Computational Methods for Astrophysical Applications

Ileyk El Mellah & Jon Sundqvist

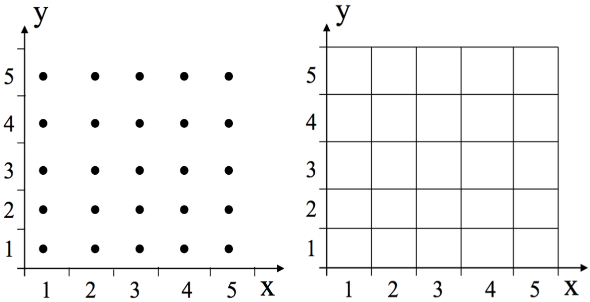
Centre for mathematical Plasma Astrophysics
Instituut voor Sterrenkunde
KU Leuven

Lesson 2 :
Finite Difference Approximation for linear hyperbolic PDE

- **Preliminary concepts**
  Mesh and data collocation
  Consistency
  Stability
- **Spatial discretization**
  Discretized functions and derivatives
  Backward, forward and central finite difference
  Truncation error and order of accuracy
- **Time advance**
  Von Neumann stability analysis
  Explicit methods
  Implicit methods
  Accuracy and positivity

Mesh

- Numerical schemes require spatial and temporal discretization



Data collocation

- Finite difference (FD): values are located at points, not necessarily regularly distributed. There is no cell.

  $\Rightarrow$ Intuitive & computationally fast but not conservative and no straightforward refinement strategy
- Finite volume (FV): values are associated to the whole cell : the value of the function is constant over the cell. Conservative by Gauss' law (a.k.a Green-Ostrogradsky).

  $\Rightarrow$ Reconstruction at interfaces required => slower

Consistency of a method

- A FD approximation of a PDE is *consistent* if and only if

$$\text{FD} \xrightarrow[\Delta t, \Delta x \to 0]{} \text{PDE}$$

$\Rightarrow$ Balsara 2.4

- Empirical order of convergence (EOC) : u analytic solution and $\tilde{u}_i$ numerical solution on 1D uniform grid x_i with $i \in [1, N_\nu = 2^\nu]$. Compute the maximal error $\epsilon_\nu = ||u - \tilde{u}||_\infty$ and deduce EOC :

$$\text{EOC}_\nu = \frac{\log\left(\epsilon_\nu / \epsilon_{\nu-1}\right)}{\log\left(N_{\nu-1} / N_\nu\right)}$$

$\Rightarrow$ quantify the overall quality of a method, on analytic test-cases

$\Rightarrow$ see Project# 1 of Köln school

$\Rightarrow$ see Balsara chapter 2, slides# 27-32

Von Neumann stability analysis

- Balsara 2.5 and intro of 2.7
- round-off errors should not grow during time progression
  - $\Rightarrow$ numerical solution = exact + round-off error $\epsilon(x, t)$
  - $\Rightarrow$ represent $\epsilon(x, t)$ in Fourier series, analyse Fourier term

$$\epsilon_i^n(k) = \hat{\epsilon}_k \mathrm{e}^{\lambda t^n} \mathrm{e}^{\mathrm{i}kx_i}$$

- numerically stable scheme $\forall$ spatial wavenumbers k if

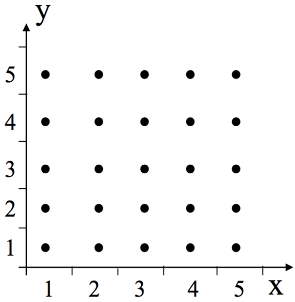
$$\left| \frac{\epsilon_i^{n+1}(k)}{\epsilon_i^n(k)} \right| = \left| \mathrm{e}^{\lambda \Delta t} \right| \leq 1$$

- Lax equivalence theorem :

consistent + stable <=> convergent

Discretized function

- Balsara 2.3
- We now want to obtain a FD discretized form of the equations to solve



$\Rightarrow$ variables evaluated at the points

Discretized spatial derivatives

- Assume $N + 1$ points regularly spaced by Δx and u_i the associated values
- Key-question: how to get a FD approximation of the spatial derivatives u_i', u_i''...?

