Hydrodynamics and VH-1

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Workshop #1

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Fluid Dynamics

Fluid Dynamics, subsuming both hydrodynamics and aerodynamics, is a continuum description of the collective behavior of a large number of particles.

The equations of fluid dynamics can be derived from kinetic theory in the limit that the collisional mean free path, λ, is much smaller than the macroscopic scales of interest, L.

Thus we are concerned with the bulk velocity of the fluid, u, while the random velocity of individual fluid particles is only considered to the extent that they form an internal energy.

Key to the behavior of fluids is that they, like solids, deform under stress. However, unlike a solid, a fluid shows no tendency to return to the former state when the stress is removed.

Continuity

Quantity of matter can be described by the mass density, which changes in time and space.

The change of ρ with time in the box requires a "flux" of mass across the boundary at velocity u.

More formally,

Applying the time independence of V on the left and divergence theorem on the right yields

Since this is true for arbitrary V,

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$$\rho\,(x,t)$$

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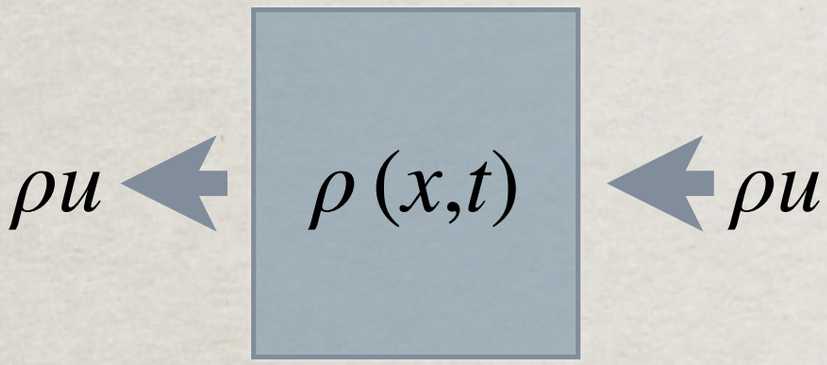


The change of ρ with time in the box requires a "flux" of mass across the boundary at velocity u.

More formally,

$$\frac{d}{dt}\int_V \rho \, dV = -\int_S (\rho\vec{u}) \cdot \vec{n} \, dS$$

Applying the time independence of V on the left and divergence theorem on the right yields

$$\int_V \frac{\partial \rho}{\partial t} \, dV = -\int_V \nabla \cdot (\rho\vec{u}) \, dV$$

Since this is true for arbitrary V,

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

Continuity Equation

Defining Derivatives

When considering a moving fluid, there are two natural frames of reference.

1) Eulerian Coordinates, which are fixed in space.

2) Lagrangian Coordinates, which move with the fluid.

To define a Lagrangian (or material) Derivative of a quantity f, we must consider both changes that are local in space and those that result from movement.

$$\frac{Df}{dt} = \frac{\partial f}{\partial t} + \vec{u} \cdot \nabla f$$

Since $\nabla \cdot (b\vec{a}) = \vec{a} \cdot \nabla b + b(\nabla \cdot \vec{a})$, the continuity equation can be transformed from

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad \text{into} \quad \frac{D\rho}{Dt} + \rho \nabla \cdot \vec{u} = 0$$

Causing Fluid to Move

We next need to understand what generates the velocity, u.

For a co-moving volume, the total momentum is $\int_V \rho u \, \mathrm{d}V$ and the time rate of change comes entirely from external forces.

These take the form of external body forces, f, e.g., gravity, and surface forces, e.g., pressure, P.

$$\frac{d}{dt}\int_V \rho\vec{u}\, dV = -\int_S P\vec{n}\, dS + \int_V \rho\vec{f}\, dV$$

Applying the Chain Rule to the left side yields,

$$\frac{d}{dt}\int_V \rho\vec{u}\, dV = \int_V \rho\frac{D\vec{u}}{Dt} dV + \int_V \vec{u}\frac{D\rho}{Dt} dV$$

$\frac{D\rho}{Dt} \to 0$

since ρV is invariant for co-moving volumes.

Applying the divergence theorem to the right side yields

$$-\int_S P\vec{n}\, dS + \int_V \rho\vec{f}\, dV = \int_V (-\nabla P + \rho\vec{f})dV$$

Euler Equation

Combining these yields

$$\int_V \rho \frac{D\vec{u}}{Dt} dV = \int_V (-\nabla P + \rho \vec{f}) dV$$

or, since this applies for arbitrary volumes,

$$\rho \frac{D\vec{u}}{Dt} = (-\nabla P + \rho \vec{f})$$

Written in terms of coordinates fixed in space, this becomes

$$\rho \left(\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} \right) = (-\nabla P + \rho \vec{f})$$

Euler Equation

To make sure we see the physics of this equation, we can rewrite this as

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \rho \vec{u}\vec{u} = -\nabla P + \rho \vec{f}$$

Viscosity

When we wrote the effect of the surface pressure as $\int_S P\,\vec{n}\,dS$, we implicitly assumed that viscosity was unimportant.

In the general case, $F_i = \int_S \Sigma_j P\,\sigma_{ij}\,n_j\,dS$, where σ_{ij} is the stress tensor, rather than $\int_S P\,n_i\,dS$.

For gases and simple liquids, we can define a dynamical viscosity, μ, in which case the stress tensor is

$$\sigma_{ij} = -P\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}(\nabla\cdot\vec{u})\delta_{ij}\right)$$

In this case, the momentum equation becomes Navier-Stokes Equation.

$$\rho\frac{D\vec{u}}{Dt} = -\nabla P + \rho\vec{f} + \mu\left(\nabla^2\vec{u} + \frac{1}{3}\nabla(\nabla\cdot\vec{u})\right)$$

μ is generally very small in astrophysics and the Reynolds number, the ratio of inertial forces to viscous forces, is large.

Mechanical Energy

The Euler equation includes a gradient of the kinetic energy, requiring an equation to evolve the kinetic energy.

Taking the dot product of u/ρ with the Euler equation

$$\frac{\vec{u}}{\rho} \cdot \rho \frac{D\vec{u}}{Dt} = \frac{\vec{u}}{\rho} \cdot (-\nabla P + \rho \vec{f})$$

provides such an equation

$$\frac{D}{Dt}\left(\frac{1}{2}\vec{u}^2\right) = -\frac{1}{\rho}\vec{u} \cdot \nabla P + \vec{u} \cdot \vec{f}$$

mechanical energy equation

Simply, the kinetic energy changes in response to work done by pressure and body forces.

