Numerical Approaches to Fluid- and Magnetohydrodyanamics in Astrophysics

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Outline

I. Approaches to plasma, from kinetic to fluid and MHD;

II. The linear advection equation: concepts & discretizations;

III. Nonlinear hyperbolic PDE: shocks and expansion waves;

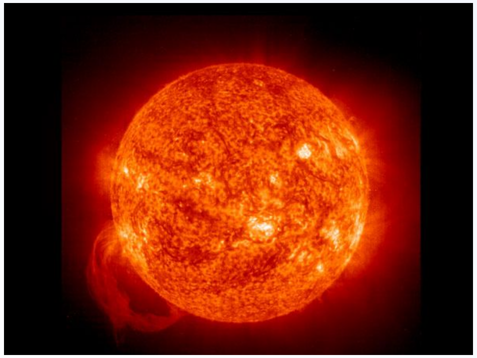
IV. Finite Volume Methods: state of the art Godunov-type codes;

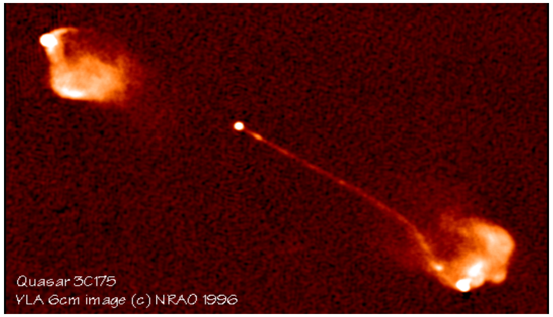
V. Beyond MHD: extending current computational models.

I. PLASMAS AS FLUIDS

Observational Evidence

- It is estimated that more than 99.9 % of matter in the Universe exists in the form of *plasma*;
- A *plasma* is a ionized gas where charged particles interact via electromagnetic forces (electric and magnetic fields);
- Examples include stars, nebulae, galaxies, supernovae, interstellar/galactic medium, jets, accretion disks, etc..
- Our knowledge limited by what we can actually observe → *emitting plasma*.





Plasma Modelling: Classical Description

$$m_i \ddot{\boldsymbol{r}}_i = e_i \left(\boldsymbol{E} + \frac{1}{c} \dot{\boldsymbol{r}}_i \times \boldsymbol{B} \right)$$

Individual particle motion

$$q(\mathbf{r}, t) = \sum_i e_i \delta \left[\mathbf{r} - \mathbf{r}_i(t) \right]$$

$$\mathbf{J}(\mathbf{r}, t) = \sum_i e_i \mathbf{v}_i \delta \left[\mathbf{r} - \mathbf{r}_i(t) \right]$$

Charge and currents

$$\boldsymbol{\nabla} \times \boldsymbol{E} = -\frac{1}{c} \frac{\partial \boldsymbol{B}}{\partial t}$$

$$\boldsymbol{\nabla} \times \boldsymbol{B} = \frac{1}{c} \frac{\partial \boldsymbol{E}}{\partial t} + \frac{4\pi}{c} \boldsymbol{J}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = 4\pi q$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$$

Maxwells' Equations

→ *Not feasible !*
(too many degress of freedom)

Plasma Modelling: Kinetic Description

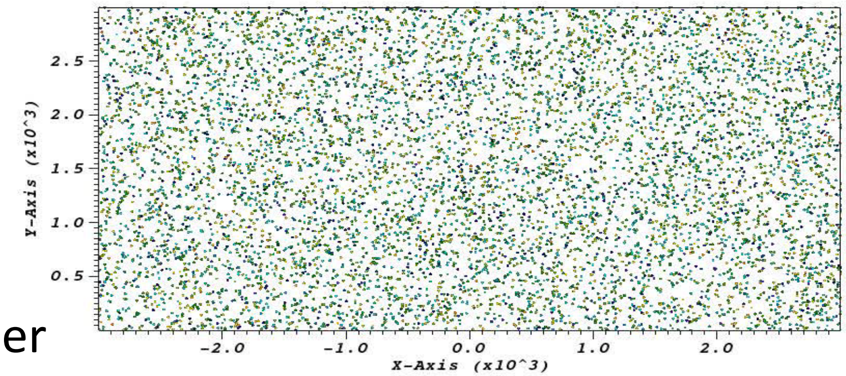
- ***Kinetic Description:***

$$\frac{\partial f}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla} f + \frac{e_0}{m}\left(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v}\times\boldsymbol{B}\right)\cdot\boldsymbol{\nabla}_{\boldsymbol{v}} f = 0.$$

*Vlasov Equation: **f(x,v,t)** is the distribution function (for a given species) giving the number density per unit element of phase space*

- ***Particle In Cell:*** (PIC) methods are based on a *finite element approach,* but with moving and overlapping elements. Distribution function of each species is given by the superposition of several elements ("superparticles"):

$$f_s(x,v,t) = \sum_p f_p(x,v,t)$$

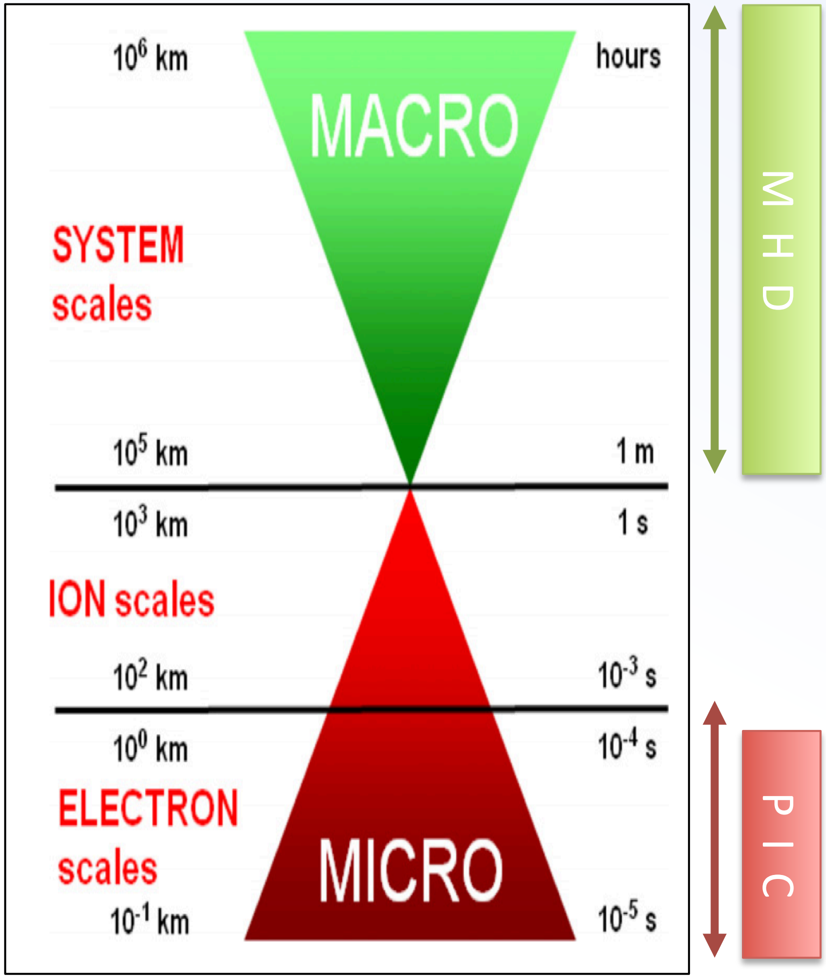


- Each element represents a large number of physical particles that are near each other in phase space.

Most consistent approach, but must resolve the plasma (electron) skin depth, $c/\omega_{\rm pe} \sim 5.4 \times 10^5\ {\rm cm}\ (n/{\rm cm}^{-3})^{-1/2}$

Kinetic Description

- ***PIC*** codes are applicable to study small-scale kinetic effects.
- Stability constraints impose a time step that is able to resolve with a cadence of about 1/10 the fastest frequency in the system.
- For space weather applications, this is commonly the electron plasma frequency, 5–7 orders of magnitude smaller than the typical scales of evolution of space weather phenomena.
- Ion scales are smaller and the electron scales much smaller, down to 100 m corresponding to typical electron Debye lengths.



Typical scales observed in the Earth magnetotail (Lapenta JCP (2012), 231).

From Kinetic to Fluid to MHD

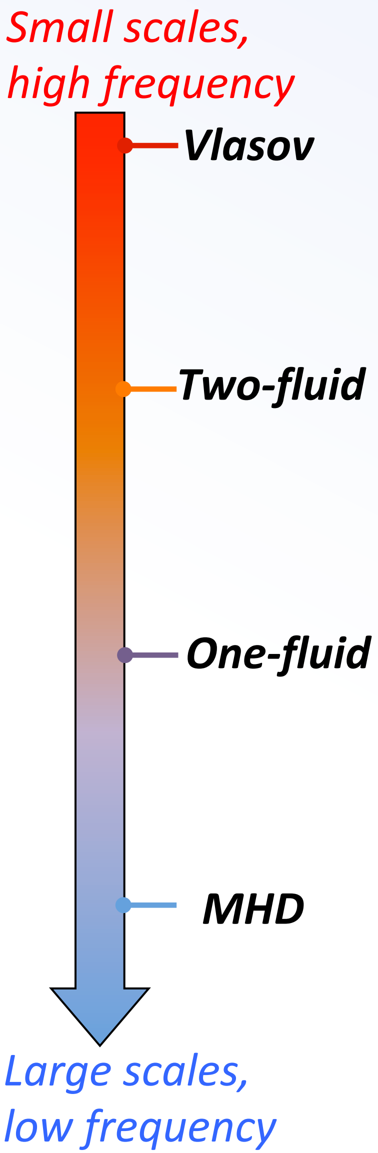
- *Vlasov / Fokker Plank* describes the time evolution, in phase space, of the plasma distribution function f(x,v,t):

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{q}{mc}\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right) \cdot \nabla_{\mathbf{v}} f = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$$

- *Two-fluid model* (ions & electrons) derived by integrating $v^n f(\mathbf{x}, \mathbf{v}, t)$ over velocity space and taking moments of increasingly higher order.

- A *one fluid model* is derived by proper average of the ions and electrons fluid equations.

- *Magnetohydrodynamics* (MHD) is a further simplification of the one fluid model.



Validity of Fluid approximations

- The fluid approach treats the system as a *continuous medium* and considering the dynamics of a small volume of the fluid.

- Meaningful to model length *scales much greater than mean free path* or individual particle trajectories.

- "Fluid element": small enough that any macroscopic quantity has a negligible variation across its dimension but large enough to contain many particles and so to be insensitive to particle fluctuations.

- *Fluid equations* involve only *moments* of the distribution function relating mean quantities. Knowledge of f(x,v,t) is not needed*.

- Still: taking moments of the Vlasov equation lead to the appearance of a next higher order moment → "loose end" → *Closure*.

Magetohydrodynamics: Assumptions

- Ideal MHD describes an electrically conducting single fluid, assuming:
  - *low frequency* $\omega \ll \omega_p, \quad \omega \ll \omega_c, \quad ,\omega \ll \nu_{pe}, \quad \omega \ll \nu_{ep}$
  - *large scales* $L \gg \frac{c}{\omega_p}, \quad L \gg R_c, \quad L \gg \lambda_{mfp},$
  - *Ignores electron mass* and finite Larmor radius effects;
  - Assume plasma is *strongly collisional* → L.T.E., isotropy;
  - *Fields* and *fluid* fluctuate on the *same time* and *length scales;*
  - Neglect charge separation, electric force and displacement current.

Ideal MHD at Last

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) &= 0 && \text{(Mass cons.)}\\
\frac{\partial (\rho\mathbf{u})}{\partial t} + \nabla\cdot\left[\rho\mathbf{u}\mathbf{u} - \frac{\mathbf{B}\mathbf{B}}{4\pi} + \left(p + \frac{\mathbf{B}^2}{8\pi}\right)\right] &= 0 && \text{(Momentum cons.)}\\
\frac{\partial E}{\partial t} + \nabla\cdot\left[\left(E + p + \frac{\mathbf{B}^2}{8\pi}\right)\mathbf{u} - \frac{(\mathbf{u}\cdot\mathbf{B})}{4\pi}\mathbf{B}\right] &= 0 && \text{(Energy cons.)}\\
\frac{\partial \mathbf{B}}{\partial t} + \nabla\cdot(\boldsymbol{u}\boldsymbol{B} - \boldsymbol{B}\boldsymbol{u}) &= 0 && \text{(Mag. flux cons.)}
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) &= 0 && \text{(Continuity)}\\
\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) &= -\nabla p + \frac{1}{c}\mathbf{J}\times\mathbf{B} && \text{(Eq. of motion)}\\
\frac{\partial (\rho e)}{\partial t} + \nabla\cdot(\rho e\,\mathbf{u}) + p\nabla\cdot\mathbf{u} &= 0 && \text{(Thermodynamics I law)}\\
\frac{\partial \mathbf{B}}{\partial t} + \nabla\times\mathbf{E} &= 0 && \text{(Faraday)}
\end{aligned}
$$

- MHD suitable for describing plasma at large scales;

$$
\begin{aligned}
\mathbf{J} &= \frac{c}{4\pi}\nabla\times\mathbf{B} && \text{(Ampere)}\\
\mathbf{E} + \frac{\mathbf{u}}{c}\times\mathbf{B} &= 0 && \text{(Ohm)}\\
\nabla\cdot\mathbf{B} &= 0 && \text{(Divergence − free)}\\
\rho e &= \rho e(\rho, p) && \text{(EoS/Closure)}
\end{aligned}
$$

- Good first approximation to much of the physics, even when some of the conditions are not met.
- Draw some intuitive conclusions concerning plasma behavior without solving the equations in detail.
- Fluid equations are *hyperbolic* conservation laws.

(Special) Relativistic Ideal MHD

- Special relativistic MHD equations:

$$
\begin{aligned}
\frac{\partial(\rho\gamma)}{\partial t} + \nabla\cdot(\rho\gamma\mathbf{v}) &= 0\,,\\
\frac{\partial\mathbf{m}}{\partial t} + \nabla\cdot[w\gamma^2\mathbf{v}\mathbf{v} - \mathbf{B}\mathbf{B} - \mathbf{E}\mathbf{E}] + \nabla p_t &= 0\,,\\
\frac{\partial\mathbf{B}}{\partial t} - \nabla\times(\mathbf{v}\times\mathbf{B}) &= 0\,,\\
\frac{\partial\mathcal{E}}{\partial t} + \nabla\cdot(\mathbf{m} - \rho\gamma\mathbf{v}) &= 0\,,
\end{aligned}
$$

$$\mathcal{E} = w\gamma^2 - p + \frac{\mathbf{B}^2 + \mathbf{E}^2}{2} - \rho\gamma$$

- Relativistic effects:
  - Bulk motion: $v \approx c$;
  - Strongly magnetized rarefied plasmas: $V_A \approx c$;
  - Extremely hot plasmas: $kT/m \approx c^2$.

- Both MHD and relaticistic MHD are *nonlinear systems of hyperbolic PDE*.

