Numerical methods for hyperbolic conservation laws

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Some references

- LeVeque 1992: Numerical Methods for Conservation Laws.
- LeVeque 2004: Finite Volume Methods for Hyperbolic Problems.
- Eymard-Gallouët-Herbin 2003: Finite Volume Methods (available online)

CONSERVATION LAWS I

- Consider PDEs in one dimension of the (strong conservation) form

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

- $f(u)$ is a flux function. IC: $u(x,0) = u_0(x)$. Systems: u is a vector
- Linear case: $u_t + Au_x = 0$, scalar version: $u_t + au_x = 0$
- An integral form of the conservation law

$$\frac{d}{dt}\int_{x_1}^{x_2} u(x,t)\,dx = -f(u(x_2,t)) + f(u(x_1,t))$$

- Another integral form

$$\int_{x_1}^{x_2}\Big[u(x,t_2) - u(x,t_1)\Big]\,dx + \int_{t_1}^{t_2}\Big[f(u(x_2,t)) - f(u(x_1,t))\Big]\,dt = 0$$

Conservation laws II

Note: solutions of the integral forms can be discontinuous
(not good news for Mr. Taylor...)

Hey! but what do you mean by "solutions"?

- Recall the *characteristics*: define $x(t)$ st

$$\begin{cases} \dfrac{d\,x(t)}{dt} & = f'(u(x(t),t)), \\ x(0) & = x_0. \end{cases}$$

Then

$$\frac{d\,u(x(t),t)}{dt} = u_x x'(t) + u_t = u_x f'(u(x(t),t)) + u_t = f(u)_x + u_t = 0$$

and so $u(x(t),t) = u_0(x_0)$

- Neat. It works if we have a smooth u... which we don't :(

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Conservation laws III

- Example: Burgers' equation

$$u_t + \left(\frac{u^2}{2}\right)_x = 0, \qquad u(x,0) = 1 - \cos(x)$$

Characteristics intersect and propagate different values

- $\Rightarrow$ no global (in x and t) solution

Weak solutions:

- for C^1 solutions, the strong and integral forms are equivalent
- If u satisfies the strong form a.e. in (a,b) then it is called a weak solution
- Hey, but I know weak forms from last week... they don't look like that
- Same idea: for any $\varphi \in C_c^\infty(\mathbb{R} \times \mathbb{R}^+)$

$$-\int_0^\infty \int_{-\infty}^\infty u\partial_t\varphi + f(u)\partial_x\varphi \, dx\, dt - \int_{-\infty}^\infty u_0(x)\varphi(x,0)\, dx = 0$$

Conservation laws IV

- The solutions of the integral form may contain jump discontinuities
- Jump discontinuities must satisfy a condition derived from the integral form (Rankine-Hugoniot)

$$\frac{f(u^+) - f(u^-)}{u^+ - u^-} = x'(t)$$

Then, if u is piecewise C^1 **and** discont. only along isolated curves **and** it satisfies the PDE when is C^1 **and** the Rankine-Hugoniot condition at the jumps, then we say u is a weak solution

- Non-conservation (or wave-speed) form

$$u_t + a(u)u_x = 0, \qquad a(u) = \frac{df}{du}$$

- Famous examples
  - $f(u) = \frac{u^2}{2}$: Burgers equation
  - $f(u) = au$: linear advection

Conservation laws V

- $f(u) = \dfrac{u^2}{u^2 + c(1-u)^2}$: Buckley-Leverett

Example: Take the Riemann problem (conservation law equipped with uniform initial conditions on an infinite spatial domain, except for a single jump discontinuity) for the Burgers eqn.

$$u_t + \left(\frac{u^2}{2}\right)_x = 0, \qquad u(x,0) = \begin{cases} 1 & x < 0 \\ -1 & \text{otherwise} \end{cases}$$

The IC is propagated in time to form a weak solution (shock discontinuity)

Example: Take the same problem, but flip the IC

$u(x,0) = \begin{cases} -1 & x < 0 \\ 1 & \text{otherwise} \end{cases}$. The propagated ICs also form a weak solution

Notice: $u(x,t) = \begin{cases} -1 & x \leq -t, \\ x/t & -t < x < t, \\ 1 & x > t, \end{cases}$ is also a weak soln. (rarefaction wave)

Conservation laws VI

Ooops! We need a third category of solutions $\longrightarrow$ Entropy Solutions

$$\int_0^\infty \int_{-\infty}^\infty E(u)\partial_t\varphi + F(u)\partial_x\varphi \, dx \, dt \geq 0,$$

with E convex and $F(u) = \int_0^u E'(v)f'(v)\,dv$

- Definitions may simplify for special fluxes:
- If $f''(u) \neq 0$ (genuinely nonlinear) then Oleinik's condition $\frac{f(u)-f(u^-)}{u-u^-} > x'(t) > \frac{f(u)-f(u^+)}{u-u^+}$ implies u is an entropy solution
- If $f''(u) > 0$ (unif. convex) or $''(u) < 0$ (unif. concave), then Lax's condition $f'(u^-) > x'(t) > f'(u^+)$ implies u is an entropy solution
- If $f'(u) > 0$ then $f'(u^-) \geq f'(u^+)$ implies u is an entropy solution
- (i.e., looking towards the "right", we can only "jump down")

Finite differences and finite volumes I

- Divide the domain into cells (intervals in 1D, the multi-D case will be discussed later)
- Grid with mesh spacing $h = \Delta x$:

- Discretize in time with time-step Δt
- As done two weeks ago, we can approximate point-values of u as $u_i^n = u(x_i, t^n)$
- Or, we can define $\bar{u}_j$ as the cell-centered average:

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

- We build numerical methods to evolve these averages (rather than point-wise samples)