This approach may seem arbitrary, but is equivalent to calculating the work done by a force as

$$uF = uma = um\frac{du}{dt} = \frac{d}{dt}\left(\frac{1}{2}u^2\right)$$

Energy Conservation

Of course, kinetic energy is not conserved, rather it is the total energy, kinetic + internal (thermal), $\frac{1}{2}u^2 + U$.

If we expand our energy equation to include the internal energy, we must add terms for the heat generated within the volume, ϵ, and the flux of heat across the boundary, F.

$$\frac{d}{dt}\int_V \left(\frac{1}{2}\vec{u}^2 + U\right)\rho\, dV = -\int_S \vec{u}\cdot P\vec{n}\, dS + \int_V \vec{u}\cdot\vec{f}\,\rho\, dV + \int_V \epsilon\rho\, dV - \int_S \vec{F}\cdot\vec{n}\, dS$$

Applying the divergence theorem to replace the surface integrals

$$\int_S \vec{F}\cdot\vec{n}\, dS = \int_V \nabla\cdot\vec{F}\, dV$$

$$\int_S \vec{u}\cdot P\vec{n}\, dS = \int_V \nabla\cdot P\vec{u}\, dV$$

Energy Equation

As in the prior derivation, the invariance of ρV for co-moving volumes simplifies the energy time derivative.

$$\frac{d}{dt}\int_V \left(\frac{1}{2}\vec{u}^2 + U\right)\rho\, dV = \int_V \rho\frac{D}{Dt}\left(\frac{1}{2}\vec{u}^2\right) + \int_V \rho\frac{DU}{Dt}\, dV$$

Once again, we can also remove the volume integral that appears in each term, yielding.

$$\rho\frac{D}{Dt}\left(\frac{1}{2}\vec{u}^2\right) + \rho\frac{DU}{Dt} = -\nabla\cdot P\vec{u} + \rho\vec{u}\cdot\vec{f} + \rho\epsilon - \nabla\cdot\vec{F}$$

Expanding the co-moving derivatives, and merging like terms, leaves

$$\frac{\partial}{\partial t}\rho(\frac{1}{2}u^2 + U) + \nabla\cdot(\rho(\frac{1}{2}u^2 + U)\vec{u}$$

$$= -\nabla\cdot P\vec{u} + \rho\vec{u}\cdot\vec{f} + \rho\epsilon - \nabla\cdot\vec{F}$$

Equation of State

The pressure, P, appears in both the momentum and energy equation, yet we have no equation for its evolution.

For all matter, there exist thermodynamic relations linking the pressure, density, temperature, internal energy, entropy…

These are the Equations of State (EoS).

The most widely known is the ideal (monatomic) gas EoS

$$P\,V = R\,T \text{ and } U = \tfrac{3}{2}\,R\,T, \text{ thus } P = \tfrac{2}{3}\,\rho\,U$$

The more generalized version is cast in terms of the adiabatic index $\gamma = C_P/C_V$, the ratio of specific heats.

$$P = (\gamma - 1)\,\rho\,U$$

where $\gamma = 5/3$ for a monatomic gas.

Polytropic Fluid

For the adiabatic case, the ideal gas EoS can be written as

$$P = \mathrm{K}\rho^{\gamma} \qquad \text{in which case} \qquad U = \frac{P}{\gamma - 1} = \frac{\mathrm{K}\rho^{\gamma}}{\gamma - 1}$$

Such EoS are often written in the form

$$P = \mathrm{K}\rho^{1+\frac{1}{n}} \qquad \text{where } n \text{ is called the polytropic index.}$$

These polytopic EoS played a large role in early calculations of stellar structure and remain useful because a number of physical states behave approximately as polytropes.

For example, both the ideal monatomic gas and a non-relativistic degenerate gas obey $P = \mathrm{K}\rho^{5/3}$.

For a relativistic degenerate gas $P = \mathrm{K}\rho^{4/3}$, and stars in radiative equilibrium also follow this relation.

The Equations We Solve

In VH-1, and many similar hydrodynamics codes, the Multi-D problem is *directionally-split* into separate 1D solutions along the representative directions. This simplifies the equations.

$$\frac{\partial \rho}{\partial t} + \frac{\partial A \rho u}{\partial V} = 0$$

To allow for different coordinate systems, we work in terms of a volume coordinate V with cell cross section A

$$\frac{\partial \rho u}{\partial t} + \frac{\partial A \rho u^2}{\partial V} = -\frac{\partial P}{\partial \chi} + \rho f$$

Gradients use a generalized spatial coordinate, χ

$$\frac{\partial \rho v}{\partial t} + \frac{\partial A \rho v u}{\partial V} = 0 = \frac{\partial \rho w}{\partial t} + \frac{\partial A \rho w u}{\partial V}$$

Momentum is also advected transversely.

$$\frac{\partial \rho E}{\partial t} + \frac{\partial A \rho E u}{\partial V} = -\frac{\partial A \rho P u}{\partial V} + \rho u f$$

Total energy $E = \frac{1}{2}(u^2+v^2+w^2) + U$

$$P = (\gamma - 1)\rho U$$

Equation of State

Spatial Differencing

Transforming continuous variables, $f(x)$, to variables represented on a discrete grid, f_j, we must approximate spatial derivates as differences. However, the choice is not unique.

For example, $\partial f/\partial x$ at $x = x_j$ can be written as

$$\left.\frac{\partial f}{\partial x}\right|_j \approx \frac{f_{j+1} - f_j}{\Delta x}$$ forward difference

$$\left.\frac{\partial f}{\partial x}\right|_j \approx \frac{f_j - f_{j-1}}{\Delta x}$$ backward difference

$$\left.\frac{\partial f}{\partial x}\right|_j \approx \frac{f_{j+1} - f_{j-1}}{2\Delta x}$$ centered difference

Higher order derivatives touch more points on the grid, e.g.,

$$\left.\frac{\partial^2 f}{\partial x^2}\right|_j \approx \frac{f_{j+1} - 2f_j + f_{j-1}}{\Delta x^2}$$

Order of Error

Different choices of derivatives affect the error that comes from mapping to a discrete grid. One can estimate this error by calculating $f_{j+1} = f(x_{j+1}) = f(x_j + \Delta x)$ and $f_{j-1} = f(x_{j-1}) = f(x_j - \Delta x)$ using the Taylor series

$$f(x+h) = f(x) + h\frac{\partial f}{\partial x} + \frac{h^2}{2}\frac{\partial^2 f}{\partial x^2} + \cdots$$

to calculate the error as a function of Δx.