II. THE LINEAR ADVECTION EQUATION:

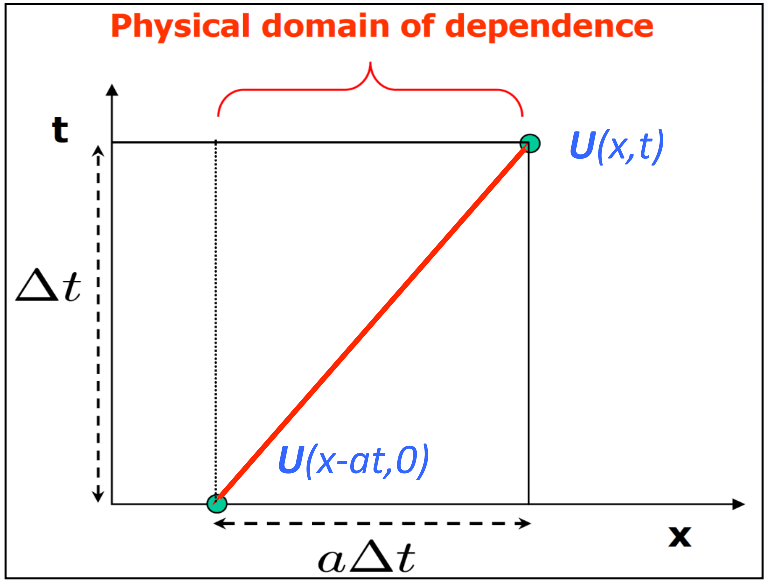
CONCEPTS AND DISCRETIZATIONS

The Advection Equation: Theory

- First order partial differential equation (PDE) in (x,t):

$$\boxed{\frac{\partial U(x,t)}{\partial t} + a\frac{\partial U(x,t)}{\partial x} = 0}$$

- Hyperbolic PDE: information propagates across domain at *finite speed*
  → method of characteristics



- Characteristic curves satisfy: $\frac{dx}{dt} = a$

- Along each characteristics:

$$\frac{dU}{dt} = \frac{\partial U}{\partial t} + \frac{dx}{dt}\frac{\partial U}{\partial x} = 0$$

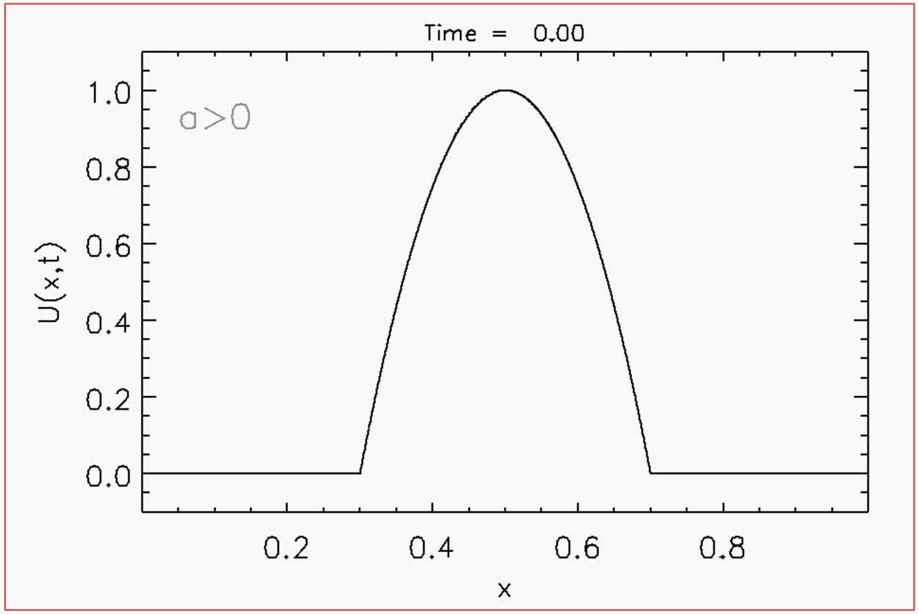
→ The solution is constant along characteristic curves.

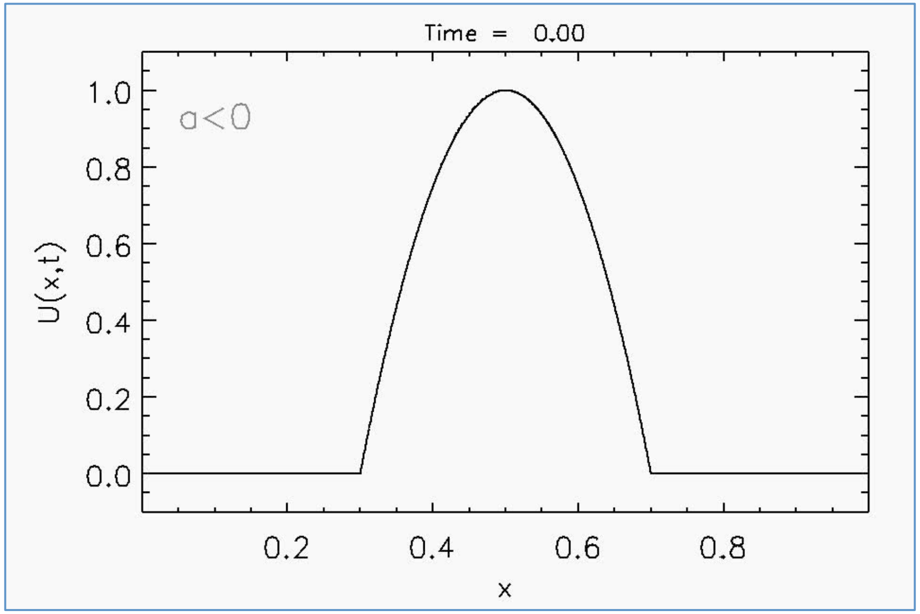
The Advection Equation: Theory

- for constant *a*: the characteristics are straight parallel lines and the solution to the PDE is a uniform shift of the initial profile:

$$U(x,t) = U(x - at, 0)$$

- The solution shifts to the right (for $a > 0$) or to the left ($a < 0$):



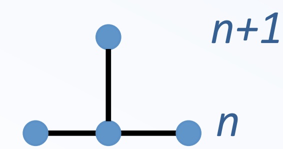


Discretization: the FTCS Scheme

- Consider our model PDE $$\frac{\partial U(x,t)}{\partial t} + a\frac{\partial U(x,t)}{\partial x} = 0$$

- Forward derivative in time: $$\frac{\partial U(x,t)}{\partial t} \approx \frac{U_i^{n+1} - U_i^n}{\Delta t} + O(\Delta t)$$

- Centered derivative in space: $$\frac{\partial U(x,t)}{\partial x} \approx \frac{U_{i+1}^n - U_{i-1}^n}{2\Delta x} + O(\Delta x^2)$$



- Putting all together and solving with respect to U^{n+1} gives

$$\boxed{U_i^{n+1} = U_i^n - \frac{C}{2}\left(U_{i+1}^n - U_{i-1}^n\right)}$$

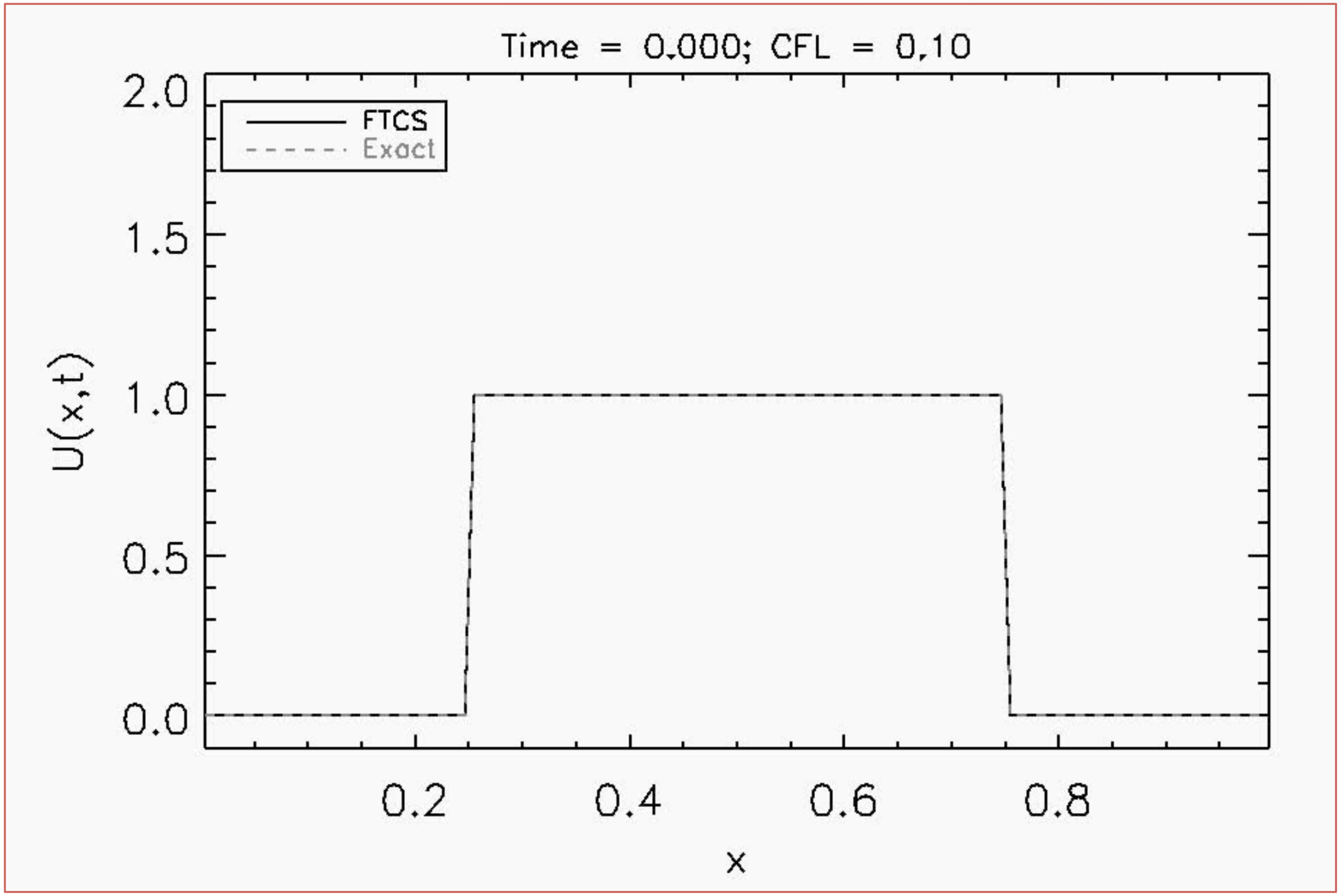
where $C = a\,\Delta t/\Delta x$ is the Courant-Friedrichs-Lewy (CFL) number.

- We call this method *FTCS* for Forward in Time, Centered in Space.

- It is an explicit method.

The FTCS Scheme

- At t=0, the ***initial condition*** is a square pulse with periodic boundary conditions:



Something isn't right… why ?

FTCS: von Neumann Stability Analysis

- Let's perform an analysis of *FTCS* by expressing the solution as a Fourier series.
- Since the equation is linear, we only examine the behavior of a single mode. Consider a trial solution of the form:

$$U_i^n = A^n e^{Ii\theta}, \quad \theta = k\Delta x$$

- Plugging in the difference formula: $\dfrac{A^{n+1}}{A^n} = 1 - \dfrac{C}{2}\left(e^{I\theta} - e^{-I\theta}\right)$

$$\Longrightarrow \quad \left|\frac{A^{n+1}}{A^n}\right|^2 = 1 + C^2 \sin^2\theta \geq 1$$

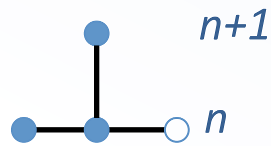
- Indipendently of the CFL number, all Fourier modes increase in magnitude as time advances.
- This method is <u>unconditionally unstable!</u>

Forward in Time, Backward in Space

- Let's try a difference approach. Consider the backward formula for the spatial derivative:

$$\frac{\partial U}{\partial x} \approx \frac{U_i^n - U_{i-1}^n}{\Delta x} + O(\Delta x) \quad \Longrightarrow \quad \boxed{U_i^{n+1} = U_i^n - C\left(U_i^n - U_{i-1}^n\right)}$$

- The resulting scheme is called FTBS:



- Apply von Neumann stability analysis on the resulting discretized equation:

$$\left|\frac{A^{n+1}}{A^n}\right|^2 = 1 - 2C(1-C)(1-\cos\theta)$$

- Stability demands $\quad \left|\frac{A^{n+1}}{A^n}\right| \le 1 \quad \Longrightarrow \quad 2C(1-C) \ge 0$

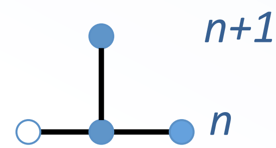
- for $a < 0$ the method is *unstable*, but
- for $a > 0$ the method is stable when $0 \le C = a\,\Delta t/\Delta x \le 1.$

Forward in Time, Forward in Space

- Repeating the same argument for the forward derivative

$$\frac{\partial U}{\partial x} \approx \frac{U_{i+1}^n - U_i^n}{\Delta x} + O(\Delta x) \quad \Longrightarrow \quad \boxed{U_i^{n+1} = U_i^n - C\left(U_{i+1}^n - U_i^n\right)}$$

- The resulting scheme is called FTFS:

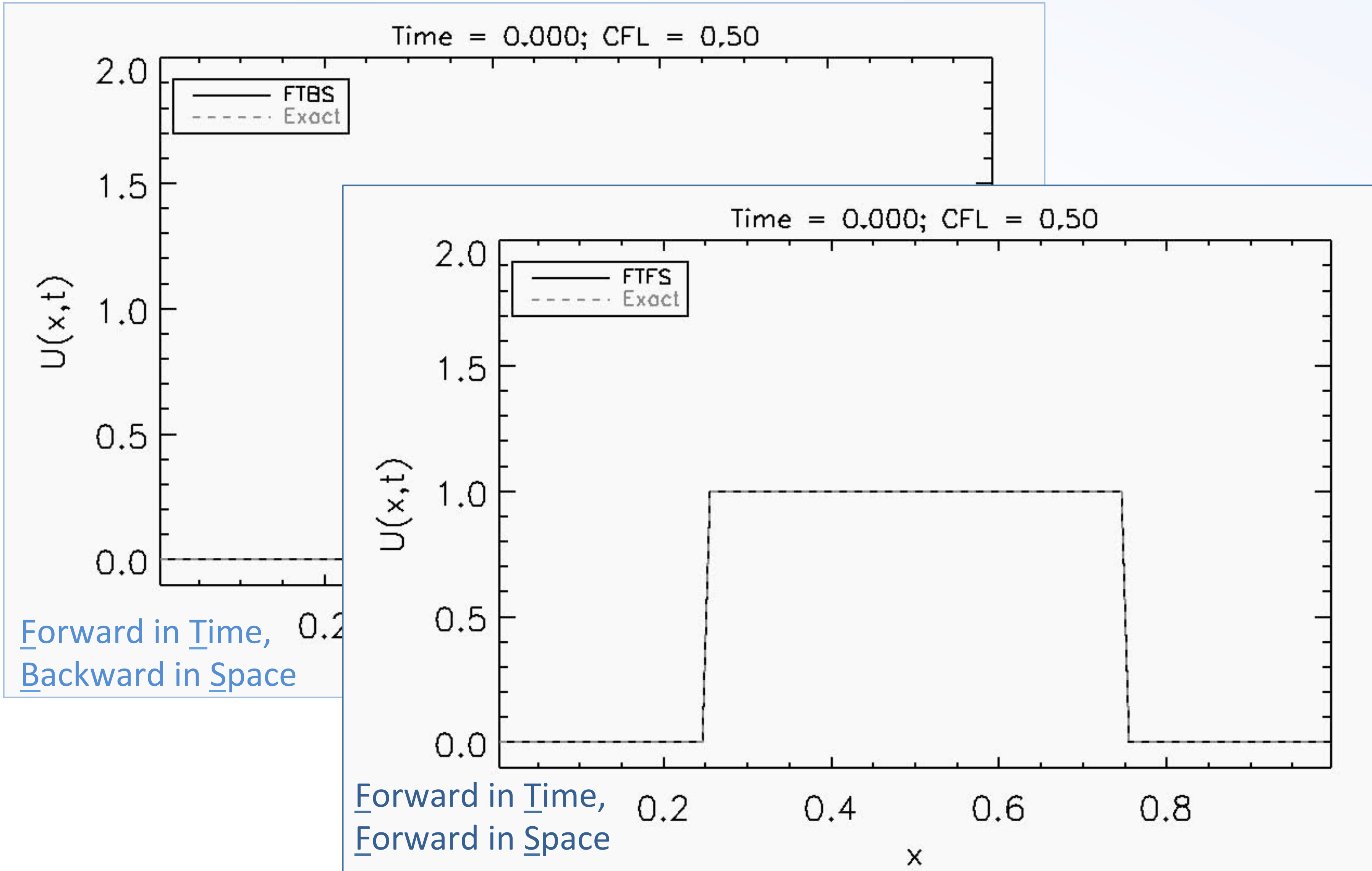


- Apply stability analysis yields $\left|\frac{A^{n+1}}{A^n}\right|^2 = 1 + 2C(1-C)(1-\cos\theta)$

- If *$a > 0$* the method will always be unstable

- However, if *$a < 0$* and *$-1 \leq C = a\,\Delta t/\Delta x \leq 0$* then this method is stable;

