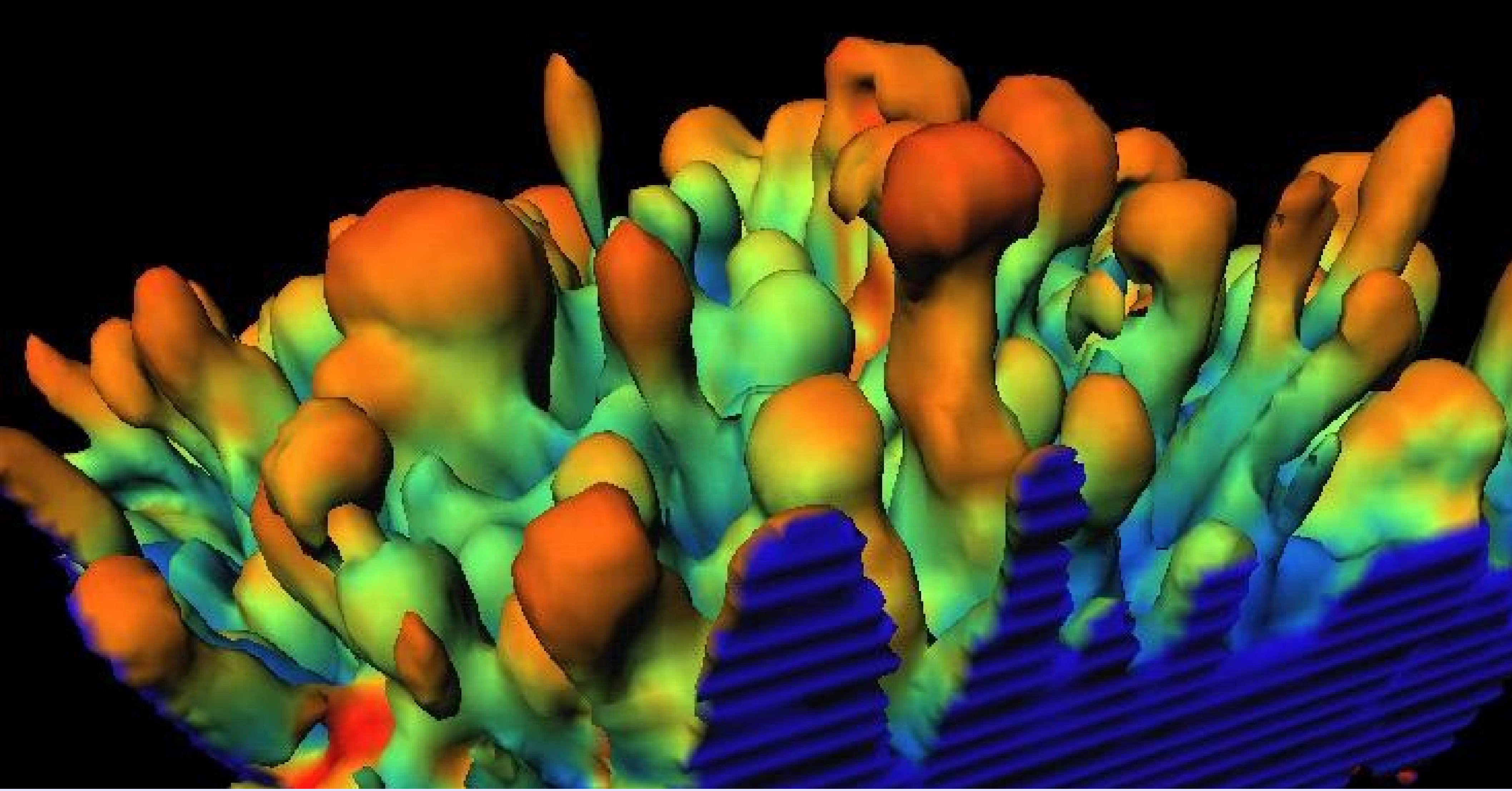


An Introduction to Computational Fluid Dynamics

Ewald Müller
Max-Planck Institut für Astrophysik

Some Basic Hydrodynamics

Hydrodynamic equations are derivable from

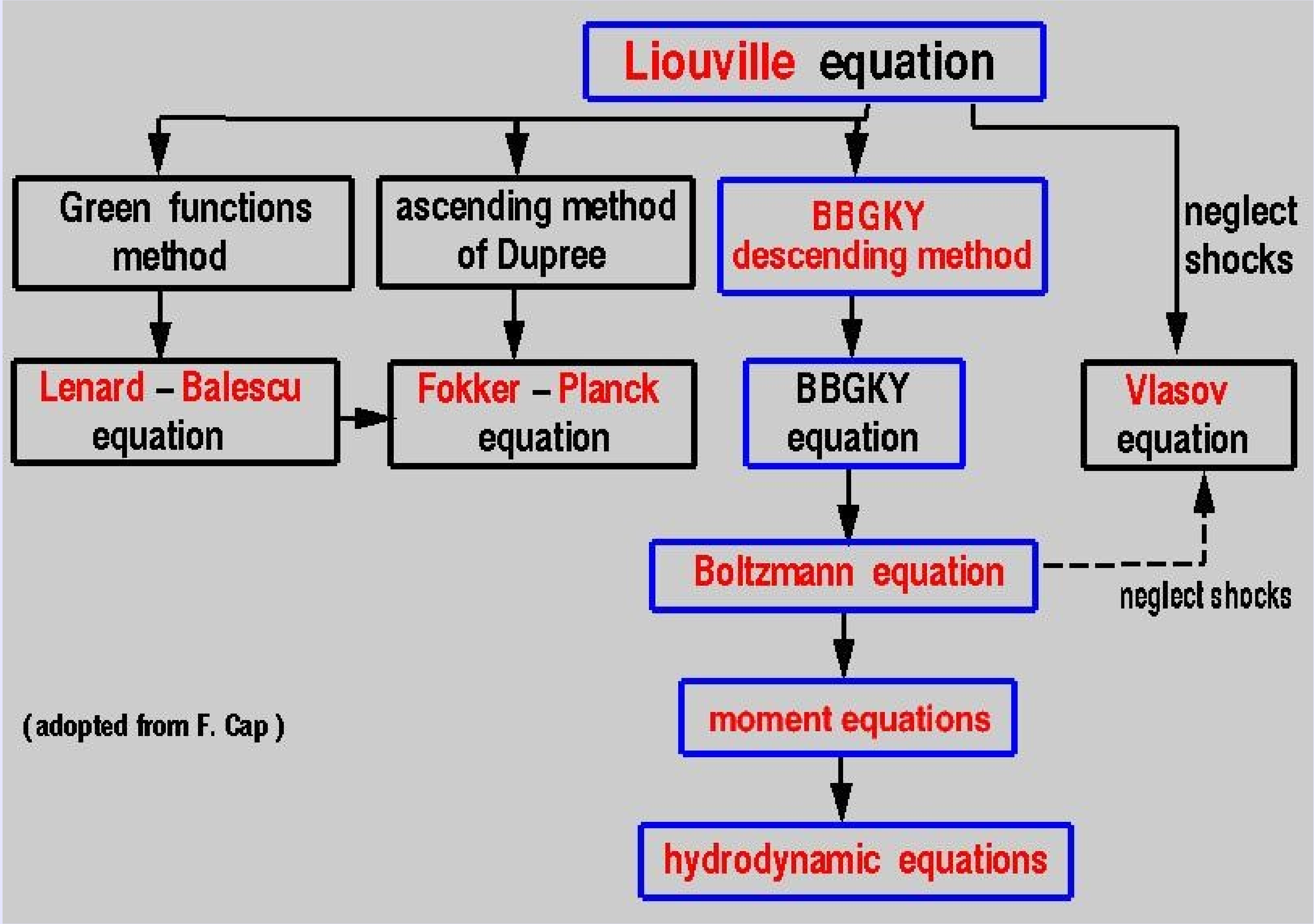
microscopic kinetic equations (Liouville, Boltzmann)

under two assumptions

(i) microscopic behaviour of single particles can be neglected ($\lambda << L$)

(ii) forces between particles do saturate (short range forces!)

---> gravity must be treated as external force!