For both forward and backward differencing the leading error in the approximation of $\partial f/\partial x$ is $\propto (\Delta x)\ \partial^2 f/\partial x^2$, thus these approximations are $O(\Delta x)$. For centered differencing, the error is $O(\Delta x^2)$ because the $\partial^2 f/\partial x^2$ terms cancel.

While having a smaller truncation error, centered differencing has a tendency to spread sharp features which is detrimental in some circumstances.

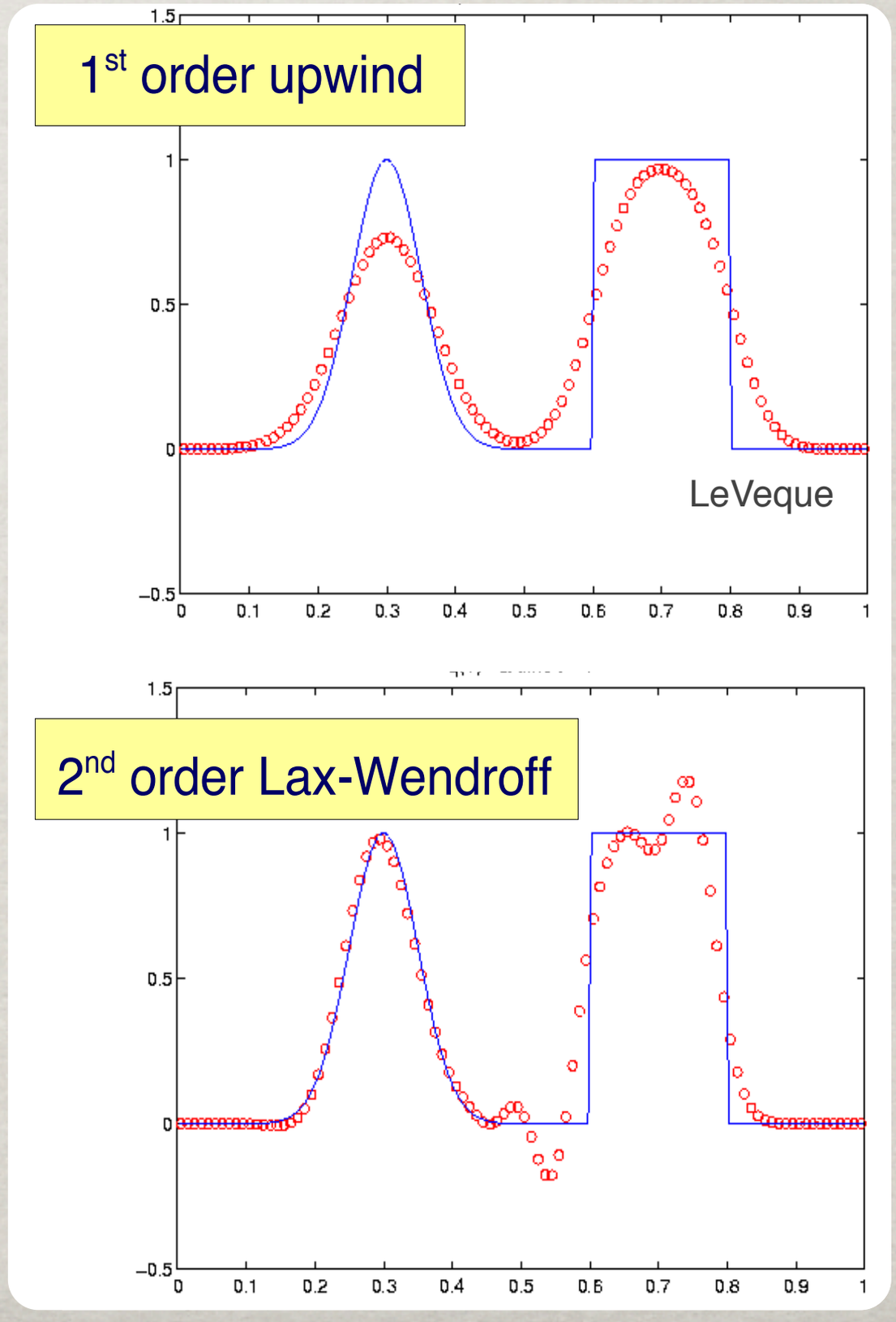
Capturing Shocks

Many problems in nuclear astrophysics include shocks and compositional (contact) discontinuities.

Simple differencing schemes are challenged by sharp flow features like these.

Low order methods tend to diffuse these features over many zones.

Higher order methods are less diffusive, but can add considerable dispersion (noise).