Stable Discretizations: FTBS, FTFS

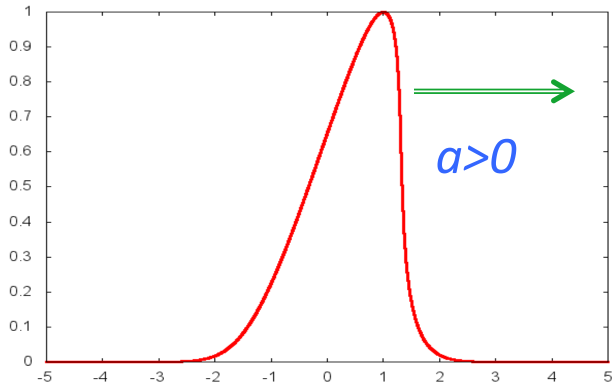


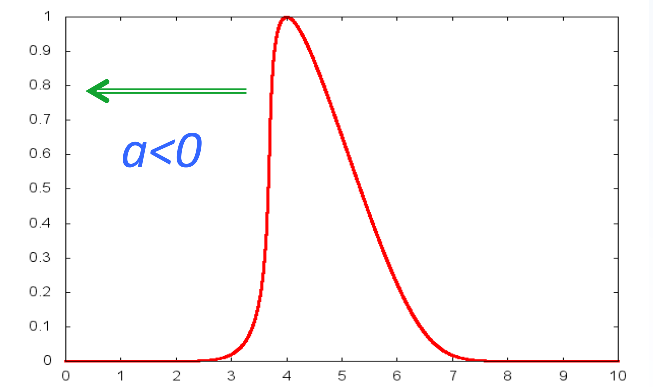
Forward in Time,
Backward in Space

Forward in Time,
Forward in Space

The 1st Order Godunov Method

- Summarizing: the stable discretization makes use of the grid point where information is coming from:





- ➔ '*Upwind*':

$$\begin{cases} U_i^{n+1} = U_i^n - \frac{a\Delta t}{\Delta x}\left(U_i^n - U_{i-1}^n\right) & \text{for} \quad a > 0 \\ U_i^{n+1} = U_i^n - \frac{a\Delta t}{\Delta x}\left(U_{i+1}^n - U_i^n\right) & \text{for} \quad a < 0 \end{cases}$$

- This is also called the first-order Godunov method;

Conservative Form

- Define the "flux" function $F^n_{i+\frac{1}{2}} = \frac{a}{2}\left(U^n_{i+1} + U^n_i\right) - \frac{|a|}{2}\left(U^n_{i+1} - U^n_i\right)$

so that Godunov method can be cast in *conservative* form

$$\boxed{U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\left(F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}\right)}$$

a > 0

$$\boxed{U_i^{n+1} = U_i^n - \frac{a\Delta t}{\Delta x}\left(U_i^n - U_{i-1}^n\right)}$$

a < 0

$$\boxed{U_i^{n+1} = U_i^n - \frac{a\Delta t}{\Delta x}\left(U_{i+1}^n - U_i^n\right)}$$

- The conservative form ensures a correct description of *discontinuities* in nonlinear systems, ensures global conservation properties and is the main building block in the development of high-order *finite volume* schemes.

The CFL Condition

- Since the advection speed *a* is a parameter of the equation, Δx is fixed from the grid, the previous inequality is a stability constraint on the time step for explicit methods

$$\boxed{\Delta t \leq \frac{\Delta x}{|a|}}$$

- Δt cannot be arbitrarily large but, rather, less than the time taken to travel one grid cell (CFL) condition.

- In the case of nonlinear equations, the speed can vary in the domain and the maximum of *a* should be considered instead.

III. NONLINEAR HYPERBOLIC PDE

Nonlinear Advection Equation

- We turn our attention to the scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

- Where *f(u)* is, in general, a nonlinear function of *u*.

- To gain some insights on the role played by nonlinear effects, we start by considering the inviscid Burger's equation:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) = 0$$

Nonlinear Advection Equation

- We can write Burger's equation also as $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$

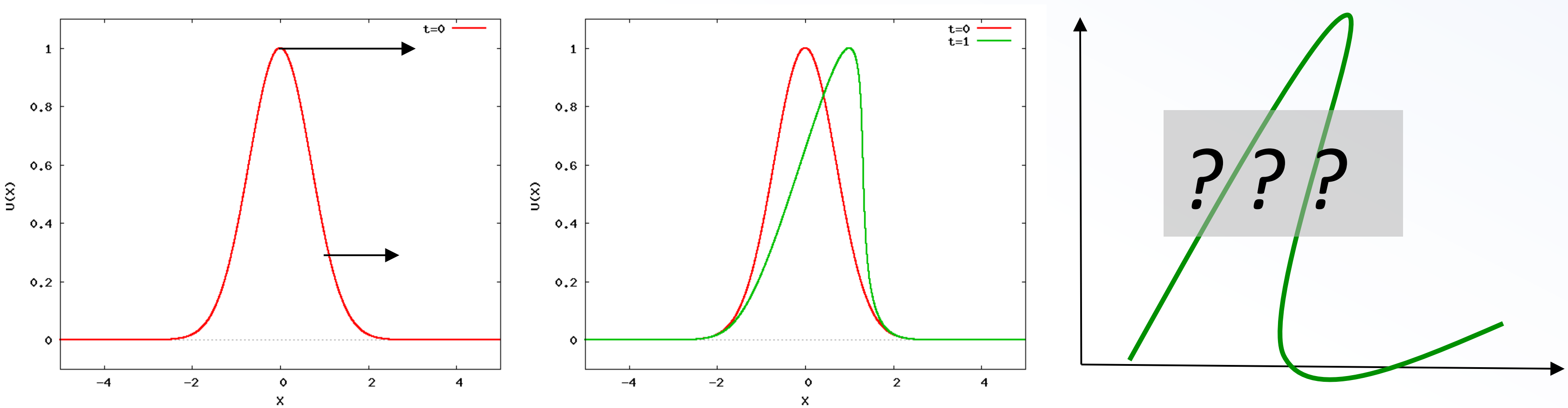
- In this form, Burger's equation resembles the linear advection equation, except that the velocity is no longer constant but it is equal to the solution itself.
- The characteristic curve for this equation is

$$\frac{dx}{dt} = u(x,t) \quad \Longrightarrow \quad \frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{dx}{dt} = 0$$

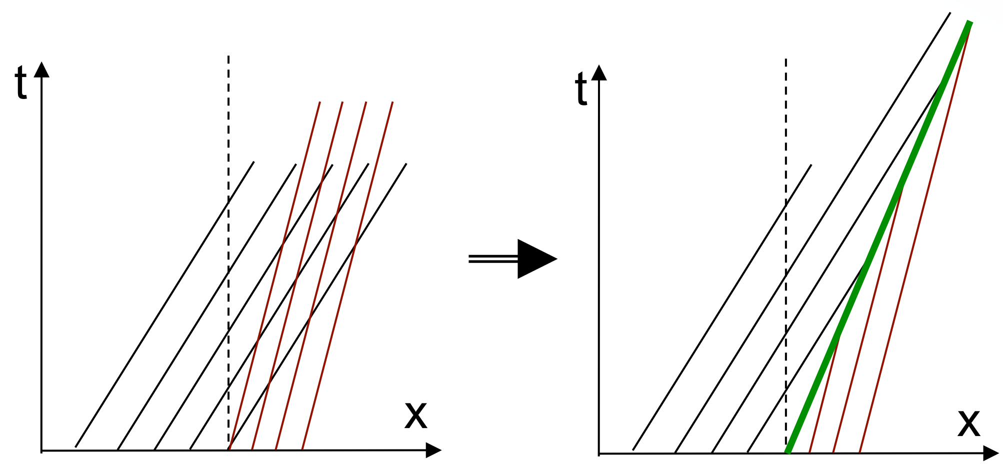
- → *u* is constant along the curve *dx/dt=u(x,t)* → characteristics are again straight lines: values of *u* associated with some fluid element do not change as that element moves.

Nonlinear Advection Equation

- From $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$ one can predict that higher values of *u* will propagate faster than lower values: → wave steepening.

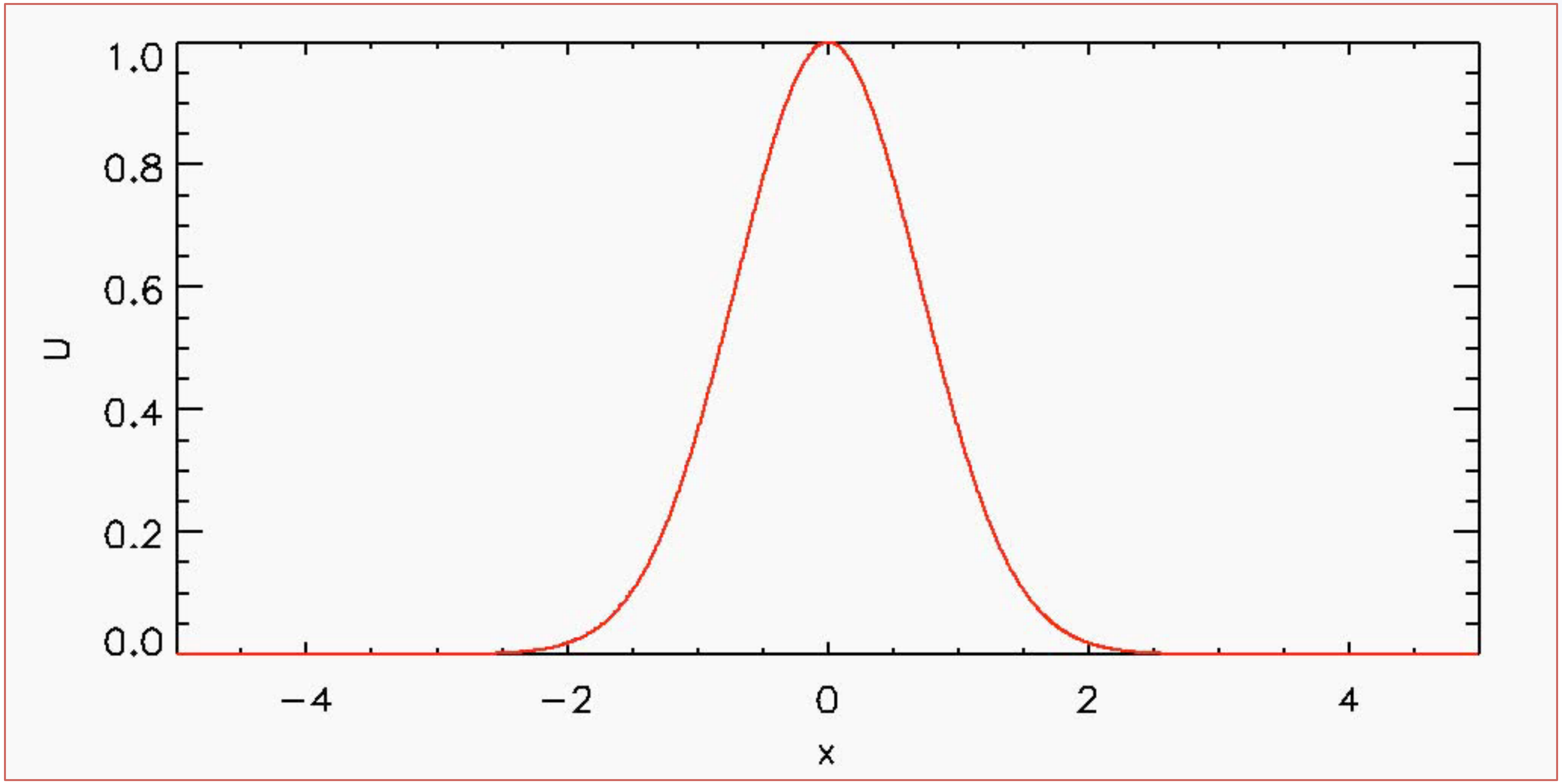


- Correct answer:
  characteristic will intersect
  creating a *shock wave*:



Nonlinear Advection Equation

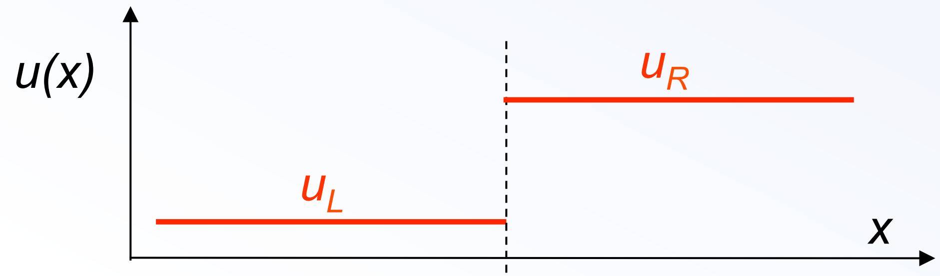
- This is how the solution should look like:



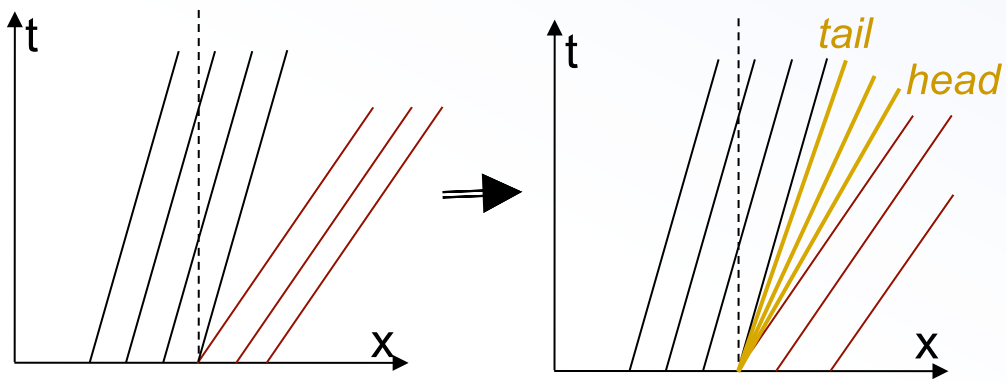
- Such solutions to the PDE are called *weak solutions*.

Nonlinear Advection Equation

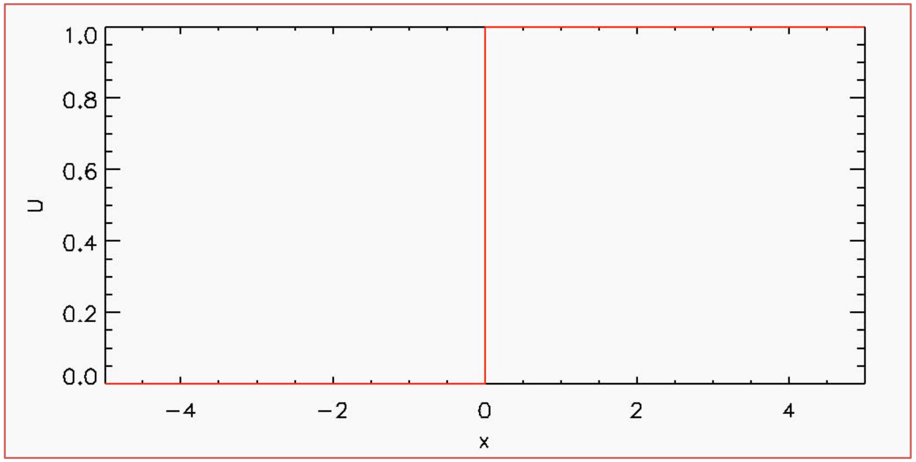
- In the opposite situation:



- Here characteristic velocities on the left are smaller than those on the right →



- The proper solution is a *rarefaction (expansion) wave*, a nonlinear self-similar wave that smoothly connects L/R states.



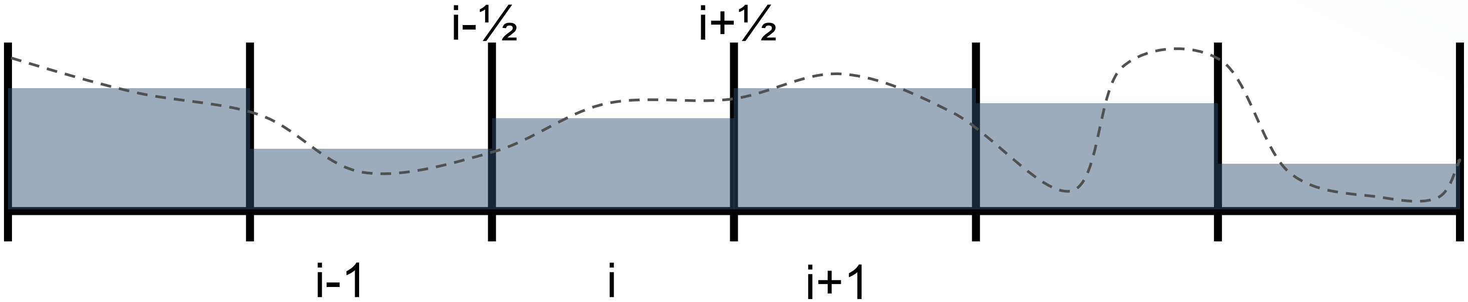
IV. FINITE VOLUME METHODS

Finite Volume Approach

- In a finite volume discretization, the unknowns are the spatial averages of the function itself:

$$\langle U \rangle_i^n = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} U(x, t^n)\, dx$$

where $x_{i-½}$ and $x_{i+½}$ denote the location of the cell interfaces.