Finite differences and finite volumes II

- Essentially a different philosophy than FD, but in simple cases leads to the same schemes
- Similar methods applied: use U_j to approximate either pointwise values u_j or cell averages $\bar{u}_j$ (depending on whether FD or FV)
- Integral form of the conservation law

$$\int_{x_1}^{x_2} \Big[u(x,t_2) - u(x,t_1) \Big] \, dx + \int_{t_1}^{t_2} \Big[f(u(x_2,t)) - f(u(x_1,t)) \Big] \, dt = 0$$

- leads to a numerical conservation law

$$\bar{u}_i^{n+1} = \bar{u}_i^n - \lambda (\hat{f}_{i+1/2} - \hat{f}_{i-1/2}),$$

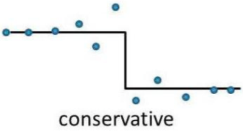
with $\lambda = \frac{\Delta t}{h}$, and where $\hat{f}$ are numerical fluxes (associated to t^n or t^{n+1}, explicit vs. implicit)

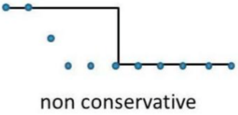
Finite differences and finite volumes III

Definition

A scheme to solve conservation laws is conservative iff

1. $\hat{f}$ is Lipschitz continuous
2. $\hat{f}(u, \ldots, u) = f(u)$





Finite differences and finite volumes IV

Conservative numerical methods automatically locate shocks correctly (however, the shape of the shock may not be reproduced correctly).

A method that explicitly enforces the Rankine-Hugoniot relation is called a shock-capturing method

Conservative methods are a simple and natural way to ensure we do not converge to non-solutions (Lax-Wndroff result):

Theorem

If the solution $\{u_i^n\}$ to a conservative scheme converges a.e. to a function $u(x,t)$, then u is a weak solution of the conservation law.

Examples of conservative schemes

- **Lax-Friedrichs**

$$\hat{f}_{i+1/2} = \frac{1}{2}\left(f(u_i) + f(u_{i+1}) - \alpha(u_{i+1} - u_i)\right), \quad \alpha = \max_u |f'(u)|$$

Finite differences and finite volumes V

- **local Lax-Friedrichs**

$$\hat{f}_{i+1/2} = \frac{1}{2}\big(f(u_i) + f(u_{i+1}) - \alpha_{i+1/2}(u_{i+1} - u_i)\big), \quad \alpha_{i+1/2} = \max_{(u_i, u_{i+1})} |f'(u)|$$

(no matter if u_i or u_{i+1} is larger)

- **Roe**'s scheme

$$\hat{f}_{i+1/2} = \begin{cases} f(u_i) & a_{i+1/2} \geq 0, \\ f(u_{i+1}) & a_{i+1/2} < 0, \end{cases} \qquad a_{i+1/2} = \frac{f(u_{i+1}) - f(u_i)}{u_{i+1} - u_i}$$

- **Enquist-Osher** scheme

$$\hat{f}_{i+1/2} = f^+(u_i) + f^-(u_{i+1}),$$

with $f^+(u) = \int_0^u \max(f'(u), 0) du + f(0)$, $f^-(u) = \int_0^u \min(f'(u), 0) du$

Finite differences and finite volumes VI

- **Lax-Wendroff** scheme (idea 1: repeatedly replace time by space derivatives using the PDE, 2: discretize space derivatives by 2nd order central FDs)

$$\hat{f}_{i+1/2} = \frac{1}{2}\left(f(u_i) + f(u_{i+1}) - \lambda f'(u_{i+1/2})[f(u_{i+1}) - f(u_i)]\right)$$

- **MacCormack** method (of "predictor-corrector" type)

$$\begin{aligned} u_i^{n+1/2} &= u_i^n - \lambda(f(u_i^n) - f(u_{i-1}^n)), \\ u_i^{n+1} &= \frac{1}{2}\left(u_i^n + u_i^{n+1/2} + \lambda\left[f(u_{i+1}^{n+1/2}) - f(u_i^{n+1/2})\right]\right) \end{aligned}$$

and $\hat{f}_{i+1/2} = \frac{1}{2}\left(f(u_i) + f(u_i - \lambda(f(u_i) - f(u_{i-1})))\right)$

What about our friends from week 3 (e.g. centered differences in space and forward Euler in time)?

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Finite differences and finite volumes VII

- Take again Burgers eqn. with $u(x,0) = \begin{cases} 1 & x < 0 \\ 0 & x \geq 0 \end{cases}$
- Entropy solution is
$$u(x,t) = \begin{cases} 1 & x \leq \frac{1}{2}t, \\ 0 & x > \frac{1}{2}t \end{cases}$$
- and notice that a max principle holds $\min_x u_0(x) \leq u(\xi,t) \max_x u_0(x)$
- For the linear advection $u_t + au_x = 0$, the friend will be disastrous!!
- For this case, upwinding can help:

  One-sided methods
$$u_i^{n+1} = u_i^n - \lambda a(u_i^n - u_{i-1}^n), \quad \text{or} \quad u_i^{n+1} = u_i^n - \lambda a(u_{i+1}^n - u_i^n)$$
  Upwinding: decide which to use point-wise, based on sign of a

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Finite differences and finite volumes VIII

- Now let's go back to the nonlinear problem (extension evident if we write it as $u_t + uu_x = 0$), and propose

$$u_i^{n+1} = u_i^n - \lambda\, u_i^n (u_i^n - u_{i-1}^n)$$

ICs $\Rightarrow$ for $i \neq i_0$, we have $u_i^0 = u_{i-1}^0$ and for $i = i_0$, $u_{i_0}^0 = 0$

- $u_i^{n+1} = u_i^n$. Bad.

