{erf}\left(\tfrac{x-at}{\sqrt{4Dt}}\right)\right)\right| dx$$

let $z = x - at$

$$\|u-v\|_1 = \int_{-\infty}^{0} \left|1 - 1 + \mathrm{erf}\left(\tfrac{z}{\sqrt{4Dt}}\right)\right| dz + \int_{0}^{\infty} \left|-1 + \mathrm{erf}\left(\tfrac{z}{\sqrt{4Dt}}\right)\right| dz$$

same integral by symmetry of erf(x).

$$= 2\int_{-\infty}^{0} \mathrm{erf}\left(\tfrac{z}{\sqrt{4Dt}}\right) dz, \quad \text{let } s = z/\sqrt{4Dt}$$

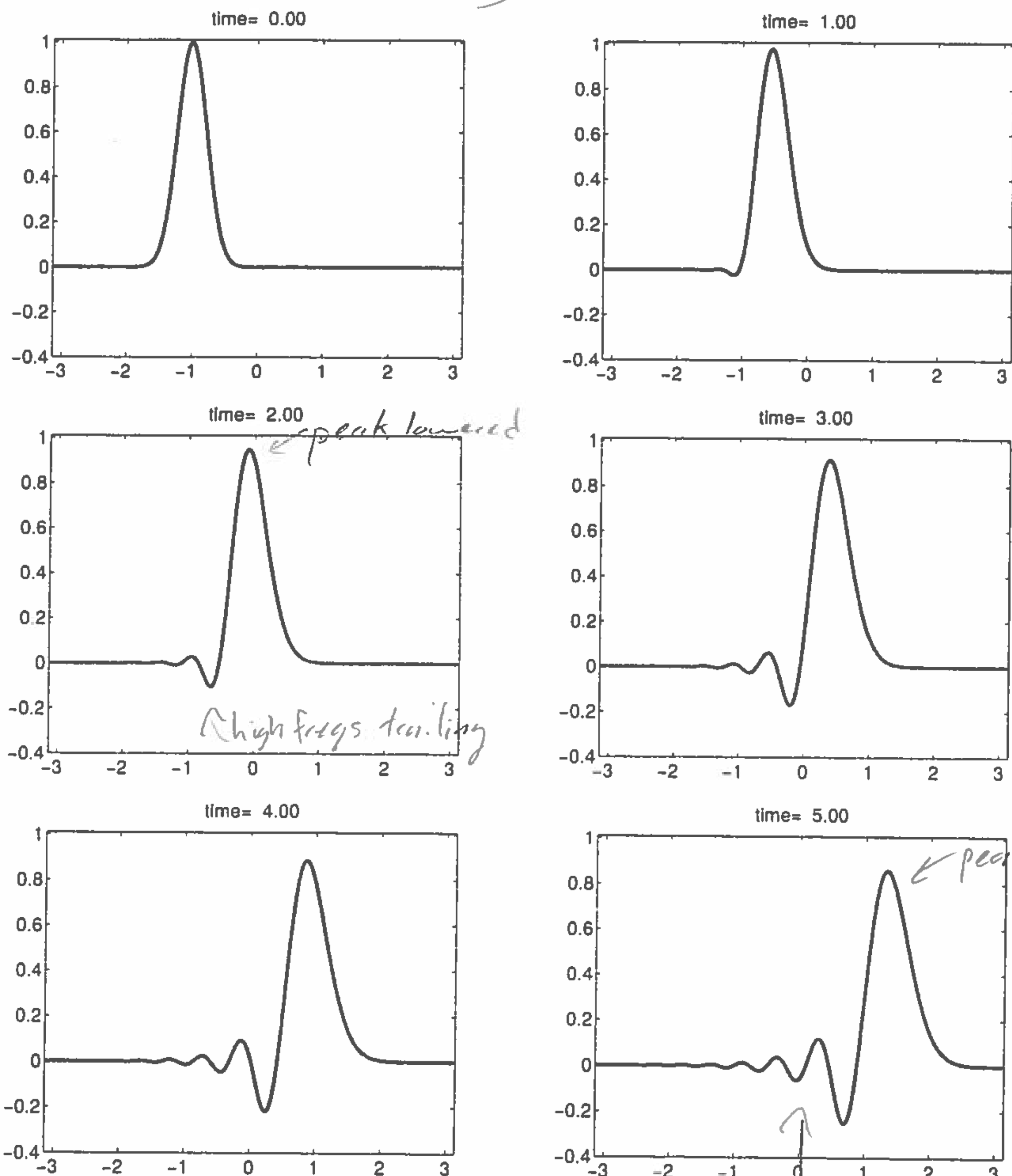
$$= 2\sqrt{4Dt}\underbrace{\int_{-\infty}^{0} \mathrm{erf}(s)\,ds}_{\text{constant}} = \mathcal{O}(\sqrt{\Delta x}).$$

Upwinding converges at order 1/2 in 1-norm for discont's initial data.

MA 128B - Lecture 22 handout - 3/3/17

μ small & negative $\Rightarrow$ high freqs. lag

Solution of $u_t + 0.5u_x = -10^{-3}\,u_{xxx}$ with Gaussian initial data



peak lowered

high freqs trailing

peak much lower

high freqs lagging

dispersion

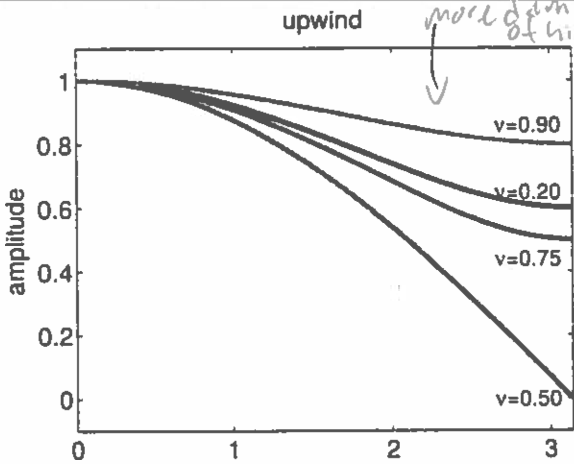
Lecture 23 - Amplitude & Phase Errors

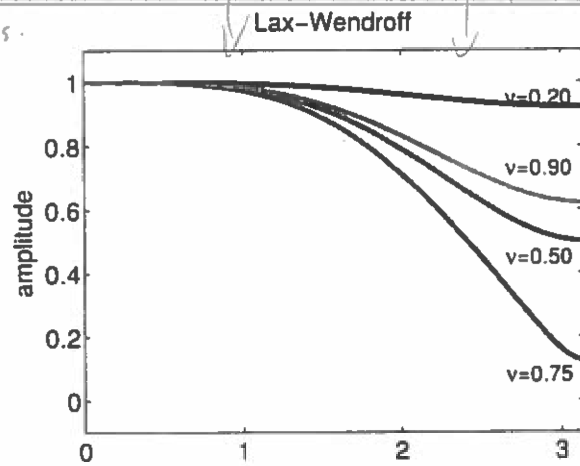
as ν goes down, more damping of high freqs.

