An introduction to finite volume methods and relativistic hydrodynamics

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Plan of this lecture

- Nonlinear hyperbolic equations
- Conservative formulations
- Brief Introduction to Relativistic hydrodynamics

Some representative examples: advection equation Before looking at the solution of the hydrodynamical equations there are some fundamental aspects of their nonlinear properties which must be clarified.

The simplest linear hyperbolic equation is the advection equation

$$\partial_t u(x,t) + \partial_x u(x,t) = 0$$

The solution is the initial data simply translated in space and time.

The propagation speeds are constant everywhere (linear nature of the equation)



Some representative examples: Burgers' equation The simplest nonlinear hyperbolic equation is Burgers' equation $\partial_t u(x,t) + u(x,t)\partial_x u(x,t) = \epsilon(x,t)\partial_x^2 u(x,t)$

where the RHS is assumed zero in the inviscid limit. Despite the remarkable similarity, the solution to this eq. is remarkably different



Some representative examples: Burgers' equation

This behaviour is referred to as "shock steepening" and is the consequence that the propagation speeds are not constant as for the advection equation but are a function of space and time (nonlinear nature of the equation).

Stated differently, the maxima time of the waves move "faster" than the minima and tend to "catch-up".

NOTE: this is a property of the equations and not of the initial data. Even smooth initial data will (eventually) shock in inviscid fluids



Why should we care?

One may think that the shock steeping may happen but on a timescale which is much longer than the one we are interested in

Furthermore, we start from continuous initial data...

Discretizing the equations in general

Let's restrict to a simpler but instructive problem: a homogeneous, flux- conservative differential equation for the scalar function u(x,t) in one dimension

$$\partial_t u(x,t) + \partial_x f[u(x,t)] = 0$$

Its generic, discretized form is (after volume and time integration)

$$\bar{u}_{j}^{n+1} = \bar{u}_{j}^{n} - \frac{\Delta t}{\Delta x} \left(\hat{F}_{j+1/2} - \hat{F}_{j-1/2} \right)$$

where $\bar{u}_i^n = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x, t^n) dx$ is an average and

 $\hat{F}_{j+1/2} \approx \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} f[u(x_{j+1/2}, t)] dt \qquad \text{``some approximation to} \\ \text{the average flux at } j+1/2''$

Any finite-difference form of (1) must represent $F_{j\pm 1/2}$ in the most accurate way. Different ways of calculating $\hat{F}_{j\pm 1/2}$ lead to different evolution schemes (FTCS, Lax, Runge-Kutta, etc..., see www.aei.mpg.de/~rezzolla)

The problem of discretization...

A generic problem arises when a Cauchy problem described by a set of *continuous* PDEs is solved in a *discretized form*: the numerical solution is, at best, *piecewise constant*



This is problematic when discretizing hydrodynamical eqs in compressible fluids.

As for Burgers' eq., the nonlinear properties generically produce, in a finite time, nonlinear waves with discontinuities (ie shocks, rarefaction waves, etc) even from smooth data!

Discontinuous initial data

Burgers' inviscid equation with discontinuous initial data offers a wellknown example of the importance of a proper writing of the equation.



Consider $\partial_t u + u \partial_x u = 0$ with $u(x,0) = \begin{cases} u_L & x \leq x_0 \\ u_R & x \geq x_0 \end{cases}$

The equation can then be written as (light blue line) $\partial_t u + u \partial_x u = 0$

or as (green line) $\partial_t u + \frac{1}{2} \partial_x u^2 = 0$

Mathematically equivalent but the numerical difference is between the right answer (blue line) or a completely wrong one!

