Numerical Methods for Astrophysical Fluid Dynamics

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Outline

I. Plasma as fluids, validity of MHD;
II. Basic Discretization Methods;
III. The Linear Hyperbolic PDE;
IV. Linear Systems of Hyperbolic PDE;
V. The Nonlinear Scalar PDE;

VI. Nonlinear Systems of (hyperbolic) PDE;
VII. Riemann Solvers;
VIII. High Order Extensions;
IX. Multidimensional Extensions & Issues;
X. Beyond Ideal MHD.

I. PLASMAS AS FLUIDS

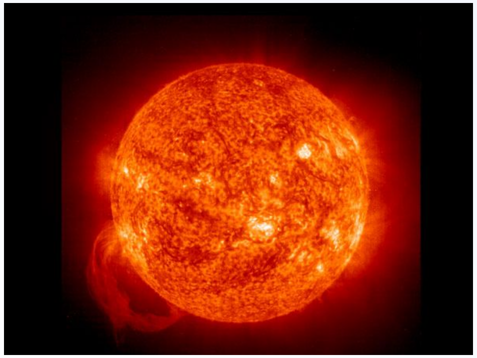
Observational Evidence

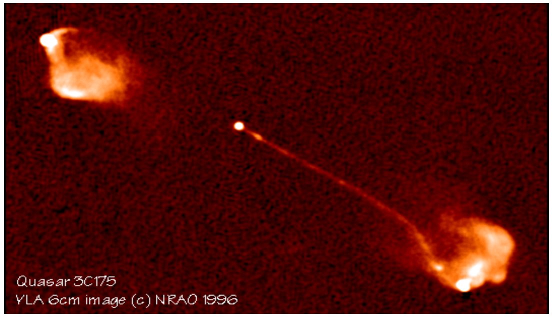
- It is estimated that more than 99.9 % of matter in the Universe exists in the form of *plasma*;

- 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*.





From Kinetic to Fluid to MHD

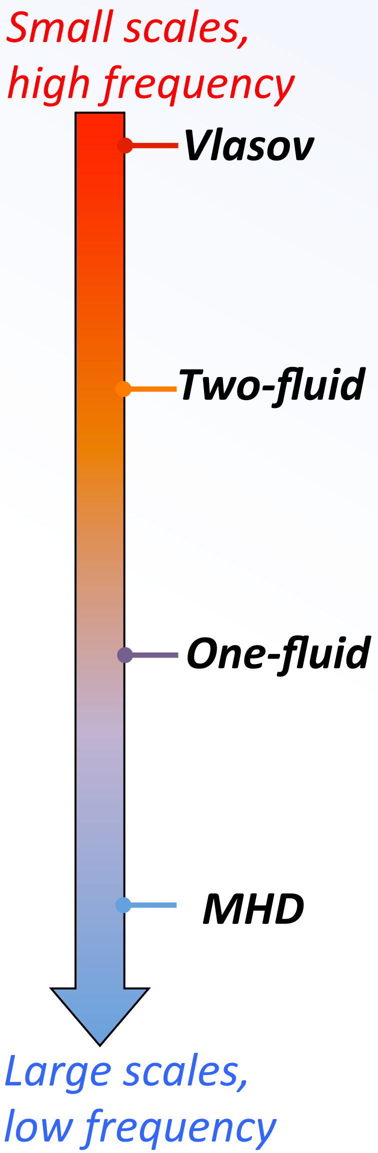
- *Vlasov / Fokker Plank* describes the time evolution, in phase space, of the plasma distribution function f(**x**,**v**,t):

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

- *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

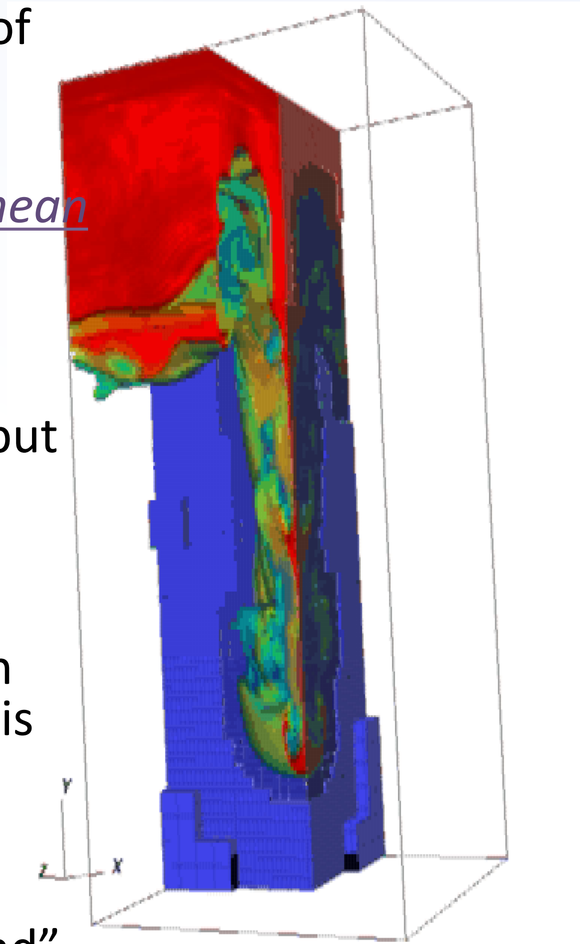
- The fluid approach treats the system as a *continuous medium* and considers the dynamics of a small volume of the fluid.

- 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

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

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

Ideal MHD at Last

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad \text{(Mass cons.)}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \left[\rho \mathbf{u}\mathbf{u} - \frac{\mathbf{B}\mathbf{B}}{4\pi} + \left(p + \frac{\mathbf{B}^2}{8\pi} \right) \right] = 0 \quad \text{(Momentum cons.)}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + p + \frac{\mathbf{B}^2}{8\pi} \right) \mathbf{u} - \frac{(\mathbf{u} \cdot \mathbf{B})}{4\pi} \mathbf{B} \right] = 0 \quad \text{(Energy cons.)}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\boldsymbol{u}\boldsymbol{B} - \boldsymbol{B}\boldsymbol{u}) = 0 \quad \text{(Mag. flux cons.)}$$

- MHD suitable for describing plasma at large scales;

- 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:

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

$$\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot [w\gamma^2\mathbf{v}\mathbf{v} - \mathbf{B}\mathbf{B} - \mathbf{E}\mathbf{E}] + \nabla p_t = 0\,,$$

$$\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) = 0\,,$$

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathbf{m} - \rho\gamma\mathbf{v}) = 0\,,$$

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

- 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. BASIC DISCRETIZATION METHODS FOR HYPERBOLIC PDE

Numerical Discretizations

- We consider our prototype first-order partial differential equation (PDE):

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

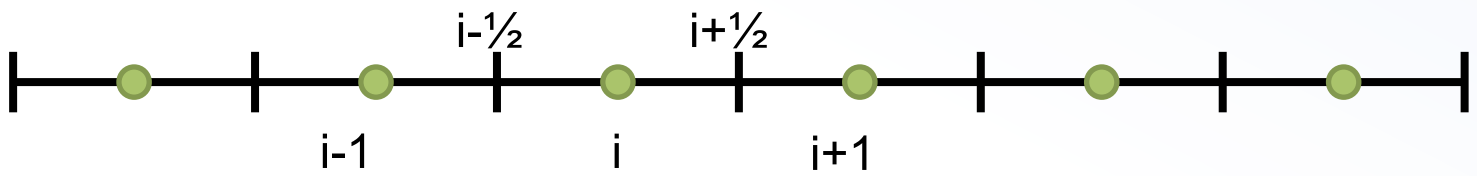
also known as a "***Conservation Law***".

- Two popular methods for performing discretization:
  - *Finite Differences* (FD);
  - *Finite Volumes* (FV);

- For some problems, the resulting discretizations look identical, but they are distinct approaches;

Finite Difference Methods

- A finite-difference method stores the solution at specific points in space and time;



- Associated with each grid point is a function value,

$$U_i^n \equiv U(x_i, t^n)$$

- We replace the derivatives in our PDE with differences between neighbour points.

Finite Difference Methods

- From Taylor expansion of the function around (x_i,t^n) we obtain, e.g.

  - *Forward* derivative (in time):

$$\frac{\partial U(x,t)}{\partial t} = \frac{U_i^{n+1} - U_i^n}{\Delta t} - \frac{\Delta t}{2}\left(\frac{\partial^2 U}{\partial t^2}\right)^n + H.O.T.$$

or simply

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

  - *Central* derivative (in space):

$$\frac{\partial U(x,t)}{\partial x} = \frac{U_{i+1}^n - U_{i-1}^n}{2\Delta x} - \frac{\Delta x^2}{6}\left(\frac{\partial^3 U}{\partial x^3}\right)_i + H.O.T.$$

or simply

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

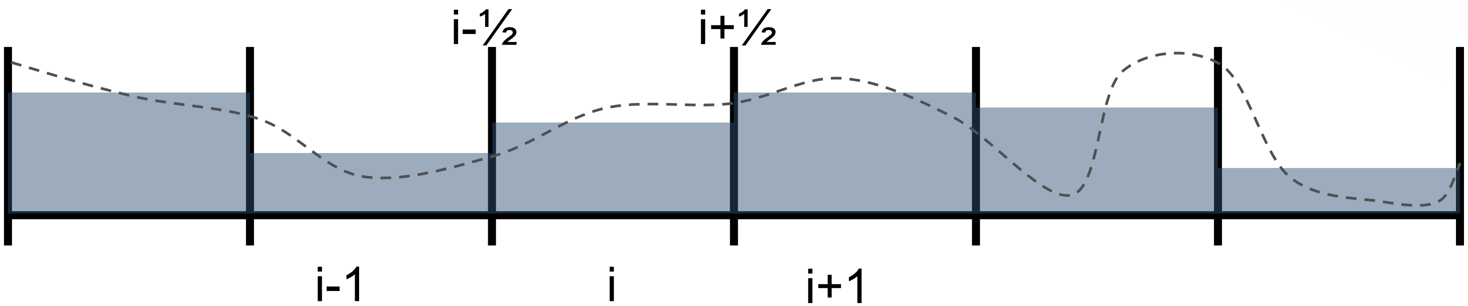
Truncation errors

Finite Volume Methods

- 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.



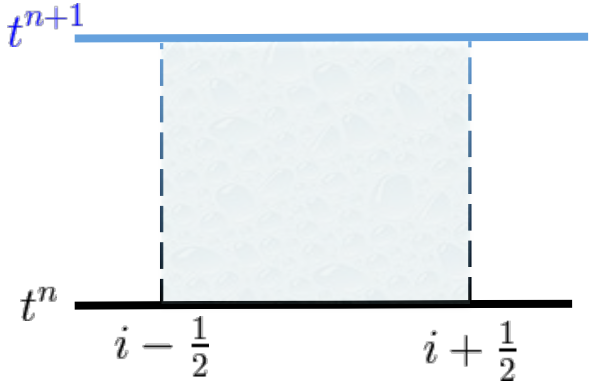
- The solution to the conservation law involves computing fluxes through the boundary of the control volumes

Finite Volume Formulation

- The *conservative form* of the equations provides the link between the *differential* form of the equation,

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0$$

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



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

Finite Volume Formulation

- Spatial integration yields

$$\int_{t^n}^{t^{n+1}} \left[\Delta x \frac{d}{dt} \langle U \rangle_i + \left(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}} \right) \right] dt = 0$$

with $\langle U \rangle_i = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} U(x,t)\, dx$ being a spatial average.

- Integration in time gives

$$\Delta x \left(\langle U \rangle_i^{n+1} - \langle U \rangle_i^n \right) + \Delta t \left(\tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \tilde{F}_{i-\frac{1}{2}}^{n+\frac{1}{2}} \right) = 0$$

where $\tilde{F}_{i\pm\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} F\left(U(x_{i\pm\frac{1}{2}}) \right) dt$ is a temporal average.

Finite Volume Formulation

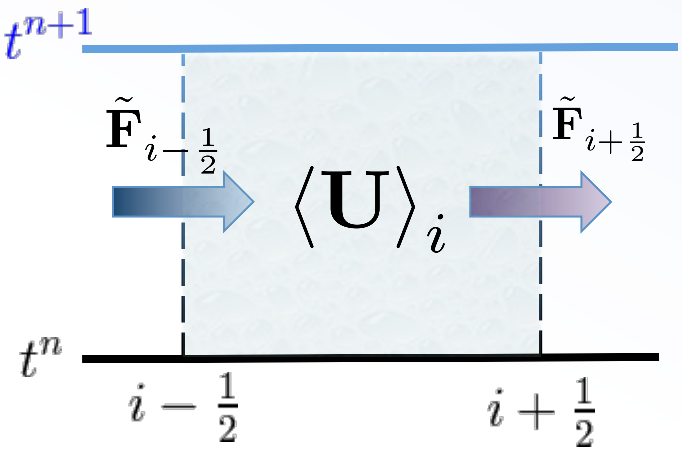
- Rearranging terms: $$\langle U\rangle_i^{n+1} = \langle U\rangle_i^n - \frac{\Delta t}{\Delta x}\left(\tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \tilde{F}_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right)$$

Integral or Conservation form

where

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

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



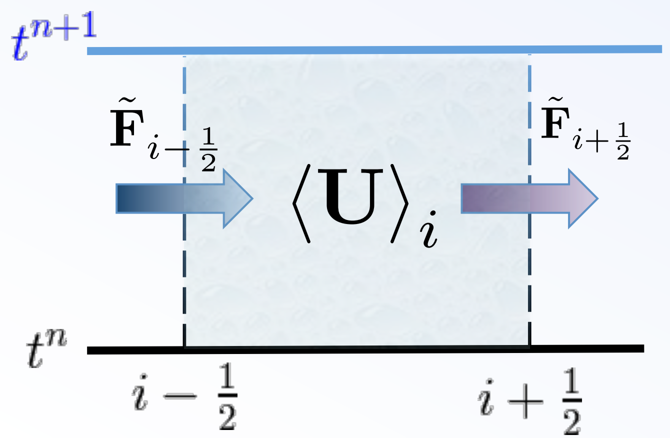
- The conservation form is an *exact* relation, no approximation introduced;
- It provides an *integral* representation of the original differential equation.
- The integral form does not make use of partial derivatives!

Importance of Conservation Form

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

- The conservation form ensure correct description of discontinuous waves in terms of speed and jumps;
- It guarantees global conservation properties (no mass / energy / momentum is created or destroyed unless a net flux exists);
- To second-order accuracy, a *finite difference* method and a *finite volume* method look essentially the same;
- Approximation introduced in the computation of the flux.

Flux computation: the Riemann Problem



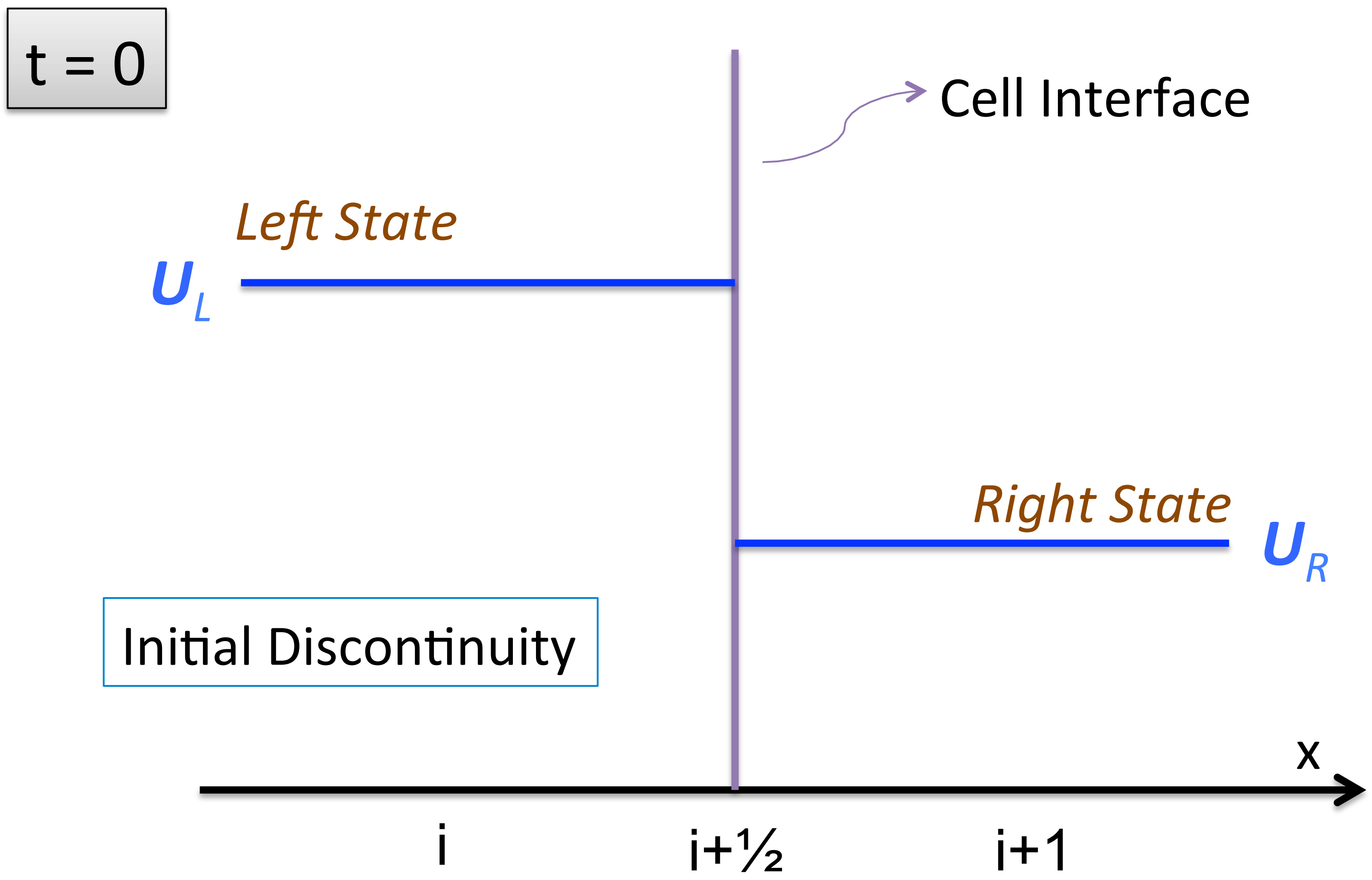
- Since the solution is known only at t^n, some kind of approximation is required in order to evaluate the flux through the boundary:

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

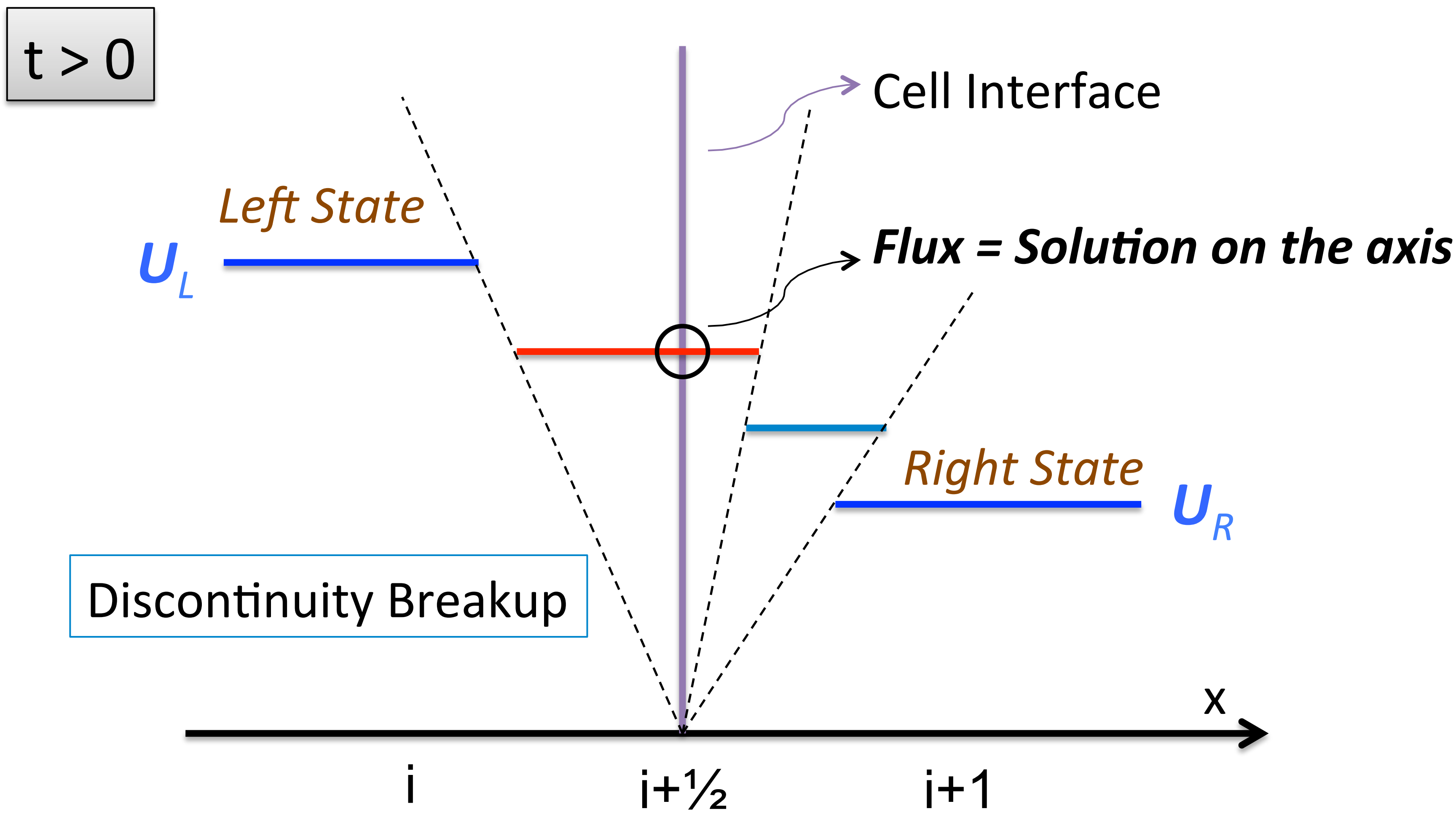
- This achieved by solving the so-called "*Riemann Problem*", i.e., the evolution of an inital discontinuity separating two *constant* states. The Riemann problem is defined by the initial condition:

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

The Riemann Problem



The Riemann Problem



III. THE LINEAR ADVECTION EQUATION:

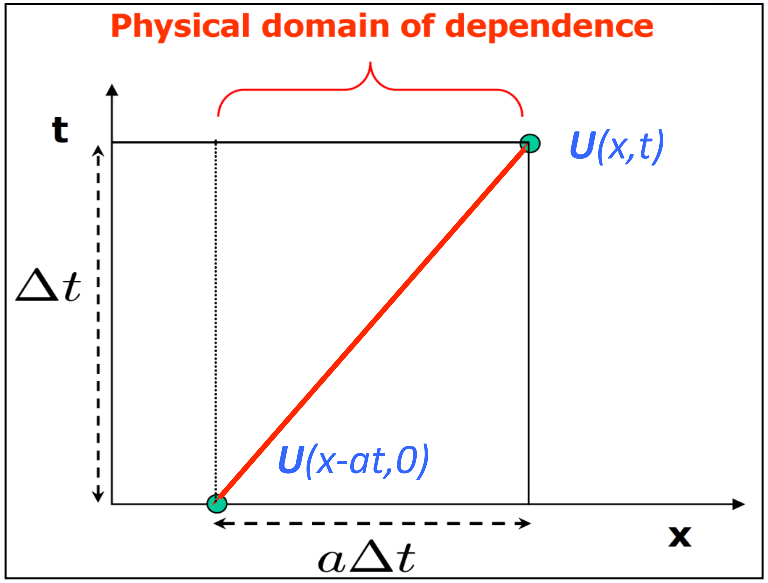
CONCEPTS AND DISCRETIZATIONS

The Advection Equation: Theory

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

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

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



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

- Along each characteristics:

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

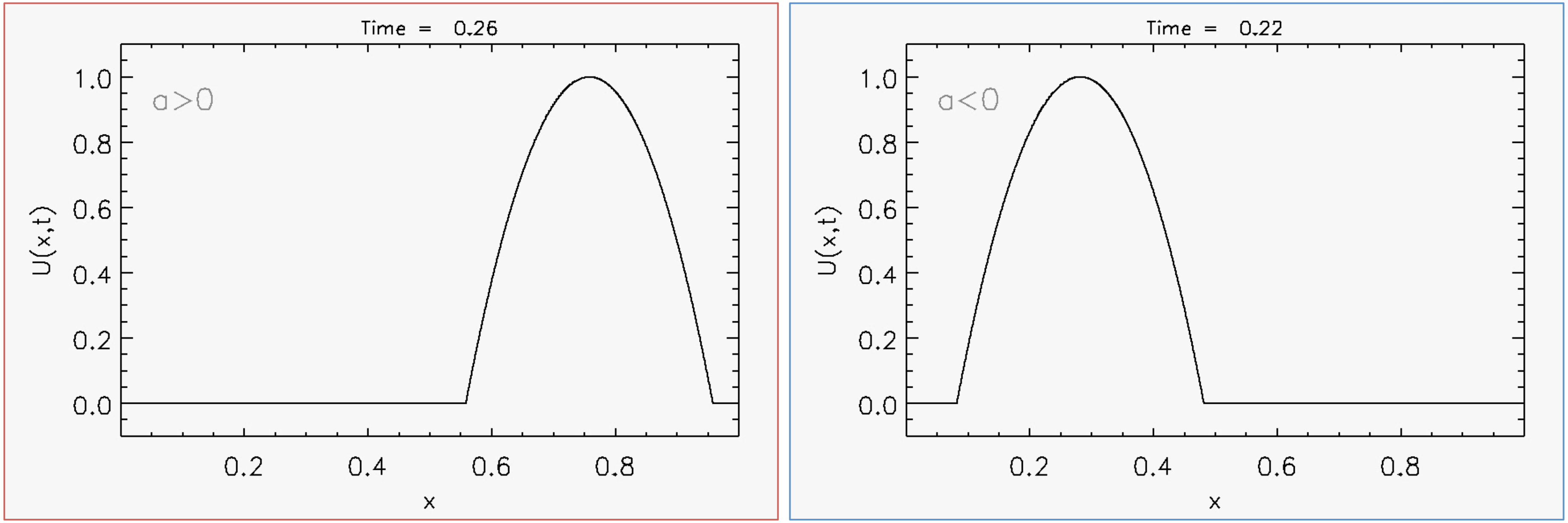
→ The solution is constant along characteristic curves.