Liouville equation
Green functions method
ascending method of Dupree
BBGKY descending method
neglect shocks
Lenard – Balescu equation
Fokker – Planck equation
BBGKY equation
Vlasov equation
Boltzmann equation
neglect shocks
moment equations
hydrodynamic equations
(adopted from F. Cap)

hydrodynamic approximation holds

--> **set of conservation laws**

simplest case: single, ideal, non-magnetic fluid; no external forces

mass:

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \vec{v}) = 0$$

momentum:

$$\frac{\partial \varrho \vec{v}}{\partial t} + \nabla \cdot (\varrho \vec{v}\vec{v} + p \underline{\underline{I}}) = 0$$

energy:

$$\frac{\partial \varrho E}{\partial t} + \nabla \cdot ([\varrho E + p]\vec{v}) = 0$$

hyperbolic system of PDEs

hydrodynamic approximation holds

general case: additional equations and/or

additional source terms

describe effects due to

- viscosity (*e.g.,* accretion disks)
- reactions (*e.g.,* nuclear burning, non-LTE ionization)
- conduction (*e.g.,* cooling of WD & NS; ignition of SNe Ia)
- radiation transport (*e.g.,* stars: photons; CCSNe: neutrinos)
- magnetic fields (*e.g.,* stars, jets, pulsars, accretion disks)
- self-gravity (stars, galaxies, Universe)
- relativity (jets, NS, BH, GRB)

eg., viscous, self-gravitating Newtonian flow

mass:

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \vec{v}) = 0$$

momentum:

$$\frac{\partial \varrho \vec{v}}{\partial t} + \nabla \cdot (\varrho \vec{v} \vec{v} + p \underline{\underline{I}} - \underline{\underline{\pi}}) = -\varrho \nabla \Phi$$

energy:

$$\frac{\partial \varrho E}{\partial t} + \nabla \cdot [(\varrho E + p) \vec{v} + \vec{h} - \underline{\underline{\pi}} \vec{v}] = -\varrho \vec{v} \nabla \Phi$$

Poisson eq.:

$$\Delta \Phi = 4 \pi G \varrho$$

Astropysical applications:

- viscosity & heat conduction often negligibly small
  (except in shock waves)

  --> inviscous Euler eqs instead of viscous Navier-Stokes eqs are solved

- numerical methods posses numerical viscosity
  (depending on grid resolution)

  --> strange situation:

  One tries to solve inviscous Euler eqs, but instead solves a viscous variant, different from Navier-Stokes eqs !!

hydrodynamic equations are incomplete

(closure relation missing)

---> equation of state required to close system

$$p = p(\varrho, T)\ , \quad \varepsilon = \varepsilon(\varrho, T)$$

discontinuous solutions of Euler eqs. exist

(weak solutions: shocks, contact discont.)

---> conservation laws in integral form

jump conditions (Rankine-Hugoniot)

flows characterizable by dimensionless numbers

Reynolds number: $Re = uL/\nu$ (ν kinematic viscosity)

measures relative strength of inertia & dissipation; often very large in astrophysics ($>10^{10}$)

For all flows there exists a critical Reynolds number, above which the flow becomes turbulent!

Prandtl number: $Pr = \nu/\kappa$ (κ: conductivity)

measures relative strength of dissipation & conduction

Hyperbolic Systems of Conservation Laws

HD eqs are special case of a system of conservation laws

$$\frac{\partial \vec{U}}{\partial t}+\sum_{j=1}^{d}\frac{\partial \vec{F}_j(\vec{U})}{\partial x_j}=0$$

with $\mathbf{x} = (x_1, \dots , x_d) \in R^d$

$\mathbf{U} = (U_1, \dots , U_p)^T$ vector of functions of **x** and t

$\mathbf{F}_j(\mathbf{U}) = (F_{1j}, \dots , F_{pj})^T$ vector of fluxes

Let D be an arbitrary domain of R^d and let $\mathbf{n} = (n_1, \dots , n_d)$ be the outward unit normal of the boundary ∂D of D. Then

$$\frac{d}{dt}\int_D \vec{U}\, d\vec{x}+\sum_{j=1}^{d}\int_{\partial D}\vec{F}_j(\vec{U})\, n_j\, dS=0$$

temporal change of state vector in domain equal to gains and losses through boundary of domain

Hyperbolic systems of conservation laws

For all $j=1, \ldots, d$ let

$$A_j(\vec{U}) = \frac{\partial \vec{F}_j(\vec{U})}{\partial \vec{U}}$$

be the Jacobian (matrix) of $F_j(U)$

System is called hyperbolic, if for any U and any $\omega = (\omega_1, \ldots, \omega_d) \in R^d$ the matrix

$$A(\vec{U}, \omega) = \sum_{j=1}^{d} \omega_j \vec{A}_j(\vec{U})$$

Has p real eigenvalues (if all distinct, system is strictly hyperbolic)

$$\lambda_1(\vec{U}, \omega) \leq \lambda_2(\vec{U}, \omega) \leq \ldots \leq \lambda_p(\vec{U}, \omega)$$

and p linearly independent (right) eigenvectors

$$\vec{r}_1(\vec{U}, \omega), \vec{r}_2(\vec{U}, \omega), \ldots, \vec{r}_d(\vec{U}, \omega)$$

Weak solutions:

U (piecewise smooth function) is weak solution of the integral form of the conservation system, if and only if two conditions hold:

(1) ***U*** is a classical solution in domains where solution is continuous

(2) Across a surface of discontinuity ***Σ*** with normal vector ***n***$=(n_t, n_{x1}, \ldots, n_{xd})$ the Rankine-Hugoniot condition holds

$$(\vec{U}_R - \vec{U}_L) n_t + \sum_{j=1}^{d} [\vec{F}_j(\vec{U}_R) - \vec{F}_j(\vec{U}_L)] n_{xj} = 0$$

For 1D systems the Rankine Hogoniot condition reduces to

$$s(\vec{U}_R - \vec{U}_L) + [\vec{F}(\vec{U}_R) - \vec{F}(\vec{U}_L)] = 0$$

where s is the speed of propagation of the discontinuity

Weak solutions:

Non-uniqueness: different weak solutions exist for the same initial data

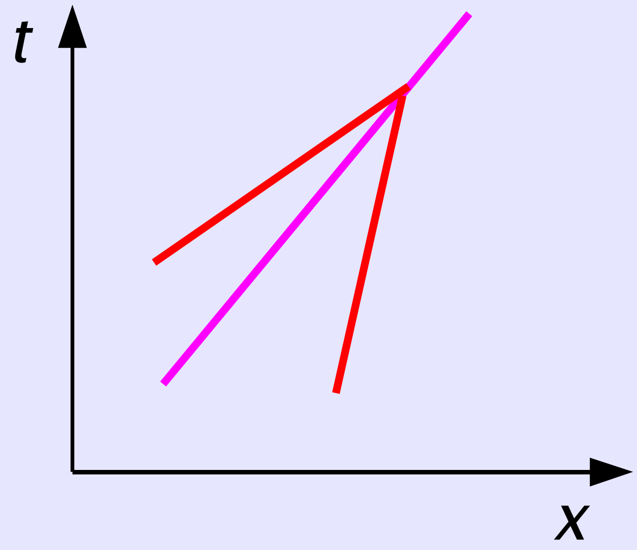
characterization of the unique physically admisible weak solution

Entropy condition (for convex fluxes, *i.e., dF/dU>0*)

scalar case

$$\frac{dF}{dU}(U_L) > s > \frac{dF}{dU}(U_R)$$

characteristics (slope = 1 / speed) approach discontinuity from both sides



Lax entropy condition for systems

discontinuties satisfying the corresponding Rankine-Hugoniot and entropy conditions are called shocks

The Art of Computational Fluid Dynamics

or

For every complex beautiful simulation result
there exists a simple, elegant, convincing,
wrong physical explanation

(adapted from Thomas Gould)

Hydrodynamic equations:

non--linear system of 1st order PDEs

one way to solve equations:

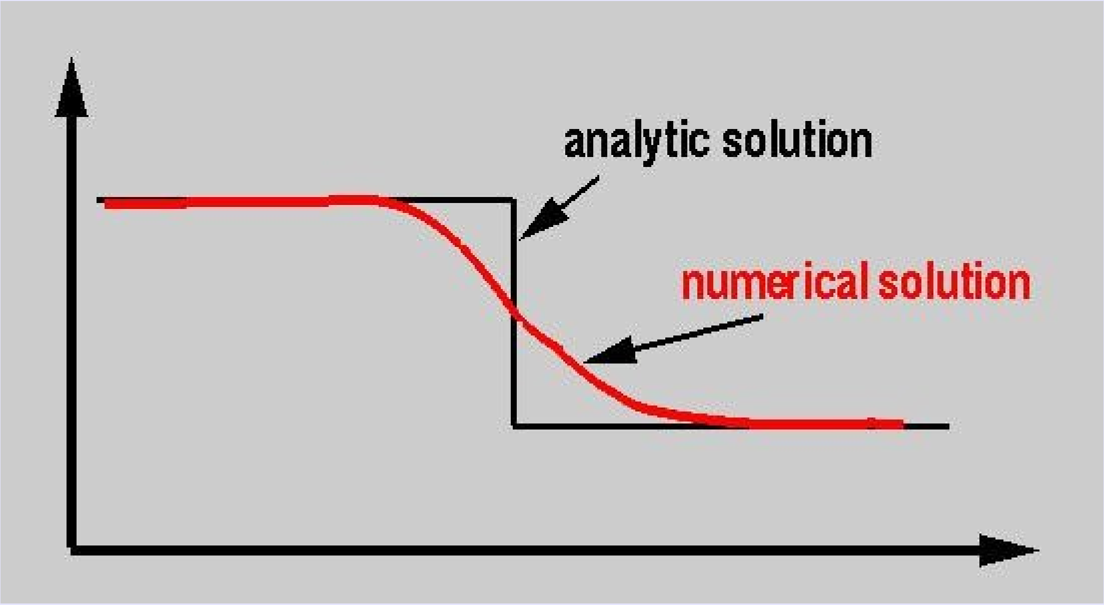
discretization in space & time

PDEs ---> set of coupled algebraic eqs

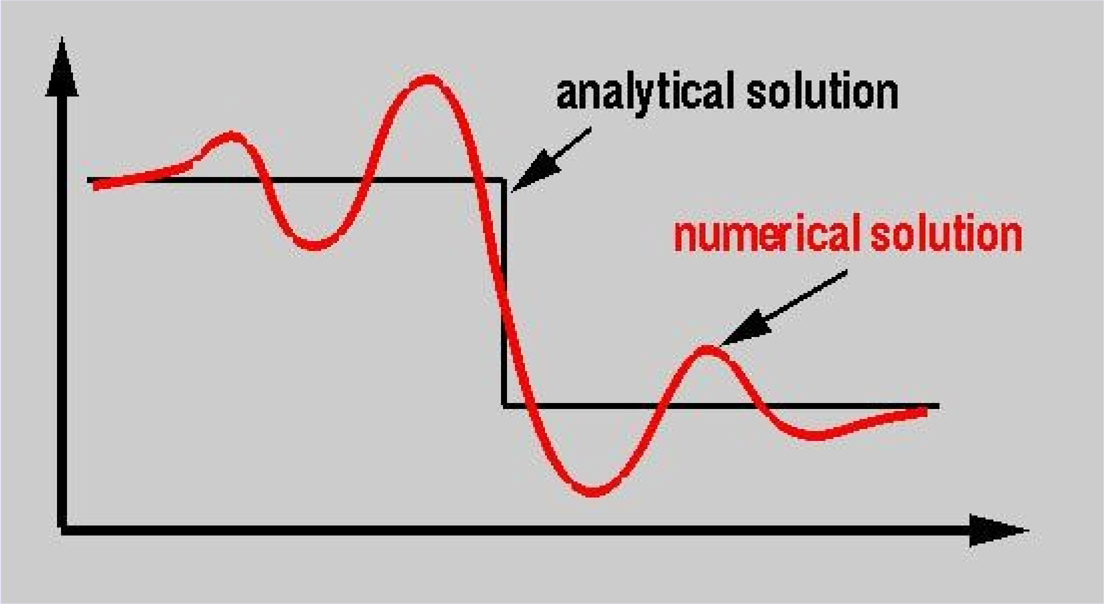
finite difference (FD), finite volume (FV), method of lines (MOL)

introduces unavoidable errors

--> It is crucial to use methods, which minimize the errors!



numerical diffusion



numerical dispersion

HD equations can be formulated with respect to
two distinct classes of coordinate systems

Eulerian <===> fixed coordinates (time independent)

Disadvantage: :numerical diffusion due to nonlinear advection terms (***v*** *grad*)

Lagrangian <===> comoving coordinates (moving with the fluid/gas)

Advantage: no numerical diffusion of mass,momentum, etc

Disadvantage: grid tangling (in case of shear or vortex flow)

--> rezoning required which causes numerical diffusion

--> major advantage lost!

===> Eulerian coordinates are to be preferred for multidimensional problems

but special efforts are necessay to minimize the inevitable numerical diffusion

---> use more accurate, high-order numerical schemes

Alternative: free-Lagrange methods

i.e. grid free methods, where gradients are evaluated without the use of any grid

---> no grid tangling, no rezoning

Most commonly used variant in astrophysics:
Smoothed Particle Hydrodynamics

Explicit and implicit methods

neglecting terms higher than 2nd order the most general (one-step) discretization of the HD eqs with respect to time is

$$\vec{U}^{n+1} = \vec{U}^{n} + L\vec{U}^{n}(1-\epsilon)\Delta t + L\vec{U}^{n+1}\epsilon\Delta t$$

Where $\vec{U}^{n} = \vec{U}(t=t^{n})$, $\vec{U}^{n+1} = \vec{U}(t=t^{n}+\Delta t)$

ϵ parameter from the intervall [0,1]

L spatial differential (difference) operator

---> special cases:

$\epsilon = 1/2$ scheme is 2nd order accurate in time

$\epsilon = 0$ new state vector $\boldsymbol{U}^{n+1}$ is explicitly defined

$\epsilon > 0$ new state vector is implicitly given

Explicit schemes are only stable, if size of time step is restricted by CFL condition (Courant, Friedrichs, Lewy)

$$\Delta t < \Delta t_{CFL} = Min_i \frac{\Delta x_i}{c_{max}}$$

c_{max}: maximum characteristic speed

i.e., information must not propagate more than one zone per time step

Implicit schemes allow arbitrarily large time steps (accuracy, convergence?) but need to solve nonlinear algebraic system (by linearization & iteration)

--> prohibitively large CPU & storage requirements for multi-d problems

CPU time ~ $(N_\nu \times N_x \times N_y \times N_z)^3$

(dimensional splitting & block elimination helps to reduce operation count!)

Consider initial value problem in one spatial dimension

$$\frac{\partial U}{\partial t} + A(U)\frac{\partial U}{\partial x} = 0 \quad \text{with} \quad U(x,0) = U_0(x)$$

- discretization of *x-t* plane into computational grid

zone width	Δx	time step	Δt
zone centers	$x_j = (j - 1/2)\,\Delta x$	time levels	$t^n = n\,\Delta t$
zone interfaces	$x_{j+1/2} = x_j + 1/2\,\Delta x$		

- finite difference/volume operator $H_{\Delta t}$

$$U^{n+1}_j = H_{\Delta t}(U^n; j)$$

Note: U^{n+1}_j depends on U^n at several zones (stencil of method)

- for conservation laws FV methods give approximation of zone average

$$\bar{U}^n_j = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} U(x, t^n)\,dx$$

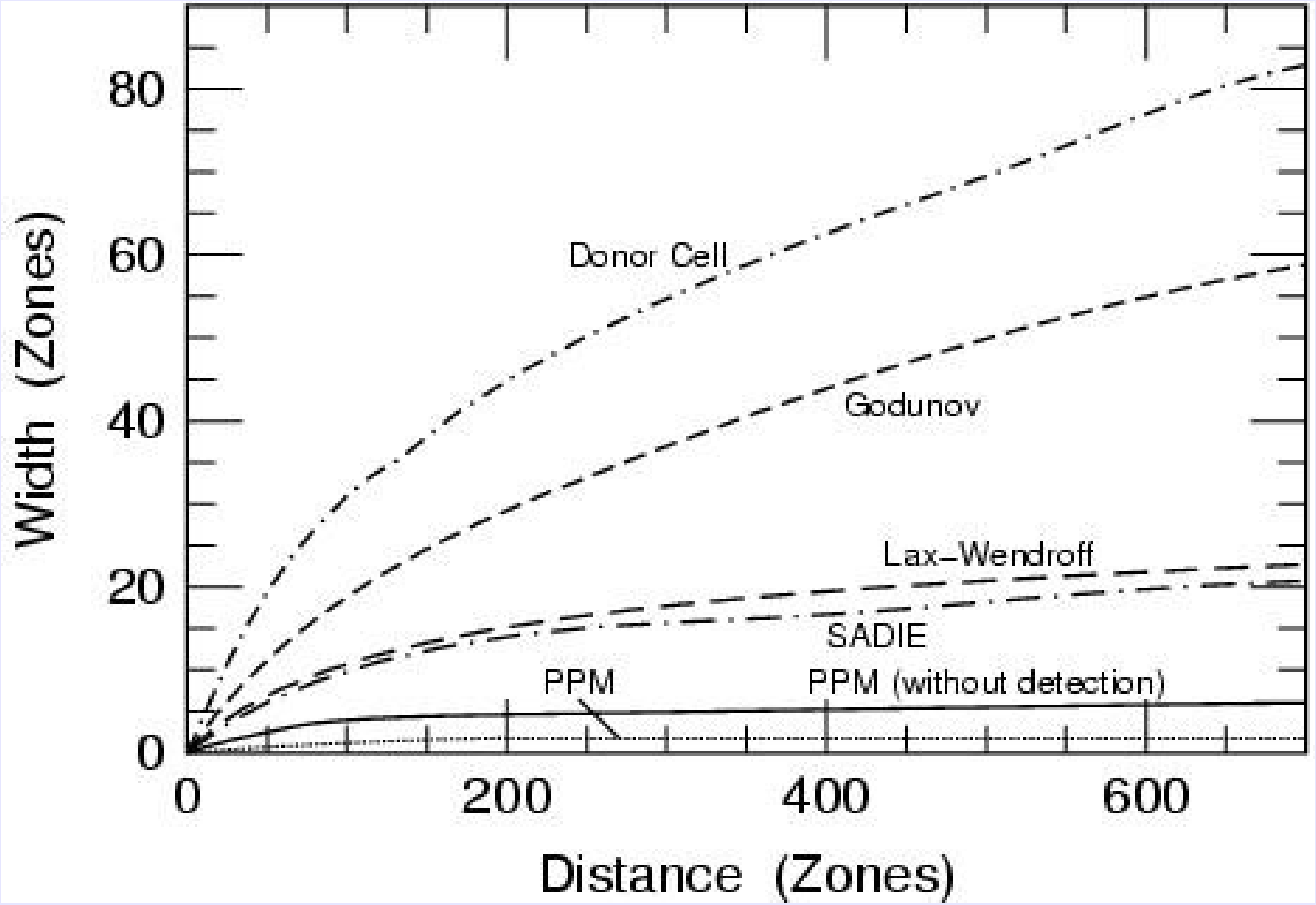
desirable & necessary properties of finite difference / finite volume schemes