Riemann Problem

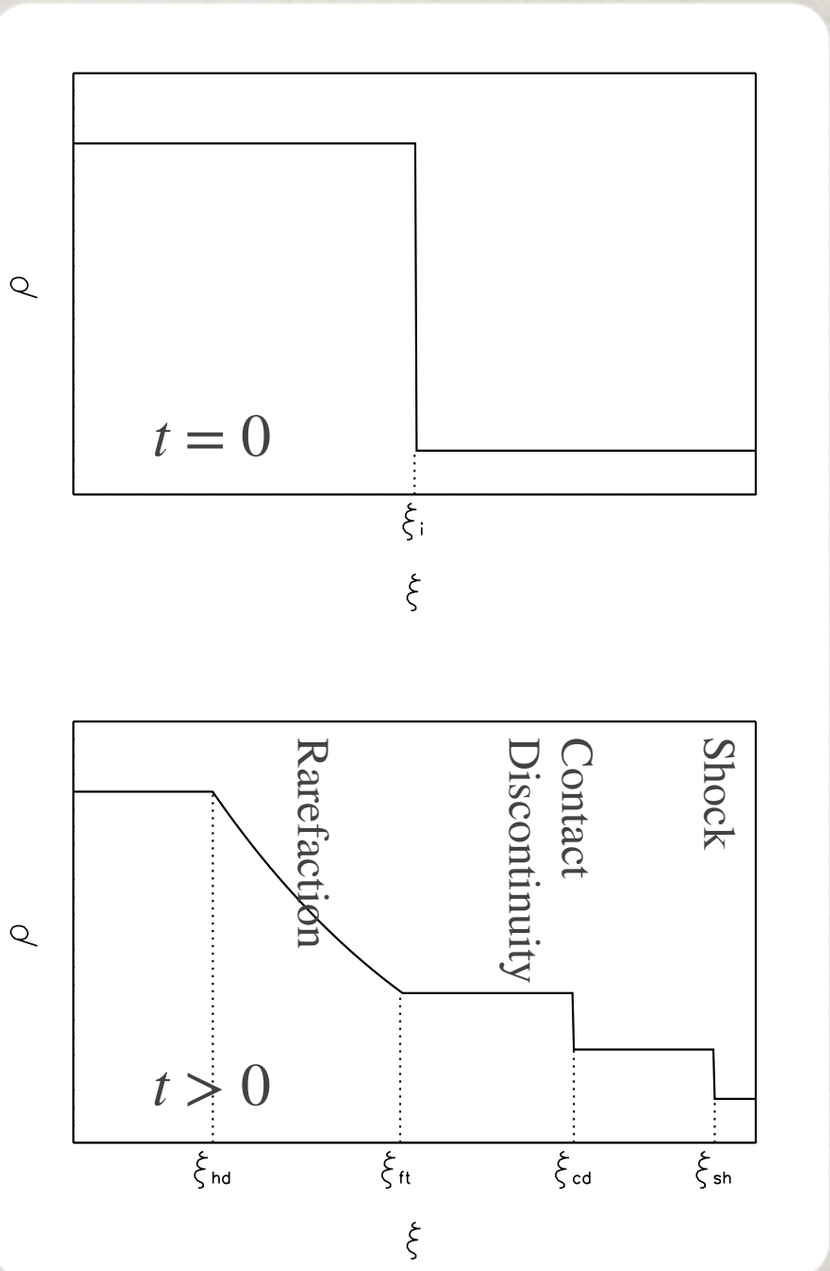
An alternative, from Godunov, is to calculate fluxes by assuming a Riemann problem at each interface.

For left wave, $P^* - P_l + W_l(u^* - u_l) = 0$

For right wave, $P^* - P_r - W_r(u^* - u_r) = 0$

where (P_r, u_r) & (P_l, u_l) characterize the unshocked right and left states, (P^*, u^*) are the unknown shocked state and

$$W_s = \rho_s c_s \left[1 + \frac{\gamma + 1}{2\gamma}\left(\frac{P^* - P_s}{P_s}\right)\right]^{1/2}$$



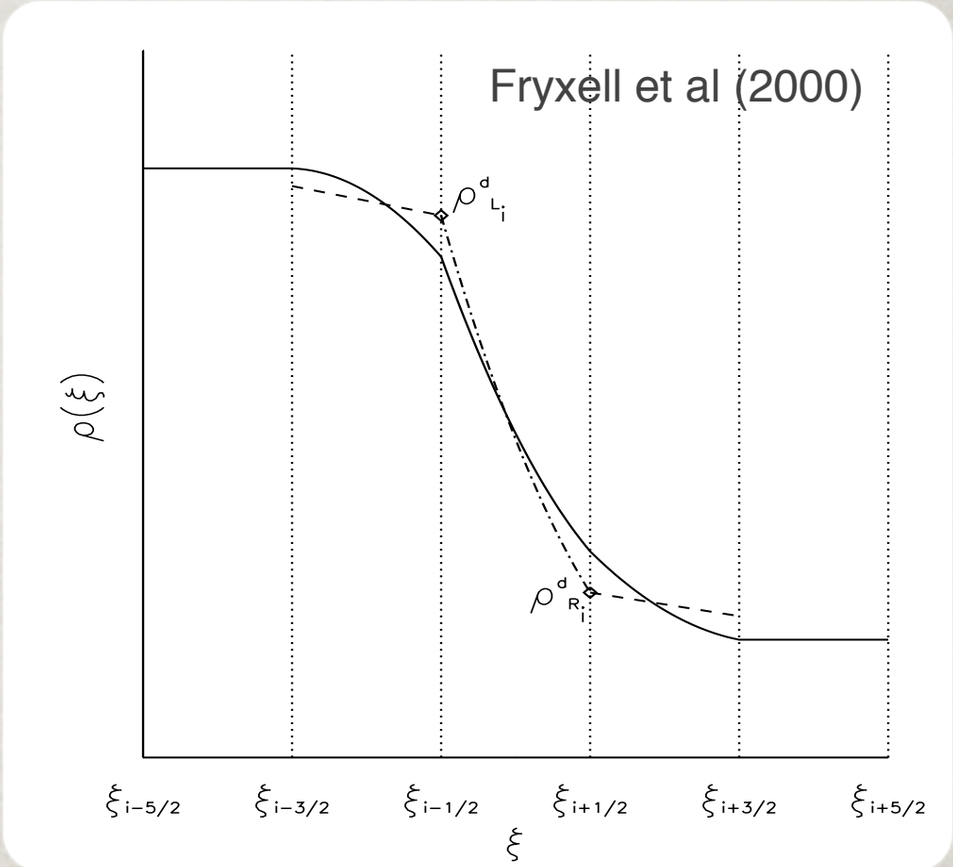
(P^*, u^*) can be calculated (iteratively) from the right and left wave equations and from these fluxes at the interfaces.