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*):

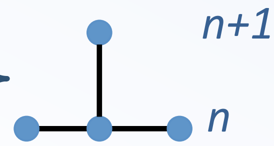


Discretization: the FTCS Scheme

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

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

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



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

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

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.

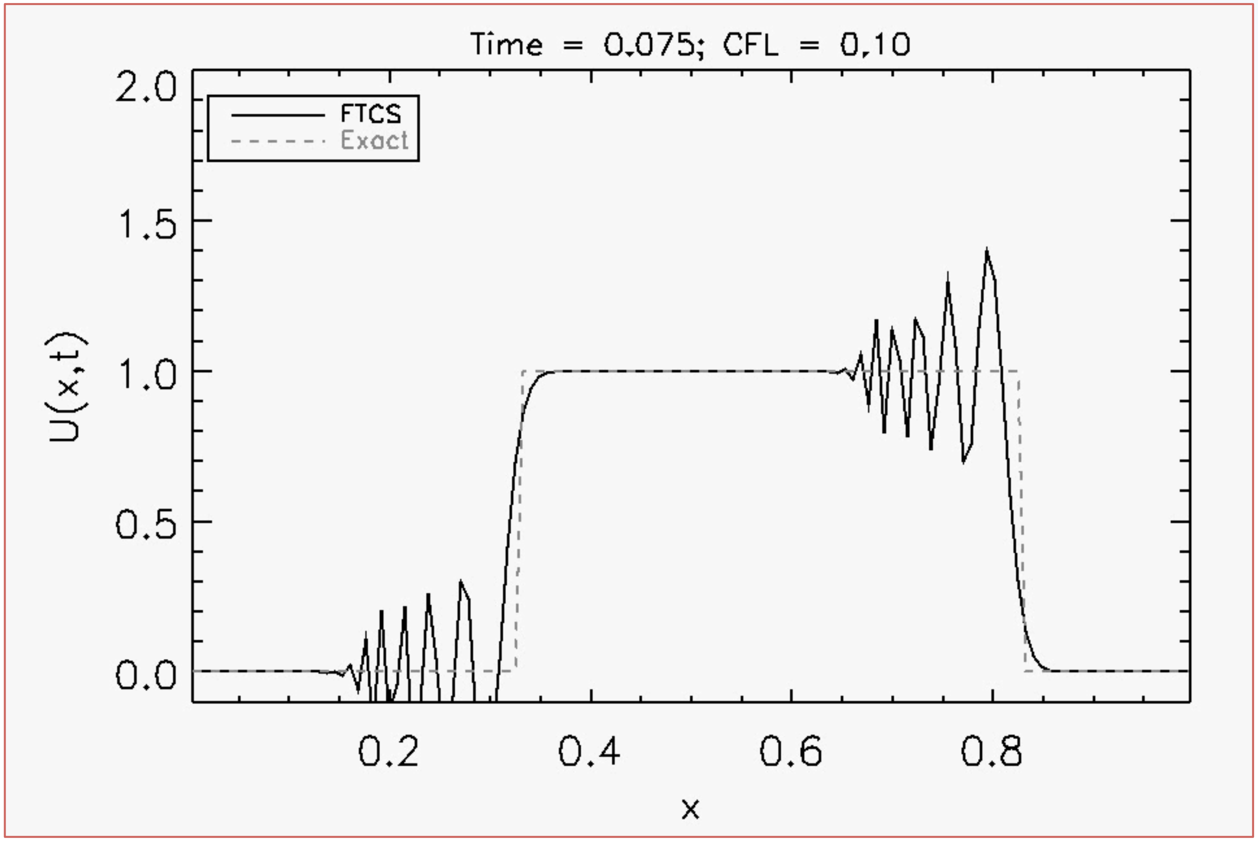
- It is an explicit method.

The FTCS Scheme

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

$$\frac{\partial U}{\partial t} \approx \frac{U_i^{n+1} - U_i^n}{\Delta t} + O(\Delta t)$$

$$\frac{\partial U}{\partial x} \approx \frac{U_{i+1}^n - U_{i-1}^n}{2\Delta x} + O(\Delta x^2)$$



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

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

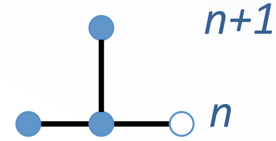
- Indipendently of the CFL number, all Fourier modes increase in magnitude as time advances.
- This method is unconditionally unstable!

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 $\left|\frac{A^{n+1}}{A^n}\right| \leq 1 \quad \Longrightarrow \quad 2C(1-C) \geq 0$

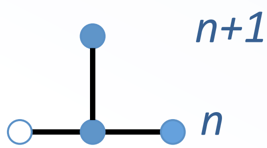
- for $a < 0$ the method is *unstable*, but
- for $a > 0$ the method is stable when $0 \leq C = a\,\Delta t/\Delta x \leq 1$.

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:

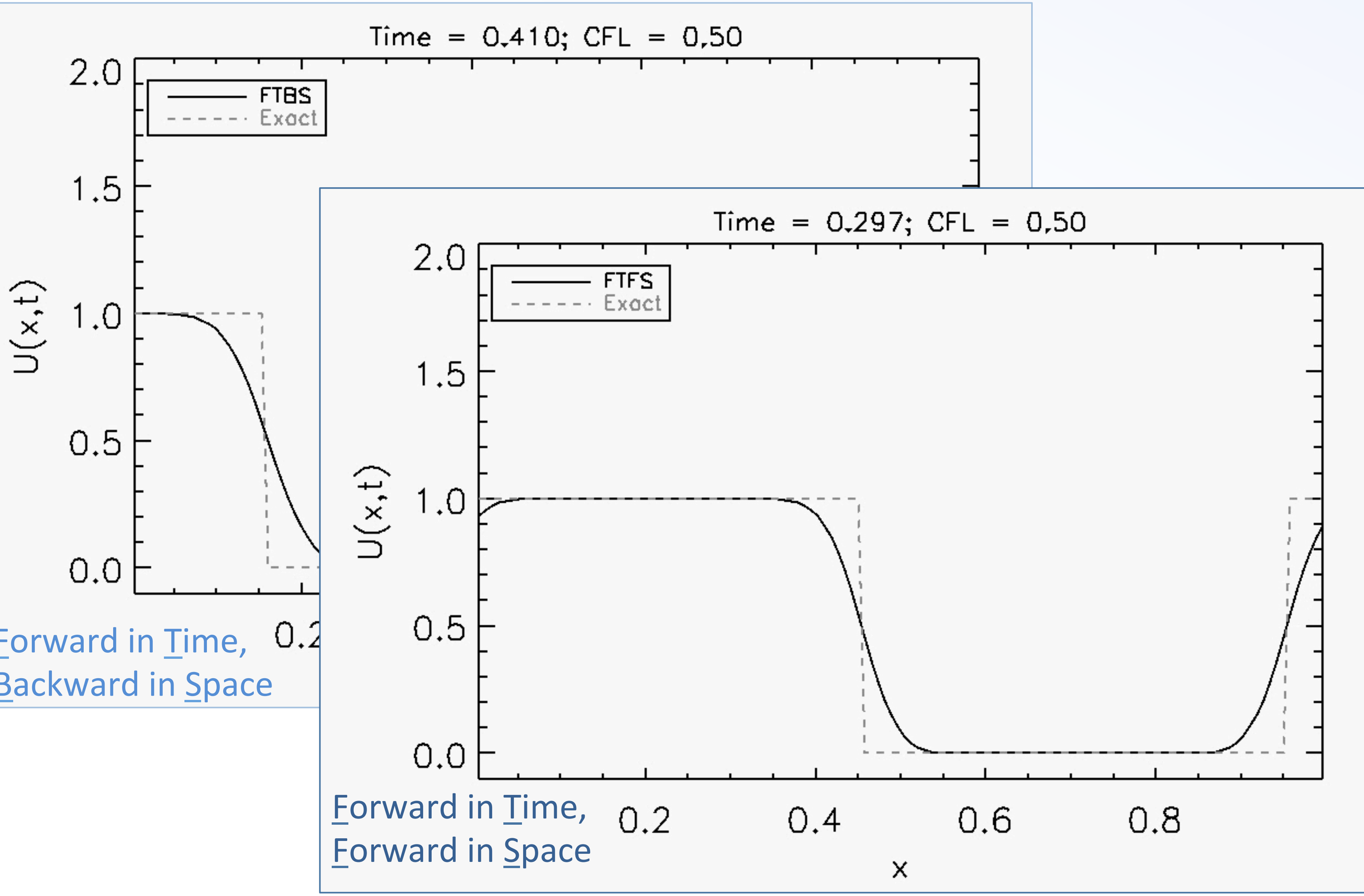


- Apply stability analysis yields $\left|\frac{A^{n+1}}{A^n}\right|^2 = 1 + 2C(1-C)(1-\cos\theta)$

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

- However, if *a < 0* and *-1 ≤ C = a Δt/Δx ≤ 0* then this method is stable;

Stable Discretizations: FTBS, FTFS



Forward in Time,
Backward in Space

Forward in Time,
Forward in Space

Stability: the CFL Condition

- Since the advection speed *a* is a parameter of the equation, Δx is fixed from the grid, the previous inequalities on $C=a\Delta t/\Delta x$ are stability constraints on the time step for explicit methods

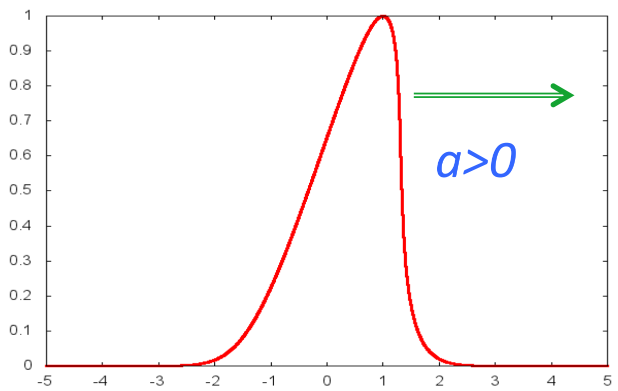
$$\Delta t \leq \frac{\Delta x}{|a|}$$

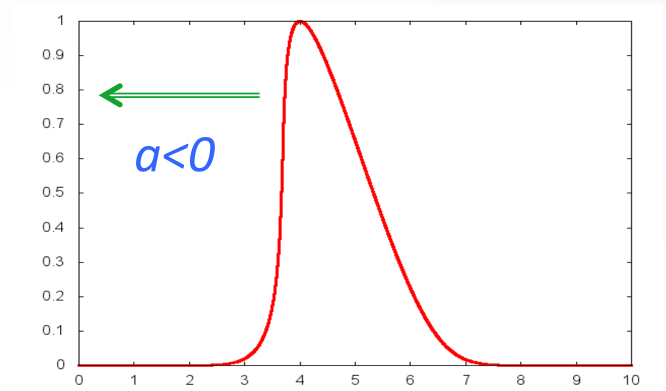
- Δt cannot be arbitrarily large but, rather, less than the time taken to travel one grid cell (→ *CFL condition*).

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

The 1st Order Godunov Method

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





- ➔ '*Upwind*':

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

- 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

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

a > 0:

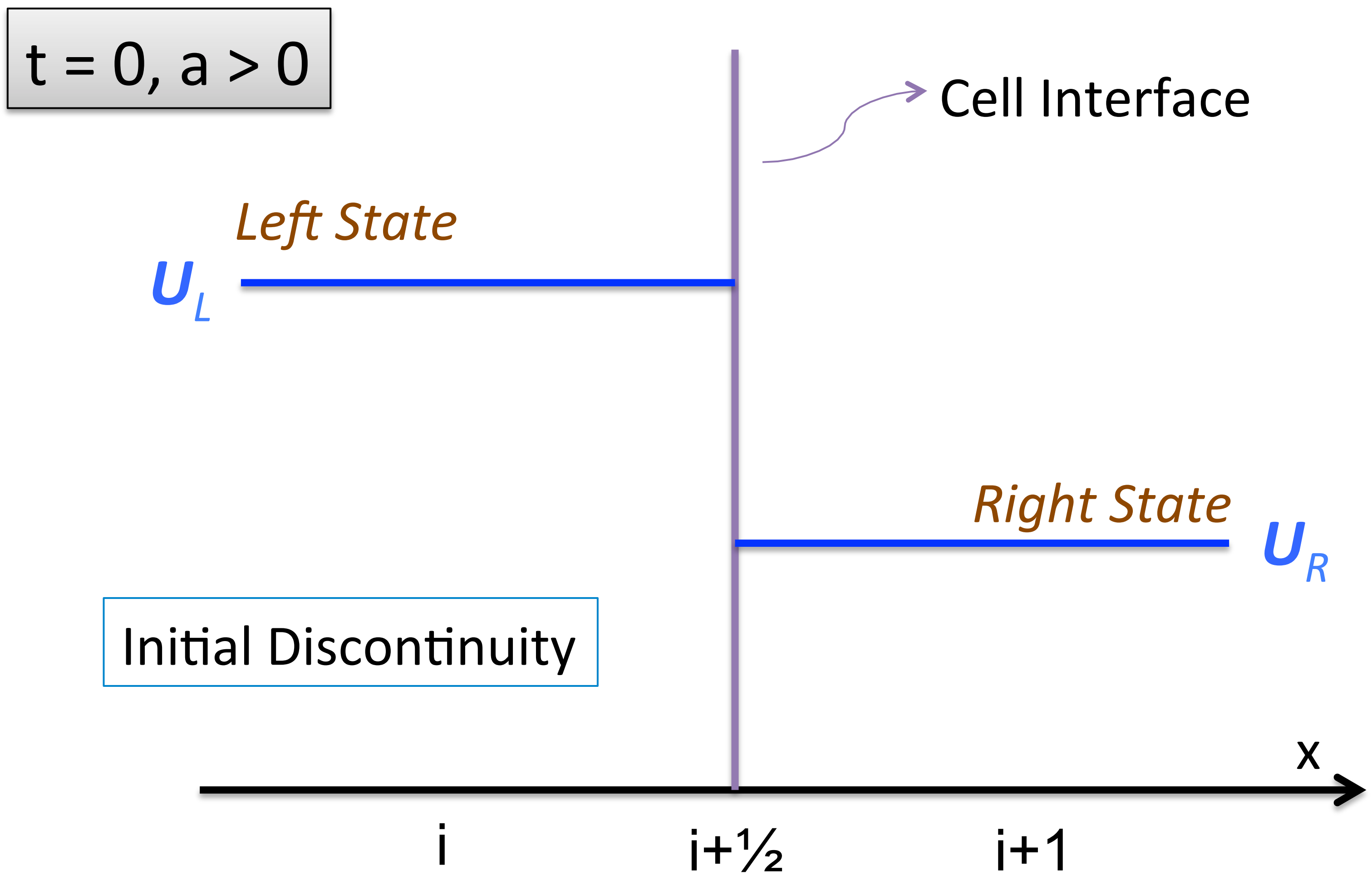
$$U_i^{n+1} = U_i^n - \frac{a\Delta t}{\Delta x}\left(U_i^n - U_{i-1}^n\right)$$

a < 0:

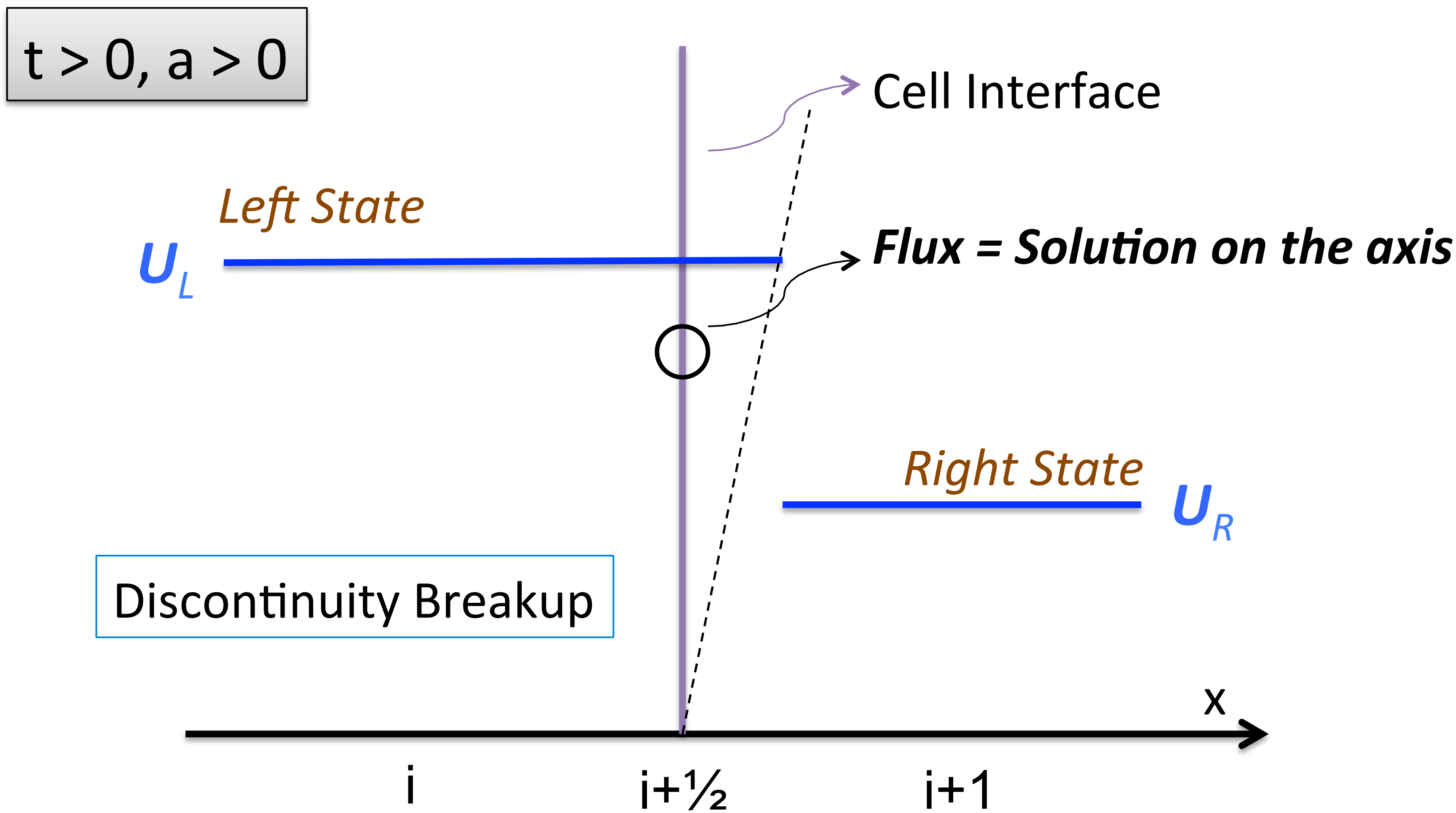
$$U_i^{n+1} = U_i^n - \frac{a\Delta t}{\Delta x}\left(U_{i+1}^n - U_i^n\right)$$

- 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 Riemann Problem



The Riemann Problem

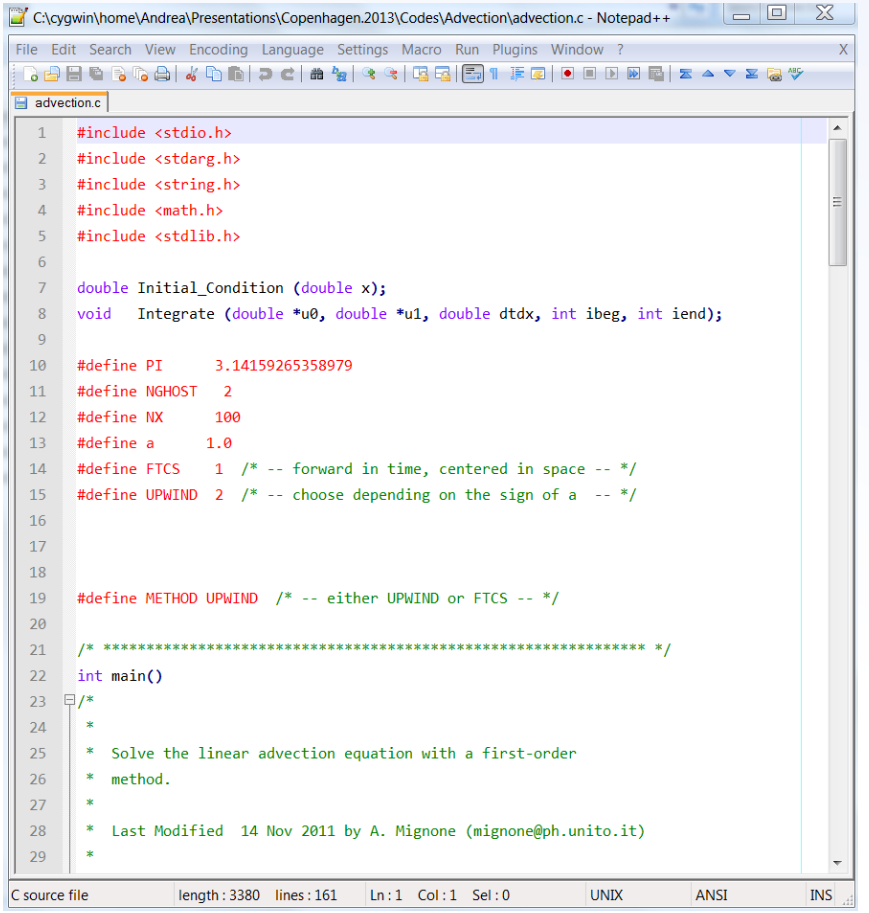


Code Example

- ***File name***: advection.c
- ***Purpose***: solve the linear advection equation using the 1st-order Godunov method.
- ***Usage***:

```
> gcc –O advection.c –o advection
> ./advection
```

- ***Output***: two-column ascii data file.