Godunov's method I

Riemann Problems

- Consider on $-\infty < x < \infty$, a piecewise constant solution with u_l for $x < 0$ (or some other reference point) and u_r for $x > 0$
- Suppose we can solve this problem: e.g., analytically or that we have some subroutine that can compute it approximately.
- Example: Burgers' eqn with shock.
- Example: Burgers' eqn with expansion fan (viscosity solution, versus other weak solutions.)

  (Getting fans correct and accurate is tricky for numerical methods, particularly for nonlinear systems.)

Godunov's idea

- Use the U_j^n values to define piecewise constant initial condition, constant over each cell. This gives us a new problem, call the solution $\tilde{u}(x, t)$. (temporary variable, just for the derivation).

Godunov's method II

- We can solve this problem exactly for small time! Consider the Riemann problem on each interface. Assume we can solve these exactly. For small time, these can be joined together to form the exact solution of this initially piecewise problem.

  (after t^{n+1} the local problems begin to interact with neighbouring cells)

- Next, average this exact solution over each cell to define the next discrete solution:

$$U_j^{n+1} := \frac{1}{h} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \tilde{u}(x, t_{n+1}) dx.$$

- Then repeat the process

Godunov's method in practice:

Godunov's method III

- Because $\tilde{u}$ is the exact solution, we can rewrite the cell-average above in terms of the integral form over the cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$ and time $[t^n, t^{n+1}]$. This gives us fluxes in/out of the cell. These define our numerical fluxes:

$$\hat{f}^n_{j+\frac{1}{2}} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} f\left(\tilde{u}(x_{j+\frac{1}{2}}, t)\right) dt.$$

- But this further reduces:

$$\hat{f}^n_{j+\frac{1}{2}} = f\left(u^*(U^n_j, U^n_{j+1})\right),$$

where u^* is a value that depends only on the initial left state $u_l = U^n_j$ and initial right states $u_r = U^n_{j+1}$.

GODUNOV'S METHOD IV

- Why? Easy to see for particularly examples (e.g., Burgers'). In general: because Riemann problem is a similarity solution, constant in $(x - x_{j+\frac{1}{2}})/t$.

  So we have a technique to build conservative numerical methods in terms of Riemann problems.

- OK, but can we simplify further? After some work, the scalar convex f case leads to:

$$\hat{f}(u_l, u_r) = \begin{cases} \min_{u_l \le u \le u_r} f(u) & \text{if } u_l \le u_r \\ \max_{u_r \le u \le u_l} f(u) & \text{if } u_l > u_r \end{cases}$$

  (and in fact its true for non-convex scalar and gives gives correct weak solution.)

Clawpack: includes collection of **fast** Fortran-based Riemann solvers for many common systems. It uses something like Godunov (with limiters to get higher-order accuracy in smooth regions.)

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Domains of dependence and CFL condition I

Generic numerical flux for an explicit method

$$\hat{f}^n_{i+1/2} = \hat{f}(u^n_{i-K_1+1}, \ldots, u^n_{i+K_2})$$

so from the integral form we get

$$u^{n+1}_i = \mathscr{U}(u^n_{i-K_1}, \ldots, u^n_{i+K_2}).$$

Similarly, for implicit methods

$$\hat{f}^n_{i+1/2} = \hat{f}(u^{n+1}_{i-L_1+1}, \ldots, u^{n+1}_{i+L_2})$$

and

$$u^{n+1}_i = \mathscr{U}(u^n_{i-K_1}, \ldots, u^n_{i+K_2}; u^{n+1}_{i-L_1}, \ldots, u^{n+1}_i, u^{n+1}_{i+L_2})$$

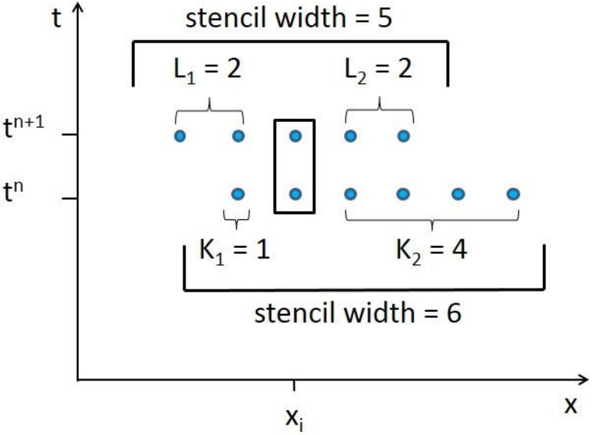
(here the solution of a system of eqns. is required at each time-step)

Stencils (direct numerical domain of dependence) of u^{n+1}_i:

$$(u^n_{i-K_1}, \ldots, u^n_{i+K_2}) \quad \text{and} \quad (u^{n+1}_{i-L_1}, \ldots, u^{n+1}_{i+L_2}),$$

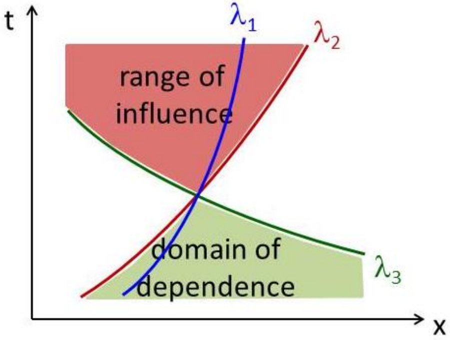
having stencil widths $K_1 + K_2 + 1$, $L_1 + L_2 + 1$, respectively.