drops off high freq slower than upwind

less dissipative than upwind

$|g(\theta)|$

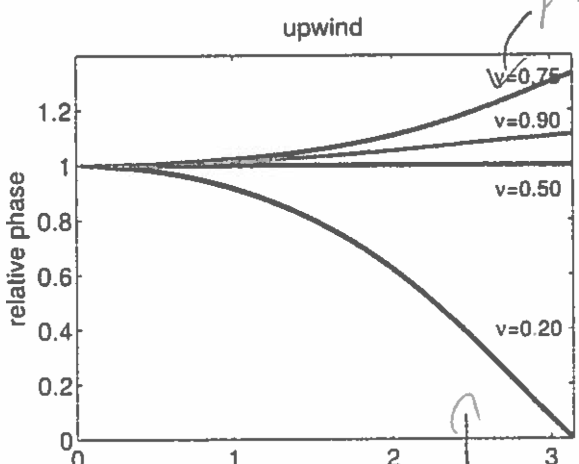


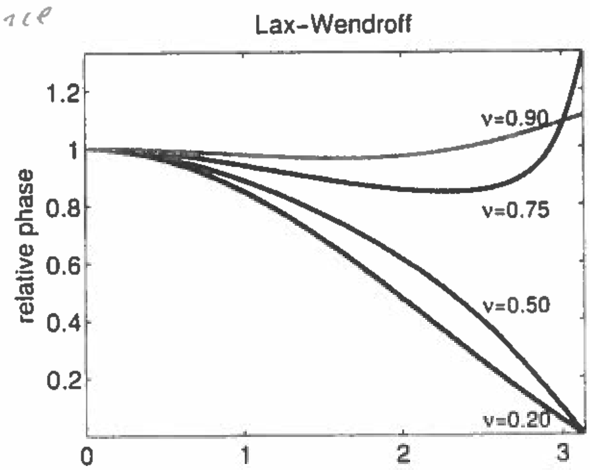


$0 \le \theta = \xi \Delta x \le \pi$

phase advance

$\frac{\psi(\theta)}{\Delta \Phi}$





phase lag

wouldn't see these b/c high freqs get wiped out by amplitude damping

phase lag in smooth modes VISIBLE

MA1110B - Lecture 23 - 3/6/17

Amplitude & Phase Errors

Von Neumann analysis: $\hat{u}^{n+1} = g(\xi)\hat{u}^n$

Look at $|g(\xi)|$ as a function of ξ to quantify amplitude error

$\theta = \xi\Delta x$. In limit of small θ (smooth initial data)

Upwinding $|g(\theta)| = 1 - \frac{1}{2}(\nu - \nu^2)\theta^2 + \mathcal{O}(\theta^4)$ $\rightarrow$ $\mathcal{O}(\Delta x^2)$ error per step $\Rightarrow$ 1^{st} order in amp.

Lax-Wendroff $|g(\theta)| = 1 - \frac{1}{8}(\nu^2 - \nu^4)\theta^4 + \mathcal{O}(\theta^6)$ $\rightarrow$ $\mathcal{O}(\Delta x^4)$ error per step $\Rightarrow$ 3^{rd} order in amp.

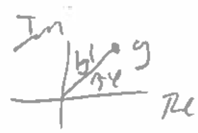
Phase Errors: $u = Ae^{i\xi(x-at)}$ is a soln to $u_t + au_x = 0$

$$Re(u) = A\cos(\underbrace{x-at}_{\text{phase}})$$

Let $\Delta\Phi$ = phase change per time step $= \xi(x - a(t+\Delta t)) - \xi(x-at) = -\xi a\Delta t$

$= -\frac{\theta}{\Delta x}a\Delta t = -\nu\theta$.

$\hat{u}^{n+1} = g(\theta)\hat{u}^n$



$\Rightarrow g(\theta) = |g|e^{i\varphi}$, $\varphi = \arg(g)$

Numerical scheme changes phase by $\varphi(\theta)$ per step.

Relative phase $\frac{\varphi(\theta)}{\Delta\Phi}$

For smooth modes, limit of small θ:

upwinding $\frac{\varphi(\theta)}{\Delta\Phi} = 1 - \frac{1}{6}(1-\nu)(1-2\nu)\theta^2 + \dots$ ← closer to 1 w/ $\nu \approx 1$

L-W $\frac{\varphi(\theta)}{\Delta\Phi} = 1 - \frac{1}{6}(1-\nu^2)\theta^2 + \dots$

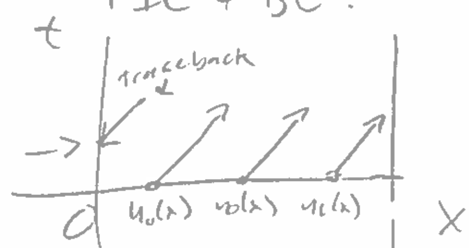
] - phase lag at same order

Boundary Conditions: $u_t + au_x = 0$ on $(0,1)$, $a > 0$

$+ IC + BC$?

Need BC at $x=0$ "inflow boundary"

wll: $\begin{cases} u_t + au_x = 0 \text{ on } (0,1) \\ u(x,0) = u_0(x) \\ u(0,t) = g(t) \end{cases}$ ← need data here



Can't specify boundary cond'n at outflow.

How to add inflow boundary numerically!