IV. LINEAR SYSTEMS OF HYPERBOLIC CONSERVATION LAWS

System of Equations: Theory

- We turn our attention to the system of equations (PDE)

$$\frac{\partial \mathbf{q}}{\partial t} + A \cdot \frac{\partial \mathbf{q}}{\partial x} = 0$$

where $\mathbf{q} = \{q_1, q_2, \ldots q_m\}$ is the vector of unknowns. *A* is a *m* × *m* constant matrix.

- For example, for m=3, one has

$$\frac{\partial q_1}{\partial t} + A_{11}\frac{\partial q_1}{\partial x} + A_{12}\frac{\partial q_2}{\partial x} + A_{13}\frac{\partial q_3}{\partial x} = 0$$
$$\frac{\partial q_2}{\partial t} + A_{21}\frac{\partial q_1}{\partial x} + A_{22}\frac{\partial q_2}{\partial x} + A_{23}\frac{\partial q_3}{\partial x} = 0$$
$$\frac{\partial q_3}{\partial t} + A_{31}\frac{\partial q_1}{\partial x} + A_{32}\frac{\partial q_2}{\partial x} + A_{33}\frac{\partial q_3}{\partial x} = 0$$

System of Equations: Theory

- The system is hyperbolic if A has real eigenvalues, $\lambda^1 \leq \ldots \leq \lambda^m$ and a complete set of linearly independent right and left eigenvectors r^k and l^k ($r^j \cdot l^k = \delta_{jk}$) such that

$$\begin{cases} A \cdot \boldsymbol{r}^k = \lambda^k \boldsymbol{r}^k \\ \boldsymbol{l}^k \cdot A = \boldsymbol{l}^k \lambda^k \end{cases} \qquad \text{for} \quad k = 1, \ldots, m$$

- For convenience we define the matrices $\Lambda = diag(\lambda^k)$, and

$$R = \left(\mathbf{r^1} | \mathbf{r^2} | \ldots | \mathbf{r^m} \right), \quad L = R^{-1} = \begin{pmatrix} \mathbf{l}^1 \\ \hline \mathbf{l}^2 \\ \hline \vdots \\ \hline \mathbf{l}^m \end{pmatrix}$$

- So that $A \cdot R = R \cdot \Lambda$, $L \cdot A = \Lambda \cdot L$, $L \cdot R = R \cdot L = I$, $L \cdot A \cdot R = \Lambda$.

System of Equations: Theory

- The linear system can be reduced to a set of decoupled linear advection equations.
- Multiply the original system of PDE's by *L* on the left:

$$L \cdot \left(\frac{\partial \boldsymbol{q}}{\partial t} + A \cdot \frac{\partial \boldsymbol{q}}{\partial x} \right) = L \cdot \frac{\partial \boldsymbol{q}}{\partial t} + L \cdot A \cdot R \cdot L \cdot \frac{\partial \boldsymbol{q}}{\partial x} = 0$$

- Define the *characteristic variables* $w = L \cdot q$ so that

$$\boxed{\frac{\partial \boldsymbol{w}}{\partial t} + \Lambda \cdot \frac{\partial \boldsymbol{w}}{\partial x} = 0}$$

- Since Λ is diagonal, these equations are not coupled anymore.

System of Equations: Theory

- In this form, the system decouples into *m* independent advection equations for the characteristic variables:

$$\frac{\partial \boldsymbol{w}}{\partial t} + \Lambda \cdot \frac{\partial \boldsymbol{w}}{\partial x} = 0 \quad \Longrightarrow \quad \frac{\partial w^k}{\partial t} + \lambda^k \cdot \frac{\partial w^k}{\partial x} = 0$$

where $w^k = \mathbf{l}^k \cdot \mathbf{q}$ (k=1,2,…,m) is a characteristic variable.

- When m=3 one has, for instance:

$$\frac{\partial w^1}{\partial t} + \lambda^1 \frac{\partial w^1}{\partial x} = 0$$

$$\frac{\partial w^2}{\partial t} + \lambda^2 \frac{\partial w^2}{\partial x} = 0$$

$$\frac{\partial w^3}{\partial t} + \lambda^3 \frac{\partial w^3}{\partial x} = 0$$

System of Equations: Theory

- The *m* advection equations can be solved independently by applying the standard solution techniques developed for the scalar equation.

- In particular, one can write the *exact analytical solution* for the *k*-th characteristic field as

$$w^k(x,t) = w^k(x - \lambda^k t, 0)$$

i.e., the initial profile of w^k shifts with uniform velocity λ^k, and

$$w^k(x - \lambda^k t, 0) = \mathbf{l}^k \cdot \mathbf{q}(x - \lambda^k t, 0)$$

is the initial profile.

- The characteristics are thus constant along the curves $dx/dt = \lambda^k$

System of Equations: Exact Solution

- Once the solution in characteristic space is known, we can solve the original system via the inverse transformation

$$\mathbf{q}(x,t) = R \cdot \mathbf{w}(x,t) = \sum_{k=1}^{k=m} w^k(x,t)\mathbf{r}^k = \sum_{k=1}^{k=m} w^k(x-\lambda^k t, 0)\mathbf{r}^k$$

- The characteristic variables are thus the coefficients of the right eigenvector expansion of *q*.
- The solution to the linear system reduces to a linear combination of *m* linear waves traveling with velocities λ^k .
- Expressing everything in terms of the original variables *q*,

$$\mathbf{q}(x,t) = \sum_{k=1}^{k=m} \mathbf{l}^k \cdot \mathbf{q}(x-\lambda^k t, 0)\mathbf{r}^k$$

Riemann Problem for Discontinuous Data

- If $\boldsymbol{q}$ is initially discontinuous, one or more characteristic variables will also have a discontinuity. Indeed, at $t = 0$,

$$w^k(x,0) = \boldsymbol{l}^k \cdot \boldsymbol{q}(x,0) = \begin{cases} w_L^k = \boldsymbol{l}^k \cdot \boldsymbol{q}_L & \text{if} \quad x < x_{i+\frac{1}{2}} \\ w_R^k = \boldsymbol{l}^k \cdot \boldsymbol{q}_R & \text{if} \quad x > x_{i+\frac{1}{2}} \end{cases}$$

- In other words, the initial jump $\boldsymbol{q}_R - \boldsymbol{q}_L$ is decomposed in several waves each propagating at the constant speed λ^k and corresponding to the eigenvectors of the Jacobian A:

$$\boldsymbol{q}_R - \boldsymbol{q}_L = \alpha^1 \boldsymbol{r}^1 + \alpha^2 \boldsymbol{r}^2 + \cdots + \alpha^m \boldsymbol{r}^m$$

where $\alpha^k = \boldsymbol{l}^k \cdot (\boldsymbol{q}_R - \boldsymbol{q}_L)$ are the *wave strengths*

Riemann Problem for Discontinuous Data

- For the linear case, the *exact* solution for each wave at the cell interface is:

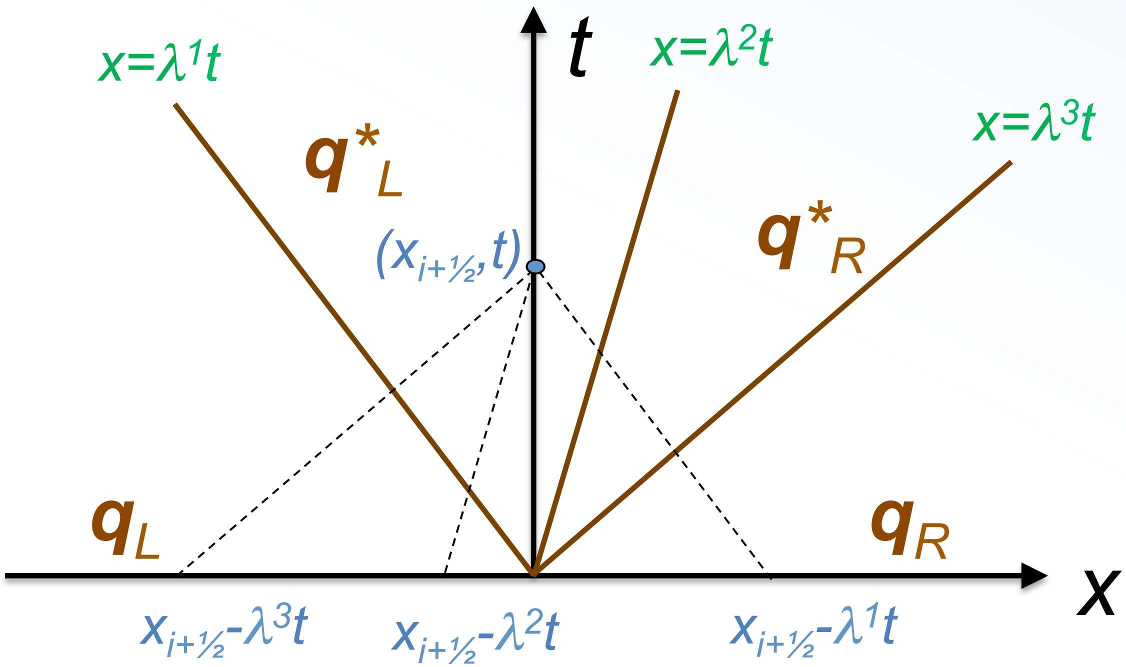
$$w^k\left(x_{i+\frac{1}{2}}, t\right) = w^k\left(x_{i+\frac{1}{2}} - \lambda^k t, 0\right) = \begin{cases} w_L^k & \text{if} \quad \lambda^k > 0 \\ w_R^k & \text{if} \quad \lambda^k < 0 \end{cases}$$

- The complete solution is found by adding all wave contributions:

$$\boldsymbol{q}\left(x_{i+\frac{1}{2}}, t\right) = \sum_{k:\lambda_k>0} w_L^k \boldsymbol{r}^k + \sum_{k:\lambda_k<0} w_R^k \boldsymbol{r}^k$$

- and the flux is finally computed as $\tilde{\boldsymbol{F}}_{i+\frac{1}{2}} = A \cdot \boldsymbol{q}\left(x_{i+\frac{1}{2}}, t\right)$

The Riemann Problem



Point ($x_{i+1/2}$,t) traces back to the right of the λ^1 characteristic emanating from the initial jump, but to the left of the other 2, so the solution is:

$$\boldsymbol{q}\left(x_{i+\frac{1}{2}}, t\right) = w_R^1 \boldsymbol{r}^1 + w_L^2 \boldsymbol{r}^2 + w_L^3 \boldsymbol{r}^3$$

Numerical Implementation

- We suppose the solution at time level *n* is known as q^n and we wish to compute the solution q^{n+1} at the next time level *n+1*.

- Our numerical scheme can be derived by working in the characteristic space and then transforming back:

$$\boldsymbol{q}_i^{n+1} = \sum_k w_i^{k,n+1} \boldsymbol{r}^k = \boldsymbol{q}_i^n - \frac{\Delta t}{\Delta x}\left(\boldsymbol{F}_{i+\frac{1}{2}}^n - \boldsymbol{F}_{i-\frac{1}{2}}^n\right)$$

where

$$\boxed{\boldsymbol{F}_{i+\frac{1}{2}}^n = A \cdot \frac{\boldsymbol{q}_{i+1}^n + \boldsymbol{q}_i^n}{2} - \frac{1}{2}\sum_k |\lambda^k| \boldsymbol{l}^k \cdot (\boldsymbol{q}_{i+1}^n - \boldsymbol{q}_i^n) \boldsymbol{r}^k}$$

is the *Godunov flux* for a linear system of advection equations.

V. NONLINEAR SCALAR 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

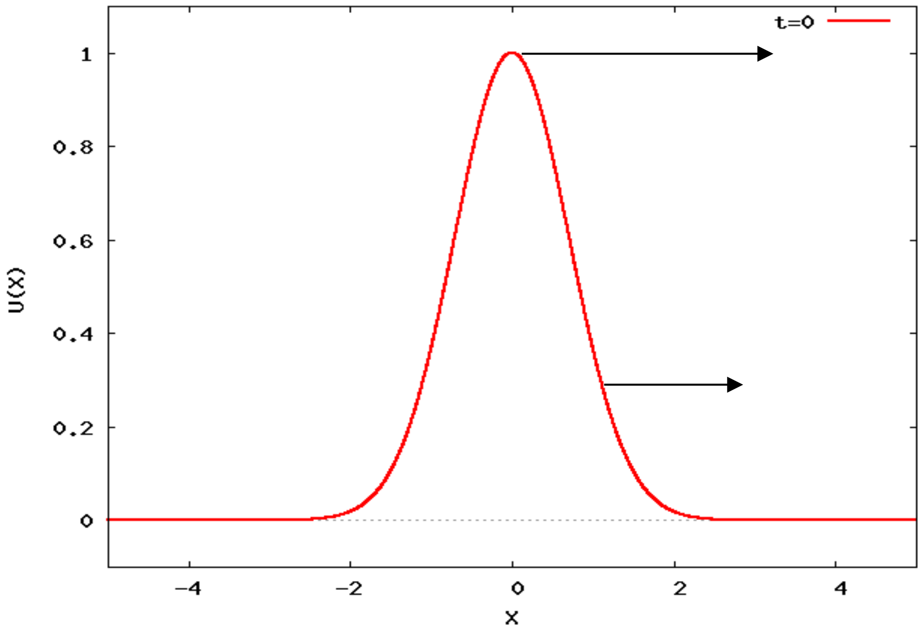
$$\frac{dx}{dt} = u(x,t) \quad \Longrightarrow \quad \frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{dx}{dt} = 0$$

- → *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

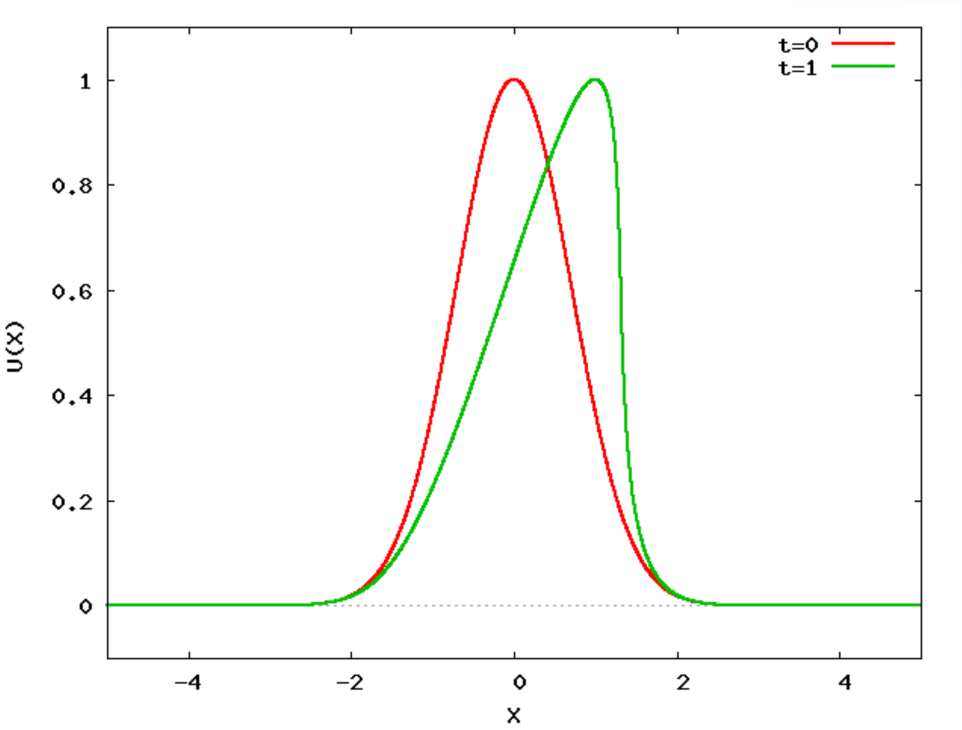
- From $$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

one can predict that, higher values of *u* will propagate faster than lower values: this leads to a *wave steepening*, since upstream values will advances faster than downstream values.



Nonlinear Advection Equation

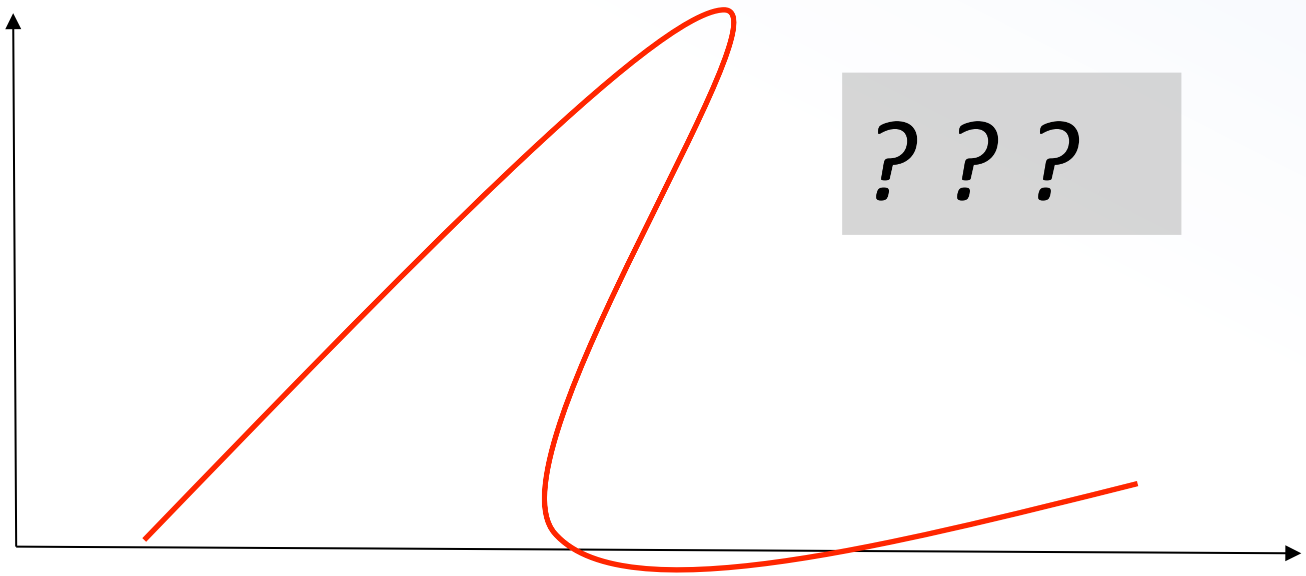
- Indeed, at t=1 the wave profile will look like:



- the wave steepens…

Nonlinear Advection Equation

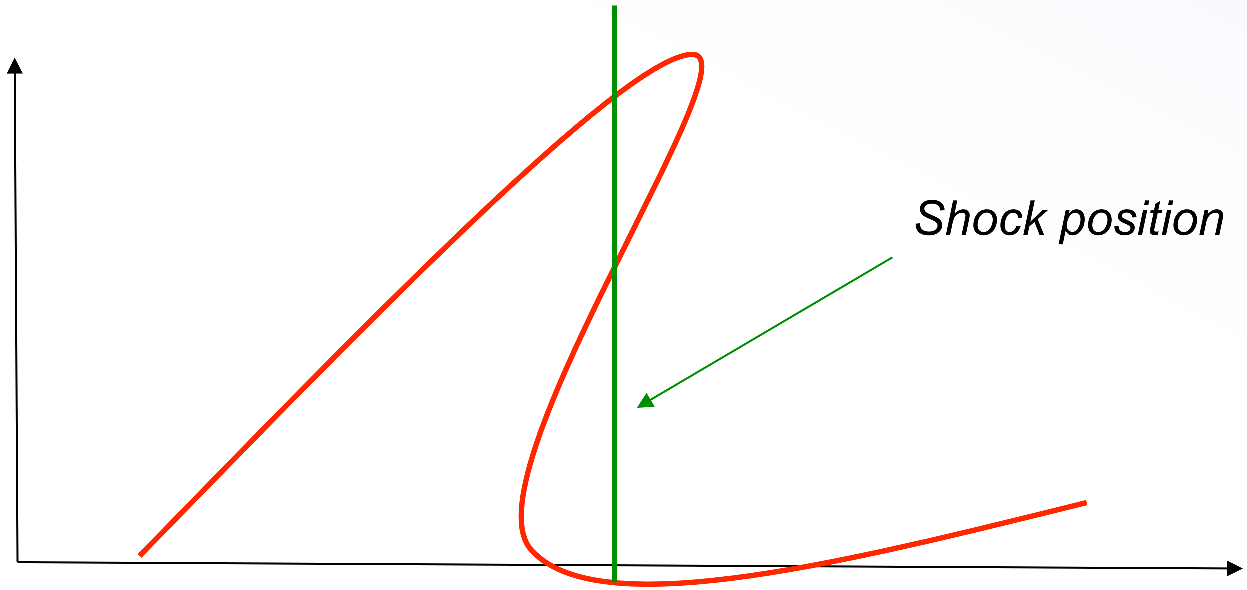
- If we wait more, we should get something like this:



- A multi-value functions ?! → Clearly ***NOT*** physical !