- The solution to the conservation law involves computing fluxes through the boundary of the control volumes

Finite Volume Formulation

- The *conservative form* links the *differential* form of the equation and its integral representation:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad \Longrightarrow \quad \int_{t^n}^{t^{n+1}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left(\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} \right) = 0$$

obtained by integrating the PDE over a time interval $\Delta t = t^{n+1} - t^n$ and cell size $\Delta x = x_{i+1/2} - x_{i-1/2}$

$$\boxed{\langle U \rangle_i^{n+1} = \langle U \rangle_i^n - \frac{\Delta t}{\Delta x} \left(\tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \tilde{F}_{i-\frac{1}{2}}^{n-\frac{1}{2}} \right)}$$

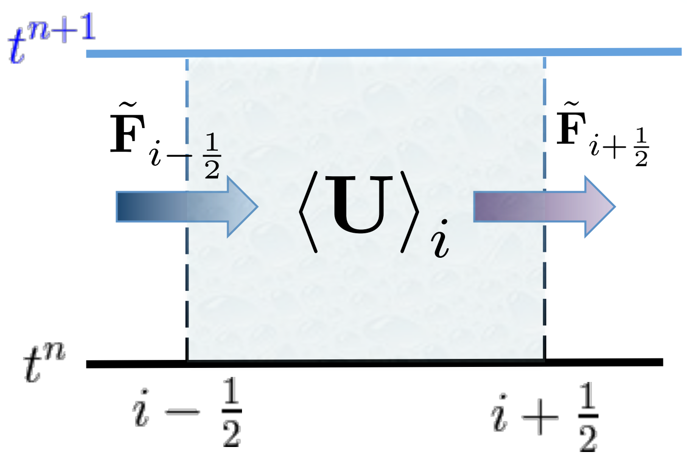
where $\tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \dfrac{1}{\Delta t} \displaystyle\int_{t^n}^{t^{n+1}} F(x_{i+\frac{1}{2}}, t)\, dt$

Finite Volume Formulation

$$\langle U \rangle_i^n = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} U(x,t^n)\,dx \qquad \tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} F(x_{i+\frac{1}{2}},t)\,dt$$

Integral form

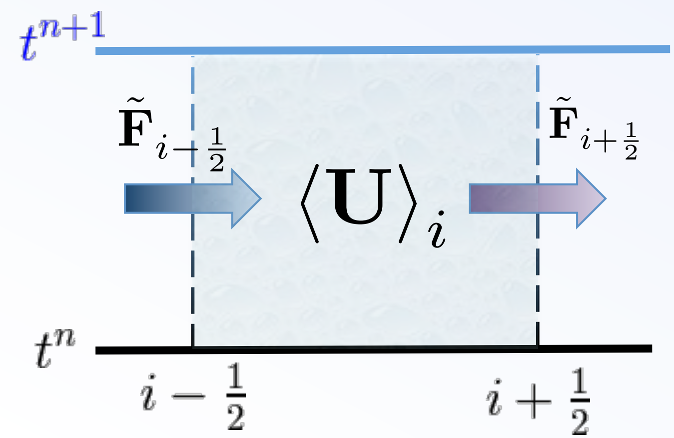
$$\boxed{\langle U \rangle_i^{n+1} = \langle U \rangle_i^n - \frac{\Delta t}{\Delta x}\left(\tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \tilde{F}_{i-\frac{1}{2}}^{n-\frac{1}{2}}\right)}$$



- This is an *EXACT* evolutionary equation for the spatial averages of *U*.
- The integral form does not make use of partial derivatives!
- Problem: how do we compute the flux ?

Flux computation: the Riemann Problem

- Since the solution is known only at t^n, some kind of approximation is required in order to evaluate the flux through the boundary:

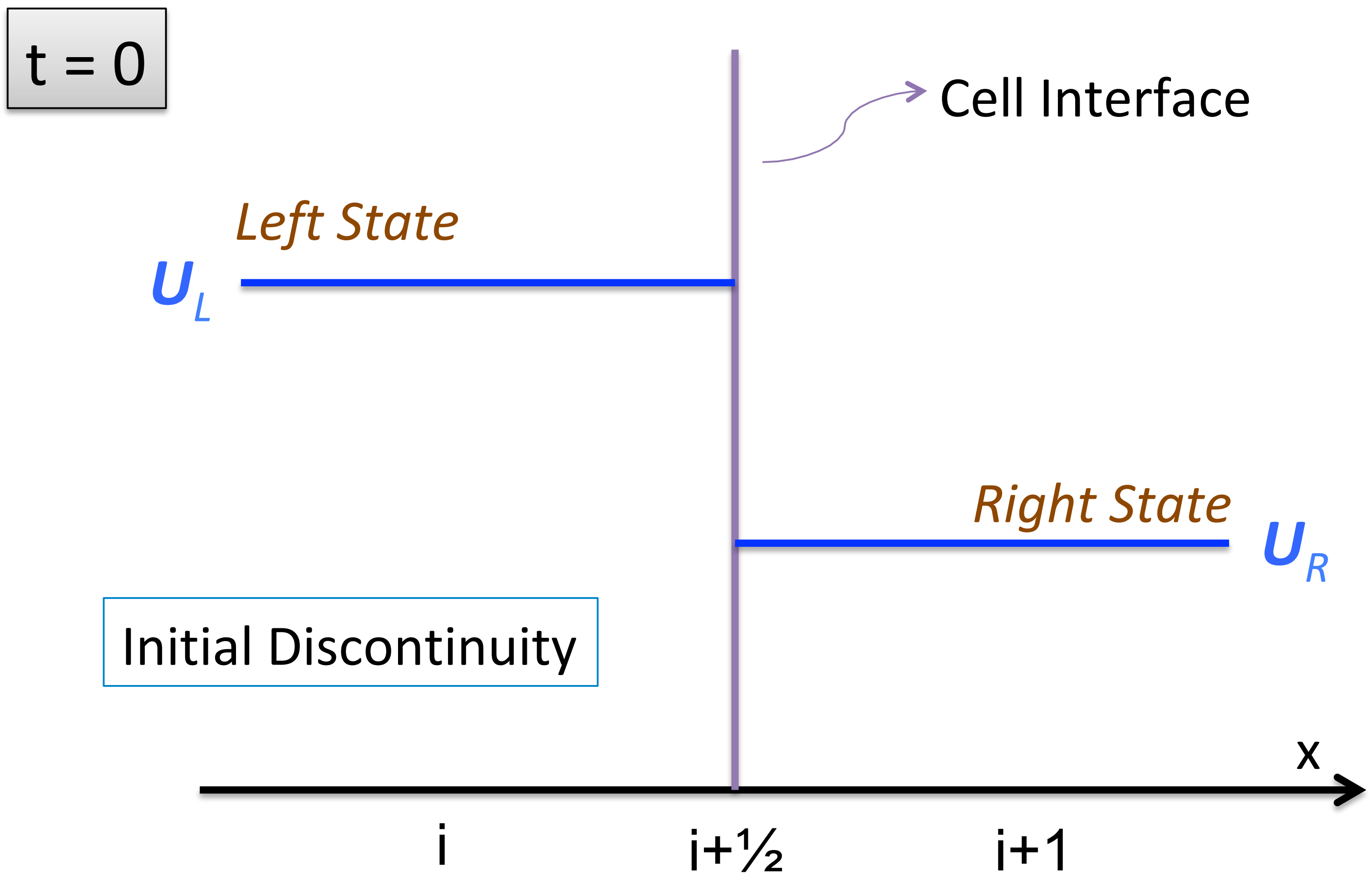


$$\tilde{F}^{n+\frac{1}{2}}_{i+\frac{1}{2}} = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} F(x_{i+\frac{1}{2}}, t)\, dt$$

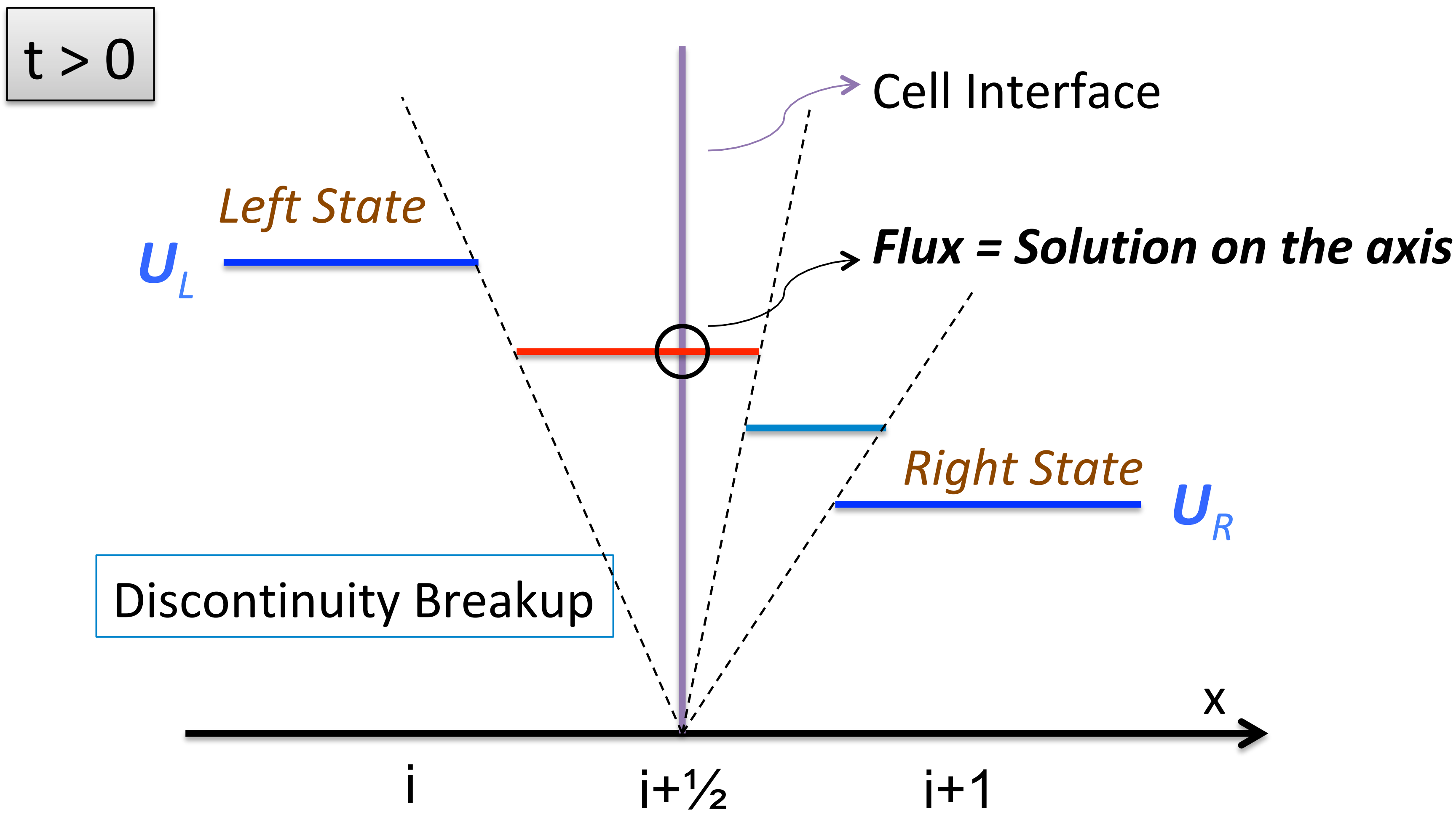
- This achieved by solving the so-called "*Riemann Problem*", i.e., the evolution of an inital discontinuity separating two *constant* states. The Riemann problem is defined by the initial condition:

$$\boxed{U(x,0) = \begin{cases} U_L & \text{for} \quad x < x_{i+\frac{1}{2}} \\ U_R & \text{for} \quad x > x_{i+\frac{1}{2}} \end{cases} \quad \Longrightarrow \quad U(x_{i+\frac{1}{2}}, t > 0) = ?}$$