Conservative form of the equations

More generally, the homogeneous partial differential equation $\partial_t u(x,t) + a[u(x,t)]\partial_x u(x,t) = 0$

is said to be in flux-conservative (FC) form if written as

 $\partial_t u(x,t) + \partial_x F[u(x,t)] = 0$

Theorems (Lax, Wendroff; Hou, LeFloch)

• FC formulation converges to the weak solution of the problem (ie a solution of the integral form of the fc form)

• NFC converges to the wrong weak solution of the problem In conservative systems (as the hydrodynamic eqs) one usually deals with a set of equations in FC form. Hence, the function uand the flux F(u) are replaced by a state vector U and a flux vector F(U)

Possible solutions to the discontinuities problem:

★ Ist order accurate schemes

• generally fine, but very inaccurate (e.g. excessive diffusion, with Lax method) or across discontinuities (e.g. upwind)

★ 2nd order accurate schemes

 generally introduce oscillations across discontinuities (not "monotonic" or TVD; see dedicated slide)

★ 2nd order accurate schemes with artificial viscosity • mimic Nature but not good in relativistic regimes

★ Godunov Methods

 good compromise between accuracy (2nd order with smooth data, 1st-order at discontinuities) but monotonic.
 Most importantly: discontinuities are exploited The importance of a conservative formulation

If the problem is linear, the importance of a conservative formulation is clear as it allows for analytic solutions.

Rewrite the flux conservative equations

 $\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) = 0$

as

$\partial_t \boldsymbol{U} + \boldsymbol{A} \partial_x \boldsymbol{U} = 0$

where $A(U) \equiv \partial F / \partial U$ is the Jacobian matrix of constant coefficients (the problem is linear). Note that the state vector U is indicated in bold because a

vector of N components

We next diagonalize A(U) so that $\Lambda = R^{-1}AR$ is the diagonal matrix of eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_N$ of the N linear equations, i.e.

$$\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_N)$$

 $R^{(i)}$ are the set of right eigenvectors of A(U) or, equivalently, the columns of the matrix R .

Note that both steps are guaranteed to be possible by the assumption we are dealing with a set of hyperbolic equations Indeed, the set of eqs

$$\partial_t U + A \partial_x U = 0$$

is said to be (strongly) hyperbolic iff A is diagonalizable with a set of real (distinct) eigenvalues λ_i and correspondingly a set of linearly independent (right) eigenvectors $R^{(i)}$ Next we can define the characteristic variables

$$m{W}\equivm{R}^{-1}m{U}$$

so that the original set of equations $\partial_t U + A \partial_x U = 0$ can be written as

$$\partial_t \boldsymbol{W} + \Lambda \partial_x \boldsymbol{W} = 0$$

Because Λ is diagonal, this is effectively a set of N decoupled ODEs along a set of specific curves in the (x, t) plane

Stated differently

$$\partial_t \bar{w}_i + \Lambda \partial_x \bar{w}_i = 0 \iff \frac{\mathrm{d}\bar{w}_i}{\mathrm{d}t} = 0 \quad \text{along} \quad \frac{\partial x}{\partial t} = \lambda_i (\boldsymbol{U}(x,t))$$

so that the characteristic variables are constant along those curves in the (x, t) plane having slope λ_i

Such curves are called characteristic curves and their slope is locally given by the characteristics speeds



Because they remain constant along characteristics, the value the characteristic variables at any time is known once the initial one is determined, i.e.

$$W^{i}(x,t) = W^{i}(x - \lambda_{i}t, t = 0)$$

Once the solution is known in terms of the characteristic variables W^i , it is simple to go back to the original state vector

$$W = R^{-1}U \implies U = RW$$

and hence

$$U(x,t) = \sum_{i=1}^{N} W^{i}(x,t) \mathbf{R}^{(i)} = \sum_{i=1}^{N} W^{i}(x-\lambda_{i}t,0) \mathbf{R}^{(i)}$$

Stated differently, the solution at any time can be seen as the linear superposition of N waves, each propagating independently at the speed given by the corresponding eigenvalue

Finite Volume Approaches

Finite-Volume methods

Godunov methods are tightly related with finite-volume methods. For simplicity, assume a 1-dim. uniform grid.

Finite-Volume Methods are based on subdividing the spatial domain into intervals ("finite volumes" or grid cells) and on keeping track of an approximation to the integral

$$\bar{u}_i^n = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x, t^n) dx$$
, where $\Delta x \equiv x_{i+1/2} - x_{i-1/2}$

over each of these volumes.

If u(x,t) is smooth, then this integral agrees with u(x,t) at the midpoint of the interval to $\mathcal{O}(\Delta x^2)$.