Burger Equation: Shock Waves

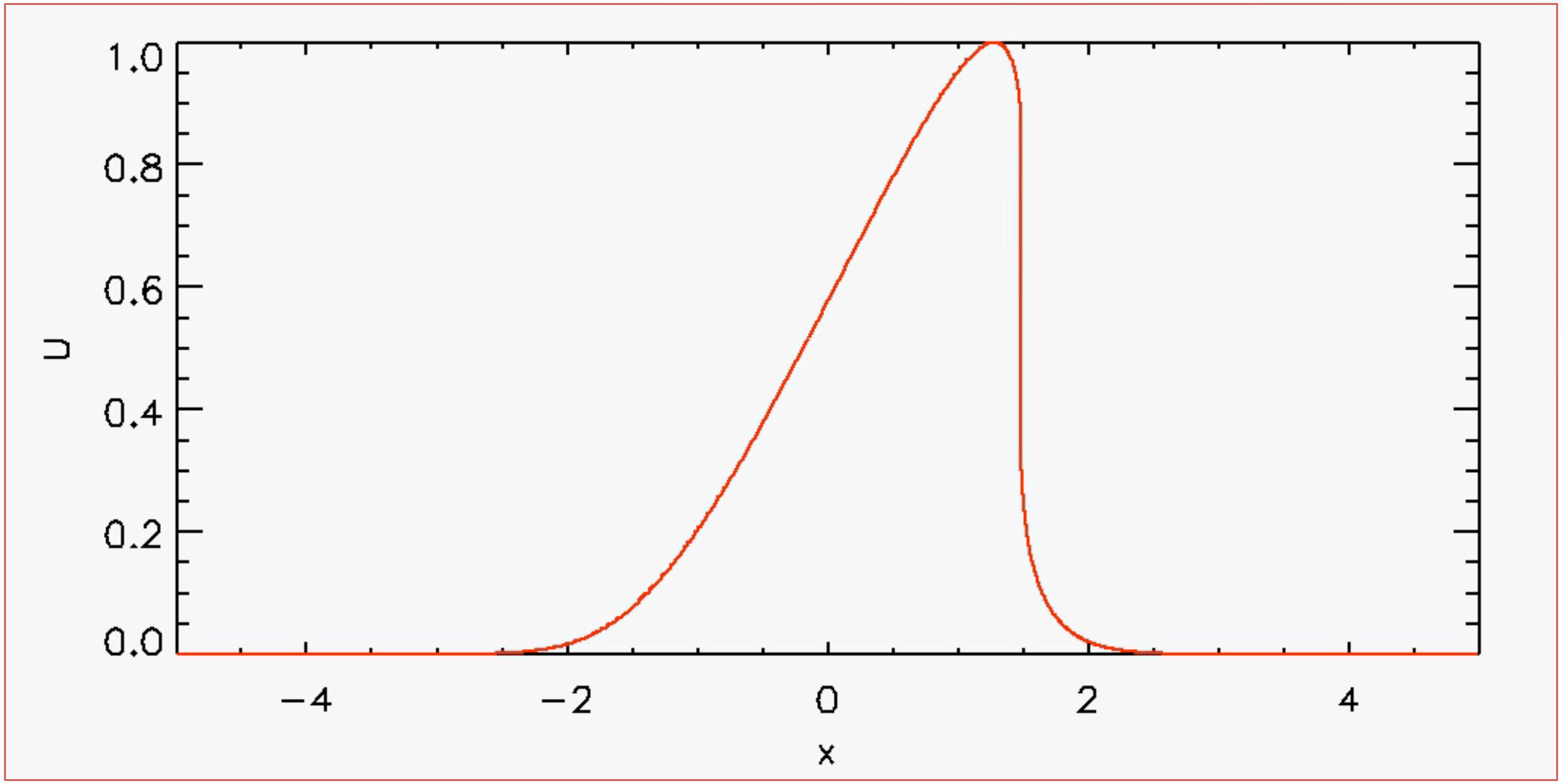
- The correct physical solution is to place a discontinuity there: a *shock wave*.



- Since the solution is no longer smooth, the differential form is not valid anymore and we need to consider the *integral form*.

Burger Equation: Shock Waves

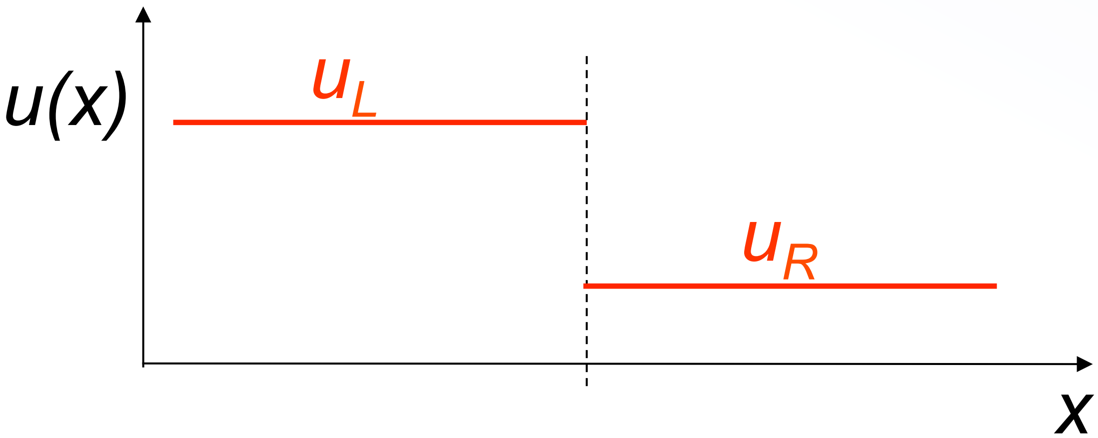
- This is how the solution should look like:



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

Burger Equation: Shock Waves

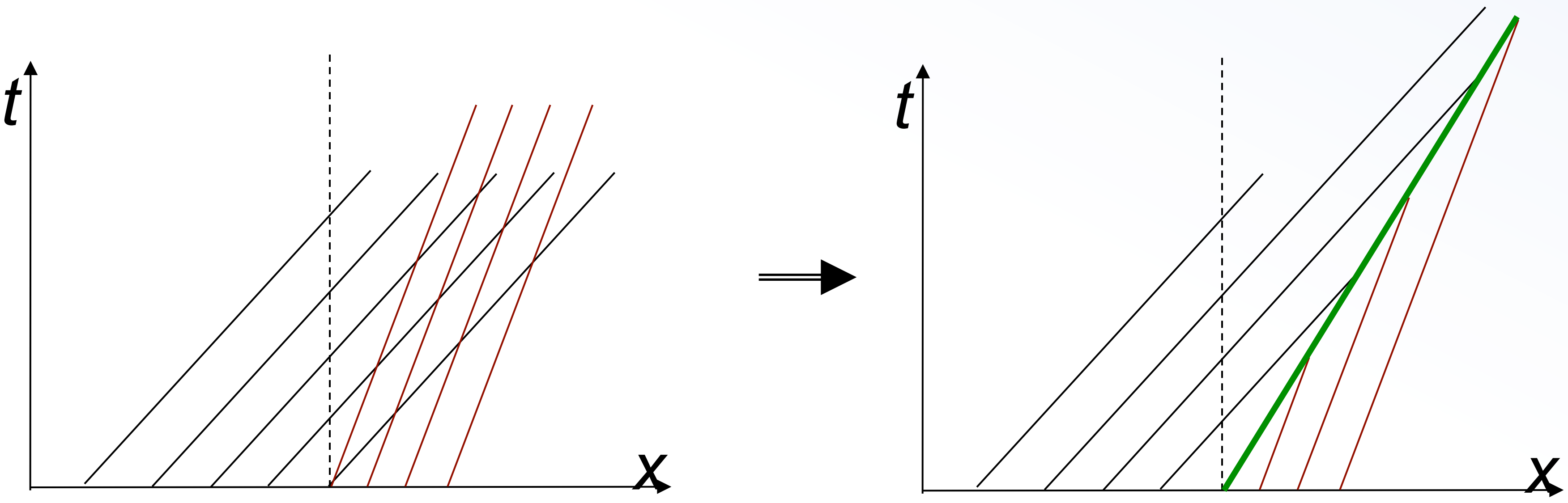
- Let's try to understand what happens by looking at the characteristics.
- Consider two states initially separated by a jump at an interface:



- Here, the characteristic velocities on the left are greater than those on the right.

Burger Equation: Shock Waves

- The characteristic will intersect, creating a *shock wave*:



- The shock speed is such that $\lambda(u_L) > S > \lambda(u_R)$. This is called the *entropy condition*.

Nonlinear Advection Equation

- The shock speed *S* can be found using the Rankine-Hugoniot jump conditions, obtained from the integral form of the equation:

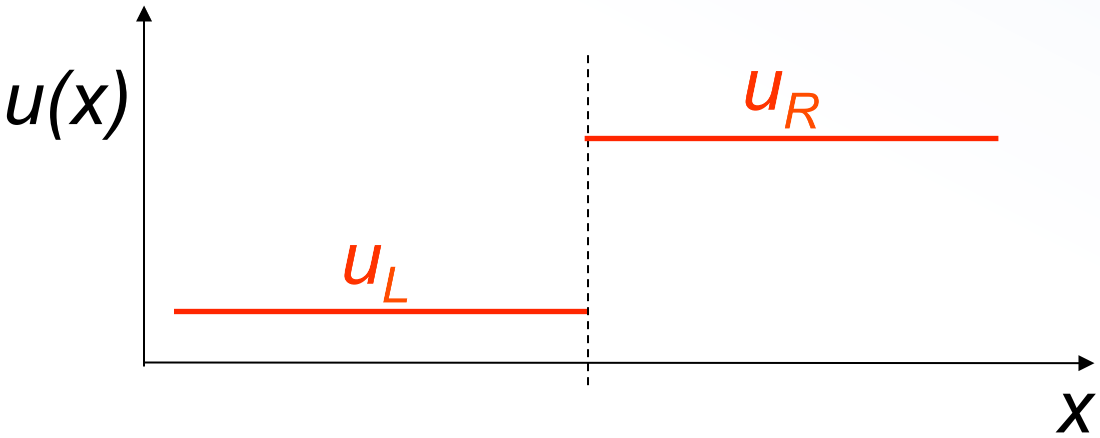
$$f(u_R) - f(u_L) = S(u_R - u_L)$$

- For Burger's equation $f(u) = u^2/2$, one finds the shock speed as

$$S = \frac{u_L + u_R}{2}$$

Burger Equation: Rarefaction Waves

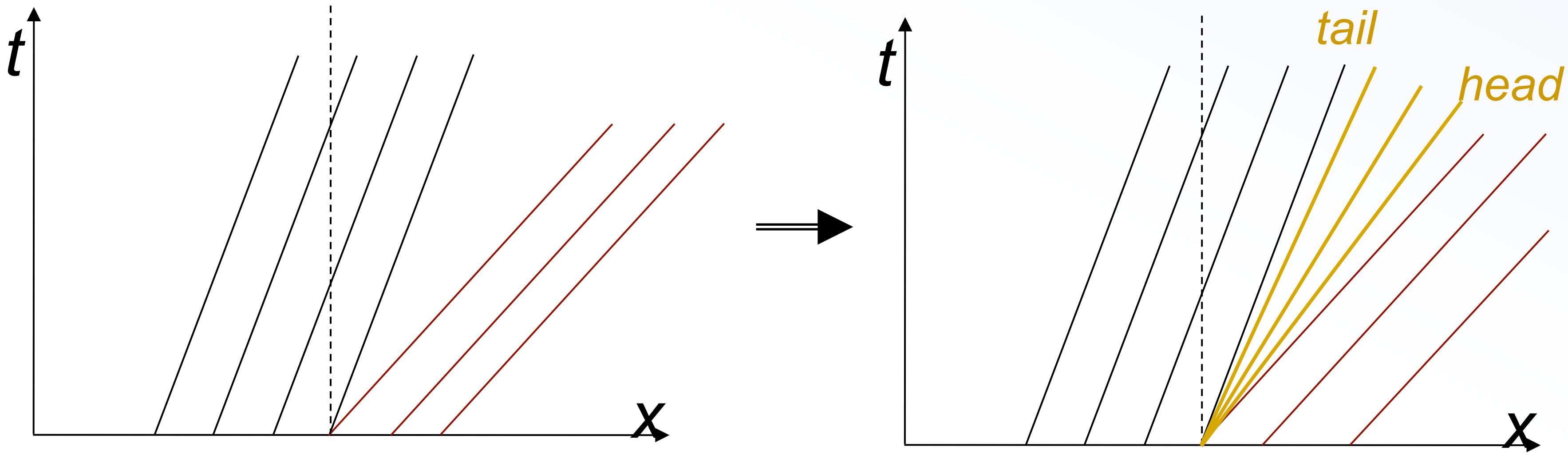
- Let's consider the opposite situation:



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

Burger Equation: Rarefaction Waves

- Now the characteristics will diverge:

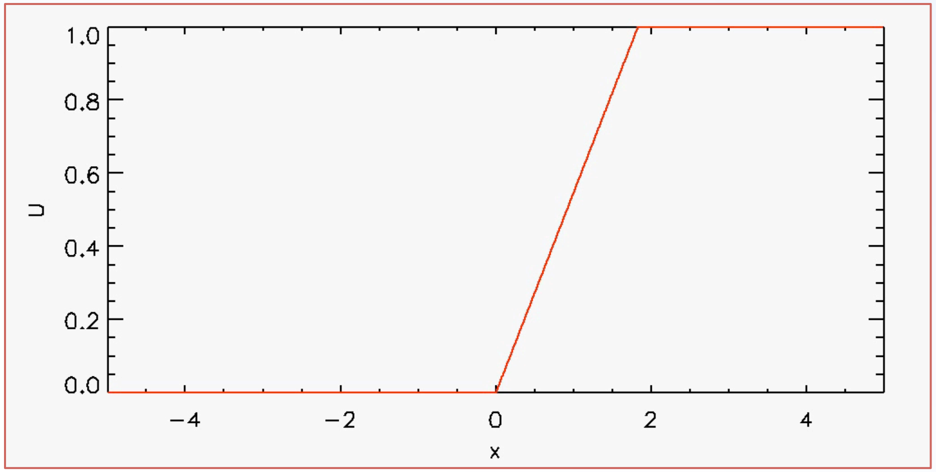


- Putting a shock wave between the two states would be incorrect, since it would violate the entropy condition. Instead, the proper solution is a *rarefaction wave*.

Burger Equation: Rarefaction Waves

- A rarefaction wave is a nonlinear wave that smoothly connects the left and the right state. It is an expansion wave.

- The solution can only be self-similar and takes on the range of values between u_L and u_R.



- The head of the rarefaction moves at the speed $\lambda(u_R)$, whereas the tail moves at the speed $\lambda(u_L)$.

- The general condition for a rarefaction wave is $\lambda(u_L)<\lambda(u_R)$

- Both rarefactions and shocks are present in the solutions to the Euler equation. Both waves are nonlinear.

Burger Equation: Riemann Solver

- These results can be used to write the general solution to the Riemann problem for Burger's equation:

  – If $u_L > u_R$ the solution is a discontinuity (*shock wave)*. In this case

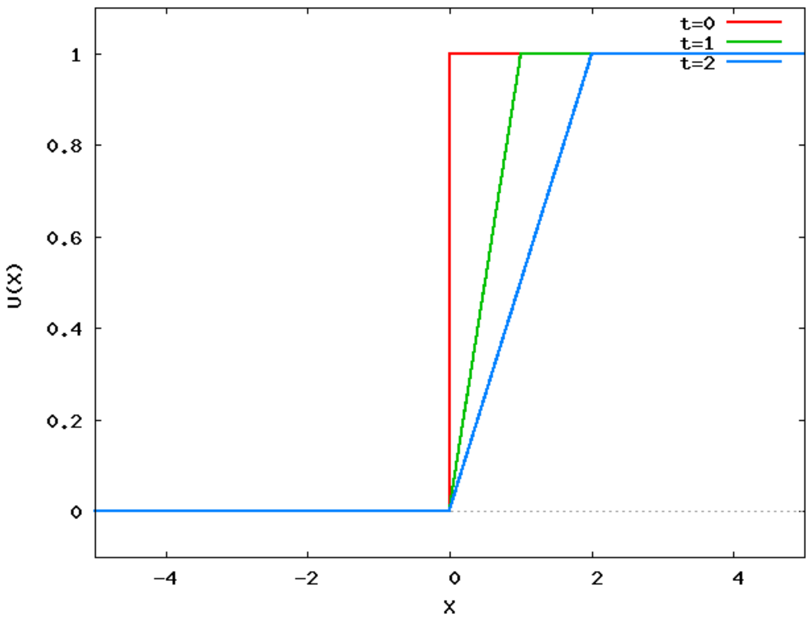
$$u(x,t) = \begin{cases} u_L & \text{if} \quad x - St < 0 \\ u_R & \text{if} \quad x - St > 0 \end{cases} , \qquad S = \frac{u_L + u_R}{2}$$

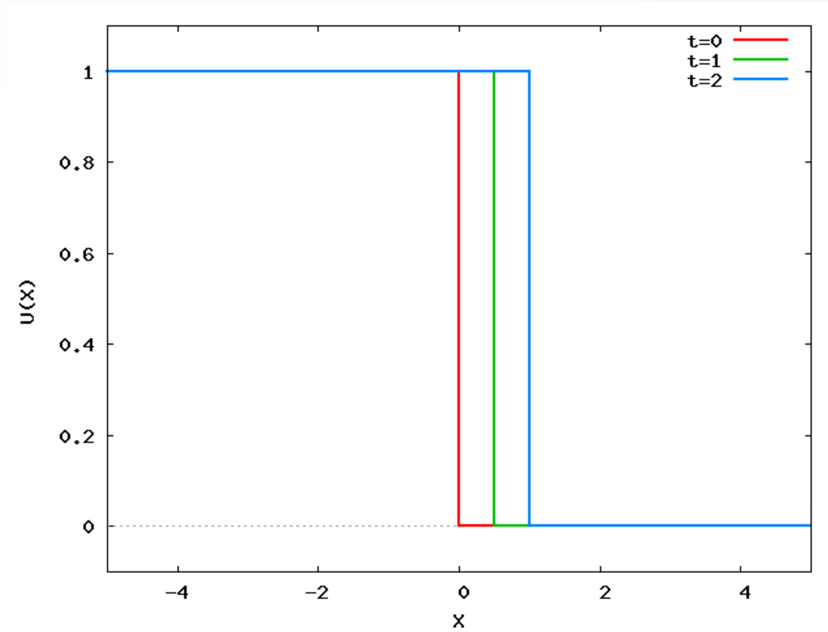
  – If $u_L < u_R$ the solution is a *rarefaction wave*. In this case

$$u(x,t) = \begin{cases} u_L & \text{if} \quad x/t \leq u_L \\ x/t & \text{if} \quad u_L < x/t < u_R \\ u_R & \text{if} \quad x/t > u_R \end{cases}$$

Nonlinear Advection Equation

- Solutions look like





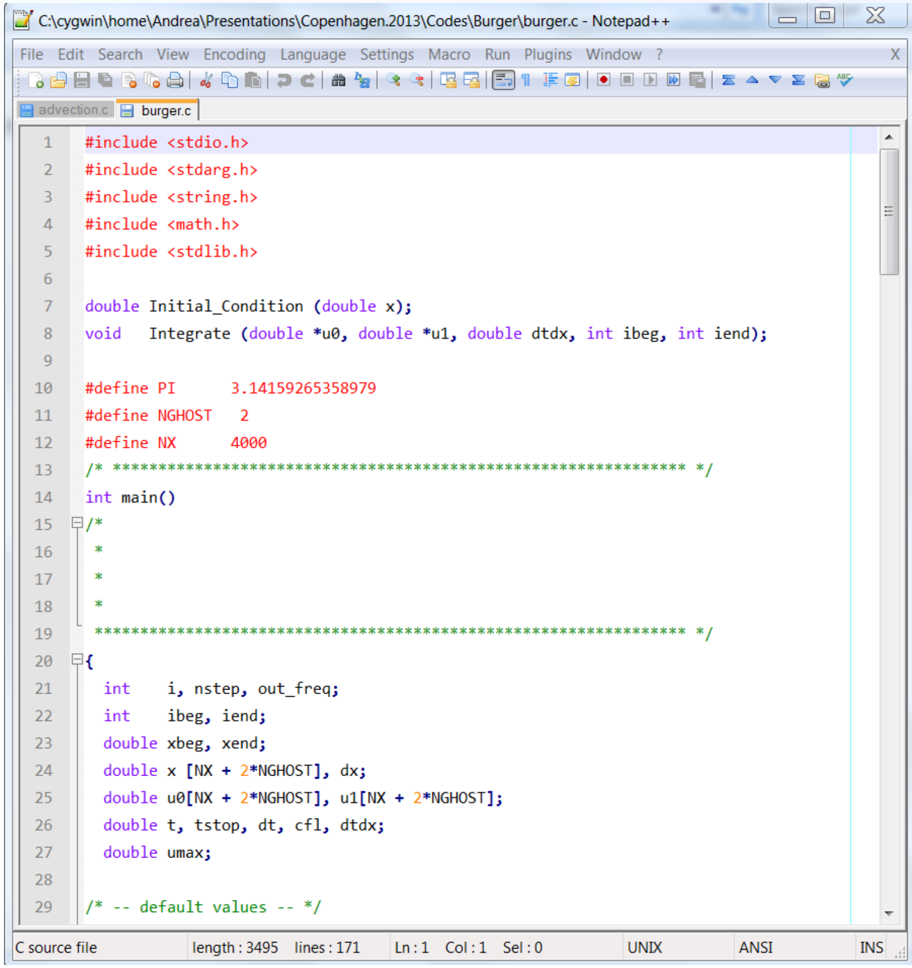
- for a rarefaction and a shock, respectively.

Code Example

- ***File name***: burger.c
- ***Purpose***: solve Burger's equation using 1st-order Godunov method.
- ***Usage***:

> gcc –O burger.c –o burger
> ./burger

- ***Output***: two-column ascii data files "data.nnnn.out"




```c
#include <stdio.h>
#include <stdarg.h>
#include <string.h>
#include <math.h>
#include <stdlib.h>

double Initial_Condition (double x);
void   Integrate (double *u0, double *u1, double dtdx, int ibeg, int iend);

#define PI      3.14159265358979
#define NGHOST   2
#define NX      4000
/* ************************************************************** */
int main()
/*
 *
 *
 *
 ************************************************************** */
{
  int    i, nstep, out_freq;
  int    ibeg, iend;
  double xbeg, xend;
  double x [NX + 2*NGHOST], dx;
  double u0[NX + 2*NGHOST], u1[NX + 2*NGHOST];
  double t, tstop, dt, cfl, dtdx;
  double umax;

/* -- default values -- */
```

VI. NONLINEAR SYSTEMS OF CONSERVATION LAW

Nonlinear Systems

- Much of what is known about the numerical solution of hyperbolic systems of nonlinear equations comes from the results obtained in the linear case or simple nonlinear scalar equations.

- The key idea is to exploit the conservative form and assume the system can be locally “frozen” at each grid interface.

- However, this still requires the solution of the Riemann problem, which becomes increasingly difficult for complicated set of hyperbolic P.D.E.

Euler Equations

- System of conservation laws describing conservation of mass, momentum and energy:

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

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot [\rho \mathbf{v}\mathbf{v} + \mathbf{I}p] = 0 \qquad \text{(momentum)}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + p)\,\mathbf{v}] = 0 \qquad \text{(energy)}$$

- Total energy density E is the sum of thermal + Kinetic terms:

$$E = \rho\epsilon + \rho\frac{\mathbf{v}^2}{2}$$

- Closure requires an Equation of State (EoS).

For an ideal gas one has $\rho\epsilon = \dfrac{p}{\Gamma - 1}$

Euler Equations: Characteristic Structure

- The equations of gasdynamics can also be written in "quasi-linear" or primitive form. In 1D:

$$\frac{\partial \mathbf{V}}{\partial t} + A \cdot \frac{\partial \mathbf{V}}{\partial x} = 0\,, \qquad A = \begin{pmatrix} v_x & \rho & 0 \\ 0 & v_x & 1/\rho \\ 0 & \rho c_s^2 & v_x \end{pmatrix}$$

where $V = [\rho, v_x, p]$ is a vector of primitive variable, $c_s = (\gamma p/\rho)^{1/2}$ is the adiabatic speed of sound.

- It is called "quasi-linear" since, differently from the linear case where we had $A = const$, here $A = A(V)$.

Euler Equations: Characteristic Structure

- The quasi-linear form can be used to find the eigenvector decomposition of the matrix *A*:

$$\mathbf{r}^1 = \begin{pmatrix} 1 \\ -c_s/\rho \\ c_s^2 \end{pmatrix}, \quad \mathbf{r}^2 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{r}^3 = \begin{pmatrix} 1 \\ c_s/\rho \\ c_s^2 \end{pmatrix}$$

- Associated to the eigenvalues:

$$\lambda^1 = v_x - c_s\,, \quad \lambda^2 = v_x\,, \quad \lambda^3 = v_x + c_s$$

- These are the characteristic speeds of the system, i.e., the speeds at which information propagates. They tell us a lot about the structure of the solution.