$a > 0$ still

~~Upwinding:~~ $u_j^{n+1} = u_j^n - \frac{a\Delta t}{\Delta x}(u_j^n - u_{j-1}^n)$

★ Dont need to do anything special to use inflow boundary. (soln given at boundary, everywhere just depends on left)

Method of Lines for Upwinding

$$\frac{du}{dt} = -\frac{a\Delta t}{\Delta x}\begin{pmatrix} 1 & & & \\ -1 & \ddots & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix} \underline{u} + \begin{pmatrix} ? \\ \vdots \\ \vdots \end{pmatrix}$$

all eigenvalues are 1. only one eigenvector] monstrously defective eigenspace

Study pseudospectrum - perturbations lead to huge eigenvalues
- very sensitive numerics / blowup common

Lax-Wendroff: $u_j^{n+1} = u_j^n - \frac{a\Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n) - \frac{a^2\Delta t^2}{2\Delta x^2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n)$

No problem at inflow boundary.

At outflow boundary, missing right data u_{j+1}^n

↳ Need to modify method at the outflow boundary

↳ Can just use Upwinding at last point.

↳ Could extrapolate to outside the domain ★ done more often

↳ Sometimes effects come from this choice

↳ Make sure outflow is really flowing out.

Systems of Eqns. $\underline{u}_t + A\underline{u}_x = 0$

A has real eigvals & is diagonalizable

e.g. turn wave eqn: $u_{tt} = c^2 u_{xx}$ into ↑ w/ variable change $q = \begin{pmatrix} u_t \\ u_x \end{pmatrix}$

$$q_t + \begin{pmatrix} 0 & c^2 \\ 1 & 0 \end{pmatrix} q_x = 0$$

L-W can do this no problem, no changes

Upwinding a system have to check "which way the wind is blowing"

↳ eigenvalue decomposition each time step.

MATH 4615 - Lecture 24 - 3/8/17

Systems of PDEs:

$$\underline{u}_t + A\underline{u}_x = 0$$ ← hyperbolic if A is constant posdef, real eigvals, diagonalizable

$$A = V\Lambda V^{-1}$$

$$\Rightarrow \underline{u}_t + V\Lambda V^{-1}\underline{u}_x = 0$$

$$V^{-1}\underline{u}_t + \Lambda V^{-1}\underline{u}_x = 0$$

let $\underline{w} = V^{-1}\underline{u}$ (using eigenvector coordinates)

$$\Rightarrow \underline{w}_t + \Lambda \underline{w}_x = 0$$ ← decoupled advection eqns.

To use upwinding, use sign of elmts of Λ

Let $\Lambda^+ = \dfrac{\Lambda + |\Lambda|}{2}$ & $\Lambda^- = \dfrac{\Lambda - |\Lambda|}{2}$

diag. matrix w/ neg. λ's set to 0. — diag matrix w/ pos λ's set to 0.

Upwinding: $$\underline{w}_j^{n+1} = \underline{w}_j^n - \frac{\Delta t}{\Delta x}\Lambda^+(\underline{w}_j^n - \underline{w}_{j-1}^n) - \frac{\Delta t}{\Delta x}\Lambda^-(\underline{w}_{j+1}^n - \underline{w}_j^n)$$

back to original variables:

$$\underline{u}_j^{n+1} = \underline{u}_j^n - \frac{\Delta t}{\Delta x}A^+(\underline{u}_j^n - \underline{u}_{j-1}^n) - \frac{\Delta t}{\Delta x}A^-(\underline{u}_{j+1}^n - \underline{u}_j^n)$$

w/ $A^+ = V\Lambda^+V^{-1}$, $A^- = V\Lambda^-V^{-1}$

or nonlinear or variable-coefficient problem, decompose differences locally
project forward differences onto left-moving eigspace of A,
project backward diffs onto right-moving eigspace of A.

Conservation Laws / Finite Volume Methods

$u_t + (f(u))_x = 0$ f is a flux function

if $f(u) = au$, recover the advection eqn.

---

if $f(u) = \frac{1}{2}u^2$, $f'(u) = u$ gives Inviscid Burger's Eqn

$\Rightarrow u_t + f'(u)u_x = 0 \rightarrow u_t + u \cdot u_x = 0$

Where did $u_t + (f(u))_x = 0$ come from?

Integral form of conservation law:

$$\frac{d}{dt}\int_{x_1}^{x_2} u\,dx = \underbrace{f(u(x_1,t))}_{\text{flux on } x_1 \text{ boundary}} - \underbrace{f(u(x_2,t))}_{\text{flux on } x_2 \text{ boundary}}$$

If u is a density, integral is total amt. of stuff in the interval $[x_1, x_2]$

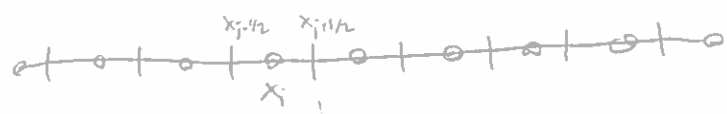
Stuff only changes from movement across boundary

Integral form can handle disconts, nonsmooth data!!!

Finite Volume Methods

Recall: in finite difference methods, $u_j \approx u(x_j)$ ← using approx values of fn. to approx derivatives

Divide domain into set of volumes C_j



$C_j = [x_{j-1/2}, x_{j+1/2}]$

Let $u_j \approx \frac{1}{|C_j|}\int_{C_j} u(x)\,dx$ ← the average value of the function over the volume/cell j.

e.g. $u_j \approx \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x)\,dx$. Note: $\frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x)\,dx = u(x_j) + O(\Delta x^2)$

u at the cell center is a 2nd order approx. to the average & vice versa

MA 448B - Lecture 24 cont'd - 3/8/17

Conservation Law: $u_t + (f(u))_x = 0$

Finite Vol. Methods: Divide domain into cells C_j

Approx $u_j \approx \frac{1}{|C_j|} \int_{C_j} u \, dx$

Cons. Law on C_j: $\underbrace{\frac{d}{dt} \int_{x_{j-1/2}}^{x_{j+1/2}} u \, dx}_{\Delta x \cdot u_j(t)} = f(u(x_{j-1/2}, t)) - f(u(x_{j+1/2}, t))$

Integrate in time from t_n to t_{n+1}

$$\Delta x (u_j^{n+1} - u_j^n) = \int_{t_n}^{t_{n+1}} f(u(x_{j-1/2}, t)) - f(u(x_{j+1/2}, t)) \, dt$$

Let $F_{j+1/2}^n = \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(u(x_{j+1/2}, t)) \, dt$

Then $\Delta x (u_j^{n+1} - u_j^n) = \Delta t (F_{j-1/2}^n - F_{j+1/2}^n)$

$$u_j^{n+1} = u_j^n + \frac{\Delta t}{\Delta x} (F_{j-1/2}^n - F_{j+1/2}^n)$$

or $$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{F_{j+1/2}^n - F_{j-1/2}^n}{\Delta x} = 0 \quad (*)$$

w/ $u_j^n = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t_n) \, dx$. this is exact, no approximation.