At each time step, we update these values using approximations to the flux through the endpoints of the intervals.

Advantages of finite-volume methods

In terms of finite-volumes, it is easier to use important properties of the conservation laws in deriving numerical methods.

In particular, we can ensure that the numerical method is conservative in a way that mimics the true solution and this is important for correctly calculating shock waves.

The quantity

$$\sum_{i=1}^{N} \bar{u}_i^n \Delta x$$

approximates the integral of u over the entire interval [a, b]

Using a method in conservative form, the discrete sum will change only due to the fluxes at the boundaries x = a and x = b. In this way conservation (eg of mass) is guaranteed provided that the boundary conditions are properly imposed. High-Resolution Shock-Capturing (Godunov) Methods

Based on a simple, yet brilliant idea by Godunov ('59). Example of how basic physics can boost research in computational physics.

Basic idea: a piecewise constant description of hydrodynamical quantities produce a collection of local Riemann problems whose solution can be found exactly.

The solution at time t_{n+1} can be constructed by piecing together the Riemann solutions, provided that the time step is short enough that the waves from two adjacent Riemann problems have not yet started to interact.

What is a Riemann problem?

It's the evolution of a fluid initially composed of two states with different and constant values of velocity, pressure and density, i.e.

$$u(x,0) = \begin{cases} u_L & x \le x_0 \\ u_R & x \ge x_0 \end{cases}$$

where u_L and u_R are the two constant "left" and "right" states



A typical example of a Riemann problem is a "shock-tube" where there is a right-moving shock and a left-moving rarefaction wave.

Not the development of a constant state between the two waves and the presence of a contact discontinuity where the density is discontinuous but pressure and velocity are not High-Resolution Shock-Capturing (Godunov) Methods

In other words, the flux $F_{j+1/2}$ discussed in the previous slides and needed to evolve the state vector to the new timelevel is in this case given by

$$\hat{F}_{j\pm 1/2} \equiv \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} F[\tilde{u}(x_{j+1/2}, t)] dt$$

where $\tilde{u}(x_{j+1/2}, t), \quad t \in [t^n, t^{n+1}]$

is the exact solution of the Riemann problem with initial data

$$\tilde{u}(x_{j\pm 1/2}, t^n) = \begin{cases} u_L(x, t^n) & \text{for } x < x_{j\pm 1/2} \\ u_R(x, t^n) & \text{for } x > x_{j\pm 1/2} \end{cases}$$

Solving the Riemann problem

The solution of such a problem is particularly simple because the states are constant. In particular, given initial data

$$u(x,0) = \begin{cases} u_L & x \le 0\\ u_R & x \ge 0 \end{cases}$$

the two constant "left" and "right" states can be decomposed in terms of the characteristic variables as

$$u_L = \sum_i^N w_L^i r^i , \qquad u_R = \sum_i^N w_R^i r^i$$

The initial data for the *i*-th characteristic $w^i(x,0) = \begin{cases} w_L^i & x \leq 0 \\ w_R^i & x \geq 0 \end{cases}$ variable will be:

and each of the *i* waves $w^i(x,t) = \begin{cases} w^i_L & x - \lambda_i t \leq 0 \\ w^i_R & x - \lambda_i t \geq 0 \end{cases}$ will propagate as

Solving the Riemann problem

The solution is written as a linear superposition of waves

$$u(x,t) = \sum_{\substack{\forall i \mid x - \lambda_i t \leq 0}}^{N} w_L^i r^i n + \sum_{\substack{\forall i \mid x - \lambda_i t \geq 0}}^{N} w_R^i r^i$$

In other words, the solution at any point (x,t) is the sum of the left states of all the waves which are to the right of (x,t) and of the right states of all the waves which are to the left of (x,t)

Once $x - \lambda_i t$ changes sign, the corresponding conserved variable changes from w_R^i to w_L^i while all the other w^i with remain constant.