Euler Equations: Riemann Problem

- By looking at the expressions for the right eigenvectors,

$$\mathbf{r}^1 = \begin{pmatrix} 1 \\ -c_s/\rho \\ c_s^2 \end{pmatrix}, \quad \mathbf{r}^2 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{r}^3 = \begin{pmatrix} 1 \\ c_s/\rho \\ c_s^2 \end{pmatrix}$$

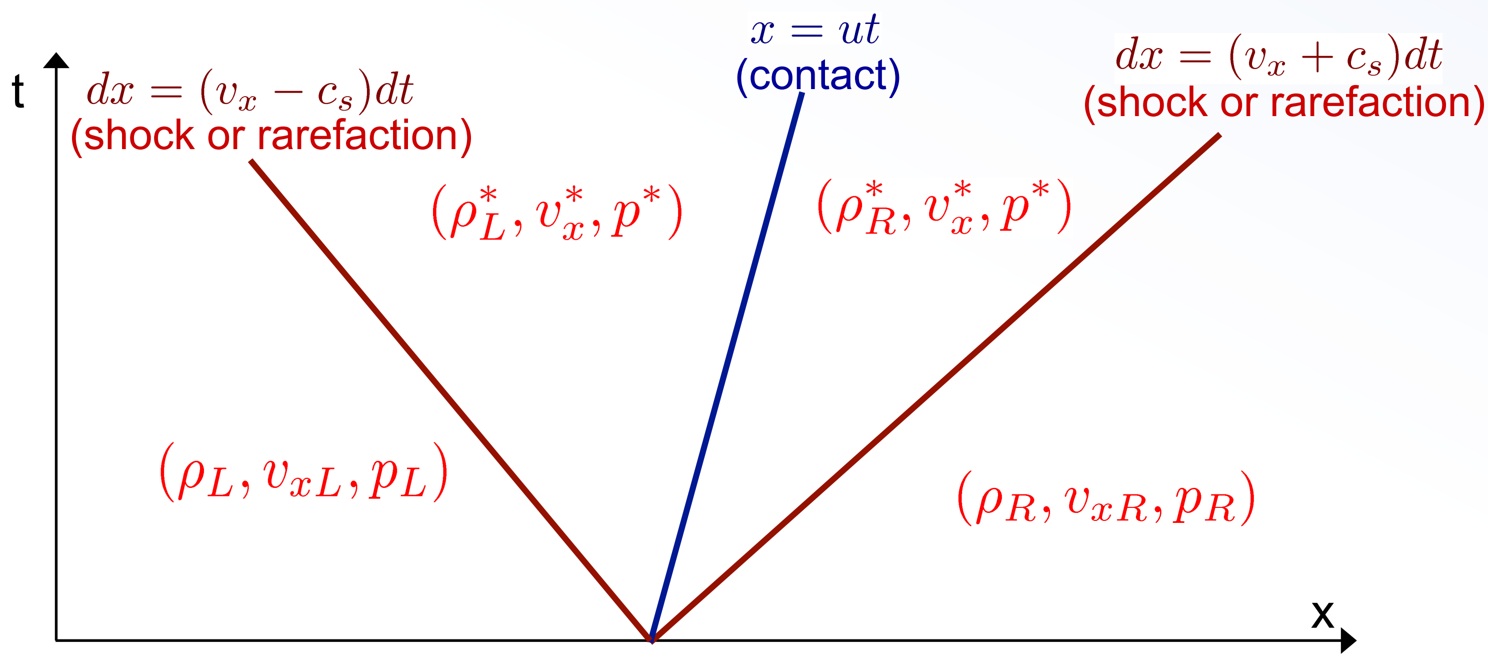
- we see that across waves 1 and 3, all variables jump. These are nonlinear waves, either shocks or rarefactions waves.

- Across wave 2, only density jumps. Velocity and pressure are constant. This defines the *contact discontinuity*.

- The characteristic curve associated with this linear wave is $dx/dt = u$, and it is a straight line. Since v_x is constant across this wave, the flow is neither converging or diverging.

Euler Equations: Riemann Problem

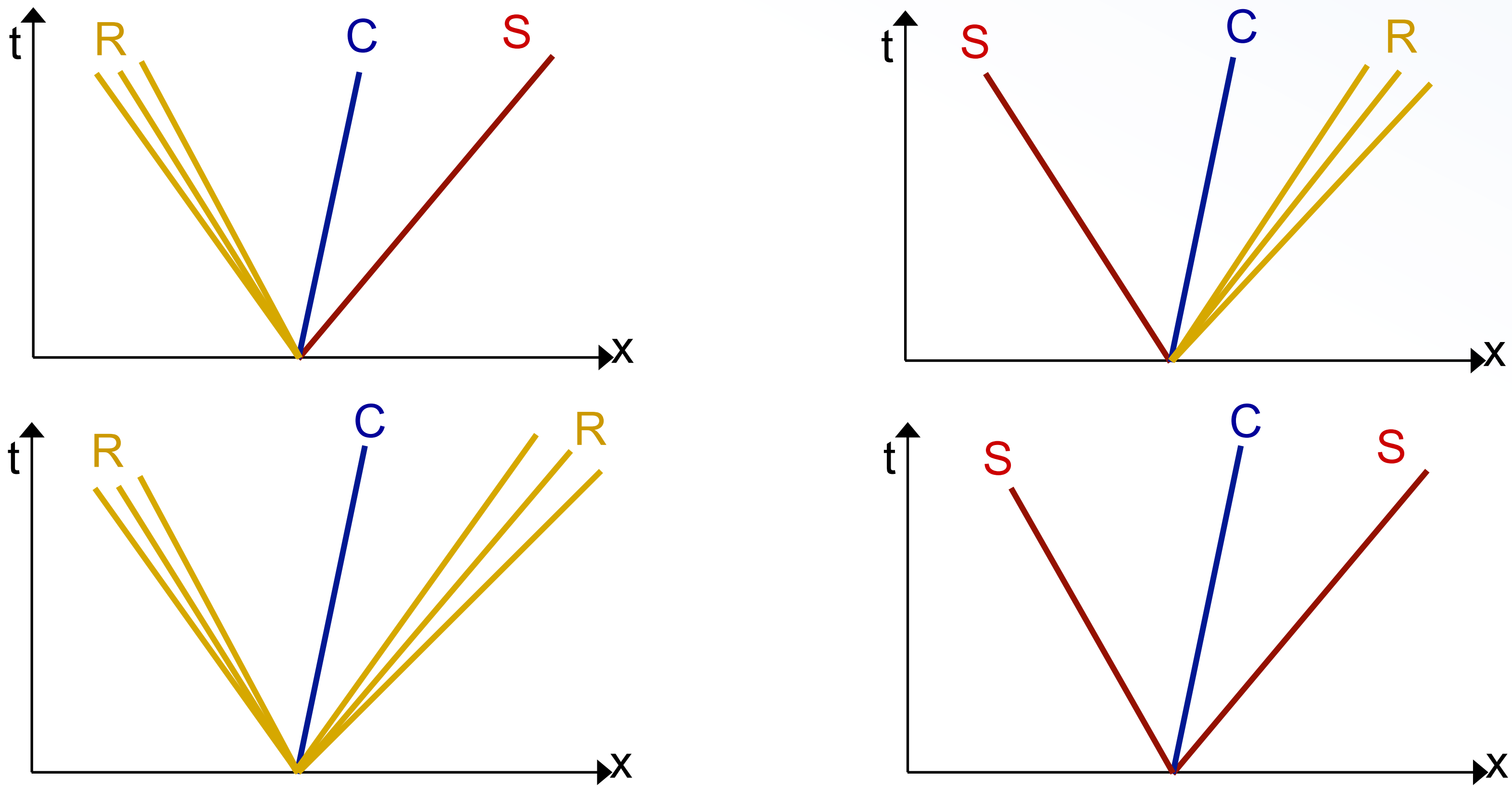
- The solution to the Riemann problem looks like



- The outer waves can be either shocks or rarefactions.
- The middle wave is always a contact discontinuity.
- In total one has 4 unknowns: $\rho_L^*, \rho_R^*, v_x^*, p^*$, since only density jumps across the contact discontinuity.

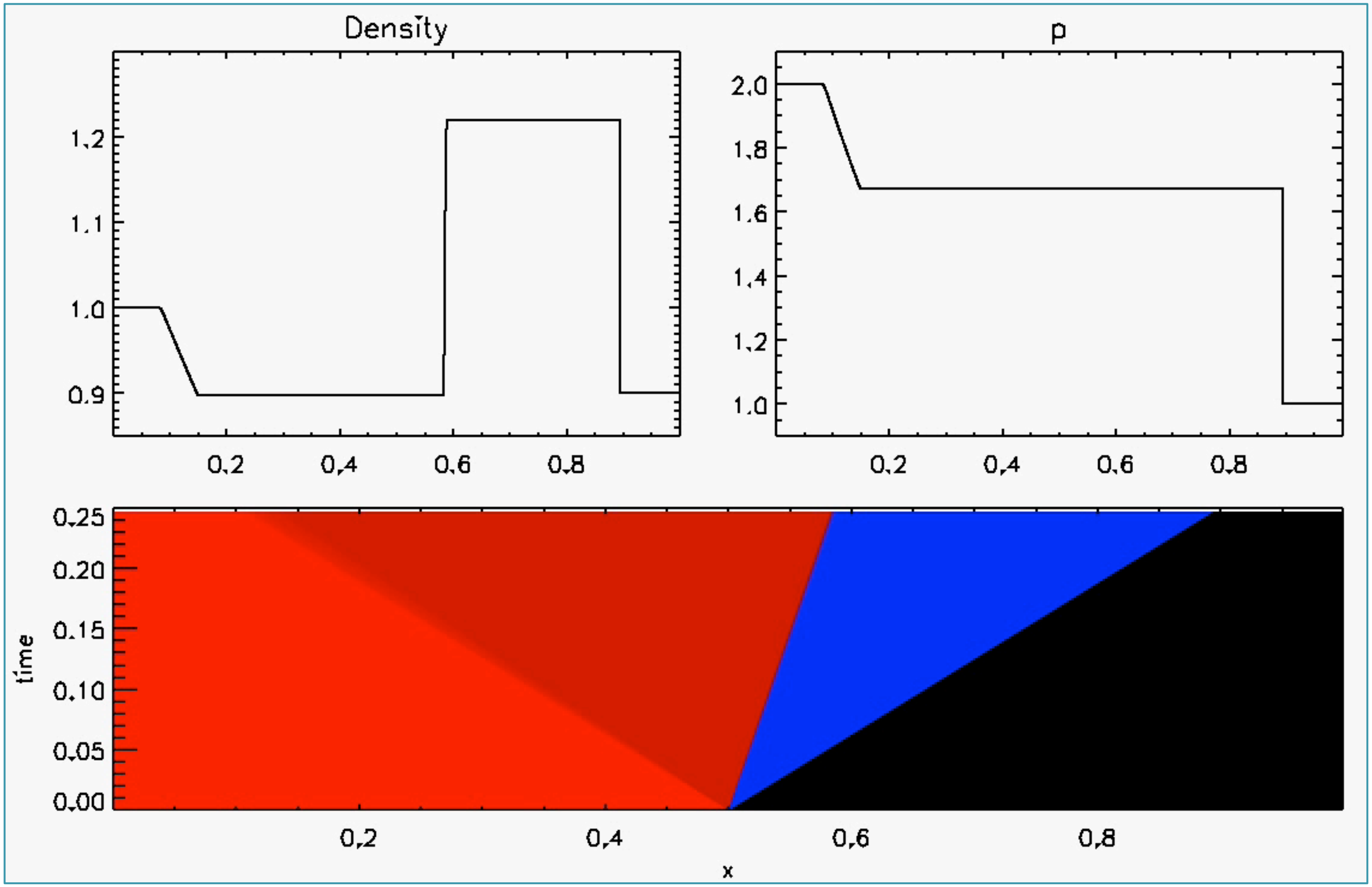
Euler Equations: Riemann Problem

- Depending on the initial discontinuity, a total of 4 patterns can emerge from the solution:



Euler Equations: Shock Tube Problem

- The decay of the discontinuity defines what is usually called the “shock tube problem”,

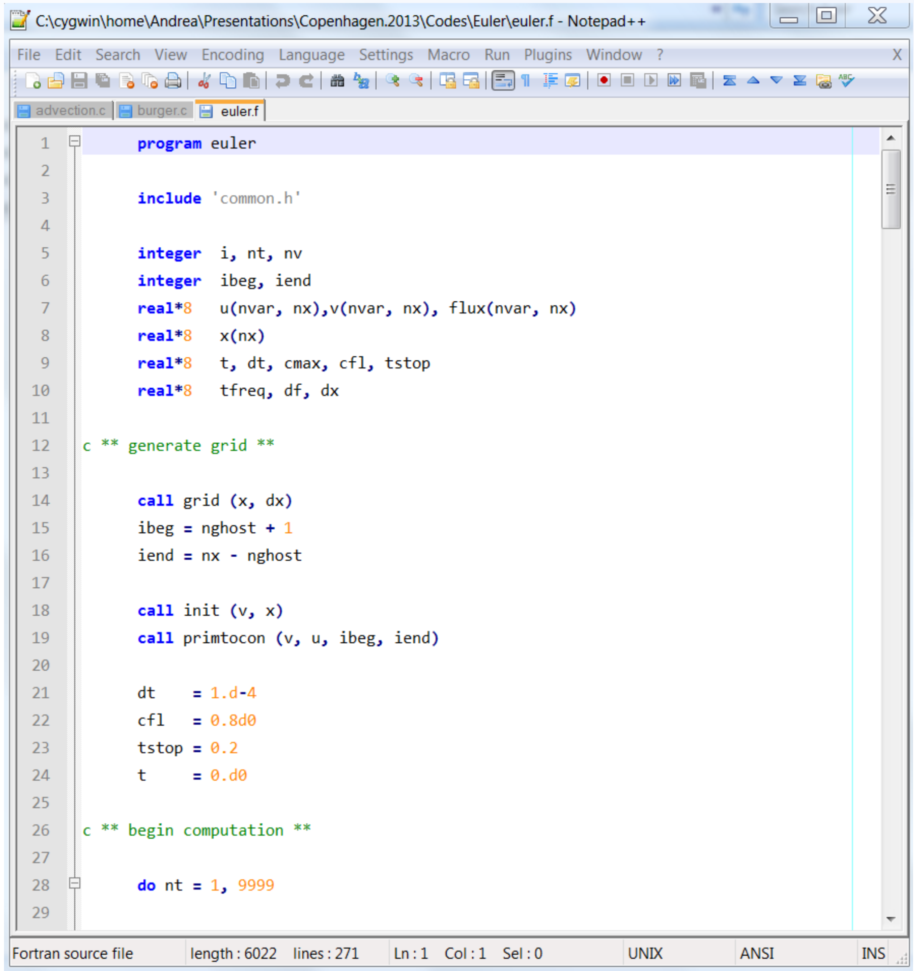


Code Example

- *File name*: euler.f
- *Purpose*: solve 1D Euler's equation
  using a 1st-order
  Lax-Friedrichs method.
- *Usage*:

> gfortran –O euler.f –o euler
> ./euler

- *Output*: 4-column ascii data files
  "data.out"



VII. RIEMANN SOLVERS

The Riemann Problem

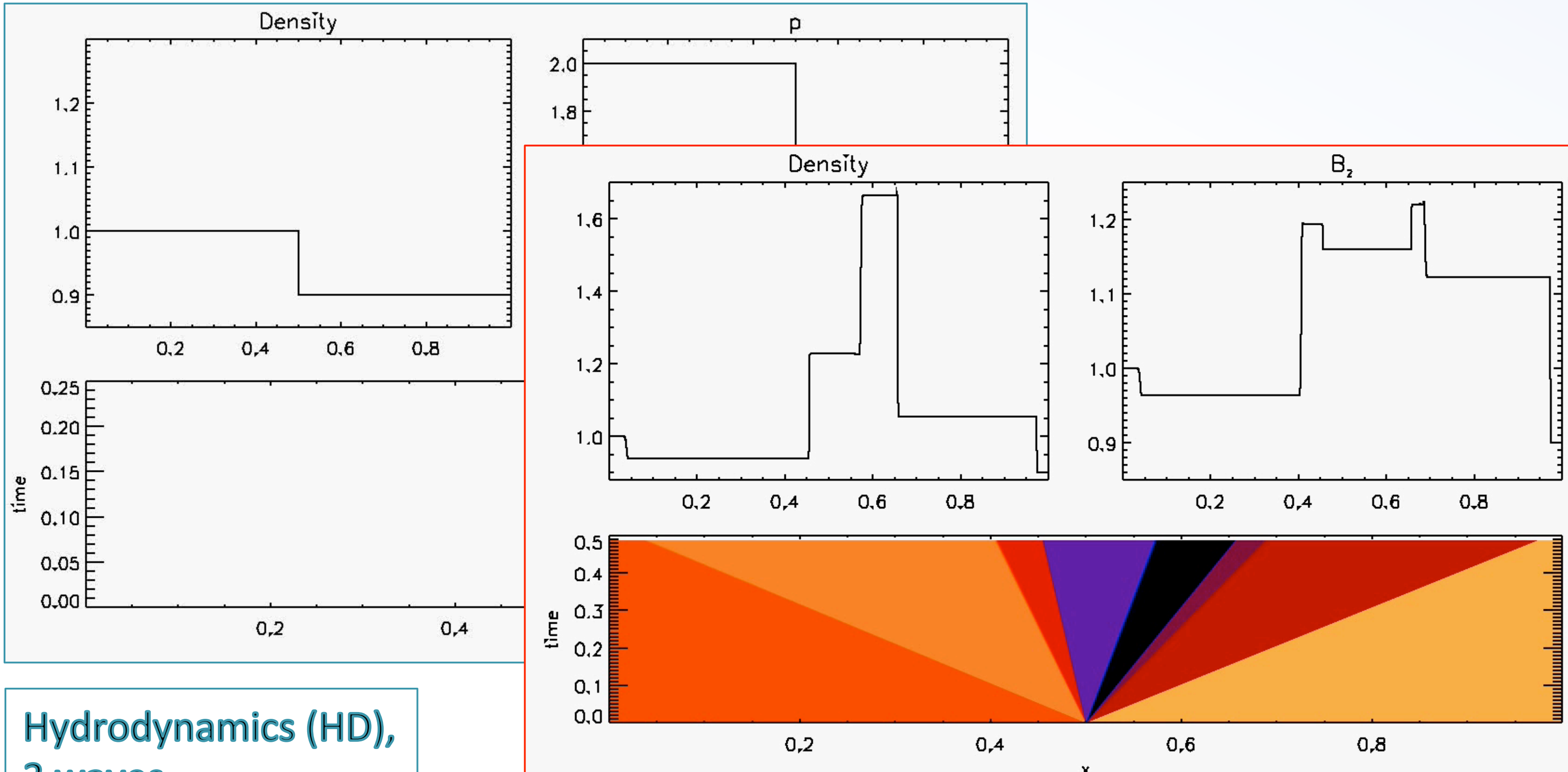
- Riemann solvers generalize the concept of "*upwind*" to *nonlinear systems of hyperbolic PDE*: *the discretization is biased towards the direction of propagation of waves*.

- The Riemann problem requires the solution of nonlinear systems of equations.

- Depending on the underlying system of PDE the solution may or may not be feasible.

The Riemann Problem

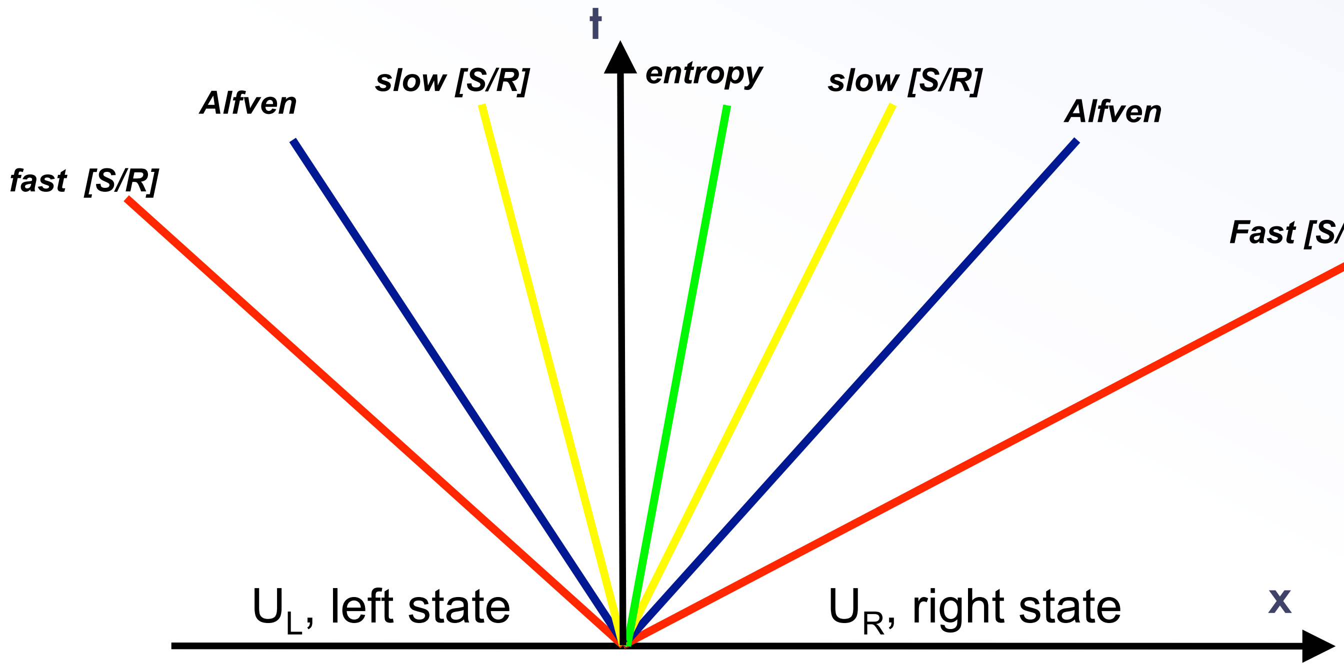
- In CFD, the solution to the Riemann problem depends on the underlying system of conservation laws:



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 $[v_x] \neq 0$

  → 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.