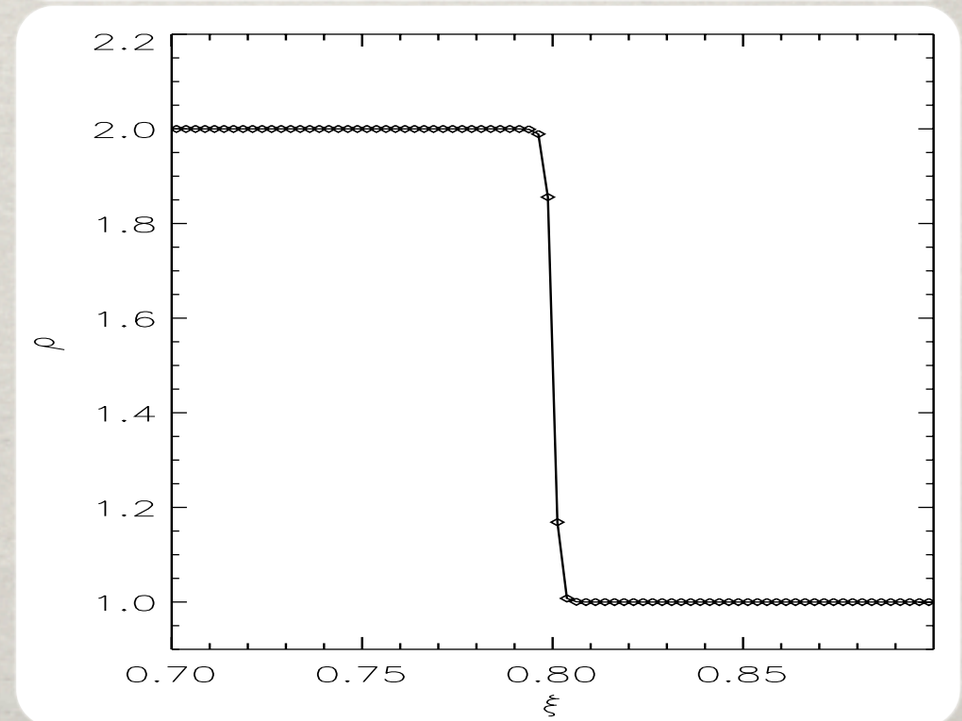
PPM

The Piecewise Parabolic Method, introduced by Colella & Woodward, improves on Godunov's method by using a piecewise parabolic reconstruction of flow variables (akin to Simpson's rule for integration) in place of piecewise constant.

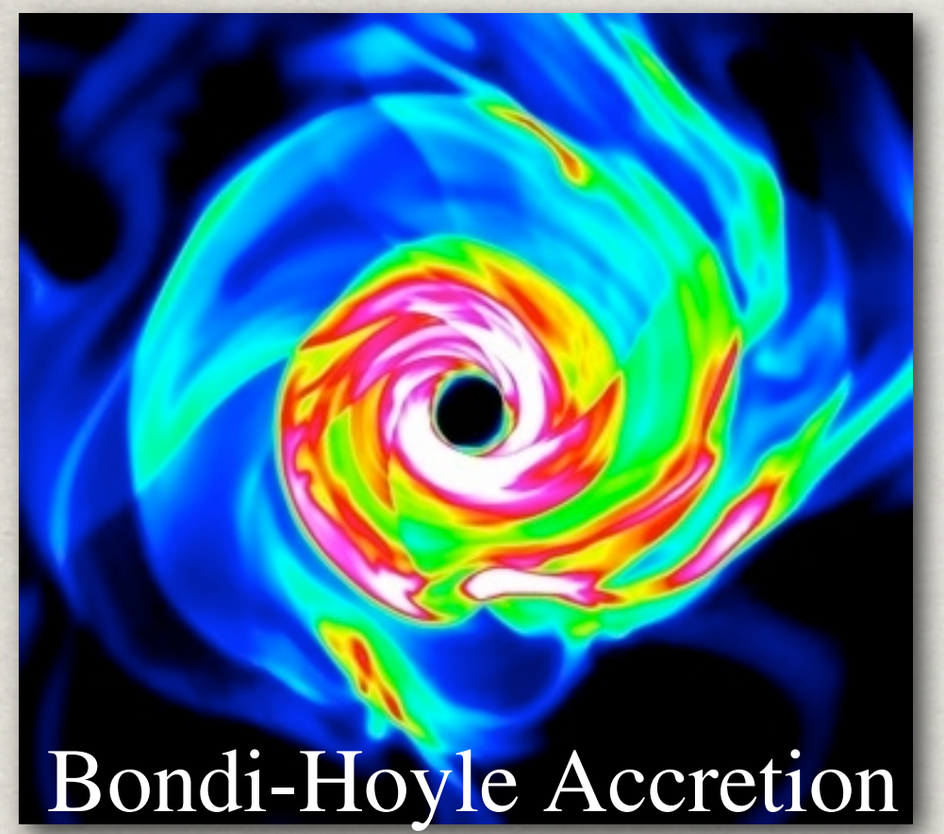
It adds explicit steeping of contact discontinuities and flattening of overly narrow shocks.

FLASH and VH-1 both incorporate implementations of PPM.