- stable and sharp resolution of flow discontinuities without excessive smearing

- consistency, i.e., convergence under grid refinement to the physically correct discontinous solution (necessary!)

- high-order accuracy (a typical 3D hydrodynamic simulation involves only ~100 zones per spatial dimension)

  is <u>essential</u> to lower computational load, because if spatial resolution: $\sim N$ ---> load $\sim N^4$ for 3D problems



diffusivity of various finite volume methods

high resolution shock-capturing methods (HRSC)

- rely strongly on hyperbolic & conservative character of HD eqs (upwind method along characteristics)

- shock-capturing ability

  * discontinuities are treated consistently & automatically

  * scheme reduces from high-order accuracy in smooth regions to 1^{st} order accuracy at discontinuities

- usually based on solution of local Riemann problems (discontinuous initial value problem) at zone interfaces

global error & convergence

- for systems of conservation laws: define the local error relative to zone average of true solution

$$E_j^n = U_j^n - \bar{U}_j^n$$

and define discrete 1-norm to evaluate global error

$$\|E^n\| = \Delta x \sum_j |E_j^n|$$

- difference scheme is conservative, if it can be written in the form

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x}[\hat{F}(U_{j-r}^n, U_{j-r+1}^n, \ldots, U_{j+q}^n) - \hat{F}(U_{j-r-1}^n, U_{j-r}^n, \ldots, U_{j+q-1}^n)]$$

for some function *F* of *r+q+1* arguments (numerical flux function)

- Theorem of Lax & Wendroff: schemes of conservation form converge (if at all) to one of the weak solutions of the original system of equations

stability

- convergence requires some form of stability
- numerical scheme is stable, if global error is bounded for all times
- for linear problems the Lax equivalence theorem holds:
  Stability is necessary and sufficient for convergence
- for nonlinear problems concept of Total Variation (TV) stability is useful

$$TV(U^n) \equiv \sum_{-\infty}^{\infty} |U_{j+1}^n - U_j^n|$$

TV stability is guaranteed, if $TV(U^n)$ is bounded.

- convergence theorem (nonlinear scalar case)
  for numerical schemes in conservation form with consistent numerical flux functions: TV stability ===> convergence

Finite volume schemes

- quasi-linear hyperbolic system of (1D) conservation laws for state vector U

$$U_t(x,t)+F_x[U(x,t)]=0$$

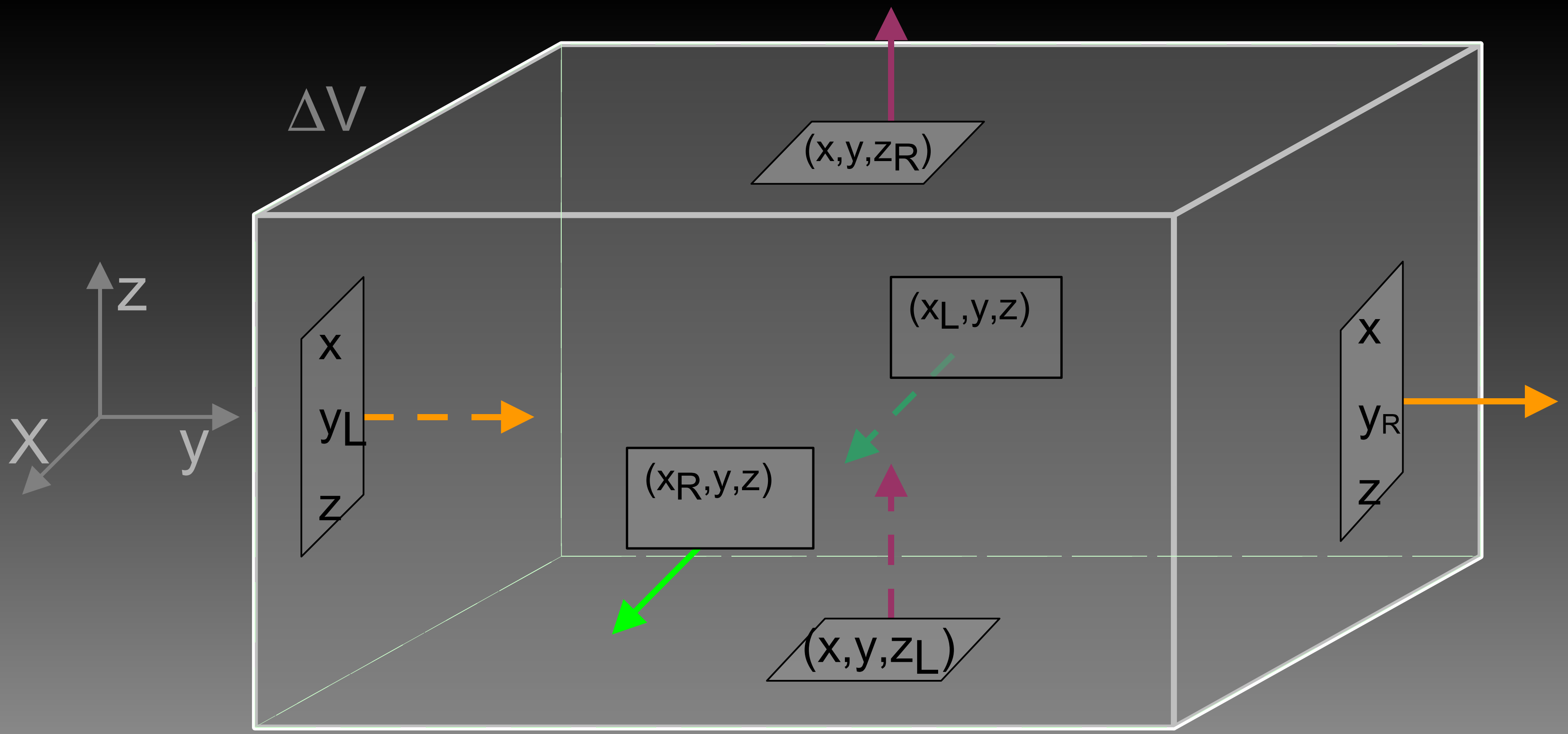
- or with the Jacobian $A(u) \equiv \partial F/\partial U$ of the flux vector F(U)

$$U_t+A(U)\cdot U_x=0$$

- integration over finite (1D spatial control) volume $[x_1,x_2]\times[t_1,t_2]$

$$\int_{x_1}^{x_2} U(x,t_2)\,dx=\int_{x_1}^{x_2} U(x,t_1)\,dx-\int_{t_1}^{t_2} F[U(x_2,t)]\,dt+\int_{t_1}^{t_2} F[U(x_1,t)]\,dt$$

integral form allows proper handling of flow discontinuities!