(*) Looks like a finite difference method, but its not!

Not an approximation until we start approxing the integrals. Approx. enters in the numerical flux function

Apply to advection eqn: Supp. $f(u) = au$

Upwinding: Choice: $F^n_{j+1/2} = \begin{cases} a \cdot u_j^n & \text{if } a \geq 0 \\ a\, u^n_{j+1} & \text{if } a < 0 \end{cases}$

numerical flux fn.
approx of flux fn.

reduces to Upwinding $\longrightarrow$

$a \geq 0 \quad u_j^{n+1} = u_j^n - \frac{a\Delta t}{\Delta x}\left(u_j^n - u_{j-1}^n\right)$

$a < 0 \quad u_j^{n+1} = u_j^n - \frac{a\Delta t}{\Delta x}\left(u_{j+1}^n - u_j^n\right)$

2-step Lax-Wendroff

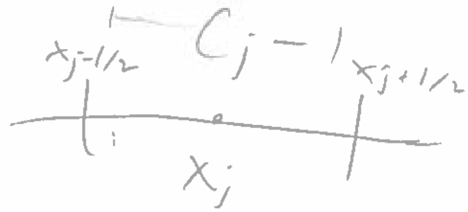
predict $u^{n+1/2}_{j+1/2}$: $\quad u^{n+1/2}_{j+1/2} = \frac{1}{2}\left(u_j^n + u_{j+1}^n\right) - \frac{\Delta t}{2\Delta x}\left(f(u_{j+1}^n) - f(u_j^n)\right)$

use to predict $F^{n+1/2}_{j+1/2} = f\left(u^{n+1/2}_{j+1/2}\right)$

Then evolve in time w/ this numerical flux fn.

MAT228B - Lecture 25 - 3/10/17

- $u_t + (f(u))_x = 0$



$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{F_{j+1/2}^n - F_{j-1/2}^n}{\Delta x} = 0$$

w/ $u_j = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t)\,dx$. F is time-averaged flux thru cell edg.

> Schemes of this form are discretely conservative.

— total amount of stuff in these 4 cells at t_n is $\Delta x \sum_{j=j_1}^{j_2} u_j^n$.

- $u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$ ← mult by Δx & sum from $j=j_1$ to $j=j_2$

$\Delta x \sum_{j=j_1}^{j_2} u_j^{n+1} = \Delta x \sum_{j=j_1}^{j_2} u_j^n - \Delta t \sum_{j=j_1}^{j_2}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$ ← telescoping sum!

$\underbrace{\Delta x \sum_{j=j_1}^{j_2} u_j^{n+1}}_{\text{stuff in interval } [j_1,j_2] \text{ at time } t_{n+1}} = \underbrace{\Delta x \sum_{j=j_1}^{j_2} u_j^n}_{\text{stuff in interval at time } t_n} - \underbrace{\Delta t\left(F_{j_2+1/2}^n - F_{j_1-1/2}^n\right)}_{\text{stuff moving across boundaries of interval}}$ ← If F's $=0$ on ends, this is $\Delta x \sum_{j=j_1}^{j_2} u_j^{n+1} = \sum_{j=j_1}^{j_2} u_j^n$

---

back to cont's: $u_t + (f(u))_x = 0$

$u_t + f'(u)u_x = 0$ Supp. $f'(u) > 0$

upwind discretization: $\frac{u_j^{n+1} - u_j^n}{\Delta t} + f'(u_j^n)\left(\frac{u_j^n - u_{j-1}^n}{\Delta x}\right) = 0$

- $u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} f'(u_j^n)(u_j^n - u_j^{n-1})$ ← sum & mult

$\Delta x \sum_{j=j_1}^{j_2} u_j^{n+1} = \Delta x \sum_{j=j_1}^{j_2} u_j^n - \Delta t \sum_{j=j_1}^{j_2} f'(u_j^n)(u_j^n - u_j^{n-1})$ ← not telescoping sum!

Not discretely conservative!

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+\frac{F_{j+1/2}^n-F_{j-1/2}^n}{\Delta x}=0 \qquad (*)$$

$$u_j^n=\frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t_n)\,dx$$ ← avg. value of fn u at time t_n over cell j

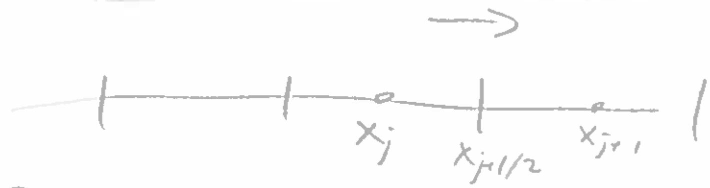
---

If $F_{j+1/2}^n=\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \underbrace{F(u(x_{j+1/2},t))}_{\text{cannot compute this exactly}}\,dt$, (*) is exact. (no approximation).

Numerical schemes defined by approximations of $F_{j+1/2}^n$

↳ Numerical fluxfunctions for $F_{j+1/2}^n$ to approx. time-averaged flux.

Supp. $f(u)=au$, $a>0$.



Approx flux by assuming the fn. u, constant over $[t_n,t_{n+1}]$. Use upwind value for $f(u)$

$\Rightarrow f(u(x_{j+1/2},t_n))=f(u(x_j,t_n))=au_j$ over the time step

General upwinding flux fn: $F_{j+1/2}^{UP}=\begin{cases} au_j^n, & a\ge 0\\ au_{j+1}^n, & a<0\end{cases}$

Upwinding is only first-order in space & time

↳ Δt error from Riemann sum integral approx.

↳ Δx error from using $u(x_j)$ over other choices.

2-step Lax-Wendroff – Approx. $f(u(x_{j+1/2},t_n))=f(u(x_{j+1/2},t_{n+1/2}))$ over time step

This gives 2^{nd} order in time approx. to the average flux.

Where do we get $u(x_{j+1/2},t_{n+1/2})$?