  $\Rightarrow$ Use Taylor series expansions

Backward, forward & central FD

- For instance, to 1st order accuracy in Δx, we have the *1st order forward difference* :

$$u_i' \sim \frac{u_{i+1} - u_i}{\Delta x}$$

$\Rightarrow$ but we also have the *1st order backward difference* :

$$u_i' \sim \frac{u_i - u_{i-1}}{\Delta x}$$

$\Rightarrow$ or the *2nd order central difference* :

$$u_i' \sim \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

- Which one to choose? Properties (e.g. stencil, accuracy)?

Truncation error and order of accuracy

- Taylor expansions linking u_i to the continuous function u :

$$u_{i+1} = u(0) + u'(0)\,\Delta x + u''(0)\,\frac{(\Delta x)^2}{2!} + u^{(3)}(0)\,\frac{(\Delta x)^3}{3!} + \dots \quad (1)$$

$$u_i = u(0) \quad (2)$$

$$u_{i-1} = u(0) - u'(0)\,\Delta x + u''(0)\,\frac{(\Delta x)^2}{2!} - u^{(3)}(0)\,\frac{(\Delta x)^3}{3!} + \dots \quad (3)$$

$$\Rightarrow\ (1)-(3) : u'(0) = \frac{u_{i+1}-u_{i-1}}{2\Delta x} + \underbrace{O\left((\Delta x)^{2}\right)}_{\text{truncation error}}$$

- Order of accuracy (o.a.) $=$ order of first truncated term

  $\Rightarrow$ (Δx–>$\Delta x/2$) => accuracy improved by $2^{\text{o.a.}}$

- Stencil : points required, increases with o.a.

2^{nd} order derivative

- Same principle

  $$(1)+(3)-2\times(2) : u''(0) = \frac{u_{i+1}-2u_i+u_{i-1}}{(\Delta x)^2} + O\left((\Delta x)^2\right)$$

  $\Rightarrow$ O.a.? Stencil?

- Exo

  $\Rightarrow$ 3^{rd}, 4^{th} & 5^{th} order central difference representations of u_i'?

  $\Rightarrow$ 2^{nd} order forward/backward differences?

Principle

- Consider the 1D linear advection equation with constant speed v :

$$\partial_t \rho + v \partial_x \rho = 0 \tag{4}$$

- Explicit time integration: values at t^{n+1} computed from available information on time level $t^n = t^{n+1} - \Delta t$

Principle

- Example: explicit forward 2nd order central difference (a.k.a. Eulerâs Forward Time Central Space, FTCS)

$$\frac{u^{n+1}-u^n}{\Delta t} = -v\frac{u^n_{i+1}-u^n_{i-1}}{2\Delta x}$$

$\Rightarrow$ rearrange to

$$u_i^{n+1} = u_i^n - v\,\frac{\Delta t}{\Delta x}\,\frac{u^n_{i+1}-u^n_{i-1}}{2} \tag{5}$$

$\Rightarrow$ 1st order accurate in time, 2nd order in space

$\Rightarrow$ Is this FD approximation consistent?

- Sandbox: Write your 1st solver using the Euler's FTCS above (and periodic boundary conditions, $\sim$ infinite simulation space). Apply it to the Riemann problem (advection of a step function). Is the numerical solution stable?

Von Neumann stability analysis

- Balsara 2.7.1
- Von Neumann stability analysis

$$e^{\lambda \Delta t} = 1 - \frac{v \Delta t}{\Delta x} \frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2} = 1 - i \frac{v \Delta t}{\Delta x} \sin(k \Delta x)$$

$\Rightarrow$ scheme is unconditionally unstable since for all k

$$\left| \frac{\epsilon_k^{n+1}}{\epsilon_k^n} \right| > 1$$

- 3 possible solutions to stabilize

$\Rightarrow$ add numerical diffusivity to damp nonphysical instability

$\Rightarrow$ impose same space-time symmetry as original PDE

$\Rightarrow$ use implicit scheme (next section)

Numerical diffusivity : the Lax-Friedrichs scheme

- adding diffusion: advection-diffusion equation has form

$$\frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x} + \mathcal{D} \frac{\partial^2 u}{\partial x^2} \quad \text{with } \mathcal{D} \text{ a diffusion coefficient}$$