Domains of dependence and CFL condition II



DOMAINS OF DEPENDENCE AND CFL CONDITION III

- A point in the $x - t$ plane is influenced only by points in a finite domain of dependence and influences only points in the range of influence

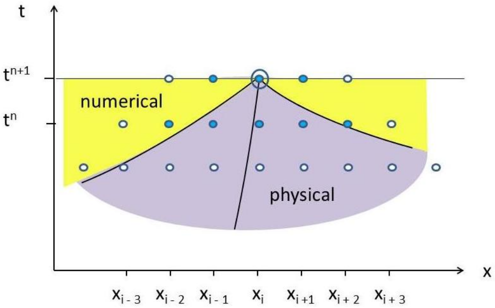


- The physical domain of dependence and physical range of influence are bounded by the waves with the highest and lowest speeds

Domains of dependence and CFL condition IV

- In a well-posed (hyperbolic) problem, the range of influence of the initial and boundary conditions should exactly encompass the entire flow in the $x - t$ plane
- Direct numerical domain of dependence of a scheme is the stencil (local set)
- Full numerical domain of dependence of a scheme is its direct numerical domain of dependence $\bigcup$ the points of the $x - t$ plane upon which the numerical values in the direct numerical domain of dependence depend upon
- The Courant-Friedrichs-Lewy or (CFL) condition: *The full numerical domain of dependence must contain the physical domain of dependence*

Domains of dependence and CFL condition V



- Schemes violating the CFL condition miss information about the exact solution and may blow up
- The CFL condition is necessary but not sufficient for numerical stability
- Precise definition (ineq. restricting the wave speed) postponed
- For systems, families of waves define the domain of dependence. We need to take the most restrictive CFL

General properties of some schemes I

Definition

Fix t. The total variation of $u(\cdot,t)$ is $TV(u(\cdot,t)) = \int_{-\infty}^{\infty} |\frac{\partial u}{\partial x}|\, dx$

(interpretation by Laney and Caughey 91: "TV(u) on an infinite domain is a sum of extrema – maxima counted positively and minima counted negatively – with the two infinite boundaries always treated as extrema and counting each once, and every other extrema counting twice")

(even simpler one: "TV is a measure of wiggliness")

Hyperbolic system $\Rightarrow$ $TV(u)$ does not increase with time

Definition

The total variation of the discrete representation of u at time t^n is (for a fixed partition)

$$TV(u^n) = \sum_{i=-\infty}^{\infty} |u_{i+1}^n - u_i^n|$$

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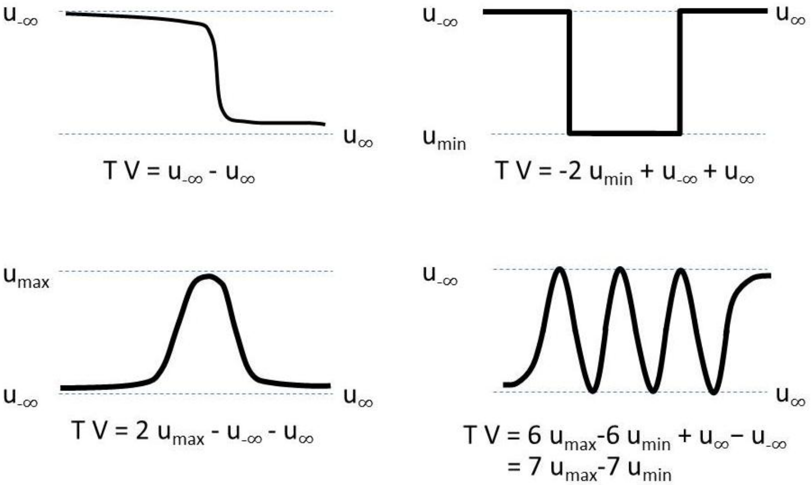
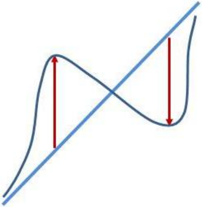
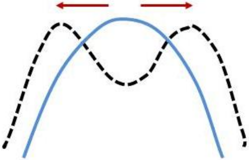
GENERAL PROPERTIES OF SOME SCHEMES II



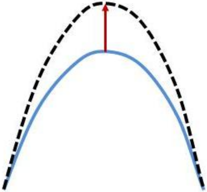
General properties of some schemes III



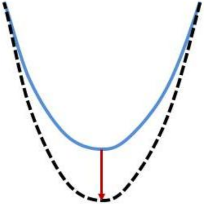
transforming a monotone region into one with a maximum and a minimum



splitting a maximum into two maxima and a minimum



amplifying a maximum



decreasing a minimum

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General properties of some schemes IV

Definition

A scheme $u^{n+1} = G(u^n)$,

$$u_i^{n+1} = u_i^n - \lambda[\hat{f}(u_{i-p}^n, \dots, u_{i+q}^n) - \hat{f}(u_{i-p-1}^n, \dots, u_{i+q-1}^n)] =: G(u_{i-p-1}^n, \dots, u_{i+q}^n)$$

is

- Total variation diminishing (TVD) if $TV(u^{n+1}) \leq TV(u^n)$
- Monotonicity-preserving if $u_{i+1}^n \geq u_i^n \ \forall i \Rightarrow u_{i+1}^{n+1} \geq u_i^{n+1} \ \forall i$
- Linear if it is linear when applied to a linear PDE
- Of type E if $\text{sign}(u_{i+1}^n - u_i^n)(\hat{f}_{i+1/2}^n - f(v)) \leq 0$ for all $v \in [u_i^n, u_{i+1}^n]$
- Monotone if G is a monotonically non-decreasing function of each argument $G(\uparrow, \uparrow, \dots, \uparrow)$

For instance,

Monotone $\Rightarrow$ E $\Rightarrow$ TVD $\Rightarrow$ Monotonicity-preserving

General properties of some schemes V

Other good features of monotone schemes

- local max principle

$$\min_{j \in \text{stencil around i}} u_j \leq G(u)_i \leq \max_{j \in \text{stencil around i}} u_j$$

- L^1–contraction

$$\left\| u^{n+1} - v^{n+1} \right\|_{L^1} \leq \| u^n - v^n \|_{L^1}$$

- Satisfaction of all entropy conditions

But, Godunov says

Theorem

Monotone schemes are at most first-order accurate.