Use 2^{nd} order acc. finite-difference method to approx $u_{j+1/2}^{n+1/2}$.

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

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Cont'd: 2-step Lax-Wendroff

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

Then use $f(u_{j+1/2}^{n+1/2})$ as numerical flux fn $F_{j+1/2}^n$

For $f(u) = au$, reduces to Lax-Wendroff

2step LW

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

$$F_{j+1/2}^{LW} = f(u_{j+1/2}^{n+1/2}) = \frac{a}{2}(u_j^n + u_{j+1}^n) - \frac{a^2\Delta t}{2\Delta x}(u_{j+1}^n - u_j^n)$$

Reduces to LW:

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^{LW} - F_{j-1/2}^{LW}\right)$$

$$= u_j^n - \frac{\Delta t}{\Delta x}\Big[\frac{a}{2}(u_{j+1}^n + u_j^n) - \frac{a^2\Delta t}{2\Delta x}(u_{j+1}^n - u_j^n)$$
$$- \frac{a}{2}(u_j^n + u_{j-1}^n) + \frac{a^2\Delta t}{2\Delta x}(u_j^n - u_{j-1}^n)\Big]$$

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

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

$\square$

High Resolution Methods:

Supp. $a>0$

$$F^{LW}_{j+1/2} = \cancel{a u_j^n - a u_j^n + \frac{a}{2}\left(u_{j+1}^n + u_j^n\right) - \frac{a^2\Delta t}{2\Delta x}\left(u_{j+1}^n - u_j^n\right)}$$

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

$$= \underbrace{a u_j^n}_{\text{upwind}} + \underbrace{\frac{a}{2}(1-\nu)\left(u_{j+1}^n - u_j^n\right)}_{2^{nd}\text{ order correction}}$$

High Resolution Scheme:

$$F = F^{up} + \left(F^{LW} - F^{up}\right)\phi$$

where ϕ is the flux limiter that depends on the soln

ϕ some smooth fn btwn 0 & 1

tune the scheme based on soln behavior

When smooth, use LW – low dispersion, phase lag

when disconts, use UP – low phase lag, dispersing.

Avoiding Wiggles

Def: Supp. $u_j^0 \geq u_{j+1}^0 \ \forall j$.

If $u_j^n \geq u_{j+1}^n \ \forall n, j$, the scheme is monotone-preserving.

Thm (Godunov's). A linear, monotonicity-preserving scheme is at-most first-order accurate.

Idea to higher order is to use a non-linear scheme. (even for linear PDEs)

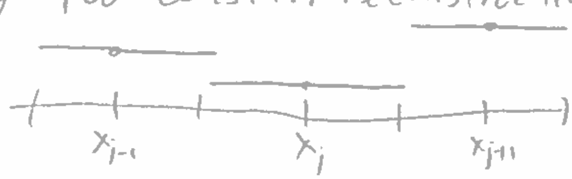
E.g., $F_{j+1/2} = F^{up}_{j+1/2} + (F^{LW}_{j+1/2} - F^{up}_{j+1/2})\phi(\underline{u}^n)$.

where ϕ is a flux-limiter.

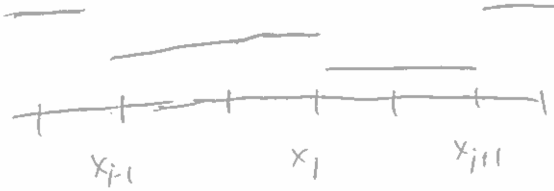
Consider hyperbolic conservation law: $u_t + (f(u))_x = 0$ for nonlinear f.

Godunov's Method: REA - reconstruct, evolve, average

1. Reconstruct a function from cell averages
   ↳ Given $u_j^n \longrightarrow \hat{u}(x, t_n)$ for $x \in [x_{j-1/2}, x_{j+1/2}]$
   e.g. PW-constant reconstruction



2. Evolve - solve the PDE exactly using reconstruction as initial data



$-r \leq 1$
$a > 0$

3. Average on each cell to update u_j^{n+1}

$$u_j^{n+1} = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} \hat{u}(x, t_{n+1})\,dx$$

☆ Easier done than said

Ex: Advection, $a>0$, $\nu \le 1$

Recall: $u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$

Only need $\tilde{u}(x_{j+1/2}, t)$ $\forall j$ to compute u_j^{n+1} using & $F_{j+1/2}^n = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(\tilde{u}(x_{j+1/2}, t))$

~~B/C $a>0$, $\nu \geq 1$ & $\tilde{u}$ is PW-constant, $\hat{u}(x_{j+1/2}, t) = u_j^n$ for $t \in [t_n, t_{n+1}]$.~~

Upwinding: $F_{j+1/2}^n = a u_j^n$

Generalize to nonlinear problems:

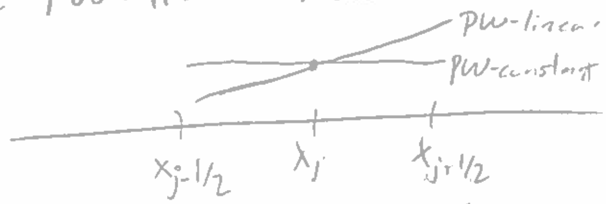
Riemann problem
$$\begin{cases} u_t + (f(u))_x = 0 \\ u(x,0) = \begin{cases} u_L, & x<0 \\ u_R, & x>0 \end{cases} \end{cases}$$

Solve Riemann problem get $\hat{u}(x_{j+1/2}, t)$

Know $F_{j+1/2}^n = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(\hat{u}(x_{j+1/2}, t))\,dt$.

Higher-Order accuracy - use more accurate reconstruction

Can use PW-linear reconstruction (average-preserving)



$$\hat{u}(x, t_n) = u_j^n + \overbrace{\sigma_j^n (x - x_j)}^{0\text{-average}}$$
on $x \in (x_{j-1/2}, x_{j+1/2})$

Average value on the cell is independent of the slope σ_j^n!

What slope to pick?

$\sigma_j^n = 0 \Rightarrow$ Upwinding. Force continuity?