- Lax-Friedrichs scheme : in (5), if we replace u_i^n by spatial average between $i-1$ and $i+1$, we get :

$$u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - v \frac{\Delta t}{\Delta x} \frac{u_{i+1}^n - u_{i-1}^n}{2}$$

which can be rearranged to form

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

$\Rightarrow$ numerical dissipation with $\mathcal{D} \equiv (\Delta x)^2/2\Delta t$

$\Rightarrow$ 1$^{\text{st}}$ order accurate in time, 2$^{\text{nd}}$ order in space

CFL condition

- perform von Neumann stability analysis for Lax-Friedrichs

$$\mathrm{e}^{\lambda \Delta t} = \cos(k\Delta x) - \mathrm{i}\,\frac{v\Delta t}{\Delta x}\sin(k\Delta x)$$

$\Rightarrow$ conditional stability requiring Courant number C

$$C \equiv \frac{|v|\Delta t}{\Delta x} \leq 1$$

$\Rightarrow$ limitation of the time step Δt for a given resolution Δx

$\Rightarrow$ Courant-Friedrichs-Lewy condition (1928)

$\Rightarrow$ necessary condition for stability

- Rk: see stencil of Lax-Friedrichs scheme in Table on slide 26
- Exo : retrieve the figures on slide# 62 of Balsara 2.7.2

$\Rightarrow$ very diffusive

The Lax-Wendroff scheme

- Lax-Friedrichs has different o.a. in space (2nd) and time (1st)
  $\Rightarrow$ 2nd order Taylor expansion in time of $u_i(t)$, yields :

$$u_i(t+\Delta t) = u_i(t) + u_i'(t)\Delta t + u_i''(t)\frac{(\Delta t)^2}{2} \tag{6}$$

$\Rightarrow$ (4) => $u_i' \sim -v\partial_x u$

$\Rightarrow$ to find u_i'', ∂_t(4) and (illegaly) switch ∂_t and ∂_x in mixed term :

$$u_i'' \sim v^2 \partial_{xx} u$$

$\Rightarrow$ finally, reinject in (6) and use a central difference for spatial derivatives :

$$u_i^{n+1} = u_i^n - \tfrac{1}{2}\frac{\Delta t}{\Delta x}\, v\,(u_{i+1}^n - u_{i-1}^n) + \tfrac{1}{2}\frac{(\Delta t)^2}{(\Delta x)^2}\, v^2\,(u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

The Lax-Wendroff scheme

- 2nd order in space and time
- Conditionally stable

  $\Rightarrow$ for $\Delta t = \Delta x / v$, we retrieve the Lax-Friedrichs scheme
- Exo : retrieve the figures on slide# 67 of Balsara 2.7.3 and compare the empirical order of convergence with respect to Lax-Friedrichs

  $\Rightarrow$ non positivity-preserving (<= monotonicity-preserving)

Space-time symmetry

- How to maintain the space-time symmetry of the PDE in the FD approximation?
  - $\Rightarrow$ use central discretisation for both time and space
  - $\Rightarrow$ leapfrog scheme

$$u_i^{n+1} = u_i^{n-1} - v \frac{\Delta t}{\Delta x} \frac{u_{i+1}^n - u_{i-1}^n}{2}$$

  - $\Rightarrow$ conditionally stable and second-order accurate
  - $\Rightarrow$ multiple time levels involved: $n-1$, n, $n+1$
  - $\Rightarrow$ potential problem: even/odd time levels may 'decouple'
- stencil of leapfrog on slide 26

First order upwind scheme

- Balsara 2.7.5
- Physically-speaking, isn't it silly that, for $v > 0$ for instance, u_i^{n+1} depends on u_{i+1}^n?