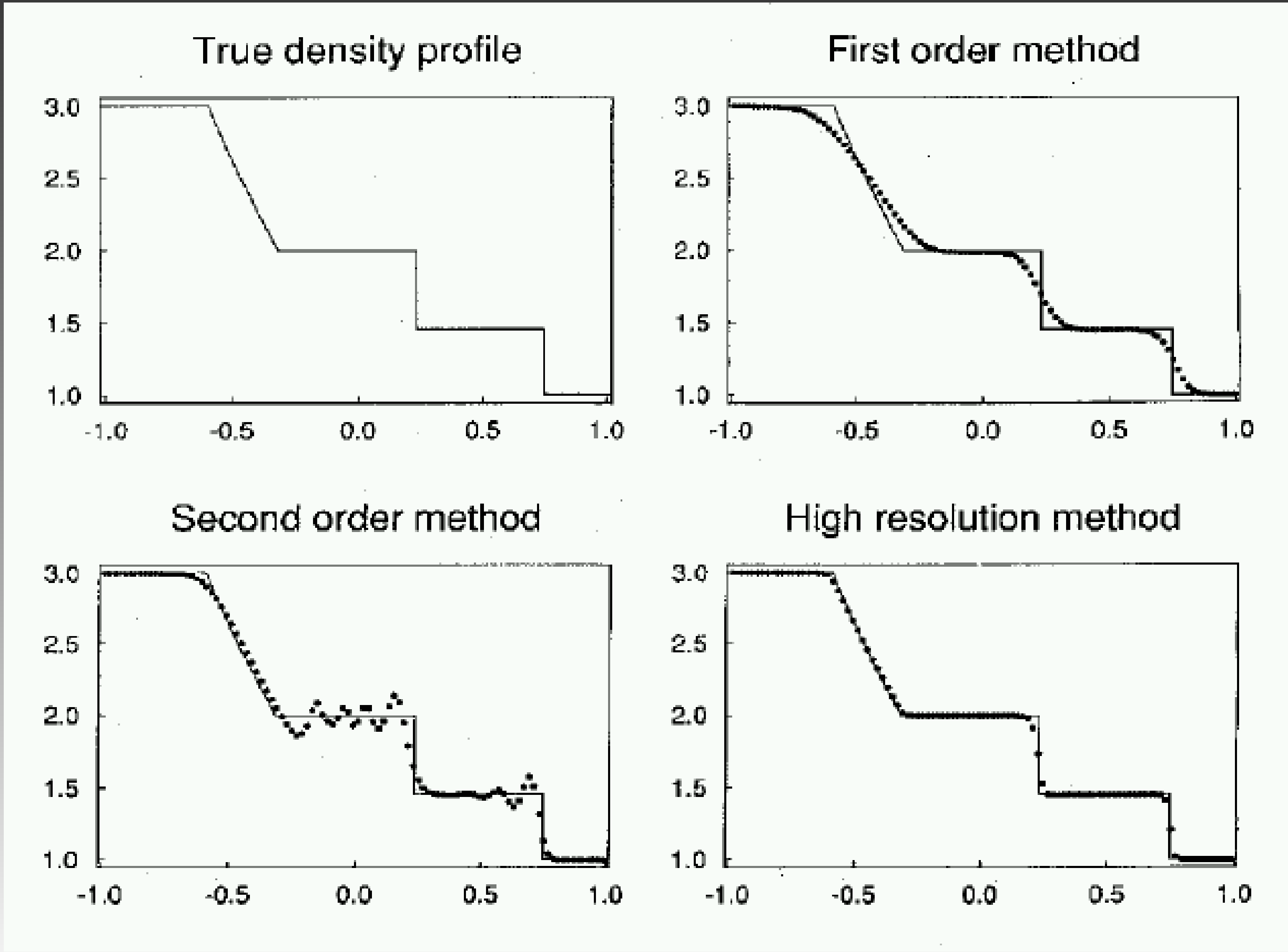
$$\bar{U}(t) = \frac{1}{\Delta V}\int_V U(\vec{x},t)d^3x \quad ; \quad \vec{F}^n(\vec{x}) = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \vec{F}\Big(U(\vec{x},t)\Big)dt$$

$$\begin{aligned}\bar{U}(t_{n+1}) - \bar{U}(t_n) = -\frac{\Delta t}{\Delta V}\Big[&\int \Big(F_x^n(x_R,y,z) - F_x^n(x_L,y,z)\Big)dydz + \\ &\int \Big(F_y^n(x,y_R,z) - F_y^n(x,y_L,z)\Big)dxdz + \\ &\int \Big(F_z^n(x,y,z_R) - F_z^n(x,y,z_L)\Big)dxdy \Big]\end{aligned}$$

(from G.Bodo)

3D flow: consider fluxes through all orthogonal volume surfaces

Handling discontinuities



Godunov Schemes

U(x,t^n) is approximated by a piecewise (on a spatial scale *Dx*) polynomial *v(x,t^n)*

$$\bar{v}(x,t^{n+1})=\bar{v}(x,t^{n})-\frac{1}{\Delta x}\left[\int_{t^n}^{t^{n+1}} F(v(x+\Delta x/2,\tau))\,d\tau-\int_{t^n}^{t^{n+1}} F(v(x-\Delta x/2,\tau))\,d\tau\right]$$

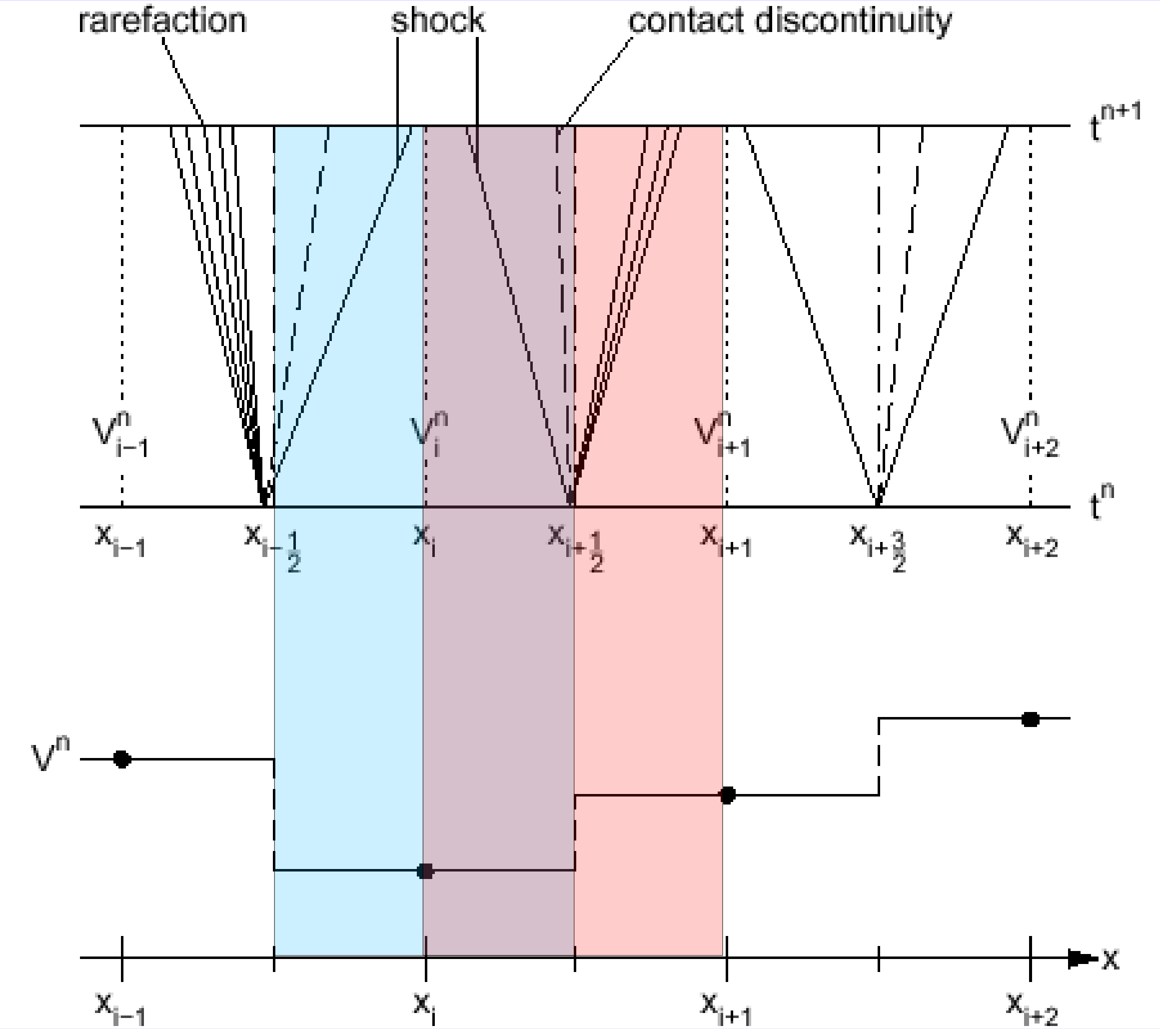
---> exact evolution of spatially averaged (approximate) state vector given by time-averaged numerical fluxes at interfaces

- construct numerical scheme by sampling at discrete grid points:

  at cell centers ---> upwind schemes
  at cell interfaces ---> central schemes

---> remaining question: How to compute numerical fluxes?

e.g., piecewise constant



upwind schemes

numerical flux at polynomial breakpoints from exact or approximate solution of local Riemann problems

(spectral information required!)

central schemes

smooth numerical flux at cell centers by quadrature

(averaging over Riemann fan)

proto-types: 1st order Godunov (upwind), Lax-Friedrichs (central)

non-oscillatory higher-order extensions of both classes exist!