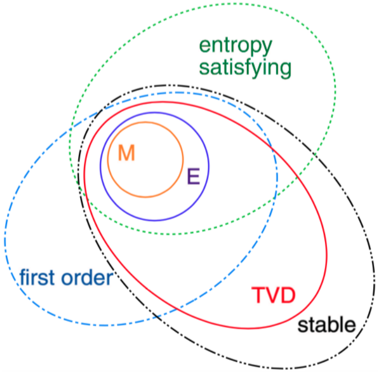
(depressing result :(, especially in view of expensive multi-D computations)

Idea: to look for a wider class of methods, but maintaining some properties of monotone schemes.

General properties of some schemes VI

Further relations:

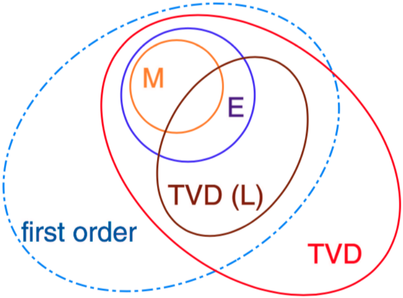
- Linear + monotonicity-preserving $\Rightarrow$ monotone scheme.
- Linear + (monotonicity-preserving or TVD) $\Rightarrow$ at most first order accurate.
- Linear + monotone $\Leftrightarrow$ linear TVD $\Rightarrow$ at most first order accurate (see below)



Goal: monotone near shocks and high order elsewhere

General properties of some schemes VII

Another bomb from Godunov: No second or high order **linear** scheme can be TVD
(that is, if you want high order TVDs, you must go nonlinear)



General properties of some schemes VIII

- Well, let's do it. Let's go nonlinear, but still TVD
- Main players here: slope limiters

But before that,

Lemma

The wave speed split form of a forward FV scheme is given by

$$\bar{u}_{i+1}^{n+1} = \bar{u}_i^n + \lambda \left[C_{i+1/2}(\bar{u}_{i+1}^n - \bar{u}_i^n) - D_{i-1/2}(\bar{u}_i^n - \bar{u}_{i-1}^n) \right].$$

If $C_{i+1/2} \geq 0$, $D_{i-1/2} \geq 0$, and $1 - \lambda(C_{i+1/2} + D_{i-1/2}) \geq 0$ (Harten's positivity condition), then the method is TVD.

Notice that D, C may depend on the $\bar{u}_i$'s...

Take the Lax-Wendroff scheme. (2nd order)

- Write it for the case of linear flux *au*:

$$\bar{u}_{i+1}^{n+1} = \bar{u}_i^n - \lambda \frac{a}{2}(\bar{u}_{i+1}^n - \bar{u}_i^n) + \lambda^2 \frac{a^2}{2}(\bar{u}_{i+1}^n - 2\bar{u}_i^n + \bar{u}_{i-1}^n)$$

General properties of some schemes IX

- Rewrite it in a split form

$$\bar{u}_{i+1}^{n+1} = \underbrace{\bar{u}_i^n - \lambda a(\bar{u}_i^n - \bar{u}_{i-1}^n)}_{\text{1st order upwind}} - \underbrace{\frac{1}{2}\lambda a(1-\lambda a)(\bar{u}_{i+1}^n - 2\bar{u}_i^n + \bar{u}_{i-1}^n)}_{\text{"anti-diffusive" flux}}$$

- Notice that

$$^{\text{LW}}\hat{f}_{i+1/2}^n = \underbrace{a\bar{u}_i^n}_{^{\text{UP}}\hat{f}_{i+1/2}^n} + \frac{a}{2}(1-\lambda a)(\bar{u}_{i+1}^n - \bar{u}_i^n)$$

- In order to get a TVD scheme, we need to limit the anti-diffusive flux. That is, we do

$$^{\text{TVD}}\hat{f}_{i+1/2}^n = a\bar{u}_i^n + \frac{a}{2}(1-\lambda a)\underbrace{\phi_{i+1/2}}_{\text{flux limiter}}(\bar{u}_{i+1}^n - \bar{u}_i^n)$$

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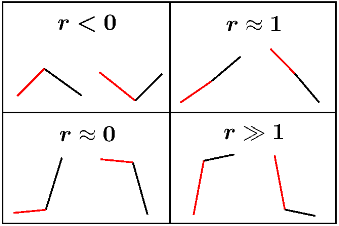
GENERAL PROPERTIES OF SOME SCHEMES X

- Therefore

$$\bar{u}_{i+1}^{n+1} = \bar{u}_i^n - \lambda a(\bar{u}_i^n - \bar{u}_{i-1}^n) - \frac{1}{2}\lambda a(1-\lambda a)[\phi_{i+1/2}(\bar{u}_{i+1}^n - \bar{u}_i^n) - \phi_{i-1/2}(\bar{u}_i^n - \bar{u}_{i-1}^n)]$$

- The limiter must be applied to the flux (to preserve conservation form)
- If $\phi = 1$ we get Lax-Wendroff (not TVD), $\phi = 0$ gives Upwind (TVD)
- The idea is to choose it close to 1, but still enforcing TVD
- Introduce the smoothness monitor $r_{i+1/2} = \dfrac{\bar{u}_i^n - \bar{u}_{i-1}^n}{\bar{u}_{i+1}^n - \bar{u}_i^n}$ and set $\phi = \phi(r)$