VH1 SIMULATIONS



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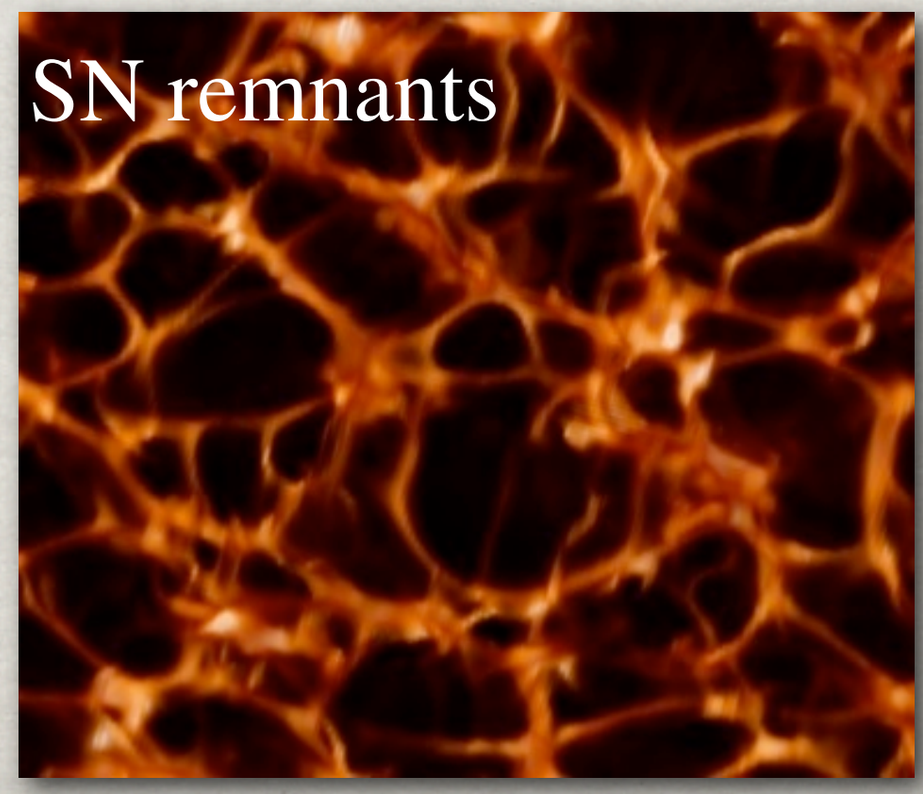
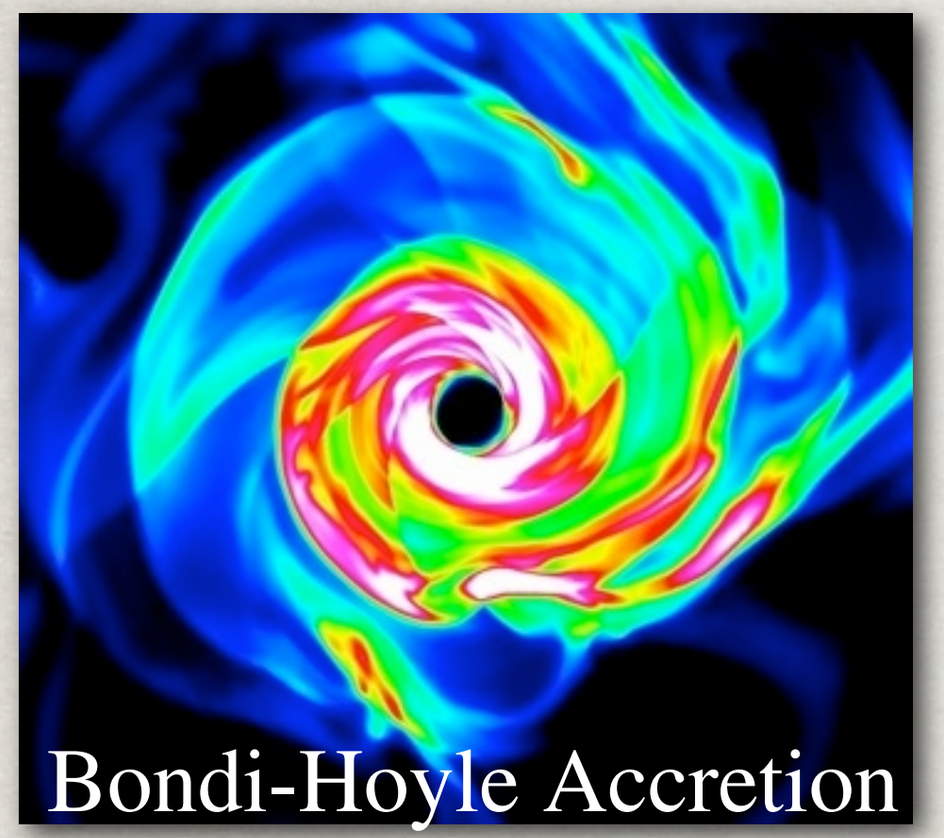
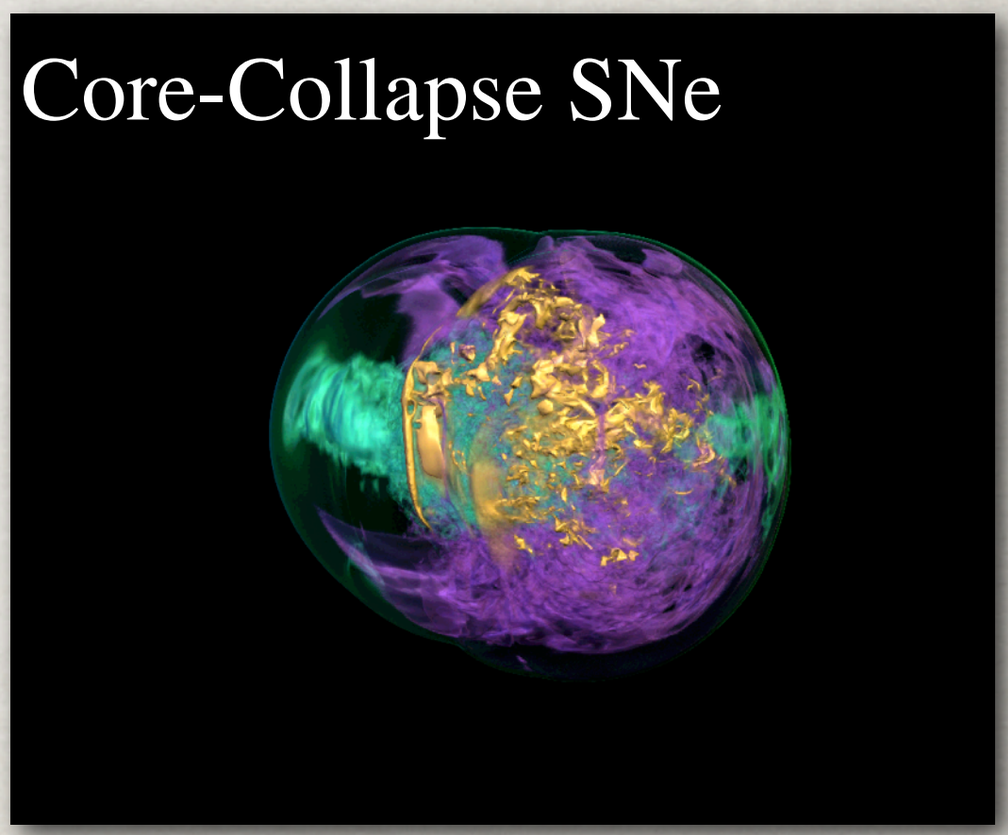
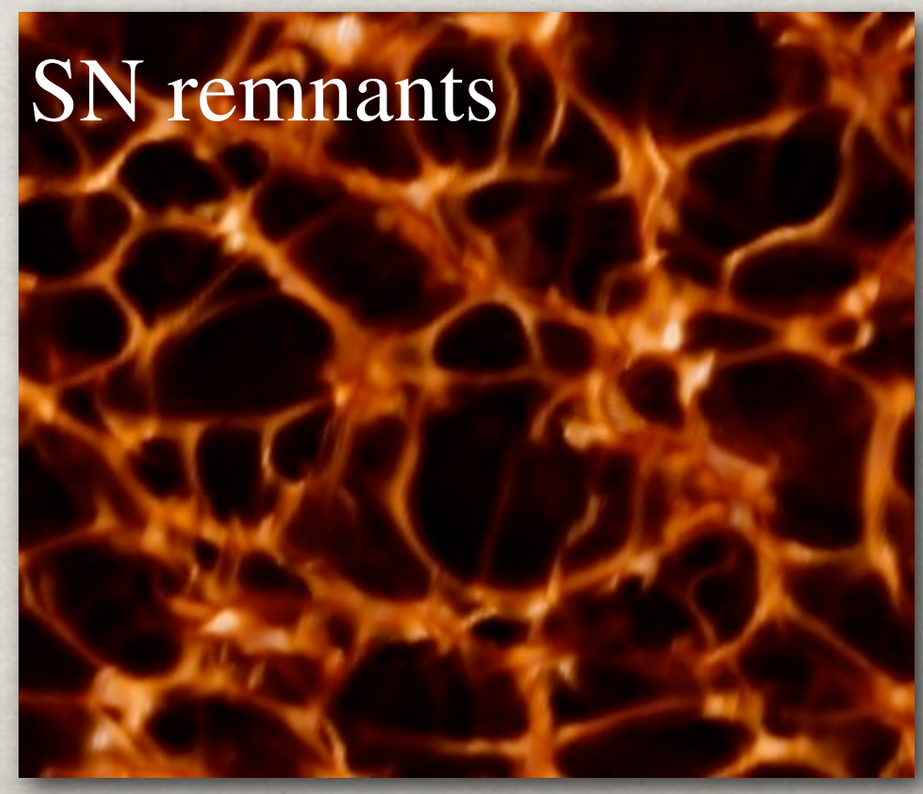