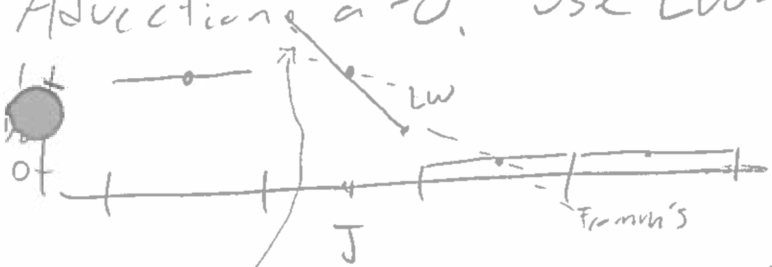
$\sigma_j^n = \dfrac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$ centered slope, for advection this is Fromm's method?

$\sigma_j^n = \dfrac{u_{j+1}^n - u_j^n}{\Delta x}$ for advection $a>0$ this is downwind slope yields Lax-Wendroff

$\sigma_j^n = \dfrac{u_j^n - u_{j-1}^n}{\Delta x}$ for advection $a>0$ this is upwind slope yields Beam-Warming

Lecture 26 cont'd

Advection $a>0$. use LW-slope for $u_j^n = \begin{cases} 1 & j \le J \\ 0 & j > J \end{cases}$



LW introduces overshoot behind the jump $\to$ wiggles behind
Fromm introduces overshoot before & after jump $\to$ wiggles both sides
Beam-Warming " after jump $\to$ wiggles in front

Don't have to use same slope function $\forall j, n$!

To get no wiggles, pick LW to right of jump & BW to left of jump.

To avoid oscillations, use a so-called limited slope

e.g. minmod slope

$$\sigma_j^n = \text{minmod}\left(\frac{u_j^n - u_{j-1}^n}{\Delta x}, \frac{u_{j+1}^n - u_j^n}{\Delta x}\right)$$

w/ $\text{minmod}(a,b) = \begin{cases} a & \text{if } |a| \le |b|, \; ab>0 \\ b & \text{if } |b| \le |a|, \; ab>0 \\ 0 & \text{if } ab \le 0 \end{cases}$

Minmod-slope avoids oscillation but is very diffusive.

A different choice is monotonized-centered slope

$$\sigma_j^n = \text{minmod}\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}, 2\left(\frac{u_{j+1}^n - u_j^n}{\Delta x}\right), 2\left(\frac{u_j^n - u_{j-1}^n}{\Delta x}\right)\right)$$

More general than minmod, less diffusive.

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$\tilde{u}(x, t_n) = u_j^n + \sigma_j^n (x - x_j)$

Advection eqn $a > 0$

compute the flux through $j-1/2$ edge

$$F_{j-1/2}^n = \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(\tilde{u}(x_{j-1/2}, t))\, dt$$

$$= \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} a \tilde{u}(x_{j-1/2}, t)\, dt$$

$$= \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} a \left(u_{j-1}^n + \sigma_{j-1}^n (x_{j-1/2} - a(t - t_n) - x_{j-1}) \right) dt$$

$$= a u_{j-1}^n + a \sigma_{j-1}^n \left(\frac{\Delta x}{2} - a \frac{\Delta t}{2} \right)$$

$$= \underbrace{a u_{j-1}^n}_{\text{upwind flux}} + \underbrace{\frac{a}{2}\left(1 - \frac{a \Delta t}{\Delta x}\right) \Delta x \sigma_{j-1}^n}_{2^{\text{nd}} \text{ order correction}}$$

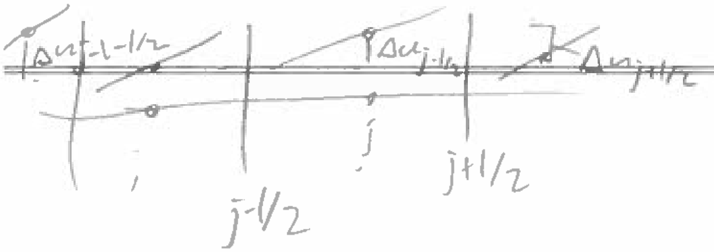
For Lax-Wendroff, $\Delta x \sigma_{j-1}^n = u_j^n - u_{j-1}^n = (\Delta u)_{j-1/2}$

For a + or −, write $F_{j-1/2}^n = F_{j-1/2}^{up} + \frac{|a|}{2}\left(1 - \frac{|a| \Delta t}{\Delta x}\right) \delta_{j-1/2}^n$

$\delta_{j-1/2}^n$ is a limited difference that depends on the solution

Need a way to measure smoothness of the solution

Let $\theta_{j-1/2} = \dfrac{(\Delta u)_{J_{up}-1/2}}{(\Delta u)_{j-1/2}}$ $\qquad J_{up} = \begin{cases} j-1 & a \geq 0 \\ j+1 & a < 0 \end{cases}$



For a smooth fn. away from extremepoints, $\theta \simeq 1$
Looking for rapid changes in soln on grid scale

Let $\delta^n_{j-1/2} = \phi(\theta_{j-1/2})(\Delta u)_{j-1/2}$ w/ ϕ the flux-limiter function

Linear schemes → $\phi = 0$ upwinding (ignore correction)
$\phi = 1$ Lax-Wendroff
$\phi(\theta) = \theta$ Beam-Warming

High resolution schemes
minmod $\phi(\theta) = \text{minmod}(1, \theta)$ picks between these 3
MC (monotonized centered) $\phi(\theta) = \max\left(0, \min\left(\frac{1+\theta}{2}, 2, 2\theta\right)\right)$
↳ better than minmod since less diffusive, more general

Superbee $\phi(\theta) = \max(0, \min(1, 2\theta), \min(2, \theta))$
Van Leer $\phi(\theta) = \dfrac{\theta + |\theta|}{1 + |\theta|}$ ↳ most sharpening

All these methods prevent oscillations!

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All the High Resolution methods are designed to be 2^{nd}-order on smooth data & to avoid introducing unphysical oscillations

The total variation of a grid function is

$$TV(\underline{u}) = \sum_j |u_{j+1} - u_j|$$

The total variation of a differentiable function is

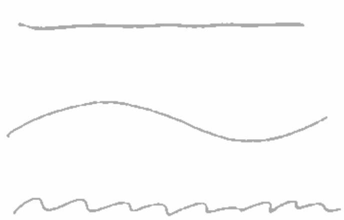
$$TV(f) = \int_a^b |f'(x)|\,dx$$

Crude way to measure how many "wiggles" in data

flat function — no variation

smooth fn — small variation

wiggly fn. — large variation



Consider $f_k(x) = e^{ikx}$ on $[0, 2\pi)$

$$TV(f_k) = \int_0^{2\pi} |ike^{ikx}|\,dx = 2\pi|k|.$$

High freq. modes have more TV.