Finally, because $F = AU = ARW = \Lambda RW = \Lambda U$, the jump in the fluxes for the *i-th* wave are

$$F_R^i - F_L^i = \lambda_i (w_R^i - w_L^i) r^i$$

rarefaction wave shock front



Solution at the time n+1 of the two Riemann problems at the cell boundaries $x_{j+1/2}$ and $x_{j-1/2}$

Spacetime evolution of the two Riemann problems at the cell boundaries $x_{j+1/2}$ and $x_{j-1/2}$. Each problem leads to a shock wave and a rarefaction wave moving in opposite directions

Initial data at the time *n* for the two Riemann problems at the cell boundaries $x_{j+1/2}$ and $x_{j-1/2}$

cell boundaries where fluxes are required

A quick primer of HRSC methods...

The numerical solution of a Riemann problem is based on three basic steps:

1) reconstruct a piecewise polynomial function from the cell averages:

 $\tilde{u}(x,t^n) = g(\bar{u}_{i+k-j}^n) \quad \forall x \in [x_{i-1/2}, x_{i+1/2}]$ A piecewise constant is the simplest reconstruction

2) evolve the hyperbolic eq. (exactly or approximately) using these initial data to obtain $\tilde{u}(x, t^{n+1})$ after a time Δt

3) **average** this solution over each grid cell to obtain a new cell average

$$\bar{u}_i^{n+1} = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \tilde{u}(x, t^{n+1}) dx$$

I) First reconstruct...



Higher accuracy is reached with a better representation of the solution.

"Reconstructing" the initial data for the Riemann problem at the cell boundaries can be made with a number of algorithms

The most interesting are the TVDs (minmod, MC, Superbee) for which the solution is

 $u(x) = \phi(u)u^{2nd-ord} + [1 - \phi(u)]u^{1st-ord}$

linear reconst.

Here ϕ is a coefficient based on the slope of u and varying from 0 (near a discontinuity) up to 1 (in smooth regions of the solution).

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- slope limiter

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2) then evolve...

As an example, Roe's approximate Riemann solver can be calculated as

$$\hat{F}_i = \frac{1}{2} \left[F_i(w_R) + F_i(w_L) - \sum_{n=1}^5 |\lambda_n| \Delta \tilde{\omega}_n \tilde{R}_n \right]$$

where w_R , w_L are the values of the primitive variables at the right/left sides of the *i*-th interface and $\{\lambda_n, \tilde{R}_n\}$ are the eigenvalues and right eigenvectors of the Jacobian matrix.

The coefficients $\Delta \tilde{\omega}_n$ measure the jumps of the characteristic variables across the characteristic field

$$U(w_R) - U(w_L) = \sum_{n=1}^{5} \Delta \tilde{\omega}_n \tilde{R}_n$$

3) finally: average, convert and build...

Once the solution in terms of the conserved variables D, S_j, τ has been obtained, it is necessary to return to the primitive variables after inverting numerically the set of equations

> $D = \rho W , \qquad \rho ,$ $S_j = \rho h W^2 v_j , \qquad \longrightarrow \qquad v_j ,$ $\tau = \rho h W^2 - \rho W - p \qquad \epsilon .$

Note: this conversion cannot be done analytically and requires the solution of a set of coupled eqs. This root-finding operation is very expensive computationally.

With the primitive variables calculated, the stress-energy tensor can be reconstructed and used on the RHS of the Einstein eqs.

This series of operations is repeated at each grid point and for each time level...

Relativistic Hydrodynamics

Numerical Relativity: how?...

In non-vacuum spacetimes (like ours!) we need to solve for the full set of equations:

$$egin{aligned} G_{\mu
u} &= R_{\mu
u} - rac{1}{2}g_{\mu
u}R = 8\pi T_{\mu
u} \ &
abla &= 0 \ , \ &
abla &= 0 \ , \ &
abla &= p(
ho, \epsilon, \ldots) \ . \end{aligned}$$

(conservation of energy – momentum) (conservation of baryon number)

(equation of state)

(field equations)

where

$$T_{\mu\nu} = T^{\text{fluid}}_{\mu\nu} + T^{\text{em}}_{\mu\nu} + \dots$$

We start again with a 3+1 split and thus a line element $ds^2 = g_{\mu\nu}dx^{\mu}dx^{\mu} = -(\alpha^2 - \beta^i\beta_i)dt^2 + 2\beta_i dx^i dt + \gamma_{ij}dx^i dx^j$ And introduce a fluid (collection of particles) with 4-velocity \boldsymbol{u}



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$$u^{\mu}u_{\mu} = -1 = n^{\mu}n_{\mu}$$

both unit and timelike, i.e.