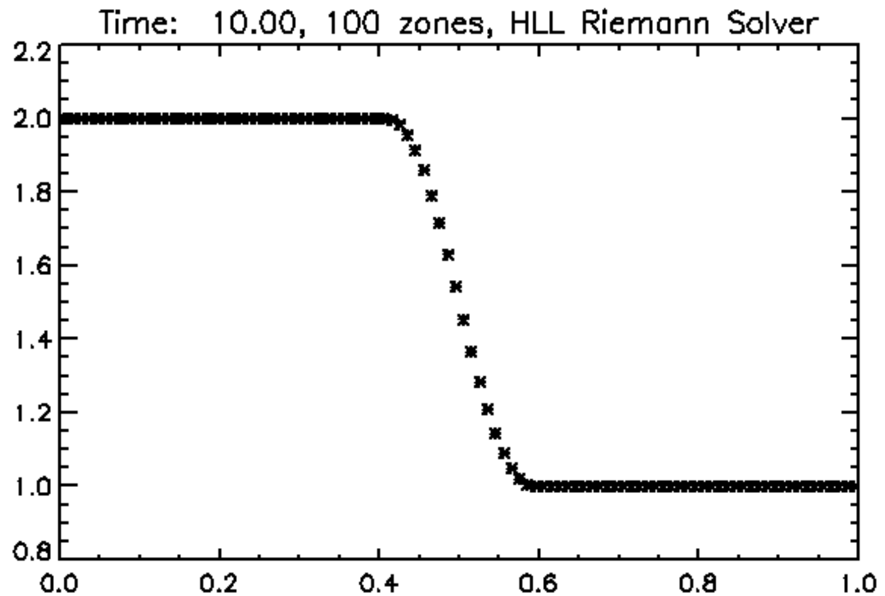
Solving the Riemann Problem

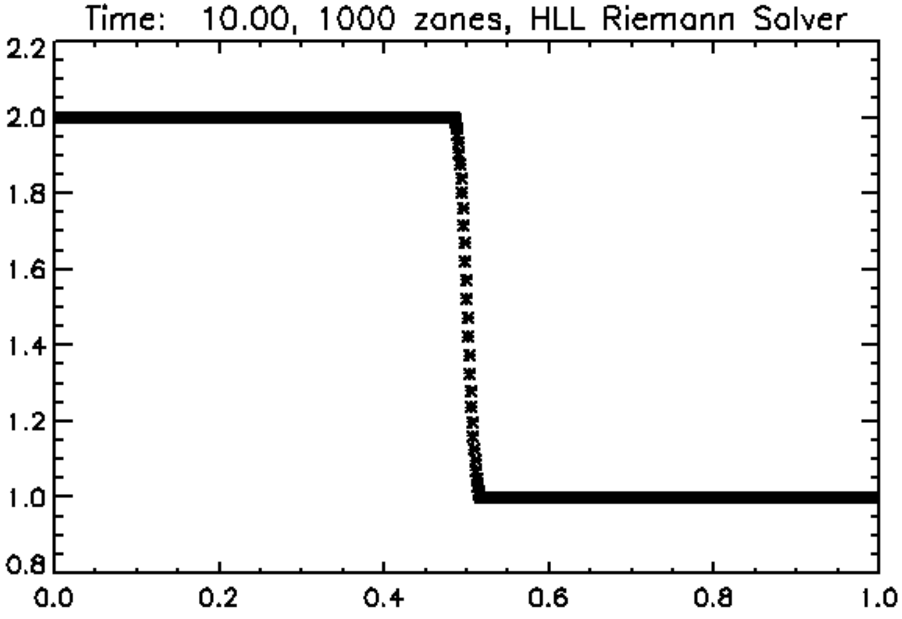
- *Exact Riemann solvers* (nonlinear)
  - Full nonlinear solution:
  - Expensive / impracticable for heavily usage in upwind codes;

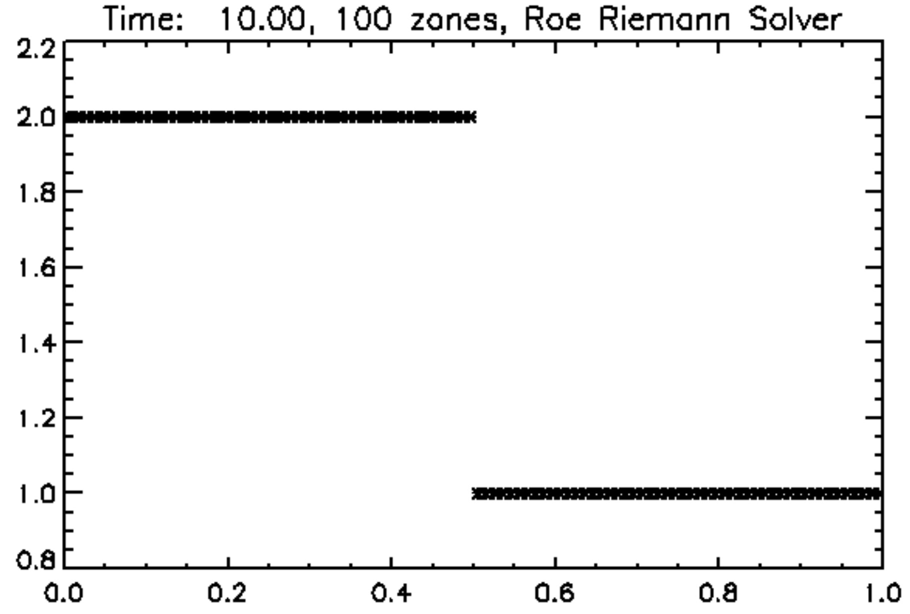
- *Linearized Riemann solvers* (Roe type)
  - require characteristic decomposition in eigenvectors
  - may be prone to numerical pathologies

- *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;

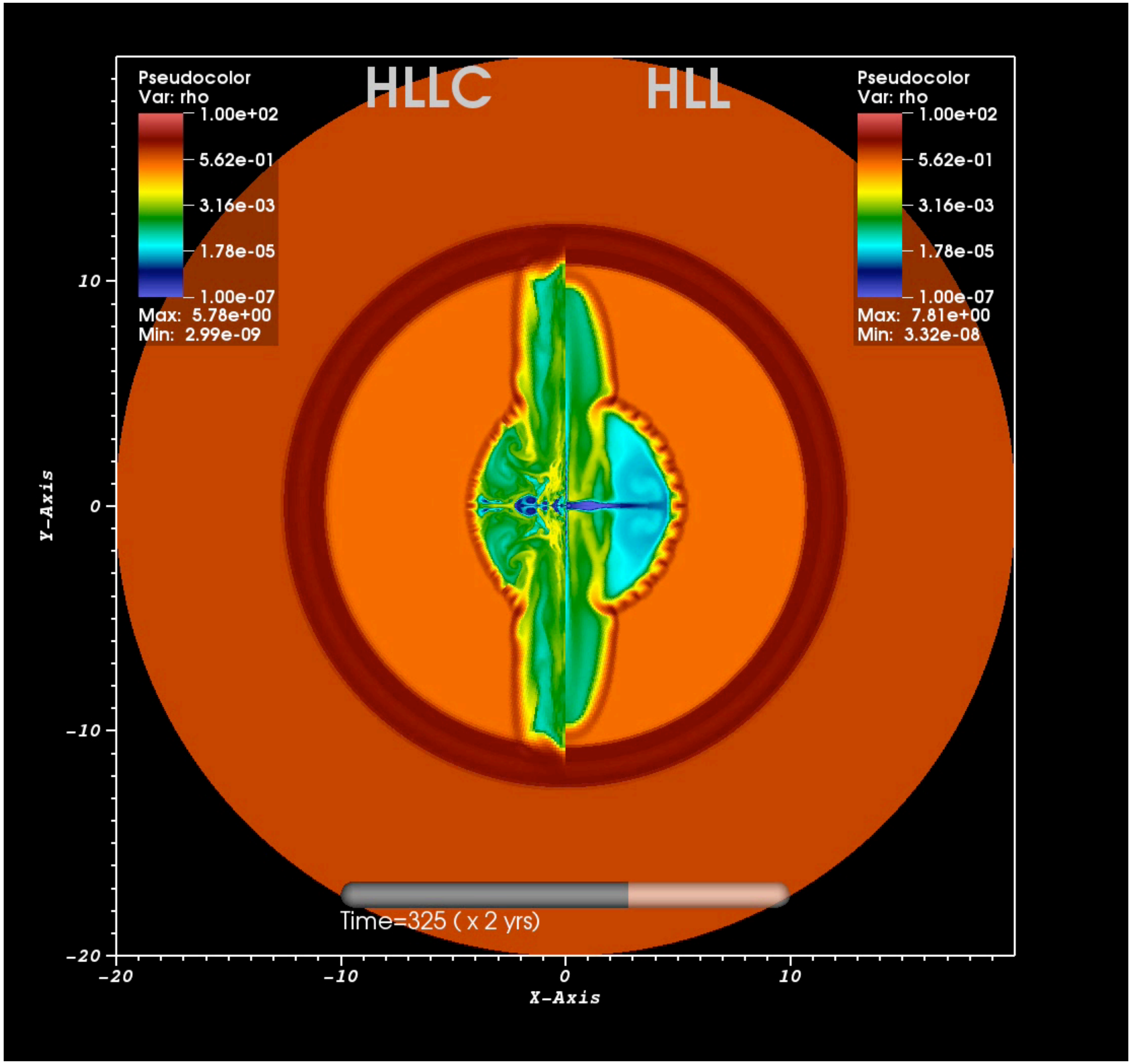
Resolution of Contact Discontinuities







A 2D Example: Axisymmetric PWN



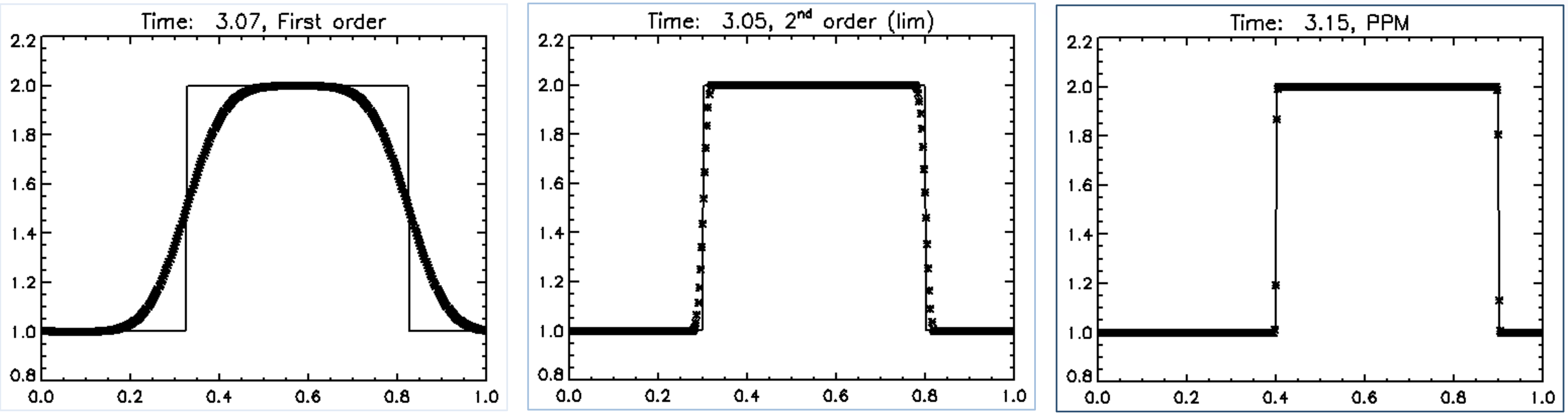
VIII. HIGH-ORDER FINITE VOLUME METHODS

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.

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*

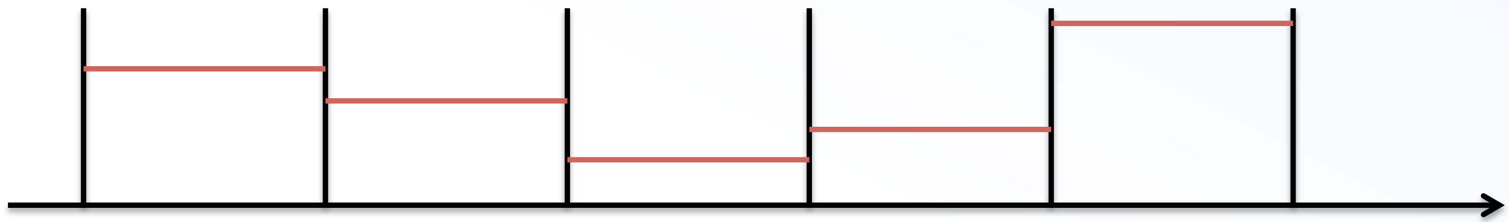


- PROS: numerical diffusion has a stabilizing effect.
- CONS: suppress small scale effect, may prevent growth of numerical instabilities when upwinding is not done correctly.

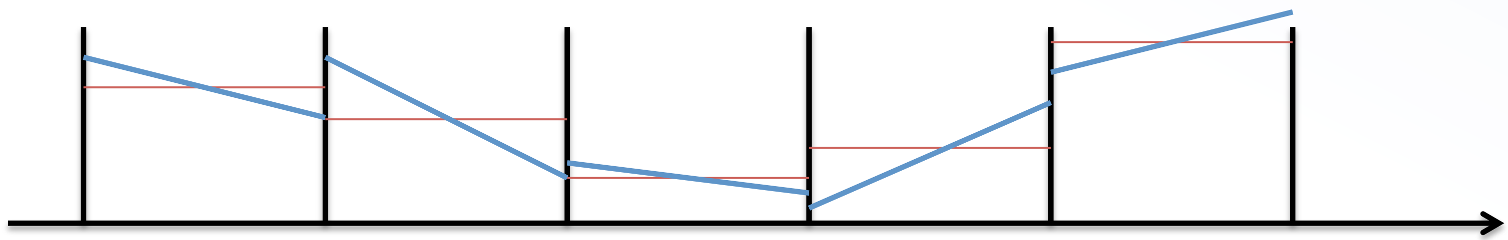
Improving spatial accuracy

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

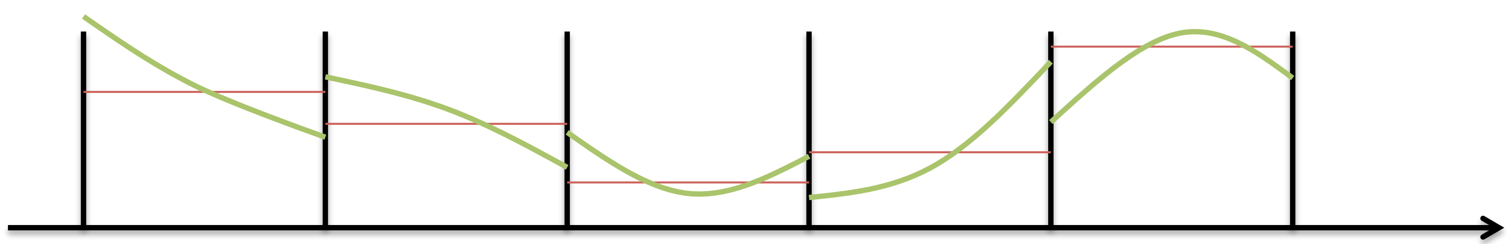
Piecewise constant



Piecewise Linear (TVD)



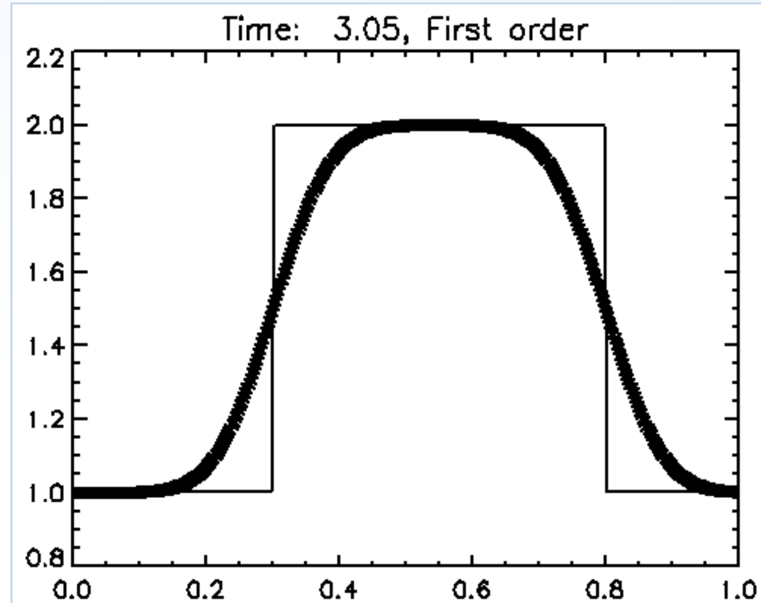
Piecewise Parabolic (PPM, WENO)



1st and 2nd Order Reconstruction

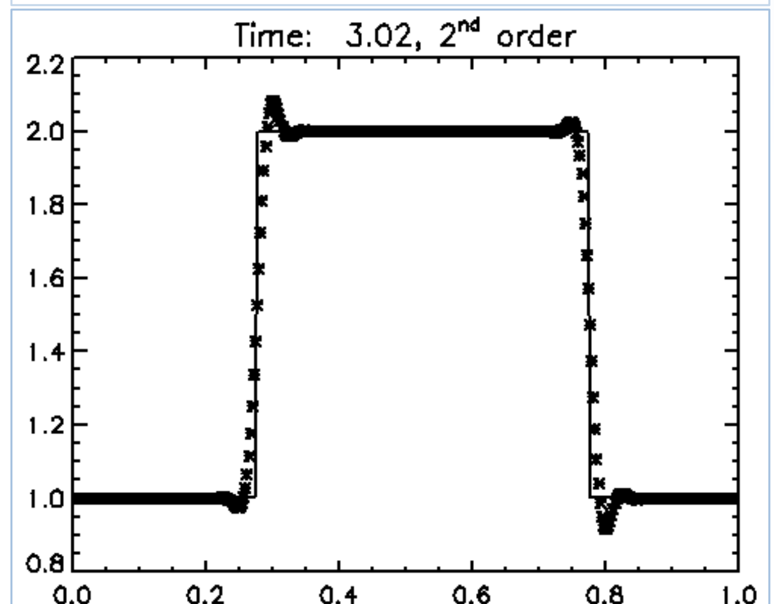
- 1st First-order reconstruction:

$$V(x) = V_i$$

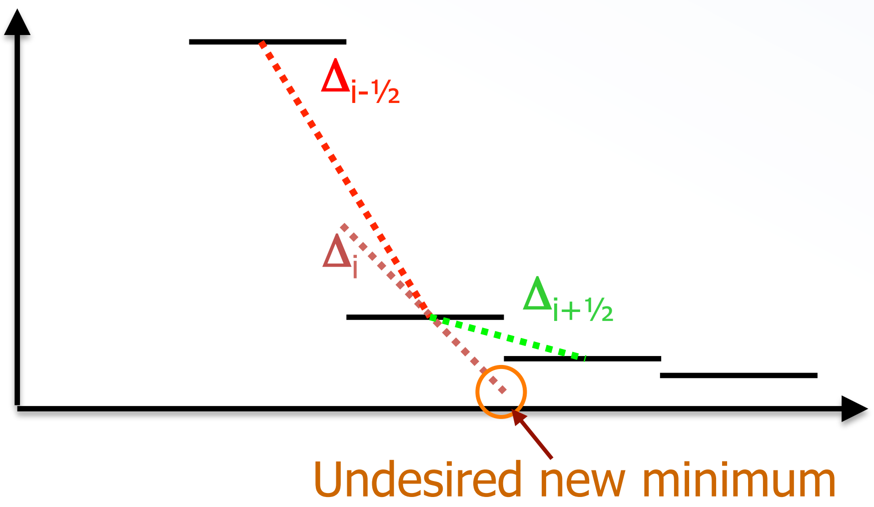


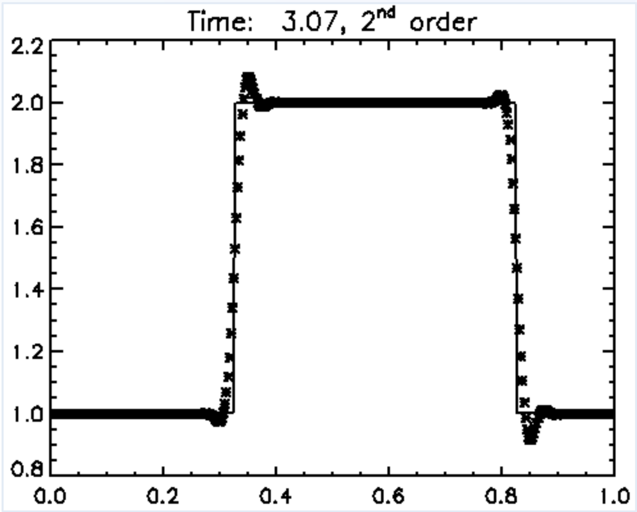
- For 2nd-order we use linear reconstrution:

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



Preventing Oscillations

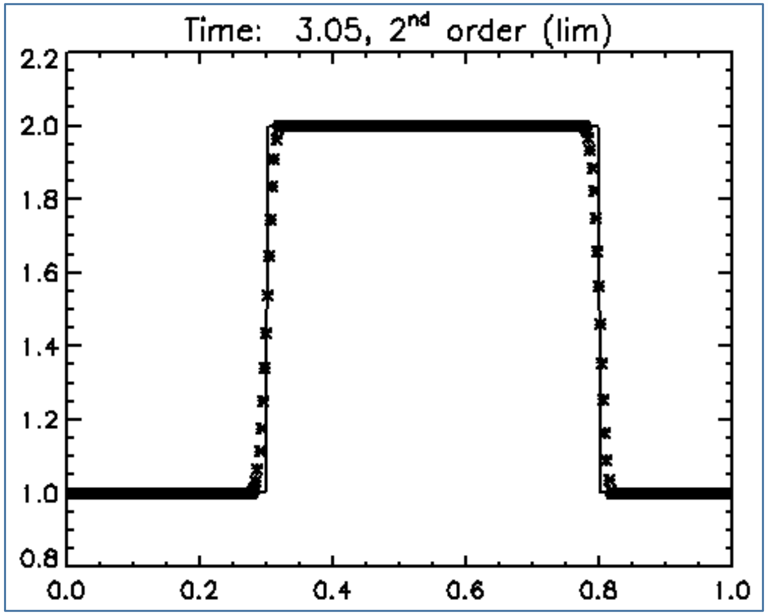




- Use slope limiters to avoid spurious oscillations: $V(x) = V_i + \frac{\delta V}{\Delta x}(x - x_i)$

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

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



High Order Integration in Time

- A simple and effective way to achieve 2nd or 3rd order accuracy in time is to treat the PDE in semi-discrete form:

$$\int \left(\frac{\partial \boldsymbol{q}}{\partial t} + \nabla \cdot \boldsymbol{F} \right) dV = 0 \quad \Longrightarrow \quad \frac{d\bar{\boldsymbol{q}}}{dt} = -\oint \tilde{\boldsymbol{F}} \cdot d\boldsymbol{S}$$

- In such a way the PDE becomes a regular ordinary differential equation (ODE) in time;

$$\frac{d\bar{\boldsymbol{q}}}{dt} = \boldsymbol{R}(\boldsymbol{q}, t) = \boldsymbol{R} \quad \Longrightarrow \quad \bar{\boldsymbol{q}}^{n+1} - \bar{\boldsymbol{q}}^{n} = \int_{n}^{n+1} \boldsymbol{R}\, dt$$

- Standard integration based on predictor/corrector schemes can then be used to solve ODEs.

Second-Order Runge-Kutta

- Using the trapezoidal method, the solution of our ODE writes:

$$\bar{\boldsymbol{q}}^{n+1} = \bar{\boldsymbol{q}}^{n} + \frac{\Delta t}{2}\left(\boldsymbol{R}^{n} + \boldsymbol{R}^{n+1}\right) + O(\Delta t^{3})$$

- the unknown $\bar{\boldsymbol{q}}^{n+1}$ appears on both side of the equation: use an estimate (predictor) for $\boldsymbol{R}^{n+1}$ with Euler method:

$$\begin{aligned}\bar{\boldsymbol{q}}^{*} &= \bar{\boldsymbol{q}}^{n} + \Delta t \boldsymbol{R}^{n} + O(\Delta t^{2}) \\ \bar{\boldsymbol{q}}^{n+1} &= \bar{\boldsymbol{q}}^{n} + \frac{\Delta t}{2}\left(\boldsymbol{R}^{n} + \boldsymbol{R}^{*}\right) + O(\Delta t^{3})\end{aligned}$$

- This is the second-order explicit Runge-Kutta method (or Heun's method) It is 2nd order accurate.