General properties of some schemes XI

-

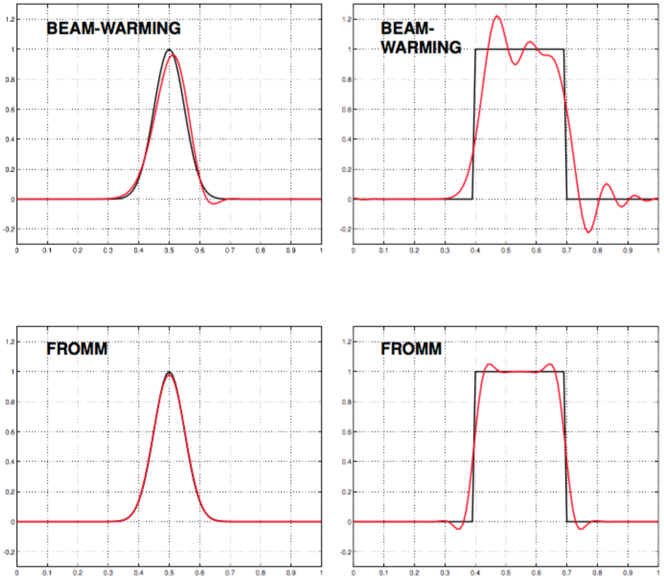
Linear methods

- Upwind: $\phi(r) = 0$ (TVD)
- Lax-Wendroff: $\phi(r) = 1$ (not TVD)
- Beam-Warming: $\phi(r) = r$
- Fromm: $\phi(r) = \frac{1}{2}(1+r)$

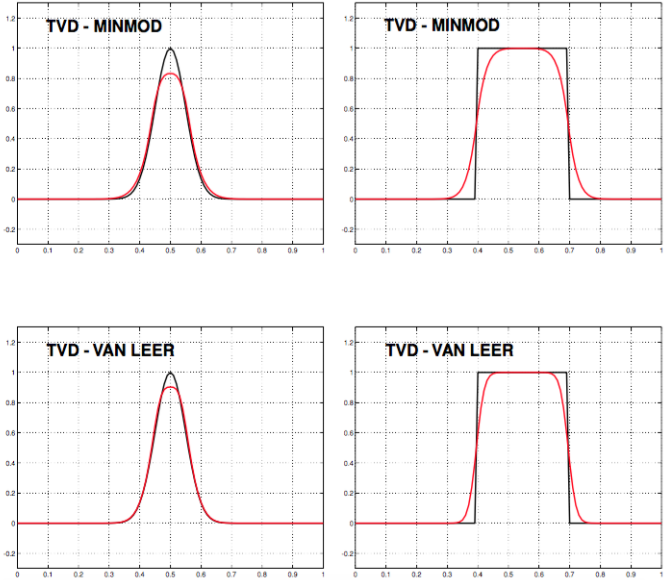
TVD limiters (all these produce 2nd order schemes when the solution is smooth and boil down to upwind at discontinuities)

- Minmod: $\phi(r) = \text{minmod}(1, r)$
- Superbee: $\phi(r) = \max(0, \min(1, 2r), \min(2, r))$
- Monotonized Centred (MC): $\phi(r) = \max(0, \min(\frac{1}{2}(1+r), 2, 2r))$
- van Leer: $\phi(r) = \frac{r+|r|}{1+r}$

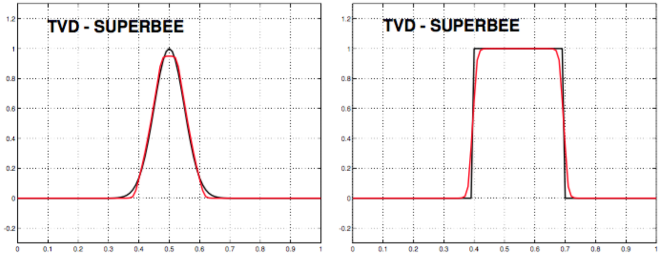
GENERAL PROPERTIES OF SOME SCHEMES XII



GENERAL PROPERTIES OF SOME SCHEMES XIII



General properties of some schemes XIV



Consist., converg., stab. & dissipation I

Let's go back to the linear conservation law (same argument extends for the nonlinear case)

Consistency. Recall the truncation error (the one obtained substituting the exact solution into the numerical scheme)

$$\tau(\Delta t, h) = \max_{i,n} |\tau_i^n|$$

- Forward or Backward Euler / centred FD: $\mathcal{O}(\Delta t + h^2)$;
- Upwind: $\mathcal{O}(\Delta t + h)$;
- Lax-Friedrichs: $\mathcal{O}(\frac{h^2}{\Delta t} + \Delta t + h^2)$;
- Lax-Wendroff: $\mathcal{O}(\Delta t^2 + h^2 + h^2 \Delta t)$.

Consist., converg., stab. & dissipation II

Convergence. A scheme is convergent (in the max norm) if

$$\lim_{\Delta t, h \to 0} \left(\max_{j,n} |u(x_j, t^n) - u_j^n| \right) = 0.$$

Other norms may be more suitable, depending on the problem.

Stability. A scheme for a hyperbolic problem is *stable* if for all T, there exist $C_T > 0$ and $\delta_0 > 0$ st

$$\|\mathbf{u}^n\|_\Delta \leq C_T \|\mathbf{u}^0\|_\Delta,$$

for all n st $n\Delta t \leq T$, for all Δt, h st $0 < \Delta t \leq \delta_0$, $0 < h \leq \delta_0$, and for any IC $\mathbf{u}_0$. C_T indep. of $\Delta t, h$.

- $\|\cdot\|_\Delta$ is some discrete norm. E.g.

$$\|\mathbf{v}\|_{\Delta,p} = \left(h \sum_{j=-\infty}^{\infty} |v_j|^p \right)^{\frac{1}{p}} \text{ for } p = 1, 2, \quad \|\mathbf{v}\|_{\Delta,\infty} = \sup_j |v_j|.$$

CONSIST., CONVERG., STAB. & DISSIPATION III

- If $\|\mathbf{u}^n\|_\Delta \leq \|\mathbf{u}^{n-1}\|_\Delta,\ n \geq 1$, then the scheme is strongly stable wrt $\|\cdot\|_\Delta$.