But they are really different: one is tracks the normal to the slice the other is the worldline of a fluid particle

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And introduce a fluid (collection Note the difference between the of particles) with 4-velocity $m{u}$ normal unit vector $m{n}$ to the slice



Note the difference between the normal unit vector n to the slice and the fluid 4-velocity u. They are both unit and timelike, i.e.

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But they are really different: one is tracks the normal to the slice the other is the worldline of a fluid particle. In addition there is always the natural time vector t

Overall, there are three 4-vectors to bear in mind: n, t, u

3+1 splitting also for the matter What we are really interested in, however, is not the 4-velocity u but rather its projection on the spatial slice, ie the 3-velocity v



Those observers with \boldsymbol{u} parallel to \boldsymbol{n} move from one slice to the next along the normal to the slice and are therefore Eulerian observers. They measure a fluid 3-velocity

$$v = rac{oldsymbol{\gamma} \cdot oldsymbol{u}}{-n \cdot oldsymbol{u}}$$

Remember in fact that in special relativity

$$u^{i} = \frac{dx^{i}}{d\tau}$$
, $v^{i} = \frac{dx^{i}}{dt} = \frac{dx^{i}}{d\tau}\frac{d\tau}{dt} = \frac{u^{i}}{u^{0}}$

The contravariant (upstairs) components of this vector are



The relativistic hydrodynamics(MHD) eqs simply express the conservation of energy, momentum, baryon number

 $\gamma \cdot (\nabla T) = 0$, (spacelike projection of divergence of T) conservation of momentum

 $n \cdot (\nabla T) = 0$, (timelike projection of divergence of T) conservation of energy

 $(\nabla \cdot \rho \boldsymbol{u}) = 0$, (divergence of mass flux)

conservation of baryon number $p = p(\rho, \epsilon)$, (equation of state EOS) thermodynamics

where

$$T^{\mu\nu} = T^{\mu\nu}_{\text{fluid}} + T^{\mu\nu}_{\text{em}} + \dots$$
$$T^{\mu\nu} = (\rho + \rho\epsilon + p + b^2)u^{\mu}u^{\nu} + \left(p + \frac{b^2}{2}\right)g^{\mu\nu} - b^{\mu}b^{\nu} + \dots$$

The Valencia (conservative) formulation

Consider for simplicity an non-magnetized ideal fluid with stress energy tensor $T^{\mu\nu} = (\rho + \rho\epsilon + p)u^{\mu}u^{\nu} + g^{\mu\nu}$ $= (e+p)u^{\mu}u^{\nu} + q^{\mu\nu}$

$$= h\rho u^{\mu}u^{\nu} + g^{\mu\nu}$$

where

 $\rho \quad (\text{rest} - \text{mass density}); \quad e = \rho(1 + \epsilon) \quad (\text{energy density}) \\ \epsilon \quad (\text{specifig internal energy}); \quad h = (e + p)/\rho \quad (\text{specific enthalpy})$

As mentioned before, the hydrodynamics eqs are then given by

$$\begin{split} \gamma^{i}{}_{\nu}T^{\mu\nu}{}_{;\mu} &= 0 , \qquad (\text{conservation of momentum}) \\ u_{\nu}T^{\mu\nu}{}_{;\mu} &= 0 , \qquad (\text{conservation of energy}) \\ \rho_{,\mu}u^{\mu} + \rho u^{\mu}{}_{;\mu} &= 0 , \qquad (\text{conservation of baryon no.}) \\ p &= p(\rho, \epsilon) , \qquad (\text{EOS}) \end{split}$$

The Valencia (conservative) formulation

The first step in rewriting the above equations in a FC form requires the identification of suitable "conserved" quantities in place of the "primitive" variables (ρ, ϵ, v^j) . A little algebra shows that these are:

$$D = \rho W ,$$

$$S_j = \rho h W^2 v_j ,$$

$$\tau = \rho h W^2 - \rho W - p$$

where $W = (1 - \gamma_{ij}v^iv^j)^{-1/2} = \alpha u^0$ is the Lorentz factor

NOTE: while the conversion primitive-to-conserved is algebraic, the inverse one is not and needs an expensive numerical solution.