Design schemes to reduce Total Variation!

High res schemes:

$$F_{j-1/2} = F^{up}_{j-1/2} + \frac{|a|}{2}\left(1 - \frac{|a|\Delta t}{\Delta x}\right)\delta_{j-1/2}$$

w/ $$\delta_{j-1/2} = \phi(\theta_{j-1/2})(u_j - u_{j-1})$$

& $$\theta_{j-1/2} = \frac{\Delta u_{J_{up}-1/2}}{\Delta u_{j-1/2}}$$

A two-level in time scheme is total variation diminishing (TVD) if

$$TV(u^{n+1}) \le TV(u^n).$$

One can show TVD $\Rightarrow$ monotonicity preserving
$\Downarrow$

~~Can show upwinding is TVD~~ ~~at most 1st order~~

LW/BW are not TVD. $\Longleftarrow$

Want to design ϕ to give a TVD scheme, but also want 2nd order for smooth data

For 2nd order, we require that $\phi(1) = 1$ ($\Leftrightarrow$ do LW/BW)
& ϕ be Lipschitz cont's at $\theta = 1$.
smooth will do, also bdd derivs

Constraints on ϕ to get TVD?

For $a > 0$, $u_j^{n+1} = u_j^n - \nu(u_j^n - u_{j-1}^n) - \frac{\nu(1-\nu)}{2}\left[\phi(\theta_{j+1/2})(u_{j+1}^n - u_j^n) - \phi(\theta_{j-1/2})(u_j^n - u_{j-1}^n)\right]$

looks like variable-rate diffusion.

or $u_j^{n+1} = u_j^n - C_{j-1}^n(u_j^n - u_{j-1}^n) - D_j^n(u_{j+1}^n - u_j^n)$

Thm: A scheme of this form is TVD if: $C_{j-1}^n \ge 0$
$D_j^n \ge 0$
$C_j^n + D_j^n \le 1$

Try $C_{j-1} = \nu - \frac{\nu(1-\nu)}{2}\phi(\theta_{j-1/2})$
$D_j = -\frac{\nu(1-\nu)}{2}\phi(\theta_{j+1/2}) < 0$ for $\phi \to [0,1]$ X bad

Trick: Write $u_{j+1} - u_j = \frac{u_j - u_{j-1}}{\theta_{j+1/2}}$ sub into scheme

Then $C_{j-1} = \nu + \frac{\nu(1-\nu)}{2}\left(\frac{\phi(\theta_{j+1/2})}{\theta_{j+1/2}} - \phi(\theta_{j-1/2})\right)$, $D_j = 0$

For TVD, require $0 \le C_{j-1} \le 1$. For CFL condition, need $\nu \le 1$.

Then if $\forall \theta_1, \theta_2 \ge 0$, $\left|\frac{\phi(\theta_1)}{\theta_1} - \phi(\theta_2)\right| \le 2$ the scheme is TVD.

cont'd

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High res scheme is CFL if $\nu \le 1$,
& TVD if $\forall \theta_1, \theta_2$, $\left| \frac{\phi(\theta_1)}{\theta_1} - \phi(\theta_2) \right| \le 2$.

Want $\phi(1) = 1$ for 2nd order, also $\boxed{\text{require } \phi = 0 \text{ for } \theta \le 0.}$
Don't know smoothness at extrema ($\theta \le 0$), so do upwinding there

To get all this, require

$$\boxed{\begin{aligned} & 0 \le \frac{\phi(\theta)}{\theta} \le 2 \\ & \& \quad 0 \le \phi(\theta) \le 2 \end{aligned} \quad \forall \theta > 0}$$

TVD region

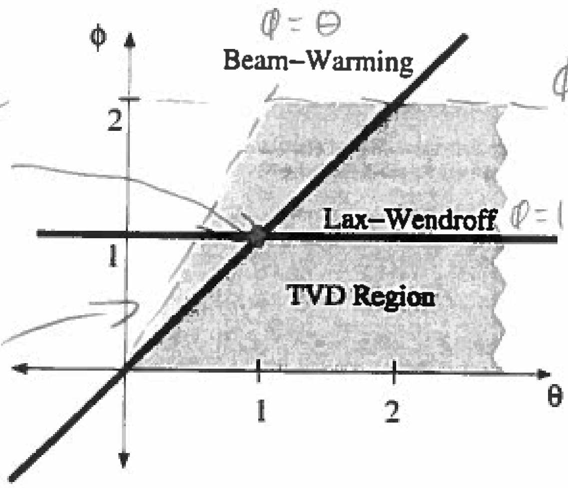
Can also restrict to ϕ btwn LW & BW $\Rightarrow$ Sweby region

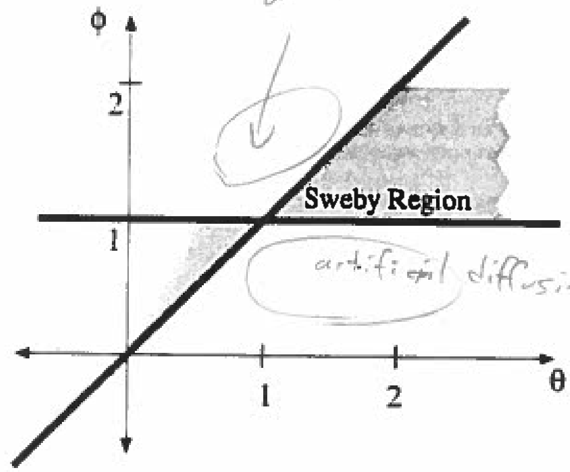
Lecture 28 handout

Plotting allowable regions for ϕ fn. to live.

require $\phi(1)=1$

$\phi \le 2\theta$

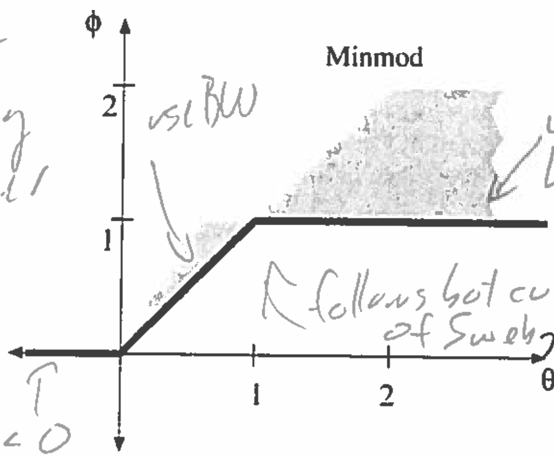




restrict to ϕ btwn LW & BW.