The Riemann Problem

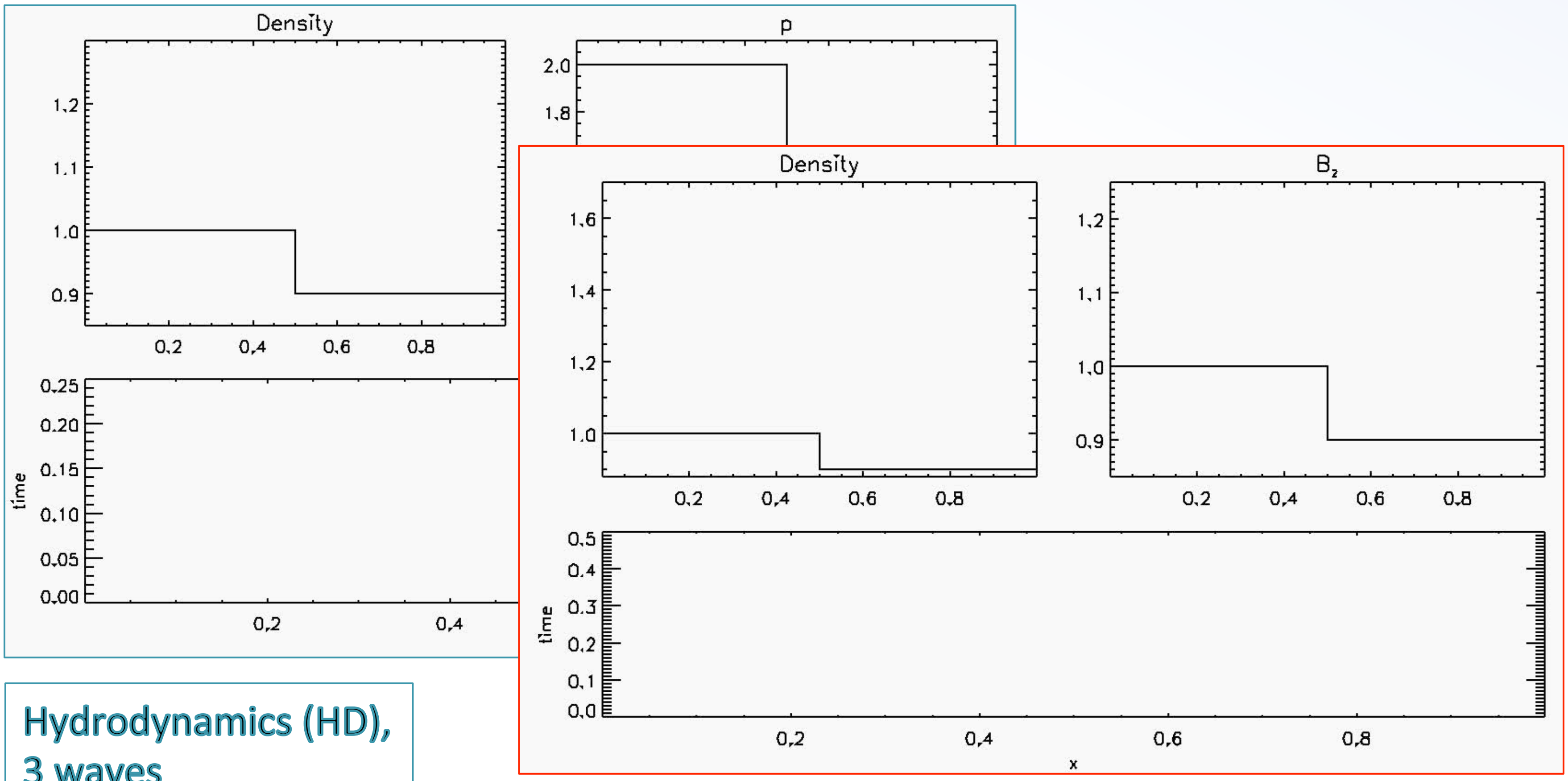


The Riemann Problem



The Riemann Problem

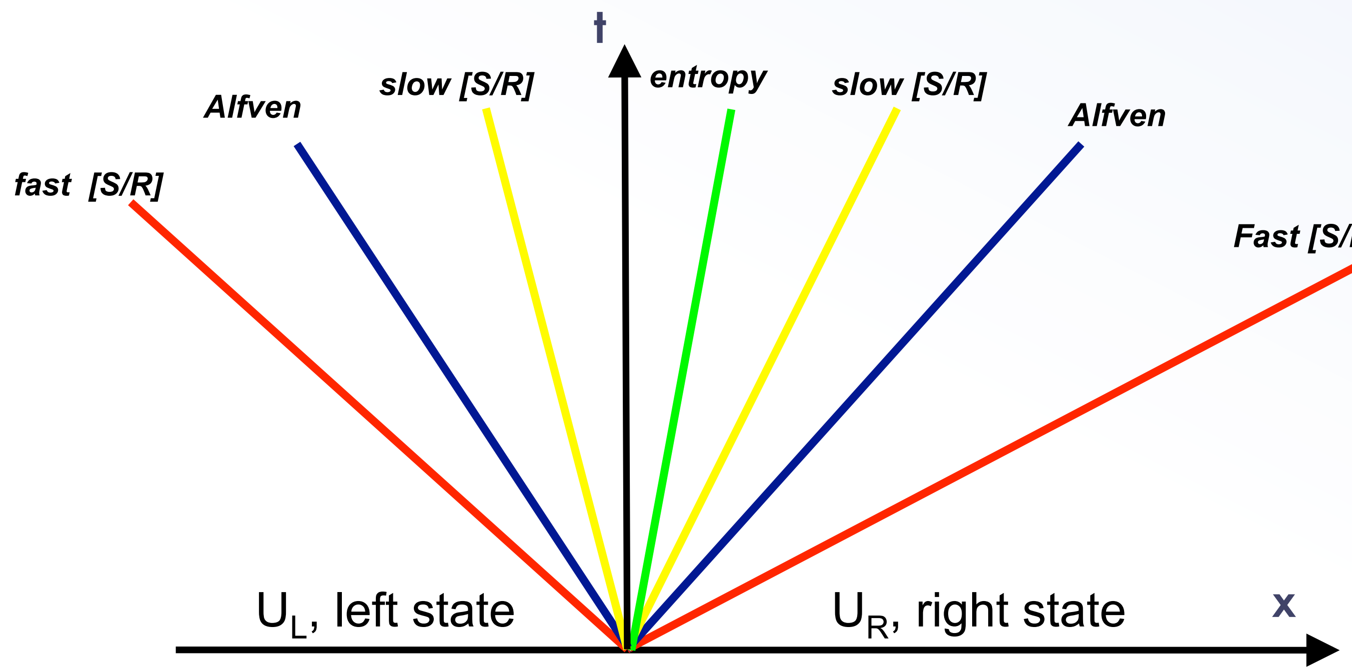
- In CFD, the solution to the Riemann problem depends on the underlying system of conservation laws:



Hydrodynamics (HD), 3 waves

Magnetohydrodynamics (MHD), 7 waves

Riemann Problem in MHD/Relativistic MHD



- 7 wave pattern, $\lambda^{(\kappa)}\left(\boldsymbol{U}_L^{(\kappa)} - \boldsymbol{U}_R^{(\kappa)}\right) = \boldsymbol{F}\left(\boldsymbol{U}_L^{(\kappa)}\right) - \boldsymbol{F}\left(\boldsymbol{U}_R^{(\kappa)}\right)$
- across the contact wave, for $B_n \neq 0$, only density has a jump;
- across Alfven waves, $[\rho] = [p_{gas}] = 0$ but normal velocity $[v_x] \neq 0$
  $\rightarrow$ magnetic field circularly / elliptically polarized.

Solving the Riemann Problem

- The full analytical solution to the Riemann problem for the Euler equation can be found, but this is a rather complicated task (see the book by Toro).
- In general, approximate methods of solution are preferred.
- The advantage of using approximate solvers is the reduced computational costs and the ease of implementation.
- The degree of approximation reflects on the ability to "capture" and spread discontinuities over few or more computational zones.

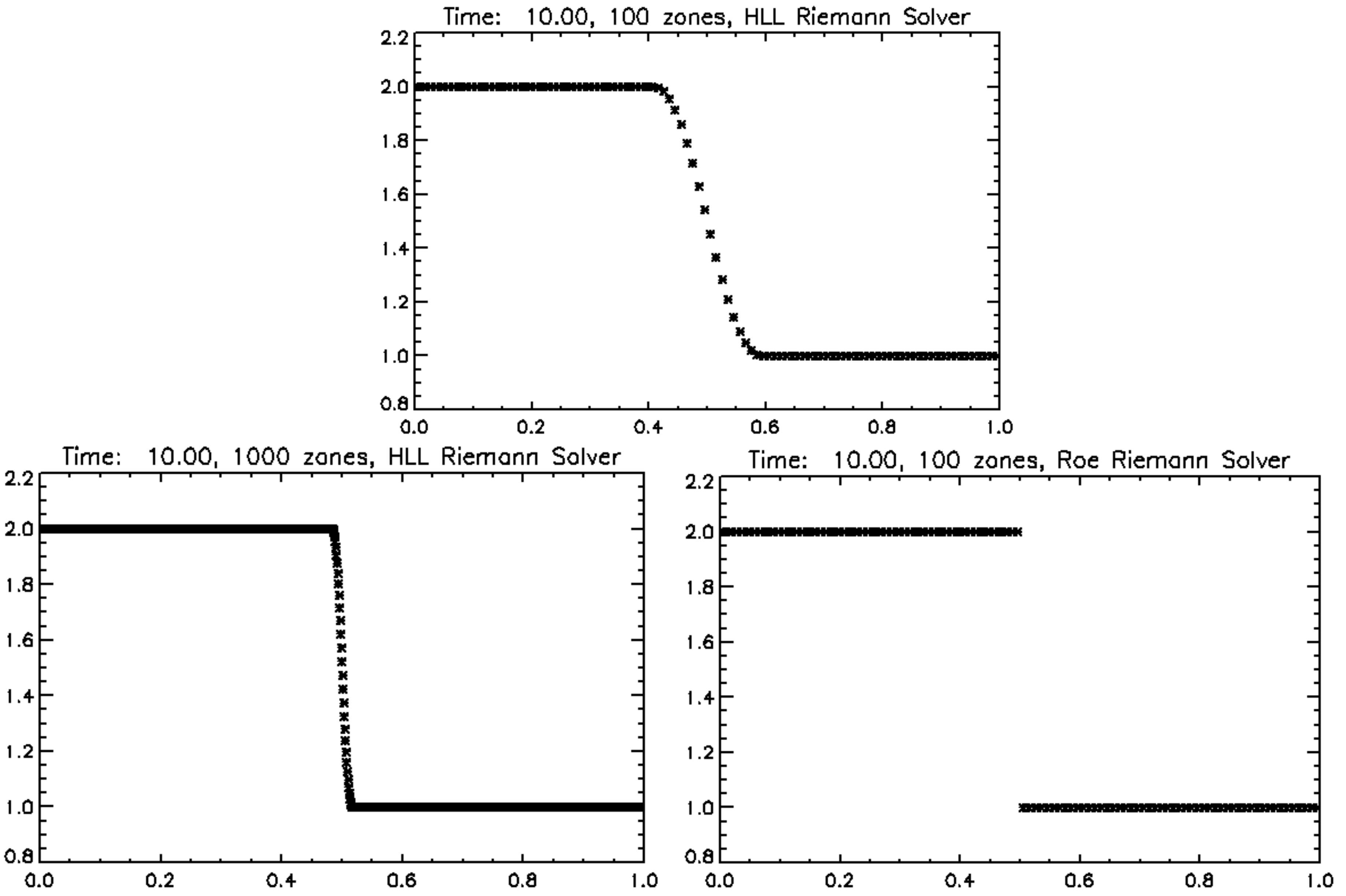
Solving the Riemann Problem

- *Exact Riemann solvers* (nonlinear)
  - Full nonlinear solution:
  - Expensive / impracticable for heavily usage in upwind codes;

- *Linearized Riemann solvers* (Roe type)
  - require characteristic decomposition in eigenvectors
  - may be prone to numerical pathologies

- *HLL-type Riemann solvers* (guess-based)
  - based on guess to the signal speeds and on the integral average of the solution over the Riemann Fan;
  - fewer waves are considered in the solution;
  - preserve positivity;

Resolution of Contact Discontinuities



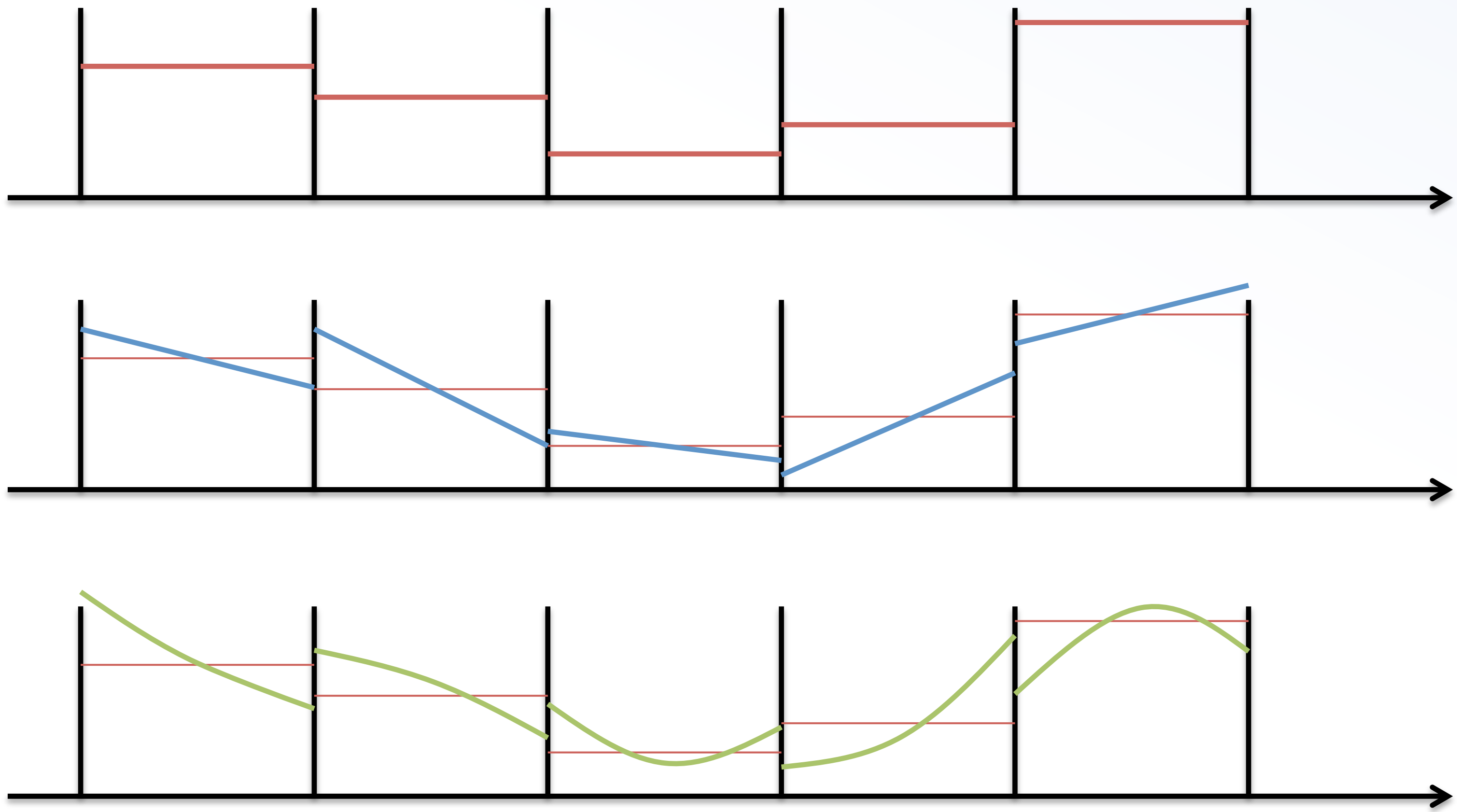
Improving spatial accuracy

- High order reconstruction can be carried inside each cell by suitable oscillation-free polynomial interpolation:

Piecewise constant

Piecewise Linear (TVD)

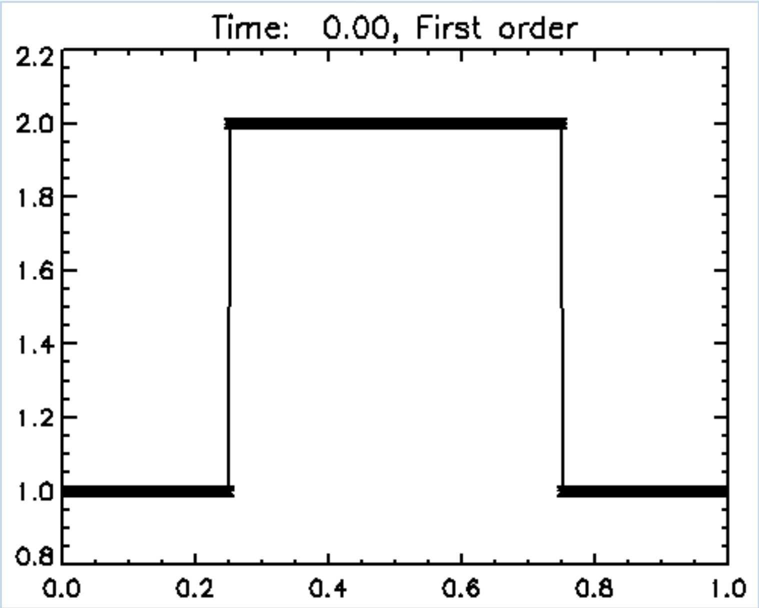
Piecewise Parabolic (PPM, WENO)



1st and 2nd Order Reconstruction

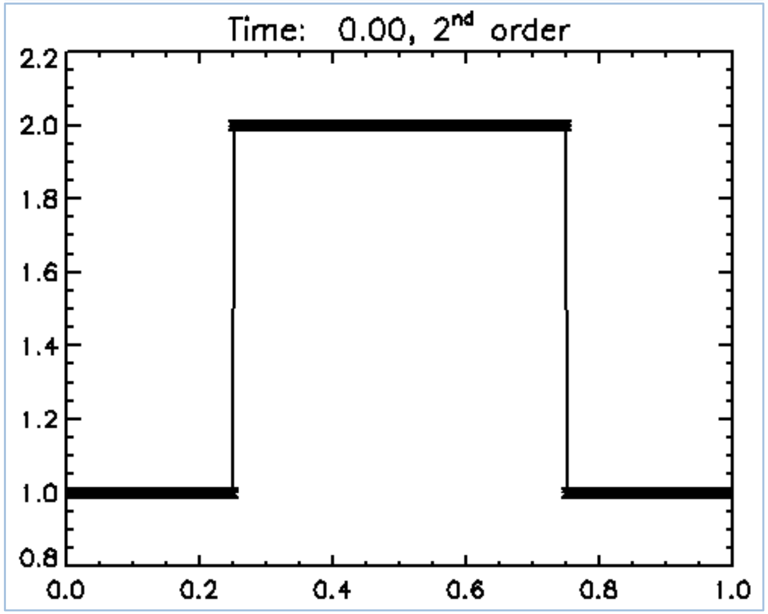
- 1st-order reconstruction:

$$\boxed{V(x) = V_i}$$

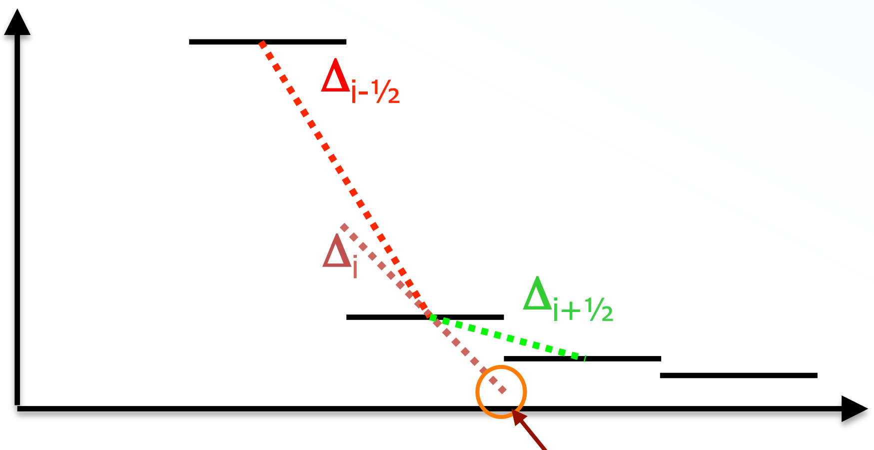


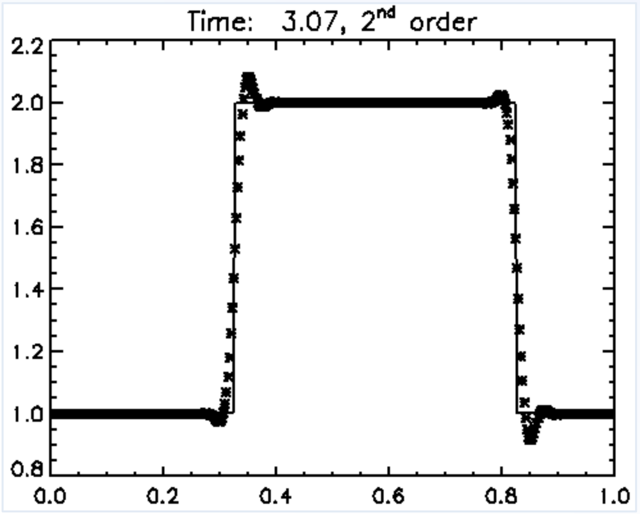
- For 2nd-order we use linear reconstrution:

$$\boxed{V(x) = V_i + \frac{\delta V}{\Delta x}(x - x_i)}$$



Preventing Oscillations

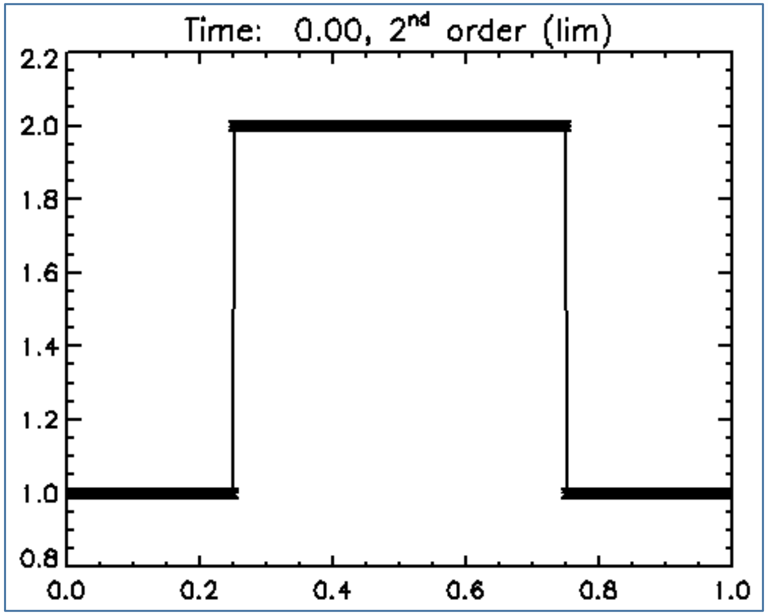




- Use slope limiters to avoid spurious oscillations: $V(x) = V_i + \frac{\delta V}{\Delta x}(x - x_i)$

$$\boxed{\delta V_i = \lim\left(\Delta_{i-1/2}, \Delta_{i+1/2}\right)}$$

$$\text{minmod}(x,y) = \begin{cases} x & \text{if} \quad |x| < |y|, xy > 0 \\ y & \text{if} \quad |y| < |x|, xy > 0 \\ 0 & \text{if} \quad xy < 0 \end{cases}$$



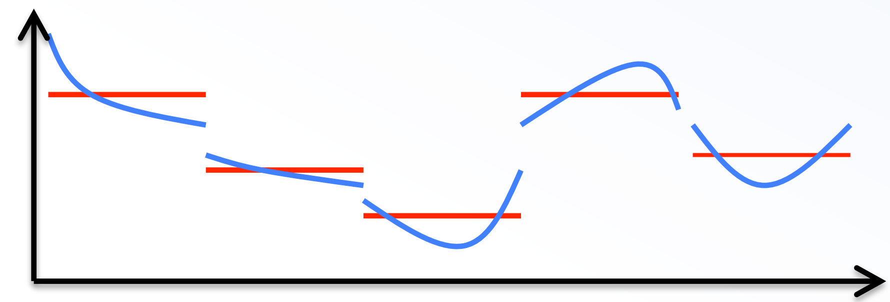
Reconstruct-Solve-Update

- Start from volume-averages

$$\langle \mathbf{U} \rangle_i^n$$

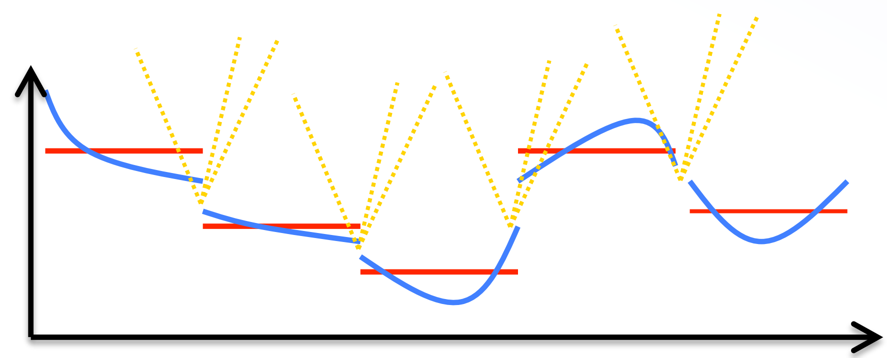
- Reconstruct interface values from zone averages using a high-order non-oscillatory polynomial:

$$\begin{cases} \mathbf{U}^L_{i+\frac{1}{2}} &= \lim_{x \to x^-_{i+\frac{1}{2}}} \mathbf{U}_i(x)\,, \\ \mathbf{U}^R_{i+\frac{1}{2}} &= \lim_{x \to x^+_{i+\frac{1}{2}}} \mathbf{U}_{i+1}(x)\,, \end{cases}$$



- Solve Riemann problems between adjacent, discontinuous states.

  → Compute interface flux.



- Update conserved variables with time stepping algorithm (e.g. RK2):

$$\boxed{\frac{d\,\langle \mathbf{U} \rangle}{dt} = -\frac{1}{\Delta \mathcal{V}} \sum_{\text{faces}} \mathbf{F} \cdot \hat{\mathbf{n}}\, dA + \langle \mathbf{S} \rangle}$$

A “Pseudo-Code”…

for each dt {

Time Stepping:

begin loop on grid zones{

$$\langle U \rangle_i^n \longrightarrow$$

Data Reconstruction

$$\longrightarrow \begin{cases} U_{i+\frac{1}{2},L} \\ U_{i+\frac{1}{2},R} \end{cases}$$

$$\begin{cases} U_{i+\frac{1}{2},L} \\ U_{i+\frac{1}{2},R} \end{cases} \longrightarrow$$

Riemann Solver

$$\longrightarrow \tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}}$$

$$\longrightarrow \langle U \rangle_i^{n+1} = \langle U \rangle_i^n - \frac{\Delta t}{\Delta x}\left(\tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \tilde{F}_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right)$$

}end loop on grid zones

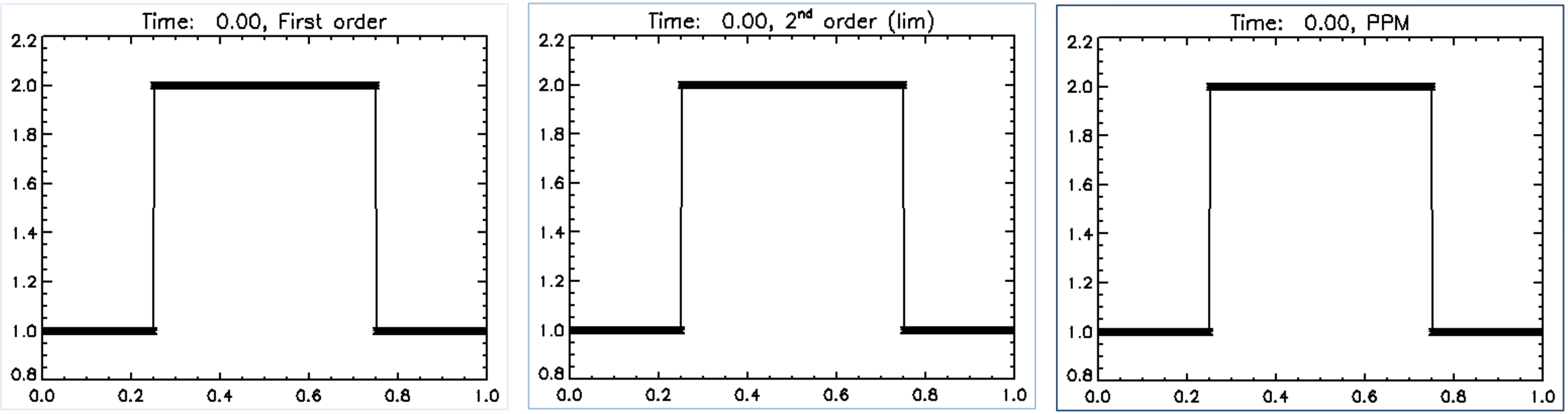
}

A Note on Numerical Diffusion

- Upwind methods have a natural, built-in numerical dissipation.
- A discretized PDE gives the exact solution to an equivalent equation with a diffusion term;
- Consider $$\frac{\partial U}{\partial t} + a\frac{\partial U}{\partial x} = 0\,, \qquad a > 0$$
  - Use upwind discretization: $$\frac{U_i^{n+1} - U_i^n}{\Delta t} + a\frac{U_i^n - U_{i-1}^n}{\Delta x} = 0$$
  - Use Taylor expansion on U_i^{n+1} and U_{i-1}^n
  - The solution to the discretized equation satisfies *exactly*
  $$\frac{\partial U}{\partial t} + a\frac{\partial U}{\partial x} = \frac{a\Delta x}{2}\left(1 - a\frac{\Delta t}{\Delta x}\right)\frac{\partial^2 U}{\partial x^2} + H.O.T.$$
  - This is an advection-diffusion equation.

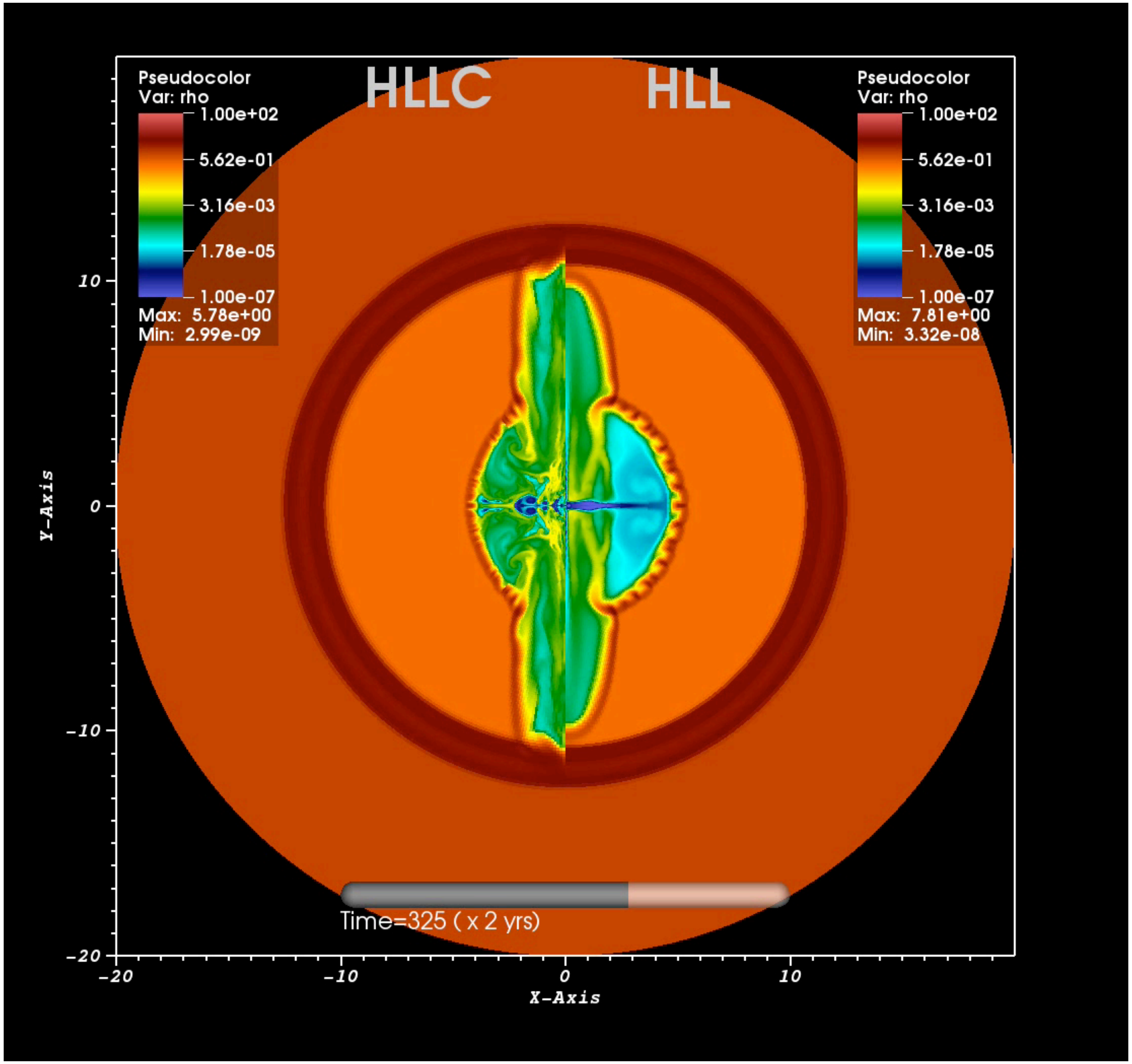
A Note on Numerical Diffusion

- Generally, the amount of numerical diffusion is controlled by the underlying grid resolution / numerical scheme:
  - spatial *reconstruction*
  - *Riemann solver* accuracy
  - (marginally) *time stepping*



- PROS: numerical diffusion has a stabilizing effect.
- CONS: suppress small scale effect, may prevent growth of instabilities

A 2D Example: Axisymmetric PWN



V. BEYOND IDEAL MHD

Beyond Ideal MHD

- The range of validity of MHD can be extended by several means, at the cost of introducing additional terms and more complex algorithms.

- One will then have to deal with *different time scales*.

- Example are:

  - *Dissipative effects* (viscosity, Ohmic dissipation, thermal conduction, etc…) → mixed hyperbolic / parabolic PDE.

  - *Extended MHD* including *generalized Ohm's law* (Hall-MHD, electron pressure) → dispersive waves, non-homogenous PDE with stiff sources (RMHD);

  - Fluid-particles *hybrid* algorithms.

Diffusion Processes

- Parabolic (diffusion) term describes transfer of momentum or energy due to microscopical processes without requiring bulk motion.
- Examples: viscosity, magnetic resistivity, thermal conduction.

$$
\boxed{
\begin{array}{rcl}
\dfrac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}) & = & 0 \\
\dfrac{\partial(\rho\boldsymbol{v})}{\partial t} + \nabla\cdot\left[\rho\boldsymbol{v}\boldsymbol{v}^T - \boldsymbol{B}\boldsymbol{B}^T\right] + \nabla p_t & = & \nabla\cdot\tau + \rho\boldsymbol{g} \\
\dfrac{\partial\mathcal{E}}{\partial t} + \nabla\cdot\left[(\mathcal{E}+p_t)\,\boldsymbol{v} - (\boldsymbol{v}\cdot\boldsymbol{B})\,\boldsymbol{B}\right] & = & \nabla\cdot\Pi_{\mathcal{E}} - \Lambda + \rho\boldsymbol{v}\cdot\boldsymbol{g} \\
\dfrac{\partial\boldsymbol{B}}{\partial t} - \nabla\times(\boldsymbol{v}\times\boldsymbol{B}) & = & -\nabla\times(\eta\boldsymbol{J}) \\
\dfrac{\partial(\rho X_\alpha)}{\partial t} + \nabla\cdot(\rho X_\alpha\boldsymbol{v}) & = & \rho S_\alpha
\end{array}
}
$$

- *No upwinding* is required since parabolic problems have infinite propagation speed → central differences are OK!