VH1 SIMULATIONS







Where?

http://astro.physics.ncsu.edu/pub/VH-1/index.php

We will follow the Quick Start guide, but we will foolishly jump right into the parallel version of VH-1. This is in blatant disregard of the (wise) advice on the the VH-1 site.

VH1

VH1 is directionally split

The flow solution along each coordinate direction is evolved independently

Many time-orderings are possible, but a standard one is to take half-timesteps in a pattern like:

x-sweep

y-sweep

z-sweep

z-sweep

y-sweep

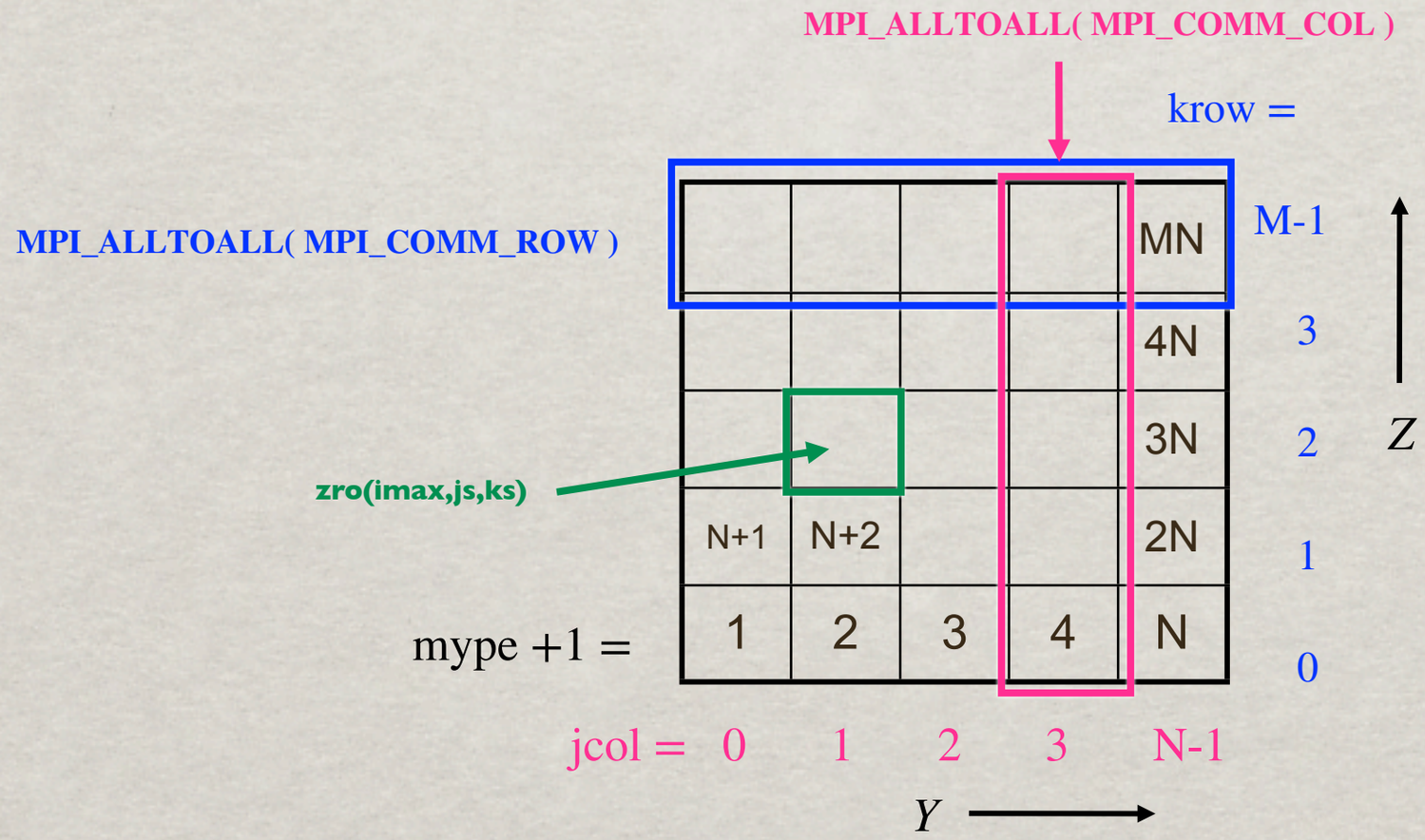
x-sweep

Implementation

This suggests an effective domain decomposition.

Contention is minimized, even though the sub-communicator ALLTOALL's amount to "everybodyTOsomebody"

Using M*N processors; *X* data starts local to proc



What does the code look like?