Von Neumann analysis.

- if $u_0(x)$ is 2π-periodic, $u_0(x) = \sum_{k=-\infty}^{\infty} \alpha_k e^{ikx}$, with α_k the $k-$th Fourier coeff. Then

$$u_j^0 = u_0(x_j) = \sum_{k=-\infty}^{\infty} \alpha_k e^{ikjh}, \quad j = 0, \pm 1, \pm 2, \cdots$$

- Applying a numerical scheme (any) yields

$$u_j^n = \sum_{k=-\infty}^{\infty} \alpha_k e^{ikjh} \gamma_k^n, \quad j = 0, \pm 1, \pm 2, \ldots, \quad n \geq 1,$$

amplification factor of the $k-$th frequency

- The amplification factor characterizes the numerical scheme

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CONSIST., CONVERG., STAB. & DISSIPATION IV

Scheme	γ_k
F Euler / Centred FD	$1 - ia\lambda \sin(kh)$
B Euler / Centred FD	$(1 + ia\lambda \sin(kh))^{-1}$
Upwind	$1 - \lvert a\rvert\lambda(1 - e^{-ikh})$
Lax-Friedrichs	$\cos kh - ia\lambda \sin(kh)$
Lax-Wendroff	$1 - ia\lambda \sin(kh) - a^2\lambda^2(1 - cos(kh))$

THEOREM

If for all T there exist $\beta \geq 0$, $m \in \mathbb{N}$ st, for a convenient choice of $\Delta t, h$, we have $|\gamma_k| \leq (1+\beta\Delta t)^{\frac{1}{m}}$ for all k, then the scheme is stable wrt $\|\cdot\|_{\Delta,2}$ with stability constant $C_T = e^{\beta T/m}$. In particular, if one can take $\beta = 0$ (and so $|\gamma_k| \leq 1$ $\forall k$), the scheme is strongly stable wrt $\|\cdot\|_{\Delta,2}$.

- Upwind: $\forall k, \quad |\gamma_k| \leq 1$ if $\quad \Delta t \leq \dfrac{h}{|a|}$ (strong stability)
- Lax-Friedrichs: strongly stable under the same condition

Consist., converg., stab. & dissipation V

- B Euler / Centred FD: $|\gamma_k| \leq 1$, for all k and for all $\Delta t, h$ (unconditionally strongly stable)
- F Euler / Centred FD: if $\beta > 0$ is such

$$\Delta t \leq \beta \frac{h^2}{a^2}$$

  then $|\gamma_k| \leq (1 + \beta \Delta t)^{1/2}$. Applying the theorem (with $m = 2$) gives stability, but under more restrictive conditions than those for the upwind scheme. No strong stability possible
- CFL condition once again:

$$\Delta t \leq \frac{h}{|a|} \quad \text{or} \quad |a\lambda| \leq 1,$$

  necessary for stability of explicit schemes.

Dissipation and dispersion. The amplification coefficients render info on the dissipation and dispersion properties of a method.

- Exact sol. of the linear PDE

$$u(x,t^n) = u_0(x - an\Delta t), \quad n \geq 0, \quad x \in \mathbb{R},$$

  where $t^n = n\Delta t$.

- The Fourier expansion of the IC gives

$$u(x_j,t^n) = \sum_{k=-\infty}^{\infty} \alpha_k e^{ikjh}(g_k)^n \quad \text{with} \quad g_k = e^{-iak\Delta t}.$$

- Simple comparison gives $\gamma_k = g_k$.
- Strong stability holds if $|\gamma_k| \leq 1$, but here we see $|g_k| = 1$, $\forall k$. Therefore γ_k is a *dissipative* coefficient
- As $|\gamma_k|$ decreases, the amplitude α_k decreases $\Rightarrow$ the dissipation of the scheme is larger

Consist., converg., stab. & dissipation VII

- Amplification (or dissipation) error of the $k-$th harmonics

$$\varepsilon_a(k) = \frac{|\gamma_k|}{|g_k|}$$

- Let $\phi_k = kh$ be the phase angle of the $k-$th harmonics
- Since $k\Delta t = \lambda \phi_k$, we have

$$g_k = e^{-ia\lambda\phi_k}.$$

- As we can rewrite γ_k in the form

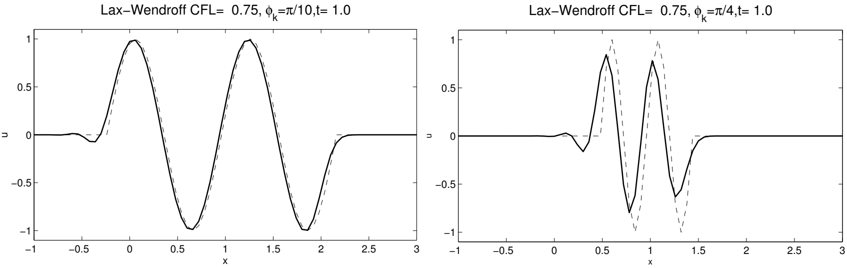
$$\gamma_k = |\gamma_k| e^{-i\omega\Delta t} = |\gamma_k| e^{-i\frac{\omega}{k}\lambda\phi_k},$$

then (comparing with the expression for g_k) the term $\frac{\omega}{k}$ represents the *speed of propagation* of the numerical solution, wrt the k-th harmonics