Explicit Scheme for Parabolic PDE

- However, explicit schemes subject to restrictive constraint:
- In 1-D with constant D: $$\frac{\partial U}{\partial t} = D\frac{\partial^2 U}{\partial x^2}$$
- Using FTCS: $$\boxed{U_i^{n+1} = U_i^n + C(U_{i-1}^n - 2U_i^n + U_{i+1}^n)}$$
- Where $C = D\Delta t/\Delta x^2$ is the (parabolic) CFL number
- Stability demands $C \leq ½ \rightarrow \Delta t \leq \Delta x^2 / (2D)$
- This is quite restrictive !

Implicit Schemes for Parabolic PDE

- Using a backward in time, centered in space (BTCS):

$$U_i^{n+1} = U_i^n + C(U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1})$$

has no stability limit (*unconditionally stable !*)

- However, it leads to an implicit (linear) system:

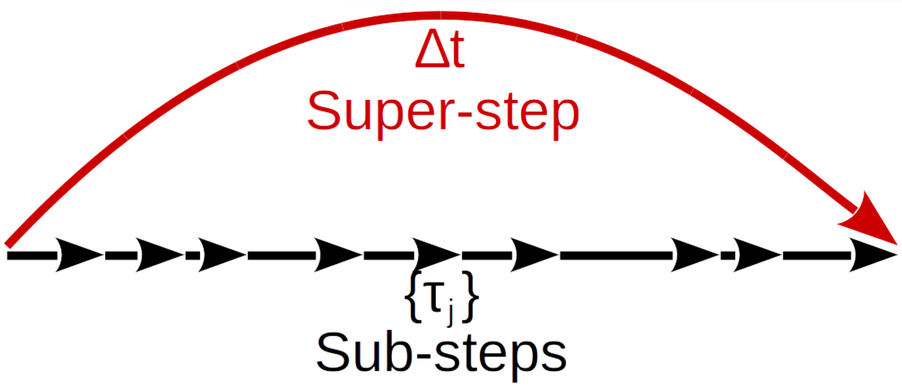
$$\mathsf{A}\{U\}^{n+1} = \{U\}^n\,, \qquad \mathsf{A} \in \mathbb{R}^{N_x \times N_x}$$

- This is a global operation and thus not can not be efficiently carried out on parallel domains.

- Alternative → Accelerated explicit methods →

Accelerated Explicit Methods

- Divide each time step Δt in *s* sub-steps based on a polynomial sequence and require stability at the end of a cycle of *s* substeps:



$$\frac{\partial U}{\partial t} = -MU \quad \Longrightarrow \quad U^{n+1} = \prod_{j=1}^{s}(\mathsf{I} - \tau_j M)U^n \equiv R_s U$$

- In practice we require the super-step to be as large as possible, exploiting properties of orthogonal polynomial, *Chebyshev* (Super Time Stepping [STS]) or *Legendre* (Runge-Kutta Legendre [RKL]).
- The scheme is still explicit !

Runge-Kutta-Legendre

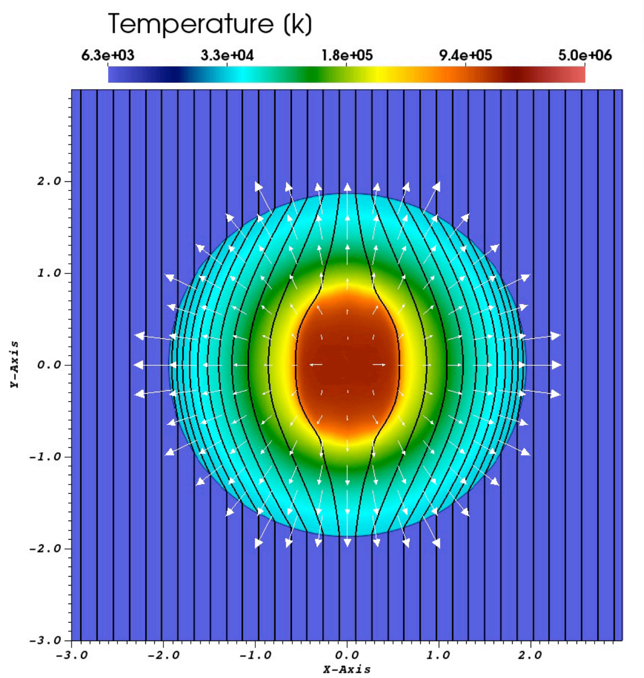
- RKL methods show better stability properties and are preferred over STS.
- Choosing s sub-steps we can cover a time step equal to

$$\boxed{\Delta t \leq \Delta t_{expl} \frac{s^2 + s - 2}{4}}$$

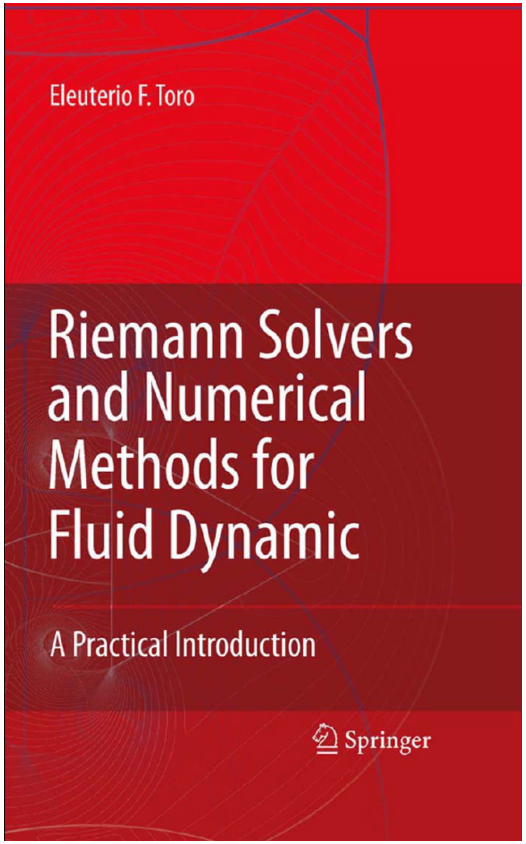
where Δt_{expl} is the standard explicit method time step.

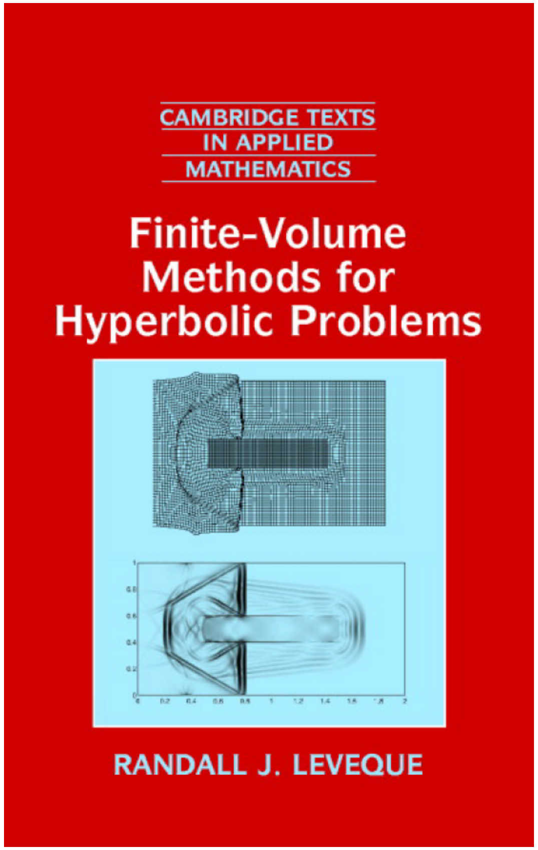
- The method is easily parallelizable.
- Scaling on 2D blast wave:

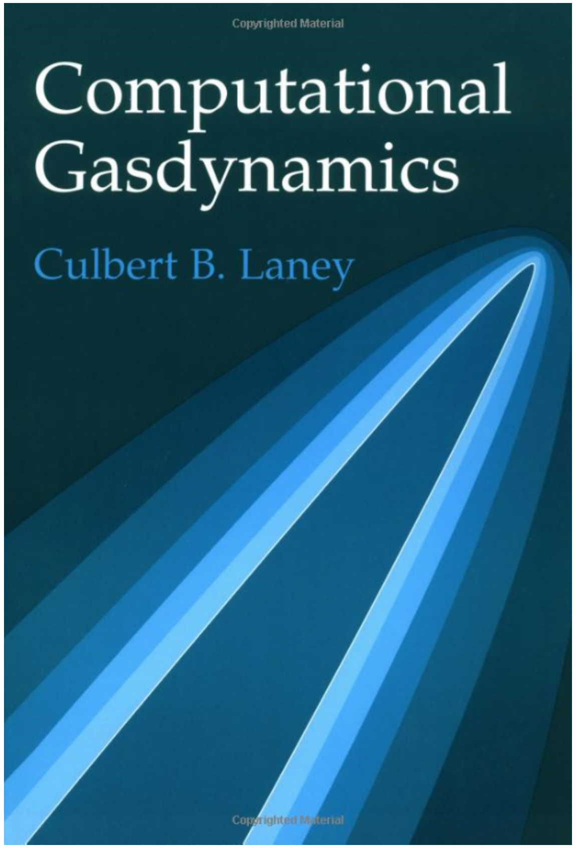
Algorithm	N_x	Execution Time $[s]$
Explicit	192	$1m : 13s$
RKL	192	$28s$
Explicit	384	$18m : 32s$
RKL	384	$5m : 19s$
Explicit	768	$4h : 21m : 15s$
RKL	768	$49m : 17s$
Explicit	1536	$3d : 5h : 13m : 10s$
RKL	1536	$10h : 4m : 55s$



Recommended Books





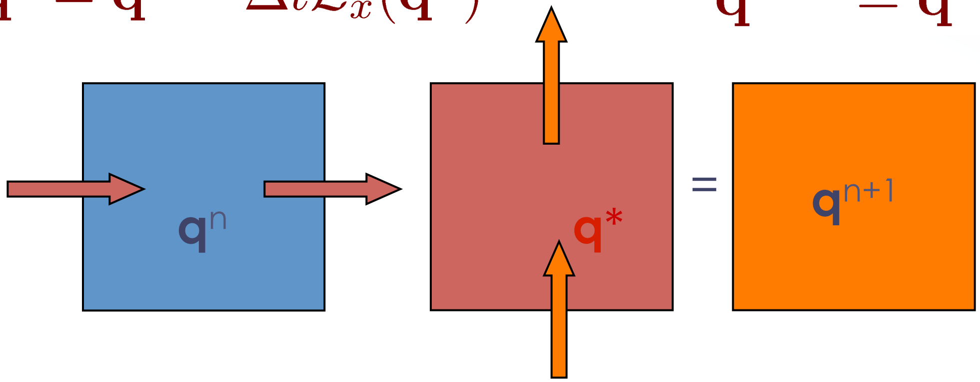


IX. MULTIDIMENSIONAL ISSUES: DIVERGENCE OF $\nabla \cdot B = 0$

Multi Dimensional Integration

- Integration in more than one dimensions can be achieved using two distinct approaches:
  - Dimensionally Split schemes: solve the PDE as a sequence of 1-D sub-problems.

$$\mathbf{q}^* = \mathbf{q}^n - \Delta t \mathcal{L}_x(\mathbf{q}^n) \qquad \mathbf{q}^{n+1} = \mathbf{q}^* - \Delta t \mathcal{L}_y(\mathbf{q}^*)$$

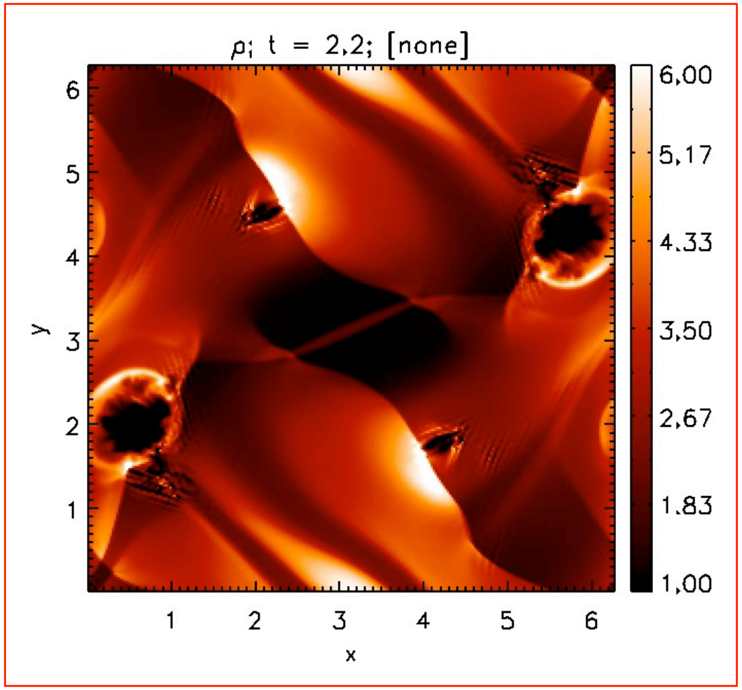


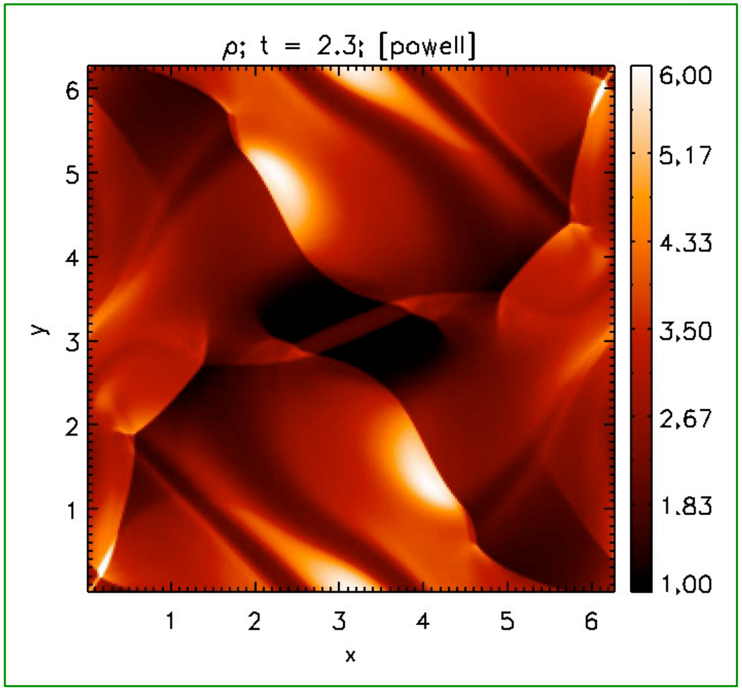
  - Dimensionally Unsplit schemes: solve the full problem in one step:

$$\mathbf{q}^{n+1} = \mathbf{q}^n - \Delta t \mathcal{L}_x(\mathbf{q}^n) - \Delta t \mathcal{L}_y(\mathbf{q}^n)$$

∇·B Condition

- Numerically, the solenoidal condition is fulfilled only at the truncation level and non-solenoidal components may be generated during the evolution:





- Magnetic monopoles cause unphysical accelerations of the plasma in the direction parallel to the field lines (BrackBill & Barnes 1980)

Cell Centered vs Staggered

- $\nabla \cdot B = 0$ cannot be satisfied for any type of discretization;

- Robustness of a method can be assessed on practical basis by extensive numerical testing.

- *Cell Centered* Methods: magnetic field treated as volume average over the zone:

    - Projection method (BrackBill & Barnes, 1980)
    - Powell's 8-wave formulation (Powell 1994, Powell et al. 1999)
    - Field CD (Toth 2000)
    - Divergence cleaning (Dedner 2002, Mignone et al. 2010)

- *Staggered* (*face-centered*) methods:

    – magnetic field has a staggered representation where field components live on the face they are normal to (Evans & Hawley 1988, Balsara 2000, 2004).

1. Projection Method

- Correct the magnetic field after the time step is completed;
- Starting from $\boldsymbol{B}^n$ we obtain $\boldsymbol{B}^*$ which is not divergence-free.

- Then, using Hodge-projection: $\boldsymbol{B}^* = \nabla \times \boldsymbol{A} + \nabla\phi$
- Taking the divergence of both sides gives

$$\nabla^2\phi = \nabla \cdot \boldsymbol{B}^*$$

which can be solved for the scalar function ϕ.