- The basic structure of the vhone.f90 looks like
  - Read indat file for job control parameters
  - Open history file for recording metadata
  - Create the simulation grid
  - Set initial conditions
  - Loop over time (time = time + dt)
    - Hydrodynamic update (directionally split)
    - Compute maximum stable time step
    - Output data to disk
- If you are not a hydro guy, there might be one surprise: unless you set `ncycend` (and it is not uncommon to set it to some really high number), the application never exits.

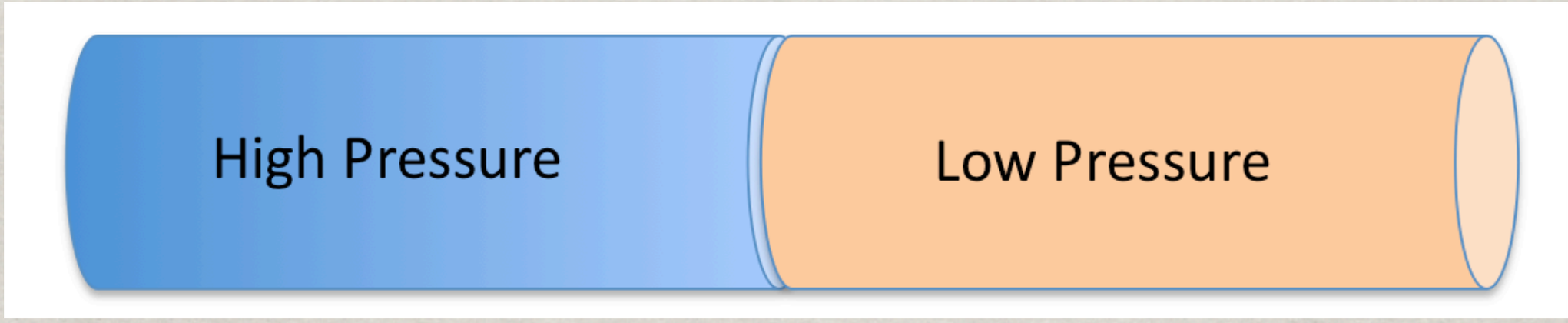
What problem are we doing?

The Sod Shock Tube

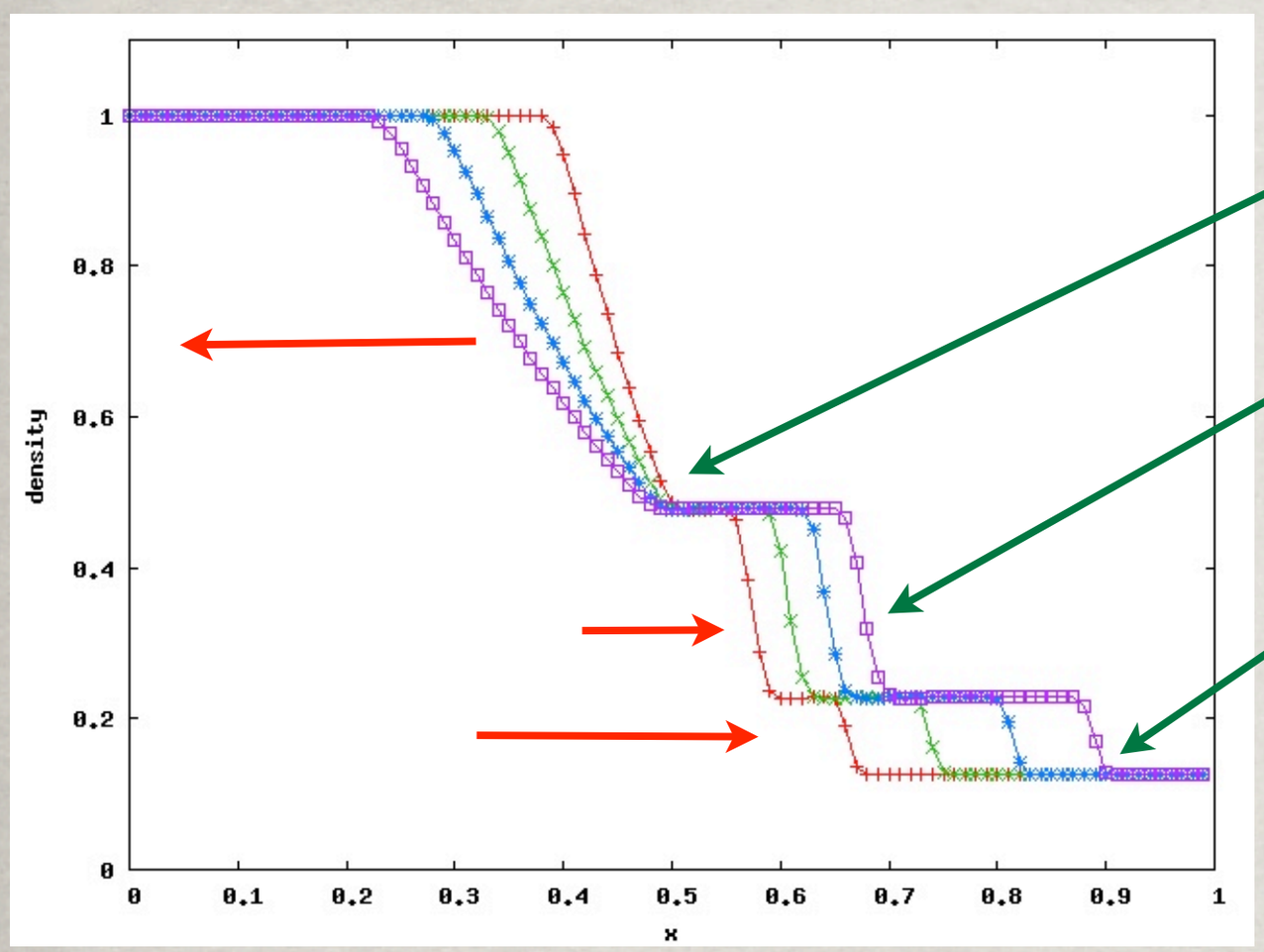
The Sod problem is a particular kind of Riemann problem

PPM uses an iterated solution of the Riemann problem at zone interfaces to evolve the fluxes

If a Godunov code does poorly on Sod, something is amiss...



Sod solution



rarefaction

contact discontinuity

shock