Riemann Problem

- consider hyperbolic system of conservation laws in one spatial dimension

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}(\vec{U})}{\partial x} = 0 \qquad with \quad \vec{U}(x,0) = \vec{U}_0(x)$$

- Riemann problem for the above system is an initial value problem with discontinuous data

$$\vec{U}_0 = \vec{U}_L \quad if\ x < 0 \qquad \wedge \qquad \vec{U}_0 = \vec{U}_R \quad if\ x > 0$$

invariant under similarity transformation: *(x, t) ---> (ax, at) , a > 0*

- Theorem of Lax: *If left and right states are sufficiently close, Riemann problem has a solution consisting of p+1 constant states separated by rarefaction waves and shocks*

$$\vec{U}_{RP}\left(\frac{x}{t}; \vec{U}_L, \vec{U}_R\right)$$

Exact Riemann solvers

iterative solution of a non-linear algebraic equation (for the pressure of the intermediate state) at each zone interface

- straightforward for ideal gas EOS (γ=const.)
- more complicated for general EOS (linear interpolation of γ)

Approximate Riemann solvers

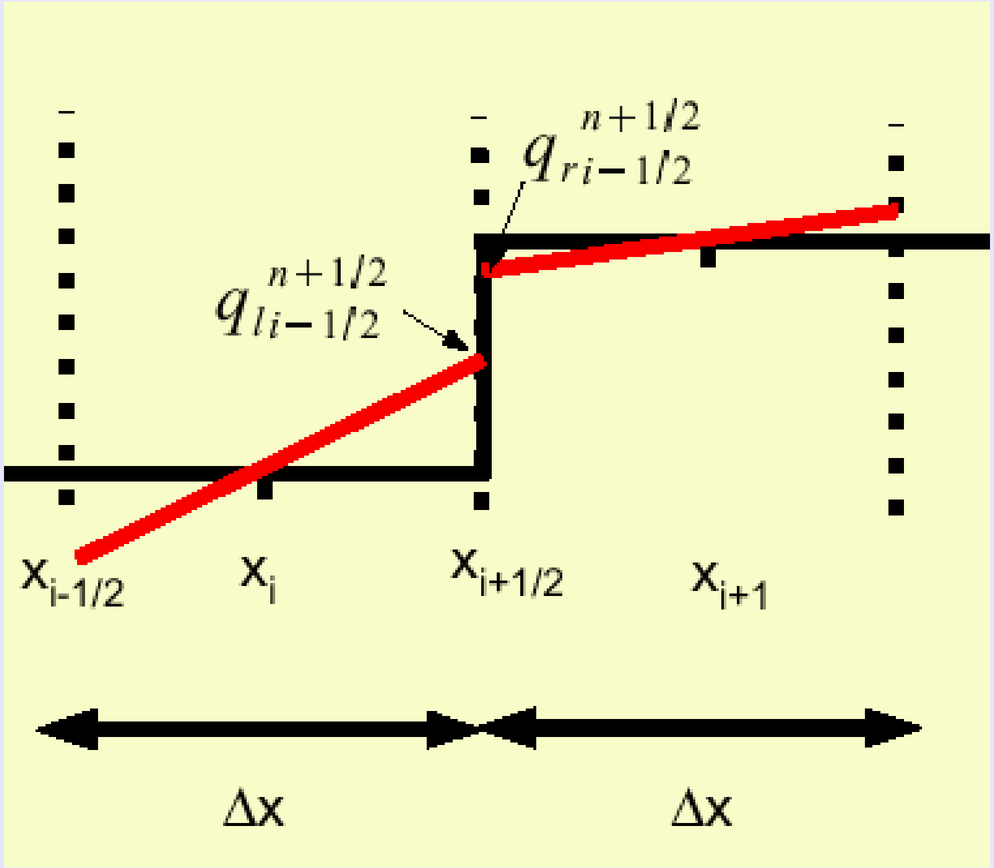
instead of solving Riemann problem exactly approximations are made, e.g.,

Roe solver: approximate RP solved exactly assuming locally constant Jacobian ---> hyperbolic system becomes linear

HLLE: exact RP is solved approximately using only maximum & minimum eigenvalues

Marquina's flux formula: exploits characteristic information to compute numerical flux function

Higher-order Godunov methods



interpolation inside cells

use slope limiters to enforce monotonicity (avoid appearance of new maxima)

higher-order interpolations used in astrophysical applications:

piecewise linear (PLM)

piecewise parabolic (PPM)

piecewise hyperbolic (PHM)

More general class of schemes

- Total Variation Diminishing schemes

$$\sum_i \left|\delta \rho^n_{i+1/2}\right| \le \sum_i \left|\delta \rho^0_{i+1/2}\right| \qquad \text{with} \quad \delta \rho^n_{i+1/2} \equiv \rho^n_{i+1} - \rho^n_i$$

---> convergence, no spurious oscillations

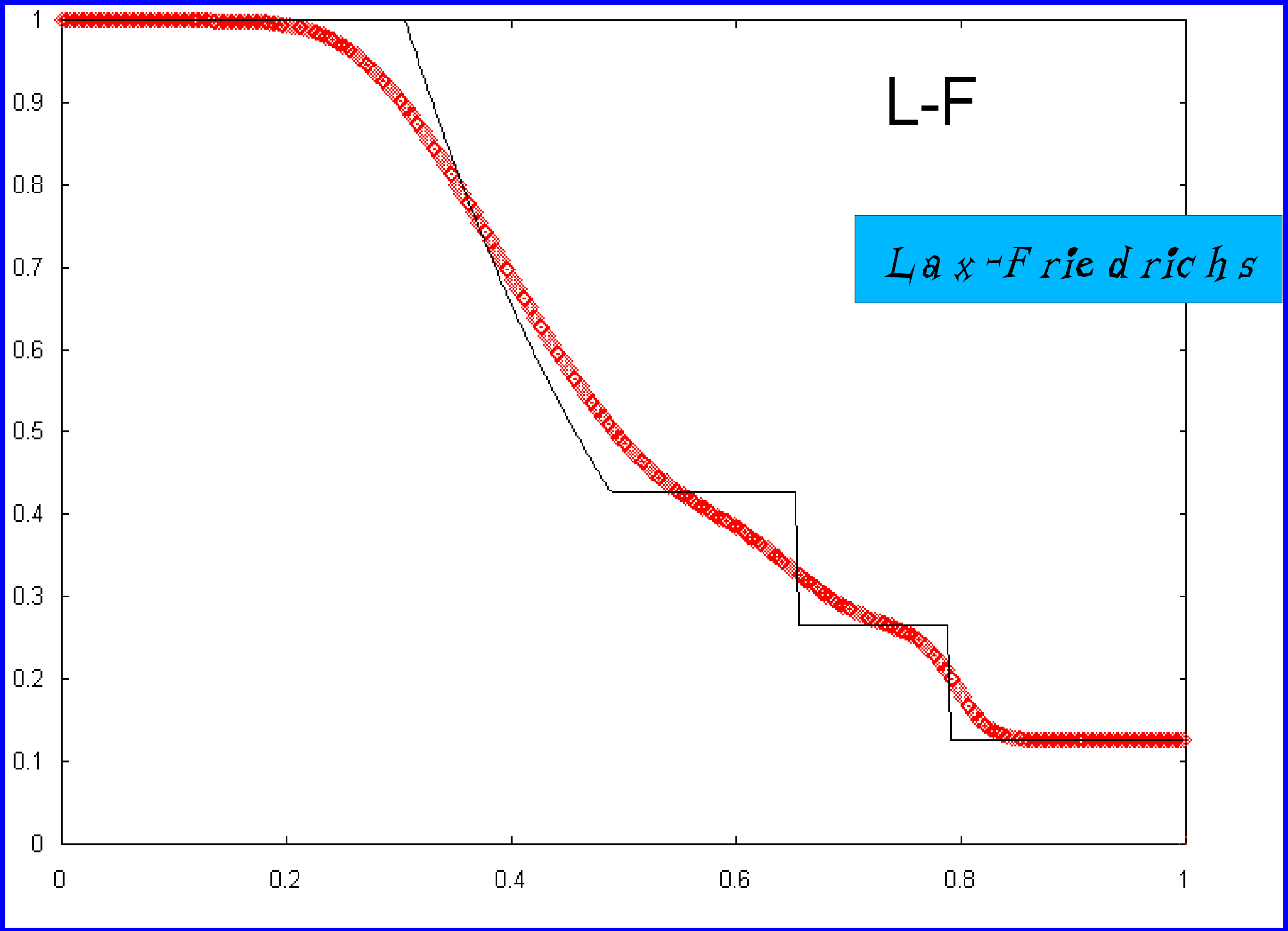
- monotone schemes at most 1st order accurate, but TVD schemes not restricted to 1st order --->