  $\Rightarrow$ Information should propagate wave speeds (see previous lesson)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -v \frac{u_i^n - u_{i-1}^n}{\Delta x}$$

$\Rightarrow$ also called the donor cell scheme

First order upwind scheme

- Positivity preserving (">0"), but 1st order accurate

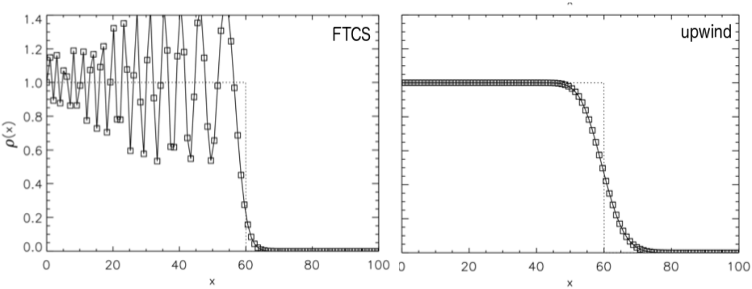


Figure 3.2: (*upper panel*) A central differencing numerical solving of the uni-dimensional linear advection equation of a step function which went wrong. The dotted line stands for the analytical solution while the markers and solid line indicate the numerical answer. (*lower panel*) The same numerical problem solved with an upwind differencing scheme. From Dullemond (2009).

Overview of explicit methods

Name	Difference Equations	Stencil
Backward Euler	$U_j^{n+1} = U_j^n - \frac{k}{2h}A(U_{j+1}^n - U_{j-1}^n)$	
One-sided	$U_j^{n+1} = U_j^n - \frac{k}{h}A(U_j^n - U_{j-1}^n)$	
One-sided	$U_j^{n+1} = U_j^n - \frac{k}{h}A(U_{j+1}^n - U_j^n)$	
Lax-Friedrichs	$U_j^{n+1} = \frac{1}{2}(U_{j-1}^n + U_{j+1}^n) - \frac{k}{2h}A(U_{j+1}^n - U_{j-1}^n)$	
Leapfrog	$U_j^{n+1} = U_j^{n-1} - \frac{k}{2h}A(U_{j+1}^n - U_{j-1}^n)$	
Lax-Wendroff	$U_j^{n+1} = U_j^n - \frac{k}{2h}A(U_{j+1}^n - U_{j-1}^n)$ $+\frac{k^2}{2h^2}A^2(U_{j+1}^n - 2U_j^n + U_{j-1}^n)$	
Beam-Warming	$U_j^{n+1} = U_j^n - \frac{k}{2h}A(3U_j^n - 4U_{j-1}^n + U_{j-2}^n)$ $+\frac{k^2}{2h^2}A^2(U_j^n - 2U_{j-1}^n + U_{j-2}^n)$	

TABLE 10.1
Finite difference methods for the linear problem $u_t + Au_x = 0$.

h=dx
k=dt

1st order schemes safe, can be > 0 BUT very diffusive
2nd order schemes accurate => great for smooth profiles (e.g. Gaussian) but terrible for discontinuous ones (e.g. top hat) because non > 0

Principle

- third cure to instability of Euler FTCS scheme: evaluate spatial derivative at t^{n+1}

$$u_i^{n+1} = u_i^n - v\,\frac{\Delta t}{\Delta x}\,\frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2}$$

$\Rightarrow$ Backwards in Time, Central in Space Euler scheme (BTCS)

$\Rightarrow$ u_i^{n+1} not expressed in terms of values at time t^n: implicit

- Stencil?

Von Neumann stability analysis

- von Neumann stability analysis for BTCS scheme

$$\left|e^{\lambda \Delta t}\right| = \frac{1}{\left|1 + i\frac{v\Delta t}{\Delta x}\sin\left(k\Delta x\right)\right|} < 1 \qquad \text{for all } k$$

  $\Rightarrow$ unconditionally stable, any time step Δt allowed
- But stability $\neq$ accuracy

  $\Rightarrow$ the larger Δt, the lower the accuracy
- BTCS is 1$^{\text{st}}$ order in time
- Implicit methods more used for elliptic PDE => not covered by the current course

Godunov's order barrier theorem

- Explicit schemes

Scheme	o.a.	Can be stable?	>0?
FTCS	1^{st}	no	yes
Lax-Friedrichs	1^{st}	yes	yes
Lax-Wendroff	2^{nd}	yes	no
Upwind	1^{st}	yes	no

"All linear positivity-preserving schemes for linear advection are condemned to be 1^{st} order accurate"

- We want :
  - $\Rightarrow$ accuracy where the variables are smooth (i.e. $\sim$Gaussian)
  - $\Rightarrow$ positivity where they are discontinuous (i.e. $\sim$top hat)