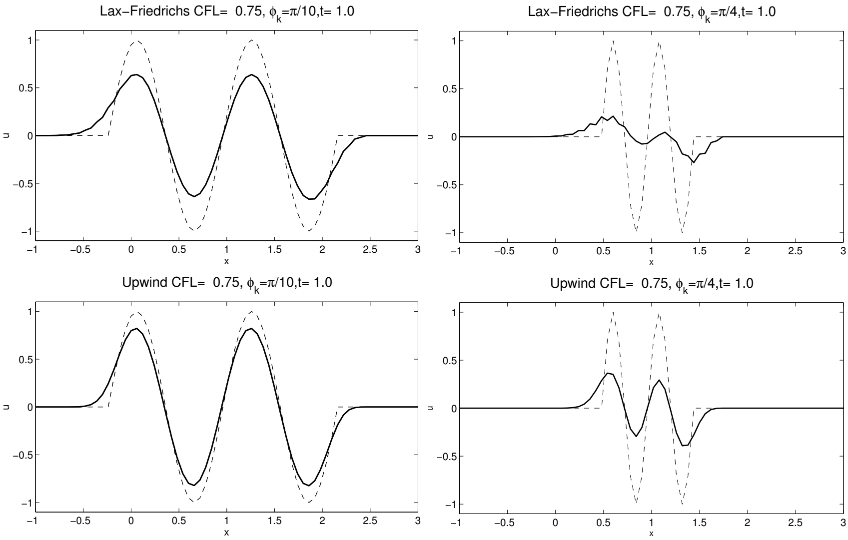
Consist., converg., stab. & dissipation VIII

- Ratio between the two speed of propagations (numerical and exact) is the dispersion error

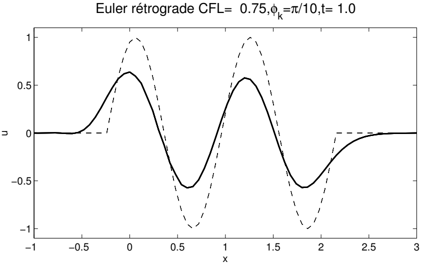
$$\varepsilon_d(k) = \frac{\omega}{ka} = \frac{\omega h}{\phi_k a}$$

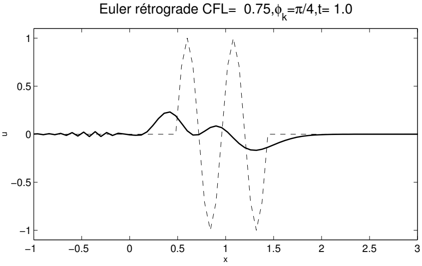


CONSIST., CONVERG., STAB. & DISSIPATION IX



Consist., converg., stab. & dissipation X





We did not discussed the reconstruction step (check it on the Red Book)

Beyond Godunov and 2nd order TVD schemes

- More efficient to go to higher order in smooth regions of the flow
- So-called spectral methods can show exponential convergence
- More flexible approaches: ultra-high-order shock-capturing schemes such as ENO, WENO, or other multistep methods (RK, SSP)
- Discontinuous Galerkin and discontinuous element methods
- Near the discontinuities it is more efficient to refine the mesh, since higher order schemes drop to first order
- Adaptive Mesh Refinement, multiresolution, multigrid, or similar adaptive techniques can be combined with conservative FD/FV methods
- h-p adaptivity (decide automatically if refining the mesh or increasing the order of the approximation)

Finite volumes in multi-D

- As in FD, we can apply tensor product extension of all the previous results to cover the 2D and 3D Cartesian cases
- Classical schemes can be also used in case of "mapped grids" (onto spheres, cylinders)
- We can also employ arbitrary polygonal (polyhedral) meshes. Flux definiton gets complicated, but the essentials are the same (at least in the conservative case)
- One has to choose between cell-centered or vertex-centered discretizations
- Extensions of limiters to 2D/3D are available for simple meshes (tets and quads)
- FV libraries: OpenFoam, OpenFVM, DUNE, CLAWPACK

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Other discretization methods

Remember the diver's picture in lecture 1.

Common items: splitting of the domain into small volumes, define balance relations on each cell, obtain and solve large (non-)linear systems

- Meshless, boundary element, lattice Boltzmann...
- Variety of applicable methods depends ideally on the problem
- Actual applicability depends typically on historical reasons
- Methods can be combined to exploit intrinsic features (hybrid strategies such as discontinuous Galerkin, finite volume-element methods, virtual discretizations, mimetic finite differences)
- Many pieces of the puzzle are still unresolved, specially when dealing with coupled, nonlinear, and multi-scale problems

Every code/method has to incorporate the steps above. But, "only so much time in a day, and only so much expertise anyone can have..."

Plus, we don't just want a simple thing, we want the state-of-the-art methods... for everything

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Anecdote

Wish list

(actual wish list given to me by some collaborators)

- Discrete integral form of model equations
- Locally accurate computation of div(phase velocities)
- Mass conservation, desirably, by construction
- Robust handling of unstructured of grids and complex geometries
- Direct computation of fluxes and velocities with arbitrary accuracy
- Flexibility to choose diverse numerical fluxes and to satisfy discrete maximum principles
- Manageable computational burden
- Massively parallel algorithms or suitability for parallelization
- Let's throw in some analysis too

Anecdote

A counter-offer – Our strategy

vs. what we could finally do

- BDF2 time stepping
- Mixed finite element (MFE) methods for momentum conservation (Navier-Stokes, Brinkman, Stokes, Darcy, Forchheimer, Elasticity)
  - Fluxes are computed directly and with the desired accuracy
  - Their finite element approximation follows BDM elements enriched with bubble functions. Pressures approximated by piecewise linear polynomials
- Discontinuous finite volume element (DFVE) methods for mass conservation or other transport eqns (concentration, volume fraction, tracer, temperature, etc)
- Piecewise constant functions on a so-called diamond grid
- Suitability for L^2-error analysis