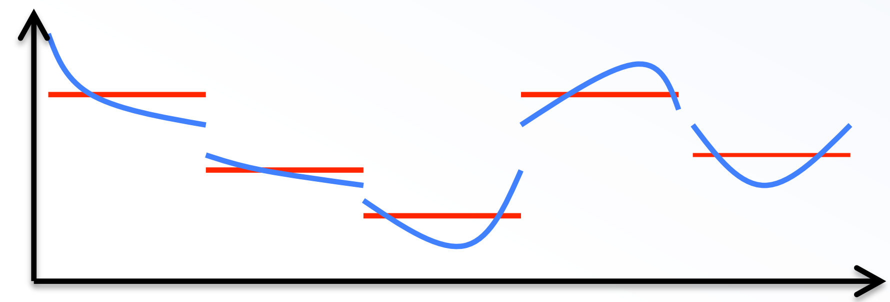
The Reconstruct-Solve-Update Algorithm

- Start from volume-averages

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

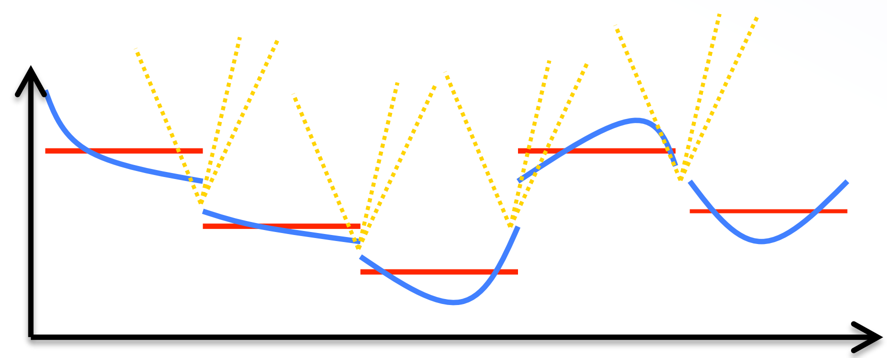
- Reconstruct interface values from zone averages using a high-order non-oscillatory polynomial:

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



- Solve Riemann problems between adjacent, discontinuous states.

  → Compute interface flux.



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

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

A “Pseudo-Code”…

for each dt {

Time Stepping:

begin loop on grid zones{

$$\langle U \rangle_i^n \longrightarrow \text{Data Reconstruction} \longrightarrow \begin{cases} U_{i+\frac{1}{2},L} \\ U_{i+\frac{1}{2},R} \end{cases}$$

$$\begin{cases} U_{i+\frac{1}{2},L} \\ U_{i+\frac{1}{2},R} \end{cases} \longrightarrow \text{Riemann Solver} \longrightarrow \tilde{F}_{i+\frac{1}{2}}^{n+\frac{1}{2}}$$

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

}end loop on grid zones

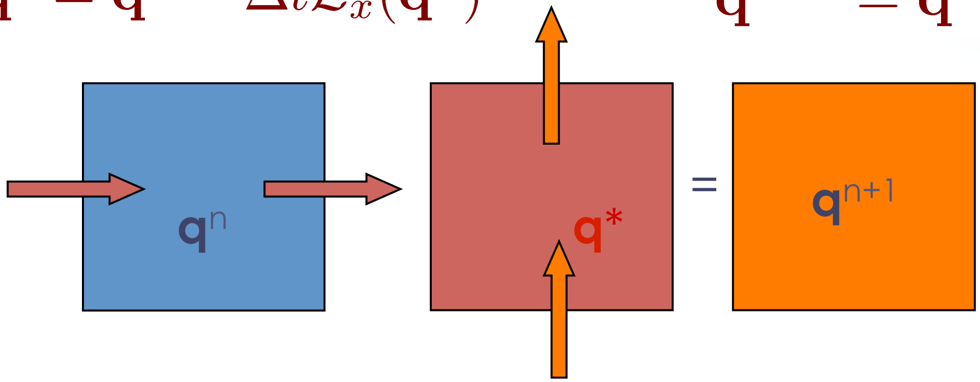
}

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.

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

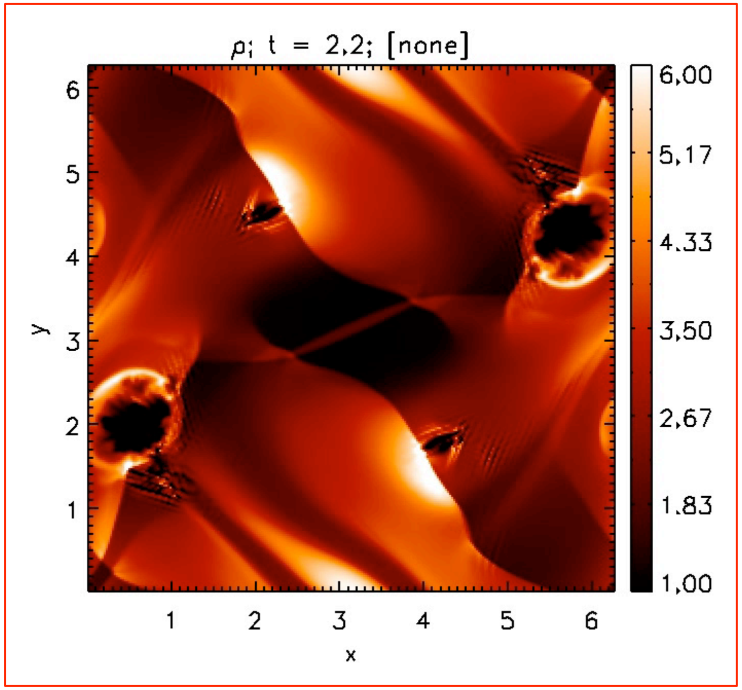


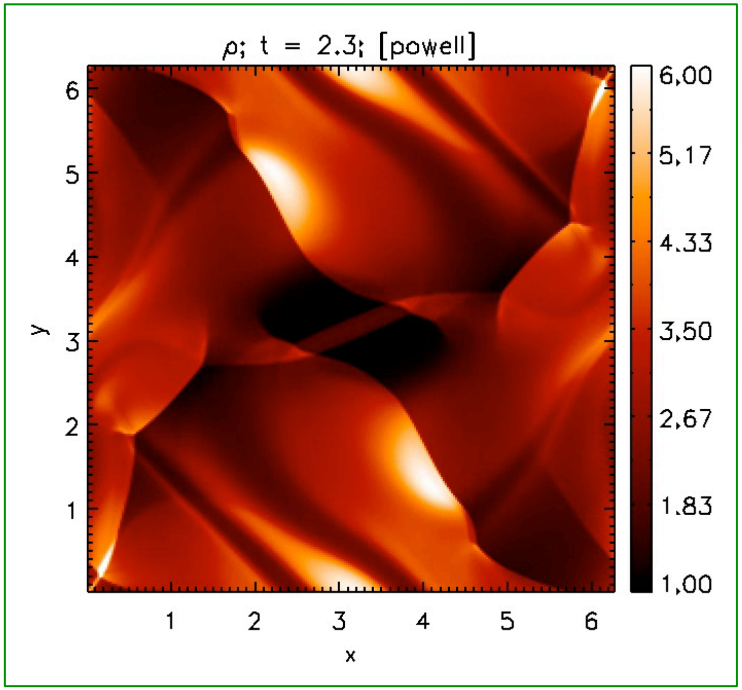
  - Dimensionally Unsplit schemes: solve the full problem in one step:

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

$\nabla\cdot B$ 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 $\nabla \cdot B$ 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:

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

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

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

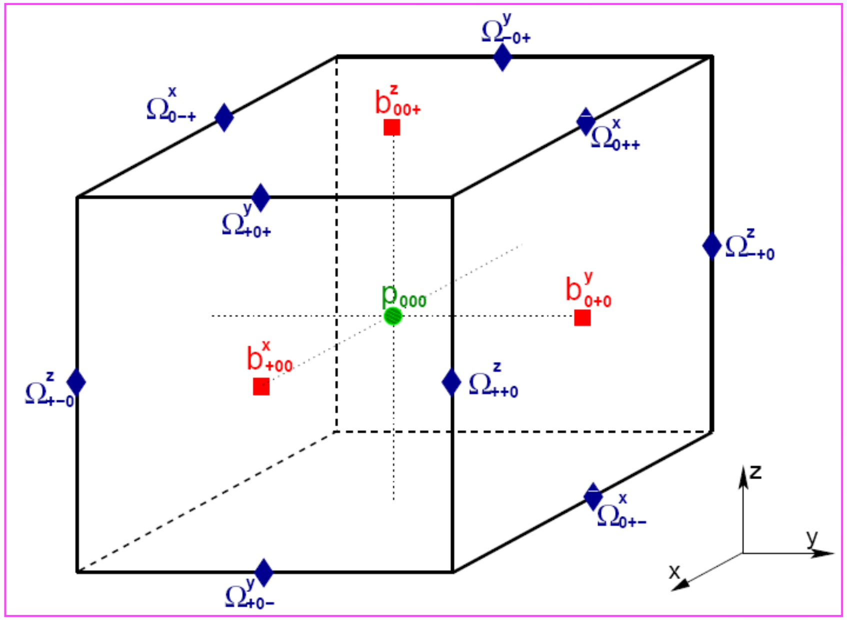
$$\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + p + \frac{\mathbf{B}^2}{2} \right) \mathbf{v} - (\mathbf{v} \cdot \mathbf{B})\mathbf{B} \right] = 0,$$

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

- 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:

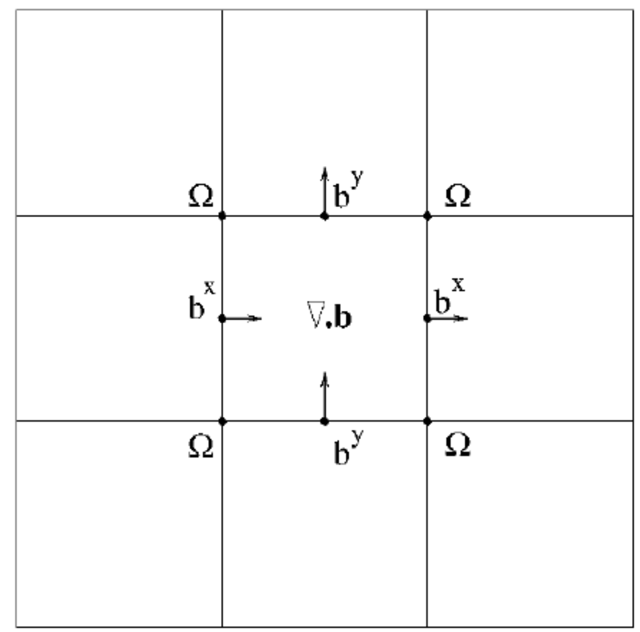
$$\int \left(\frac{\partial \boldsymbol{b}}{\partial t} + \nabla \times \boldsymbol{\mathcal{E}} \right) \cdot d\boldsymbol{S}_d = 0 \quad \Longrightarrow \quad \frac{db_{x_d}}{dt} + \frac{1}{S_d} \oint \boldsymbol{\mathcal{E}} \cdot d\boldsymbol{l} = 0$$

4. Constrained Transport in 2D

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

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

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



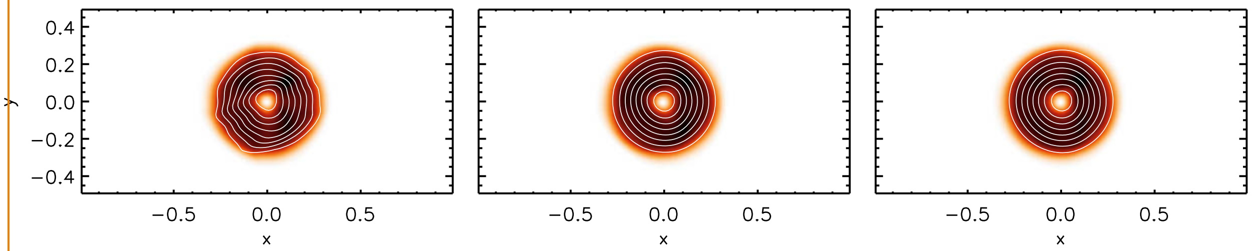
- It is easy to show that the numerical divergence of ***b*** defined by

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

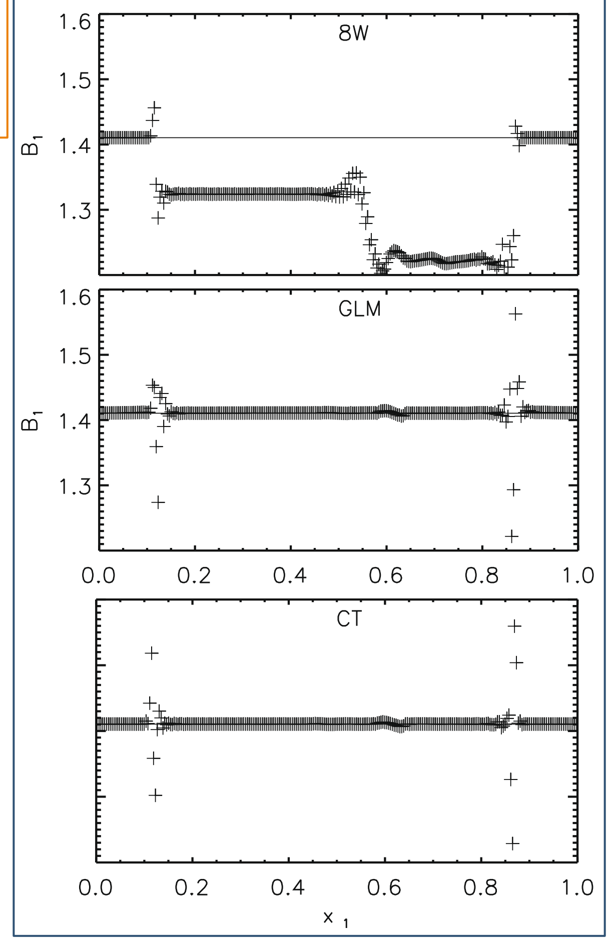
does not change due to perfect cancellation of term to machine accuracy (Toth, 2000).

Scheme Comparison

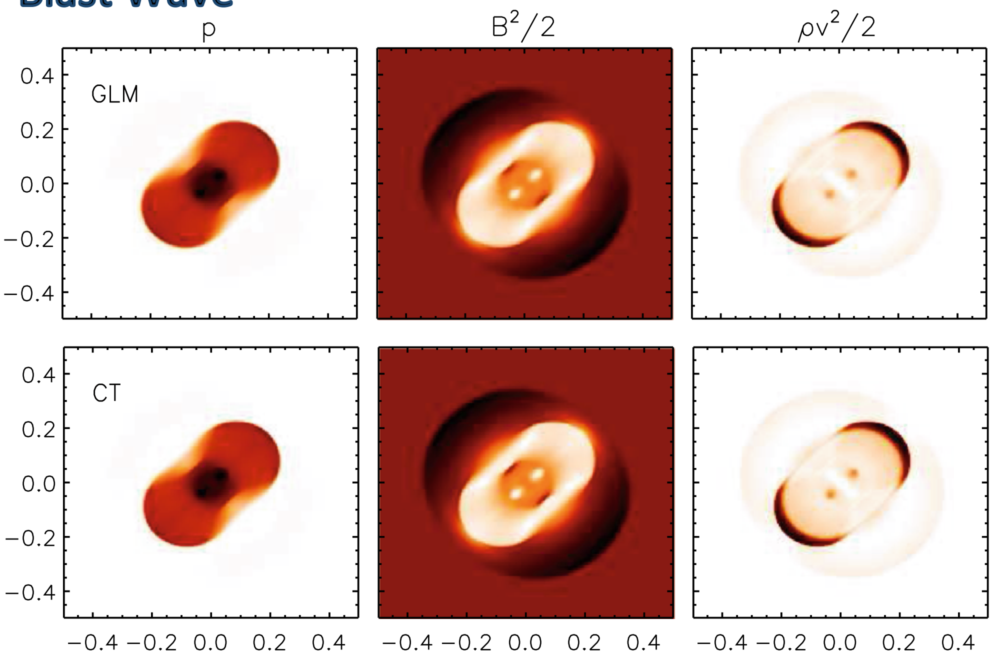
Field Loop advection



Rotated Shock Tube



Blast Wave



$\nabla \cdot B$ 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)

X. 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.

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

- *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: $$U_i^{n+1} = U_i^n + C(U_{i-1}^n - 2U_i^n + U_{i+1}^n)$$
- Where $C = D\Delta t/\Delta x^2$ is the (parabolic) CFL number
- Stability demands $C \leq ½$ → $\Delta t \leq \Delta x^2 / (2D)$
- This is quite restrictive !

Implicit Schemes for Parabolic PDE

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

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

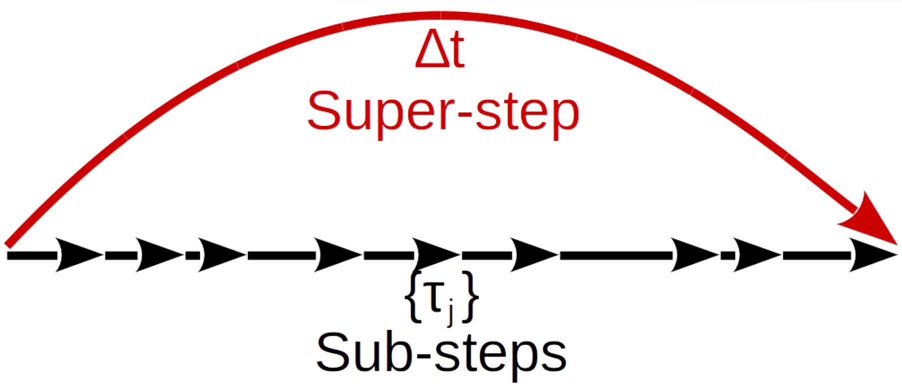
  has no stability limit (*unconditionally stable !*)
- However, it leads to an implicit (linear) system:

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

- 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

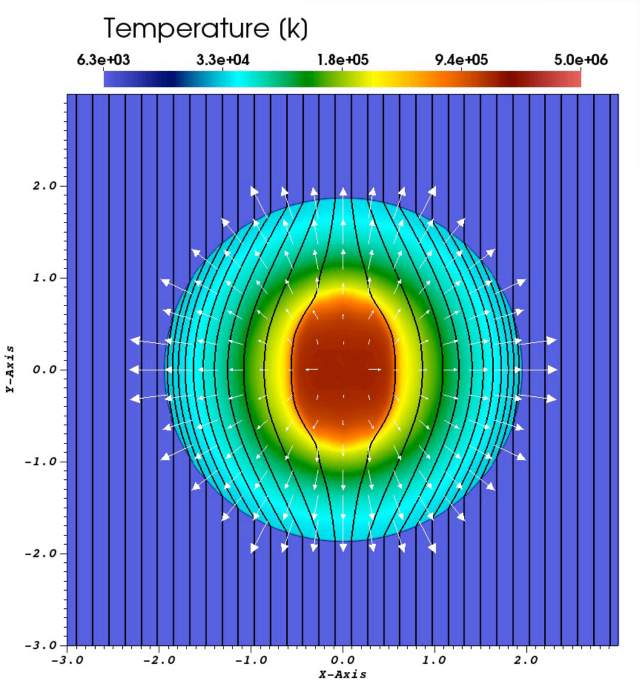
- RKL methods show better stability properties and are preferred over STS.
- Choosing s sub-steps we can cover a time step equal to

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

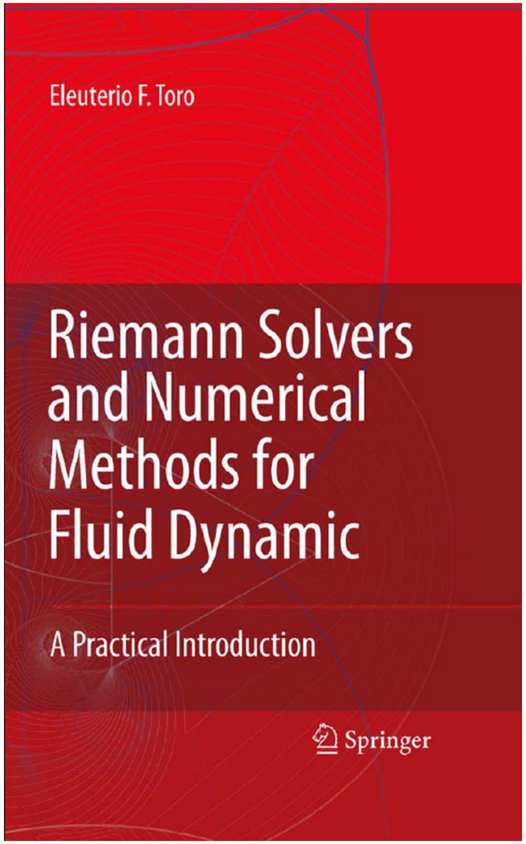
where Δt_{expl} is the standard explicit method time step.

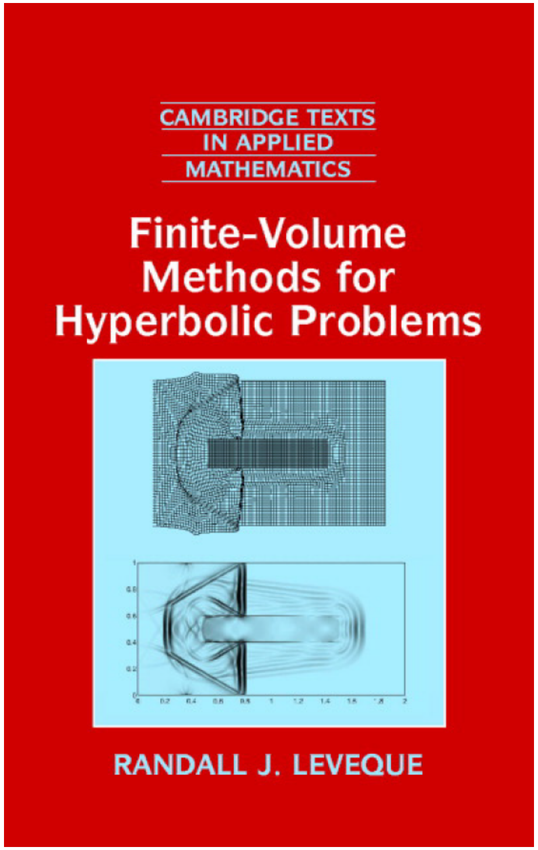
- The method is easily parallelizable.
- Scaling on 2D blast wave:

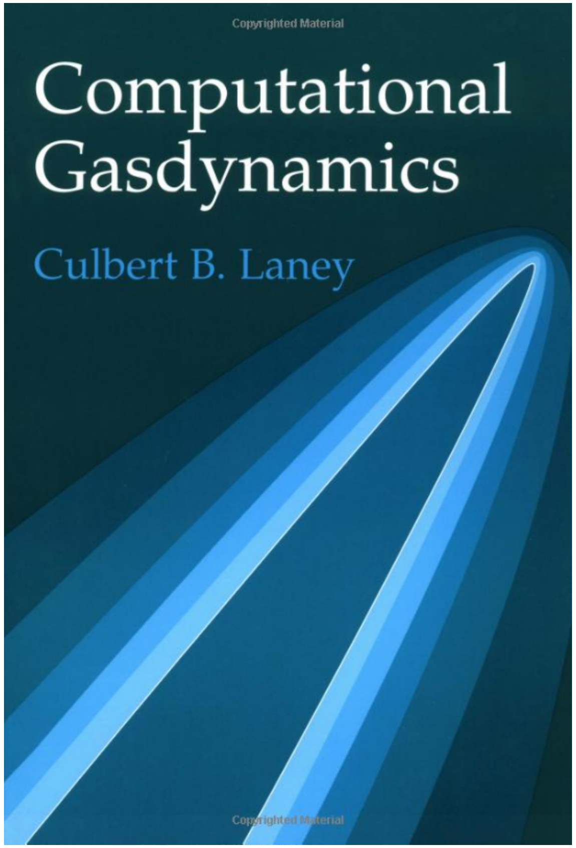
Algorithm	N_x	Execution Time [s]
Explicit	192	$1m : 13s$
RKL	192	$28s$
Explicit	384	$18m : 32s$
RKL	384	$5m : 19s$
Explicit	768	$4h : 21m : 15s$
RKL	768	$49m : 17s$
Explicit	1536	$3d : 5h : 13m : 10s$
RKL	1536	$10h : 4m : 55s$



Recommended Books







Recommended Codes

PLUTO[1,2]

→ a modular parallel code providing a *multi-physics* as well as a *multi-algorithm* framework for the solution of mixed hyperbolic/ parabolic conservation laws in astrophysics;