In this way one obtains the "Valencia" formulation (Banyuls et al. 97) of the relativistic hydrodynamics equations $\frac{1}{\sqrt{-g}} \left\{ \partial_t \left[\sqrt{\gamma} \mathbf{F}^0(\mathbf{U}) \right] + \partial_i \left[\sqrt{\gamma} \mathbf{F}^i(\mathbf{U}) \right] \right\} = \mathbf{s}(\mathbf{U}) ,$

where
$$\sqrt{-g} = \sqrt{\det(g_{\mu\nu})} = \alpha \sqrt{\det(\gamma_{\mu\nu})} = \alpha \sqrt{\gamma}$$
 and
 $\mathbf{F}^0(\mathbf{U}) = (D, S_j, \tau)^T$,

$$\mathbf{F}^{i}(\mathbf{U}) = [D(\alpha v^{i} - \beta^{i}), S_{j}(\alpha v^{i} - \beta^{i}) + p\delta_{j}^{i}, \tau(\alpha v^{i} - \beta^{i}) + pv^{i}]^{T}$$

$$\mathbf{s}(\mathbf{U}) = \left| 0, T^{\mu\nu} \left(\partial_{\mu} g_{\nu j} + \Gamma^{\delta}_{\mu\nu} g_{\delta j} \right), \alpha \left(T^{\mu 0} \partial_{\mu} \ln \alpha - T^{\mu\nu} \Gamma^{0}_{\nu\mu} \right) \right| \,.$$

NOTE: the source terms do not contain derivatives of the hydrodynamical quantities (leaving intact the principal part) and vanish in a flat spacetime

$$(-g)^{-1/2}\partial_t(\sqrt{\gamma}\rho W) + \partial_i(\sqrt{-g}\rho W v^i) = 0,$$

general relativistic

$$\begin{aligned} (-g)^{-1/2}\partial_t(\sqrt{\gamma}\rho hW^2v^j) + \partial_i(\sqrt{-g}(\rho hW^2v^iv^j + p\delta^{ij})) &= \\ T^{\mu\nu}(\partial_\mu g_{\nu j} - \Gamma^{\delta}_{\ \mu\nu}g_{\delta j}), \end{aligned}$$

$$(-g)^{-1/2}\partial_t(\sqrt{\gamma}(\rho hW^2 - p - \rho W)) + \partial_i(\sqrt{-g}v^i(\rho hW^2 - \rho W)) = \alpha(T^{\mu 0}\partial_\mu(\ln \alpha) - T^{\mu \nu}\Gamma^0_{\mu \nu}),$$

$$\partial_t(\rho W) + \partial_i(\rho W v^i) = 0,$$

special relativistic

 $\partial_t(\rho h W^2 v^j) + \partial_i(\rho h W^2 v^i v^j + p \delta^{ij}) = 0,$

 $\partial_t(\rho hW^2 - p - \rho W) + \partial_i(v^i(\rho hW^2 - \rho W)) = 0$

 $\begin{aligned} \partial_t \rho + \partial_i (\rho v^i) &= 0 , \\ \partial_t (\rho v^j) + \partial_i (\rho v^i v^j + p \delta^{ij}) &= 0 , \\ \partial_t (\rho \epsilon + \rho v^2/2) + \partial_i (v^i (\rho \epsilon + \rho v^2/2 + p)) &= 0 \end{aligned}$

Newtonian non self-gravitating fluid

Summary

The solution of the hydrodynamics equations requires special care because of the nonlinear nature of the equations

Even smooth initial data tends to steepen and shock; in addition any discretization leads to small discontinuities

Using a flux-conservative formulation is essential if modelling discontinuities

MRSC methods are particularly suited to study discontinuities since they treat the discontinuities across cell interfaces as local Riemann problems

HRSC methods are based on three different steps: reconstruct, evolve, average