- The magnetic field is then corrected as $\boldsymbol{B}^{n+1} = \boldsymbol{B}^* - \nabla\phi$
- Cons: requires the solution of a Poisson equation.

2. Powell's Method (8 wave)

- Start from the primitive form of the MHD equations without discarding the ∇·B term → quasi-conservative form

$$
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
$$

$$
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u} + \left(p + \frac{\mathbf{B} \cdot \mathbf{B}}{2\mu_0} \right) \mathbf{I} - \frac{\mathbf{B}\mathbf{B}}{\mu_0} \right) = -\frac{1}{\mu_0} \mathbf{B} \nabla \cdot \mathbf{B}
$$

$$
\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{B} - \mathbf{B}\mathbf{u}) = -\mathbf{u} \nabla \cdot \mathbf{B}
$$

$$
\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + p + \frac{\mathbf{B} \cdot \mathbf{B}}{2\mu_0} \right) \mathbf{u} - \frac{1}{\mu_0} (\mathbf{u} \cdot \mathbf{B}) \mathbf{B} \right] = -\frac{1}{\mu_0} (\mathbf{u} \cdot \mathbf{B}) \nabla \cdot \mathbf{B}
$$

2. Powell's Method (8 wave)

- The non-conservative form is discretized by introducing an 8^{th} wave in the Riemann solver associated with jumps in the normal component of magnetic field.

- With the non-conservative formulation $\nabla\cdot\mathbf{B}$ errors generated by the numerical solution do not accumulate at a fixed grid point but, rather, propagate together with the flow.

- For many problems the 8-wave formulation works.

- However, in problems containing strong shocks, the non-conservative source terms can produce incorrect jump conditions and consequently the scheme can produce incorrect results

3. Hyperbolic Divergence Cleaning

- The divergence constraint is coupled to Faraday's law by introducing a new scalar field function ψ (generalized Lagrangian multiplier).
- The second and third Maxwell's equations are thus replaced by

$$\begin{cases} \nabla \cdot \mathbf{B} = 0, \\ \dfrac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}), \end{cases} \quad \Rightarrow \quad \begin{cases} \mathcal{D}(\psi) + \nabla \cdot \mathbf{B} = 0, \\ \dfrac{\partial \mathbf{B}}{\partial t} + \nabla \psi = \nabla \times (\mathbf{v} \times \mathbf{B}), \end{cases}$$

where $\mathcal{D}$ is a linear differential operator.

- An efficient method may be obtained by choosing $\mathcal{D}(\psi) = c_h^{-2}\partial_t \psi + c_p^{-2}\psi$ yielding a mixed hyperbolic/parabolic correction.
- Direct manipulation leads to the telegraph equation:

$$\frac{\partial^2 \psi}{\partial t^2} + \frac{c_h^2}{c_p^2}\frac{\partial \psi}{\partial t} = c_h^2 \Delta \psi$$

→ errors are propagated to the domain at finite speed c_h and damped at the same time.

3. Hyperbolic Cleaning

- The resulting system is called the generalized Lagrange multiplier (GLM-MHD) and includes 9 evolution equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot \left[\rho \mathbf{v}\mathbf{v}^T - \mathbf{B}\mathbf{B}^T + \mathsf{I}\left(p + \frac{\mathbf{B}^2}{2} \right) \right] = 0,$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v}\mathbf{B}^T - \mathbf{B}\mathbf{v}^T) + \nabla \psi = 0,$$

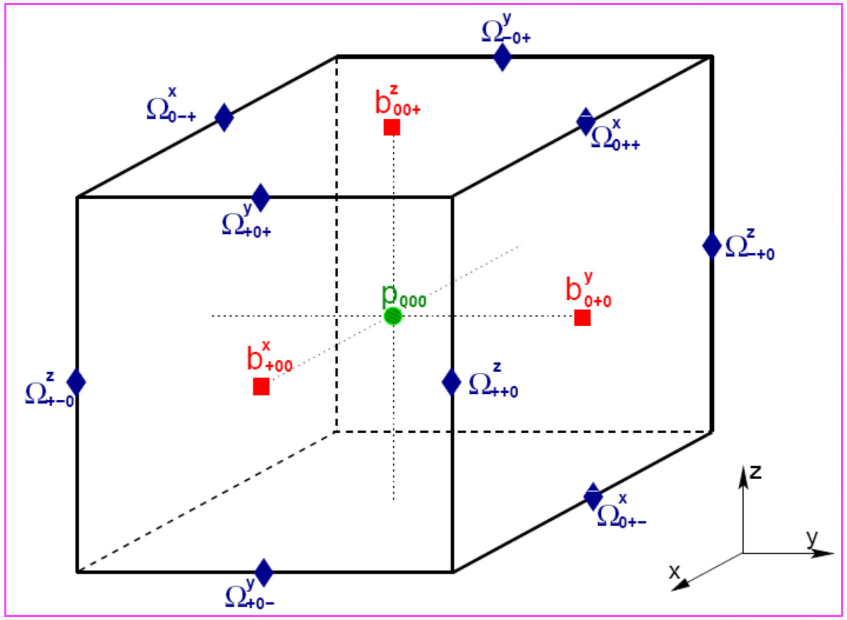
$$\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + p + \frac{\mathbf{B}^2}{2} \right) \mathbf{v} - (\mathbf{v} \cdot \mathbf{B})\mathbf{B} \right] = 0,$$

$$\frac{\partial \psi}{\partial t} + c_h^2 \nabla \cdot \mathbf{B} = -\frac{c_h^2}{c_p^2} \psi,$$

- Divergence errors propagate with speed c_h even at stagnation points where $v = 0$.

4. Constrained Transport

- Staggered magnetic field treated as an area-weighted average on the zone face.



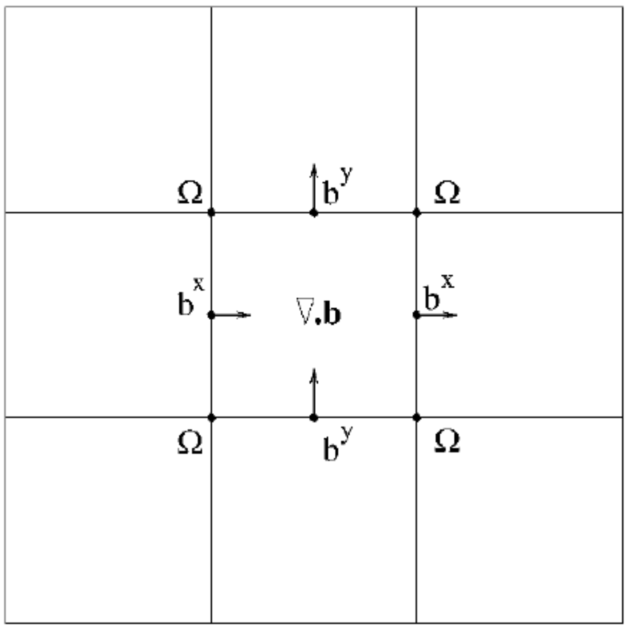
- Thus, different magnetic field components live at different location;

- A discrete version of Stoke's theorem is used to update them:

$$\int \left(\frac{\partial \boldsymbol{b}}{\partial t} + \nabla \times \boldsymbol{\mathcal{E}} \right) \cdot d\boldsymbol{S}_d = 0 \quad \Longrightarrow \quad \frac{db_{x_d}}{dt} + \frac{1}{S_d} \oint \boldsymbol{\mathcal{E}} \cdot d\boldsymbol{l} = 0$$

4. Constrained Transport in 2D

- In 2D, the emf is placed at cell corners.
- The discrete Stoke's theorem becomes



$$b^{x,n+1}_{j+1/2,k} = b^{x,n}_{j+1/2,k} - \Delta t \frac{\Omega_{j+1/2,k+1/2} - \Omega_{j+1/2,k-1/2}}{\Delta y}$$

$$b^{y,n+1}_{j,k+1/2} = b^{y,n}_{j,k+1/2} + \Delta t \frac{\Omega_{j+1/2,k+1/2} - \Omega_{j-1/2,k+1/2}}{\Delta x}$$

- It is easy to show that the numerical divergence of ***b*** defined by

$$(\nabla \cdot \boldsymbol{b})_{j,k} = \frac{b^x_{j+1/2,k} - b^x_{j-1/2,k}}{\Delta x} + \frac{b^y_{j,k+1/2} - b^y_{j,k-1/2}}{\Delta y}$$

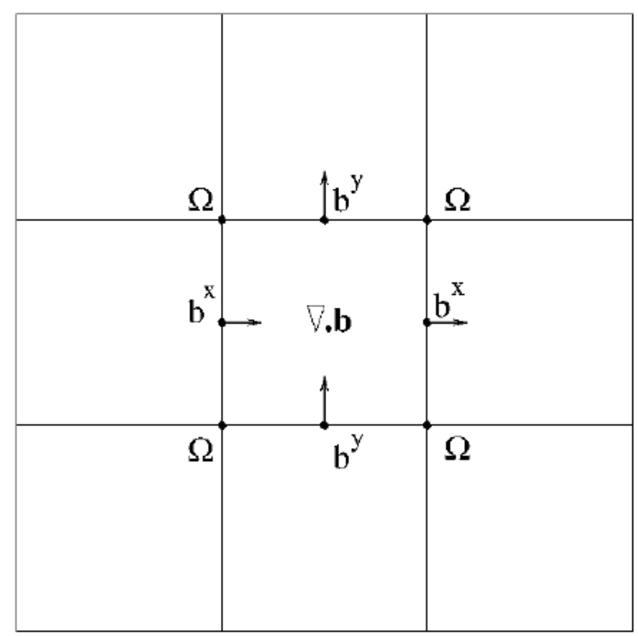
does not change due to perfect cancellation of term to machine accuracy (Toth, 2000).

4. Constrained Transport in 2D

- In 2D, the emf is placed at cell corners.
- The discrete Stoke's theorem becomes

$$b^{x,n+1}_{j+1/2,k} = b^{x,n}_{j+1/2,k} - \Delta t \frac{\Omega_{j+1/2,k+1/2} - \Omega_{j+1/2,k-1/2}}{\Delta y}$$

$$b^{y,n+1}_{j,k+1/2} = b^{y,n}_{j,k+1/2} + \Delta t \frac{\Omega_{j+1/2,k+1/2} - \Omega_{j-1/2,k+1/2}}{\Delta x}$$



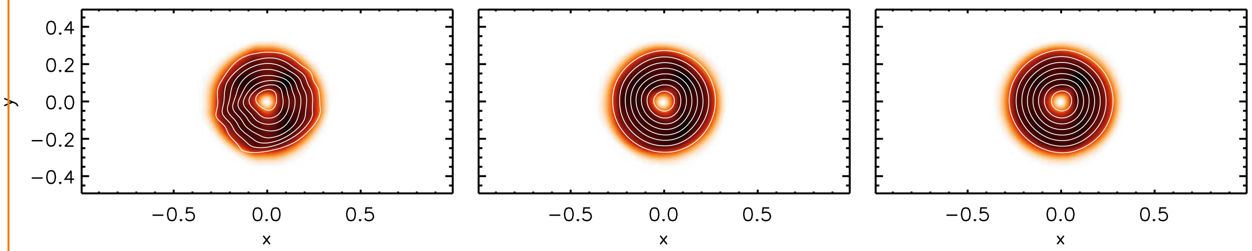
- It is easy to show that the numerical divergence of ***b*** defined by

$$(\nabla \cdot \boldsymbol{b})_{j,k} = \frac{b^x_{j+1/2,k} - b^x_{j-1/2,k}}{\Delta x} + \frac{b^y_{j,k+1/2} - b^y_{j,k-1/2}}{\Delta y}$$

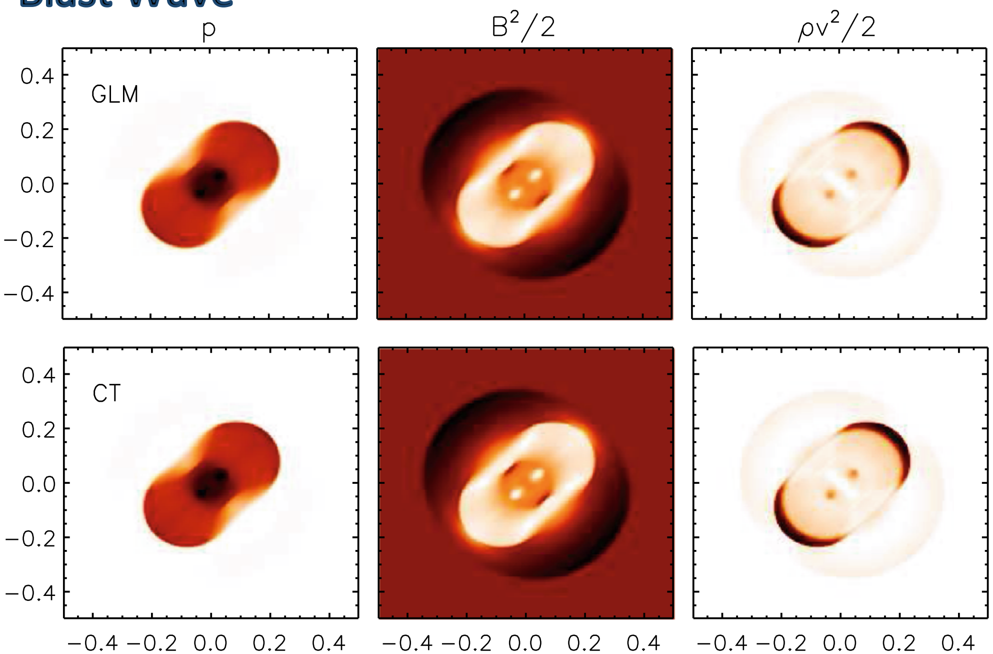
does not change due to perfect cancellation of term to machine accuracy (Toth, 2000).

Scheme Comparison

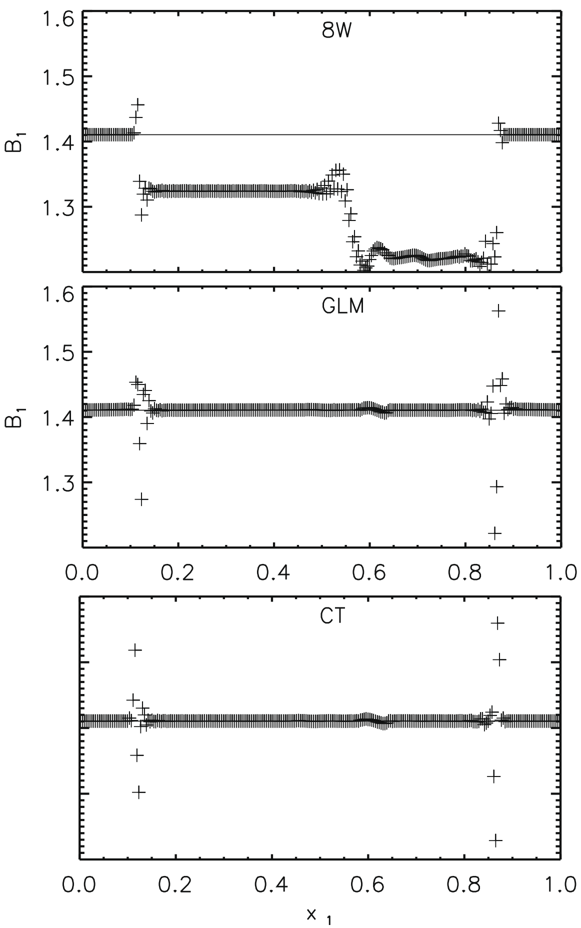
Field Loop advection



Blast Wave



Rotated Shock Tube



$\nabla \cdot B$ Condition

	Cell-Centered	*Staggered*
Pros	■ keeps "native" code discretization ■ better for I.C. and B.C. ■ easier to extend to AMR grids ■ Can be used in dimensionally split schemes	■ keep $\nabla \cdot B = 0$ to machine accuracy ■ elegant and consistent discretization ■ lead to perfectly consistent, well posed Riemann problems
Cons	■ require monopole control algorithm ■ 8 wave / Projection: ➢ Jump of B at face → Riemann problem ➢ Break conservation (??)	■ tricky extension to AMR ■ more work on B.C. and I.C. ■ Require solution of multi D Riemann problems (UCT, L. Del Zanna & Londrillo)

THE END