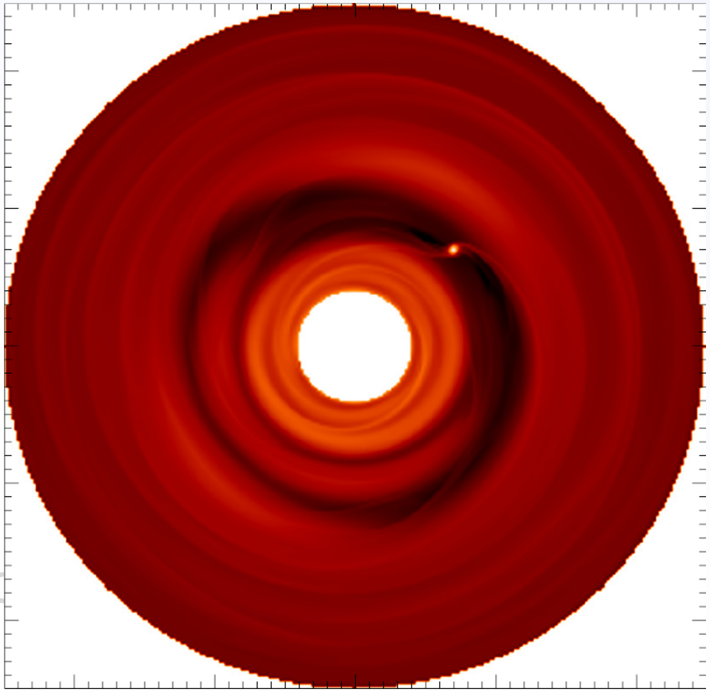
http://plutocode.ph.unito.it

(v. 4.2)

[1]Mignone et al. ApJS (2007), 170, 228-242; [2]Mignone et al, ApJS (2012), 198, 7

PLUTO Application Gallery

- Planet Formation
- Stellar Jets
- Radiative shocks
- Extragalactic Jets
- Jet Launching
- Magnetospheric accretion & star-disk Interaction
- Magneto-rotational instability (MRI) & ac
- Relativistic Shock dynamics
- Fluid instabilities CD, KH, RT, etc…



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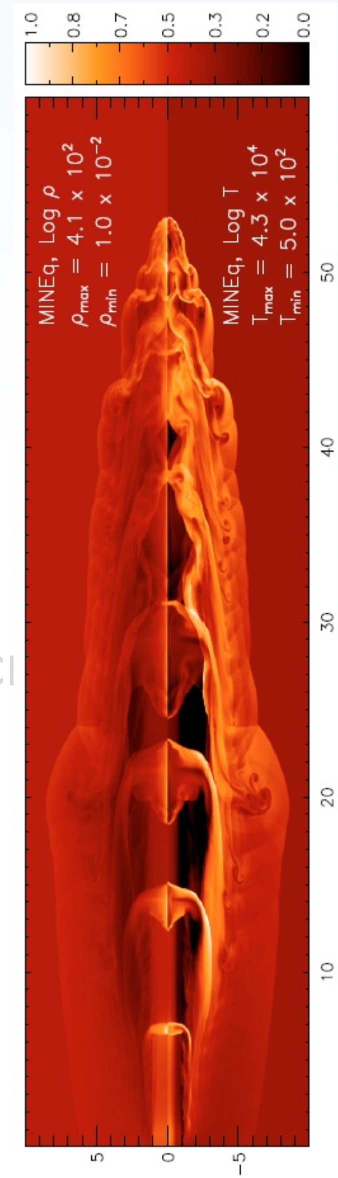

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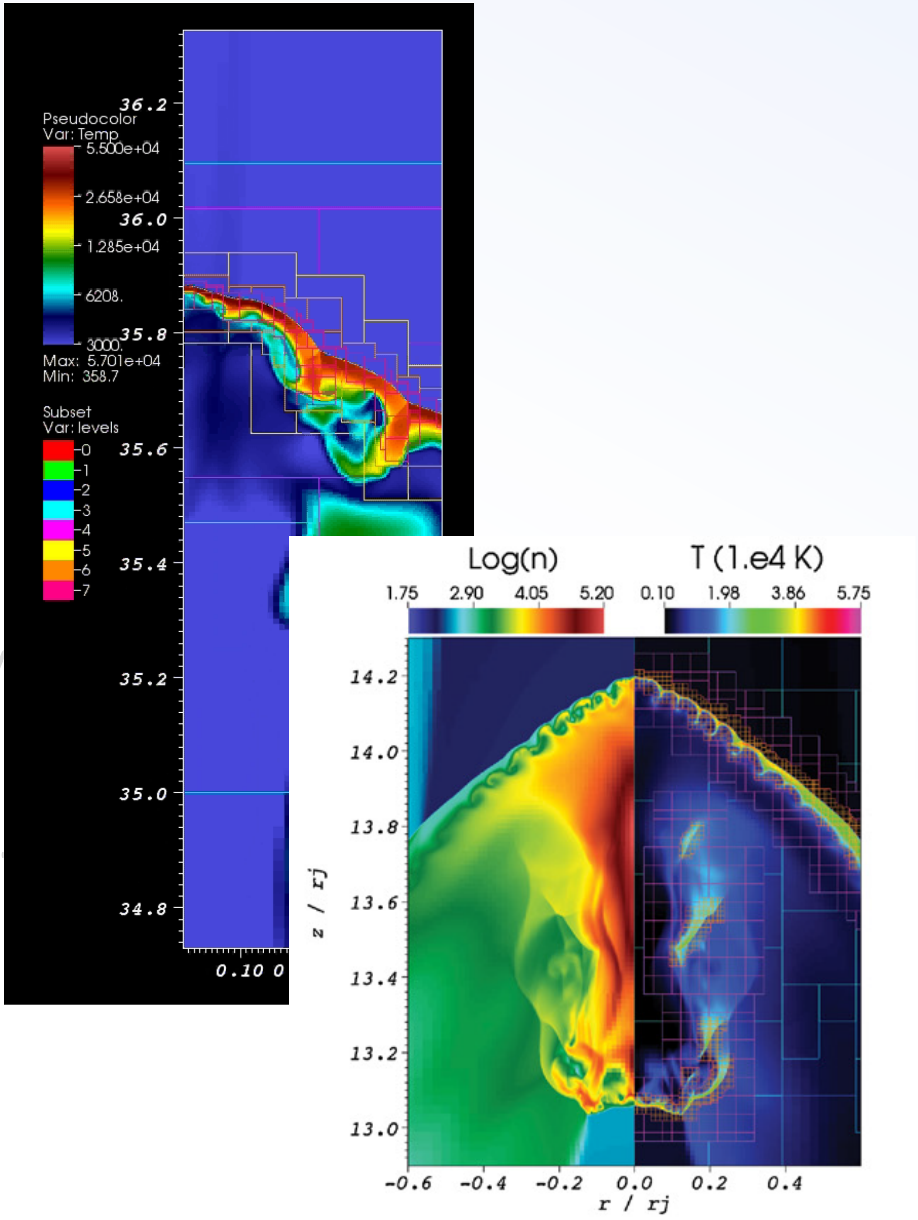

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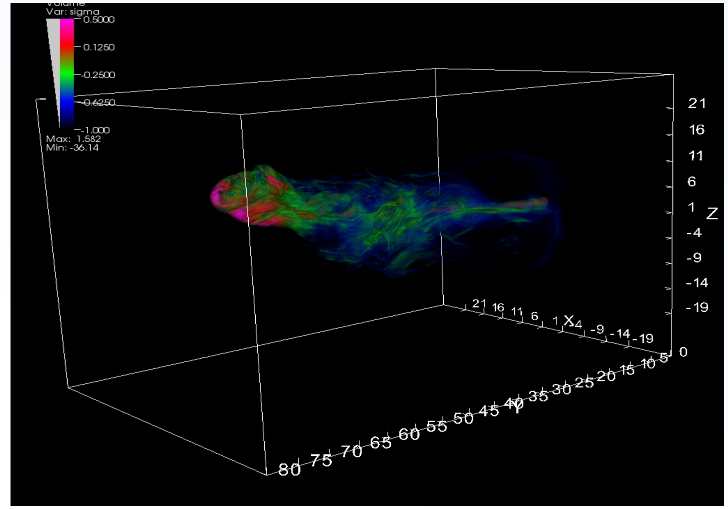
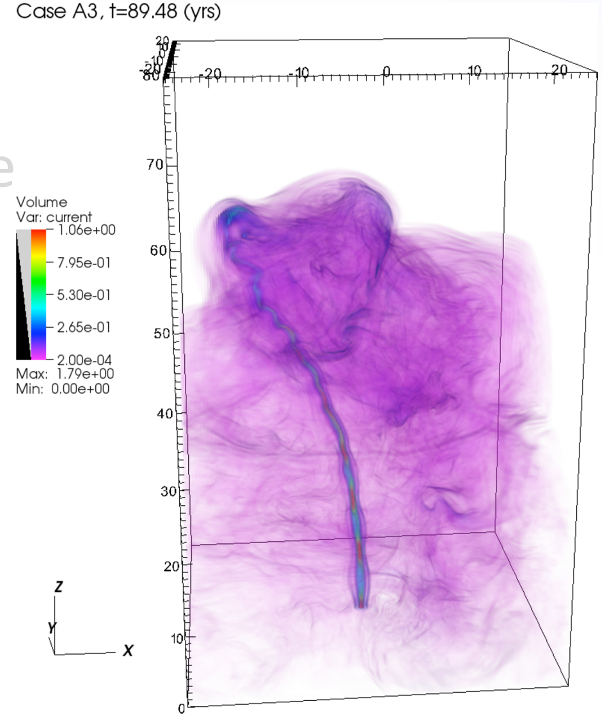


Case A3, t=89.48 (yrs)



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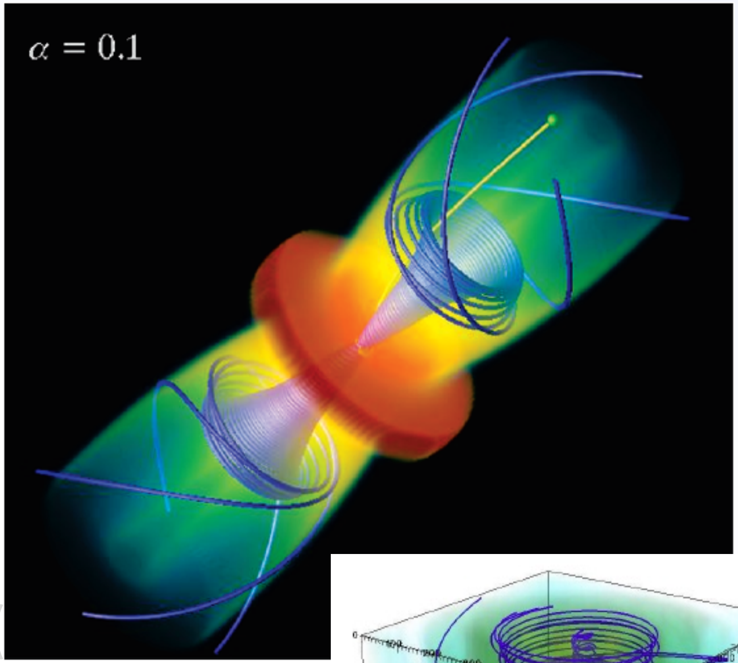

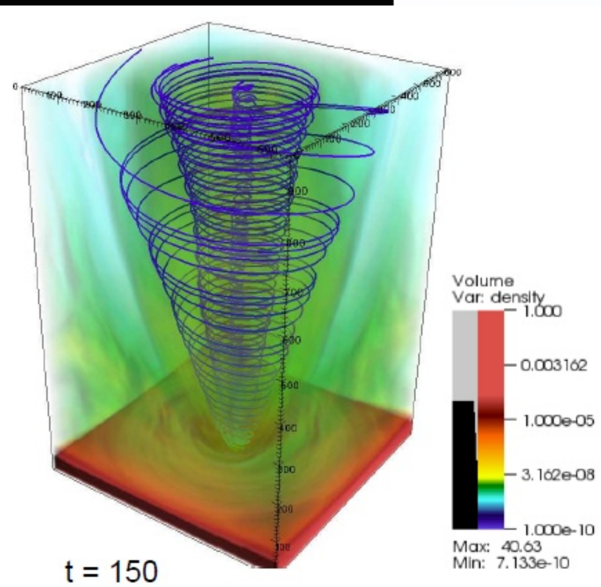

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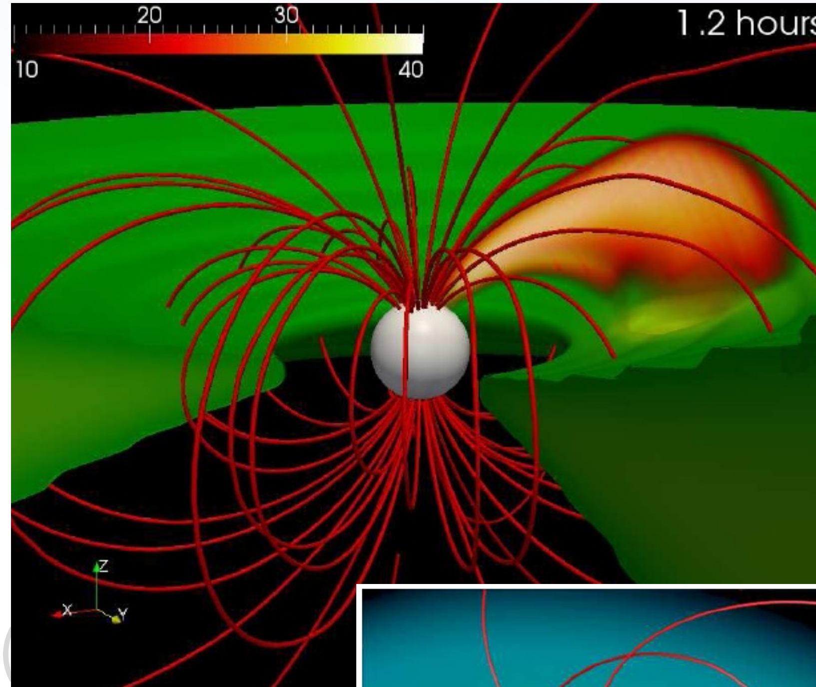

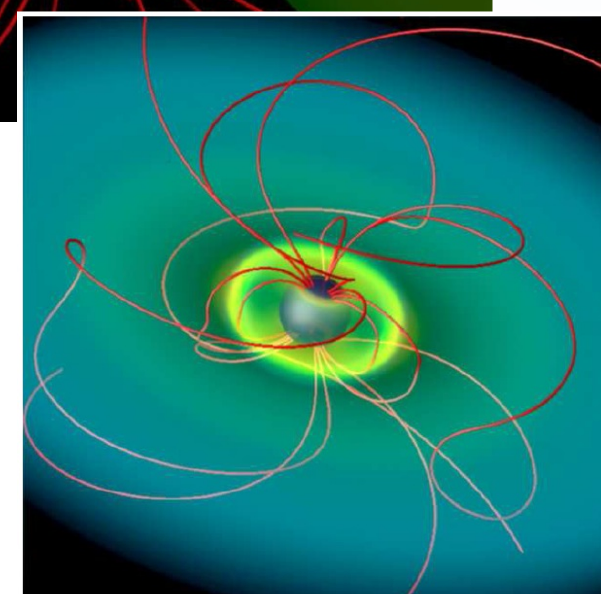

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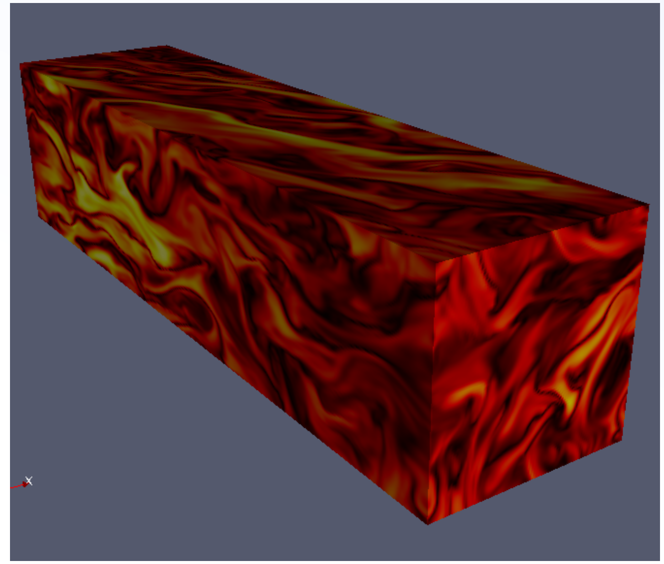

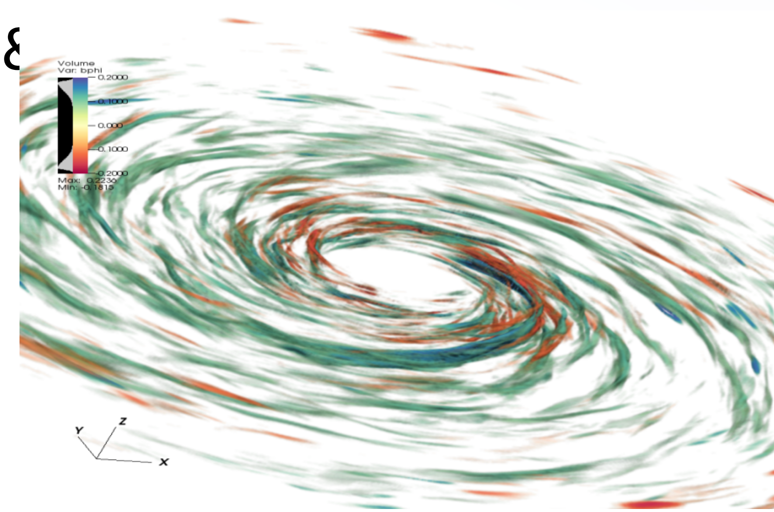

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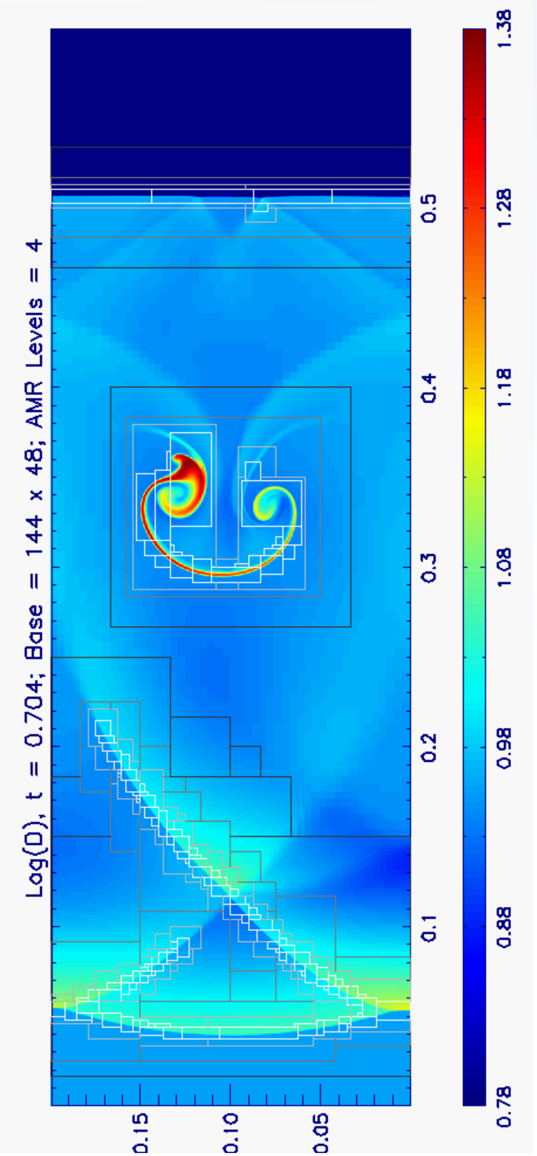

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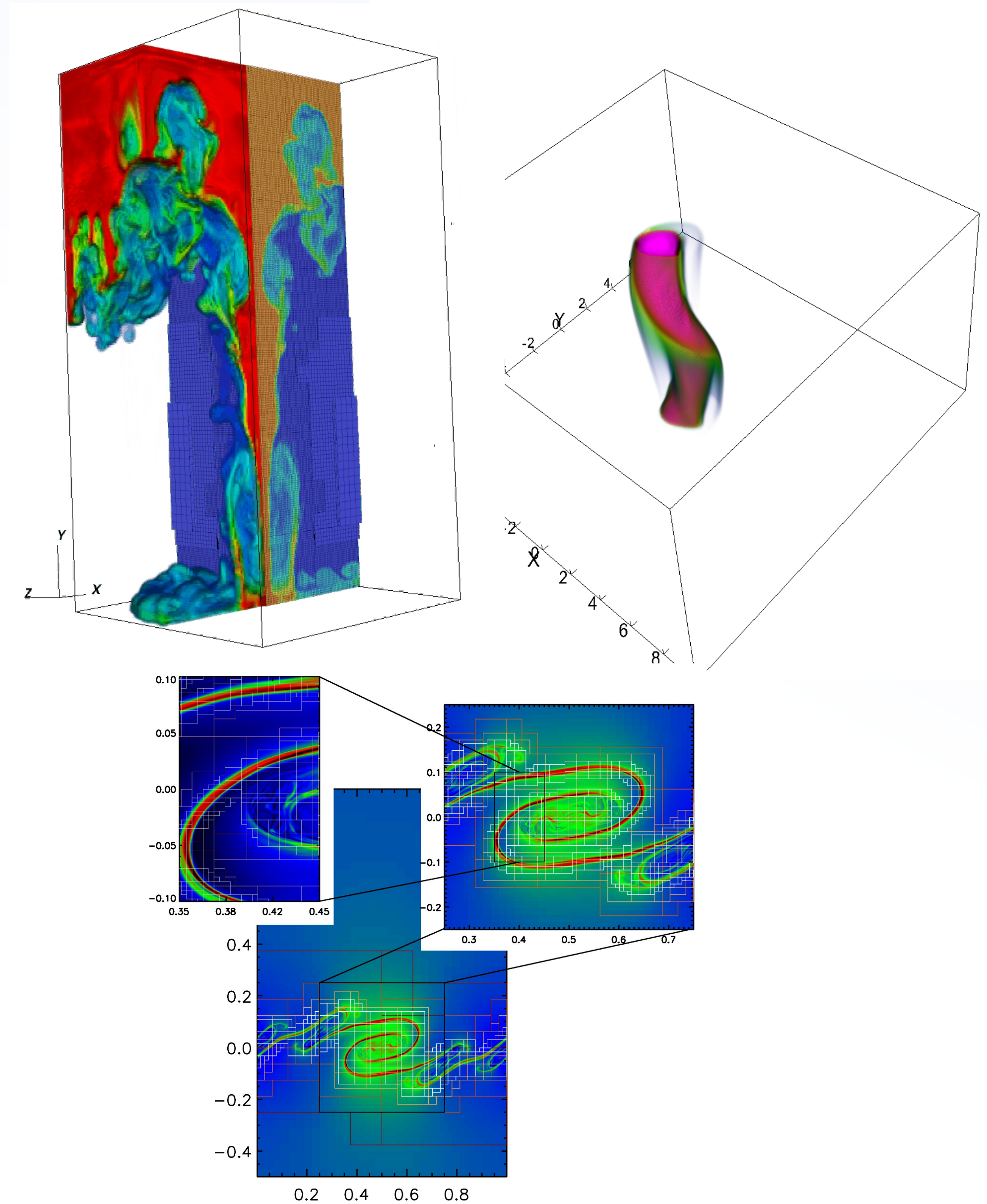

THE END