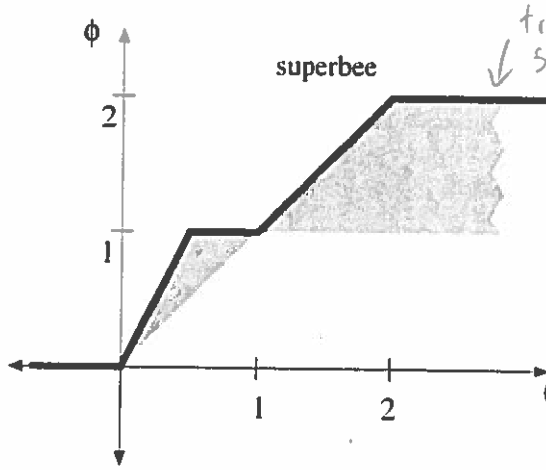
most limiting limiter

most diffusive



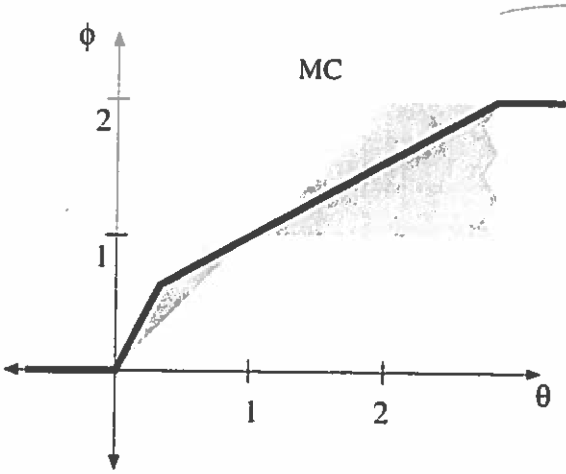
$\theta < 0$ use upwinding.

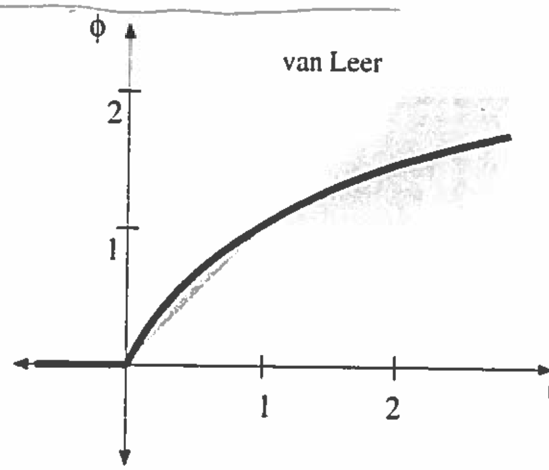
traces top of Sweby region.



least limiting, most sharpening

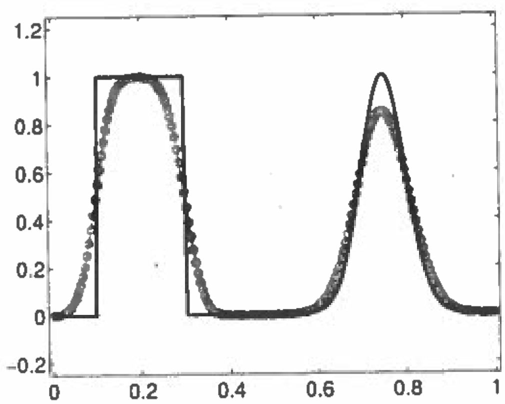
Middle of the road limiters



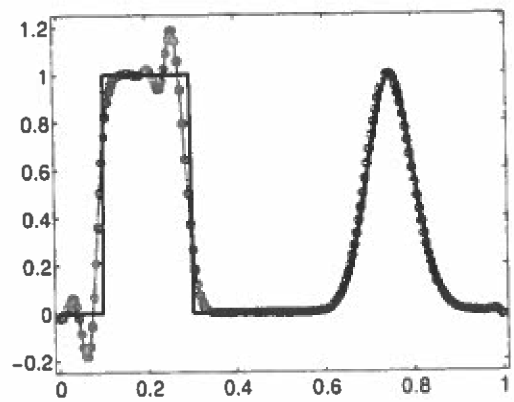


Numerical solutions of $u_t + u_x = 0$ on $(0, 1)$ with periodic boundaries at time 2.

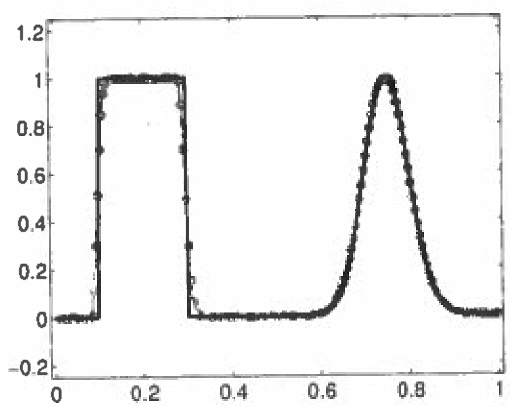
upwinding



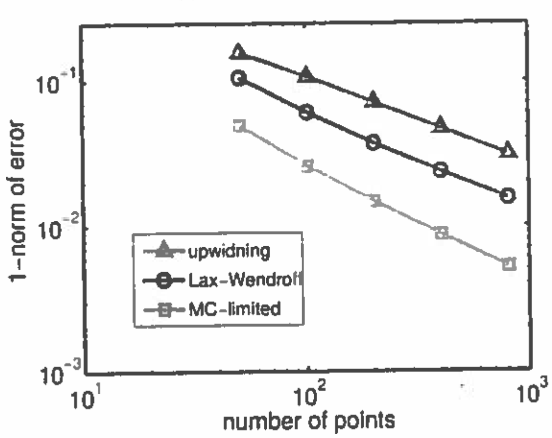
Lax-Wendroff



MC Limited



refinement



error on 100 point grid