upwind TVD schemes: 2nd order: FCT, MUSCL, Harten (NO)
3rd order: PPM, ENO

central TVD schemes with min-mod-limiter (NOCD)

2nd order: Nessyahu & Tadmore ('90)
3rd order: Tadmore ('98)

Sod's shock tube test problem (N=400, CFL=0.3)



(ρ, u, E):

$\mathbf{U}_L = (1, 0, 2.5)$

$\mathbf{U}_R = (0.125, 0, 0.25)$

from A.Serrano

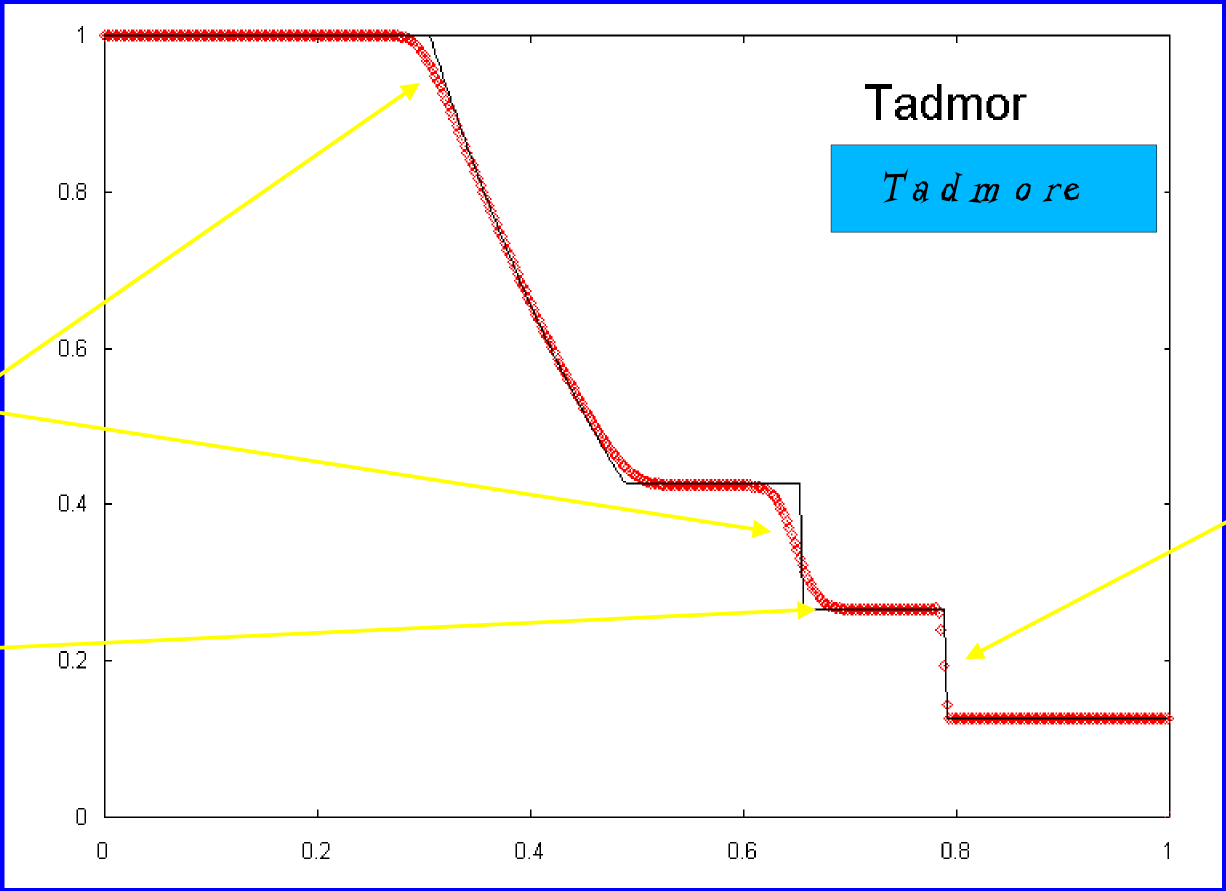
1st order central difference scheme

simple, but very diffusive everywhere

Sod's shock tube test problem (N=400, CFL=0.3)

diffusion

large diffusion



3 cells in the shock

from A.Serrano

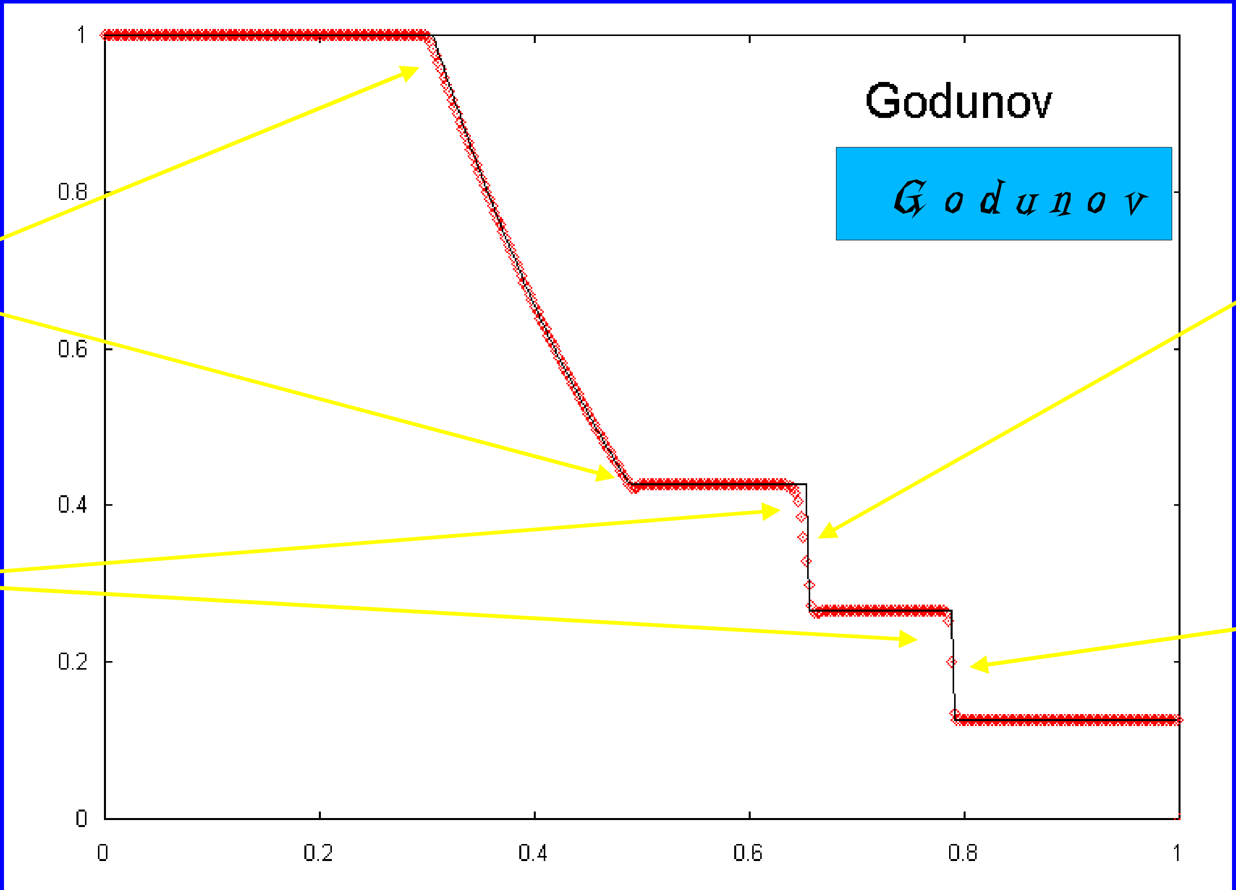
2nd order central difference scheme

good at shocks, very diffusive at contacts

Sod's shock tube test problem (N=400, CFL=0.3)

very good resolution

small undershoots



very well resolved contact

3 cells in the shock

from A.Serrano

Riemann solver, 1st order reconstruction

accurate description of all wave structures

Computer resources required:

- floating point operations

  3 - 20 variables

  10^3 - 10^8 zones (present record: $2048^3 \sim 8\ 10^9$)

  10^3 - 10^6 timesteps

  10^2 - 10^3 Ops/zone/variable/timestep

---> 10^{10} - 10^{18} operations / simulation

- central memory up to several 100 Gbytes

- present day computer

100 Mflops (PC) [~ CRAY-1 in 1980 !]

3 Tflops (´supercomputer´, *e.g.,* 1024 PE IBM Power 4)

~ 30 Tflops (Earth Simulator, Japan, ~5000 NEC-SX6)

---> 1D simulation: ~ few minutes on PC

3D simulation: ~ many weeks on supercomputer

- output data: ~ Gbyte / model ---> data analysis

~ Tbyte / simulation is non trivial!

Relativistic Hydrodynamics

numerical complexity arising in RHD:

- **strong non-linearity** (due to coupling by W and h)
- **unlimited shock compression** (large jumps)
- **Lorentz contraction** (narrow flow structures)
- **recovery of primitive variables** (iteration required)

---> High-Resolution Shock-Capturing methods

- exploit hyperbolic and conservative character of PDEs
- analytic solution of general relativistic Riemann problem known (Marti & Müller 1994), but used only for tests or for 1D flows (ODE has to be solved !)
- careful treatment of “dangerous” terms when *v/c --> 1*

Appropriate RHD codes

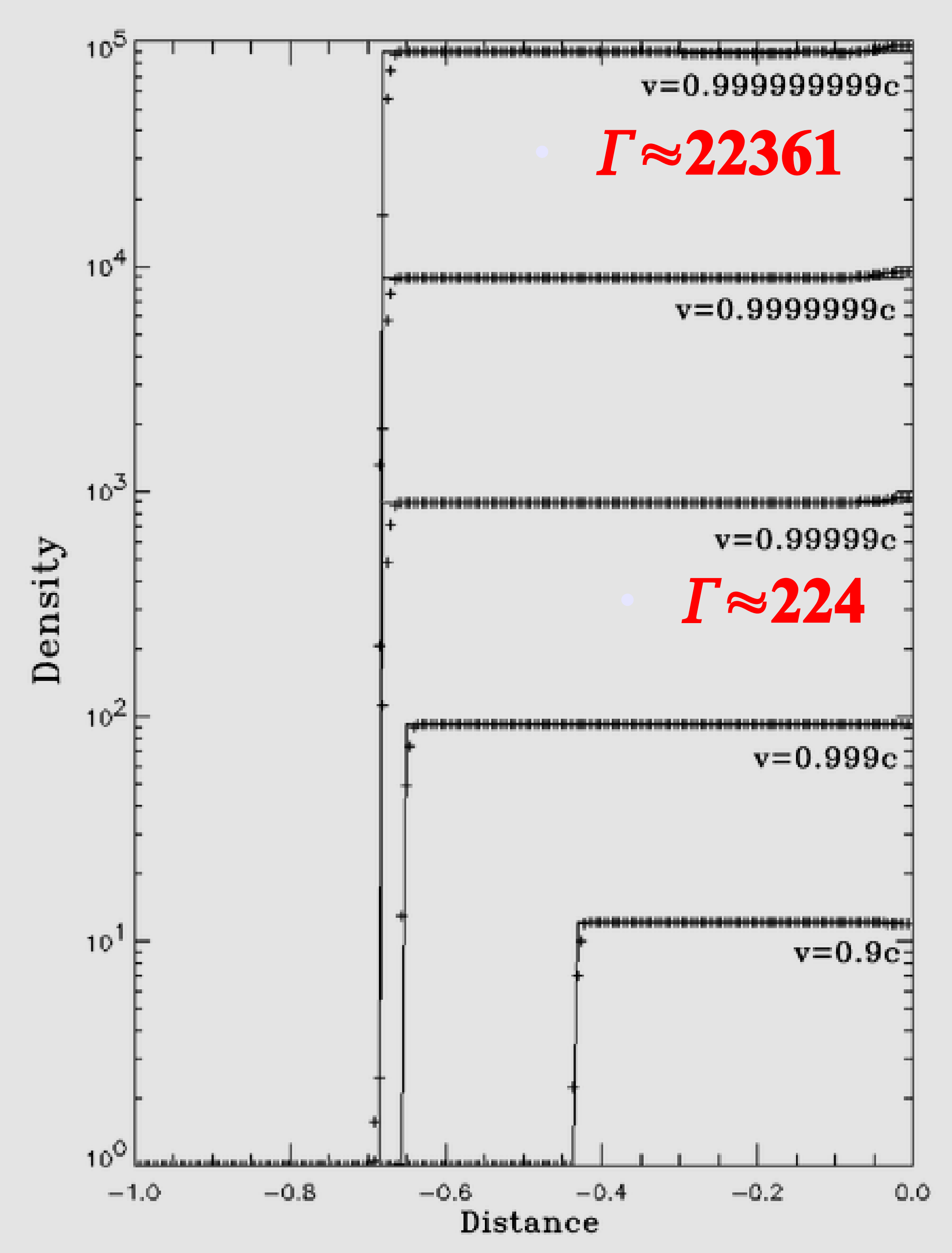
are able to handle

ultra-relativistic flows

ie. Lorentz factors

$\Gamma > 100$

Shock reflection test problem



GENESIS RHD code: Aloy, Ibánez, Marti & Müller '99

General relativistic hydrodynamics:

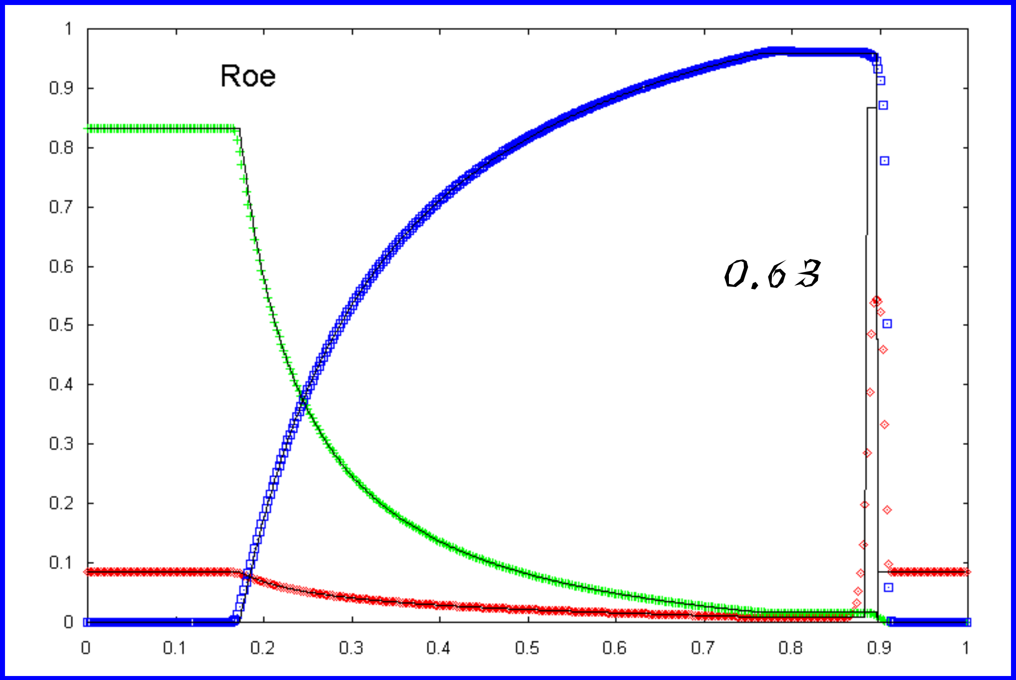
also formulated as hyperbolic system, but with source terms and geometric factors due to spacetime curvature

- Cowling approximation (flow in fixed general spacetime)
- full GRHD: integration of general relativistic HD eqs. together with Einstein field eqs. (3+1 ADM)

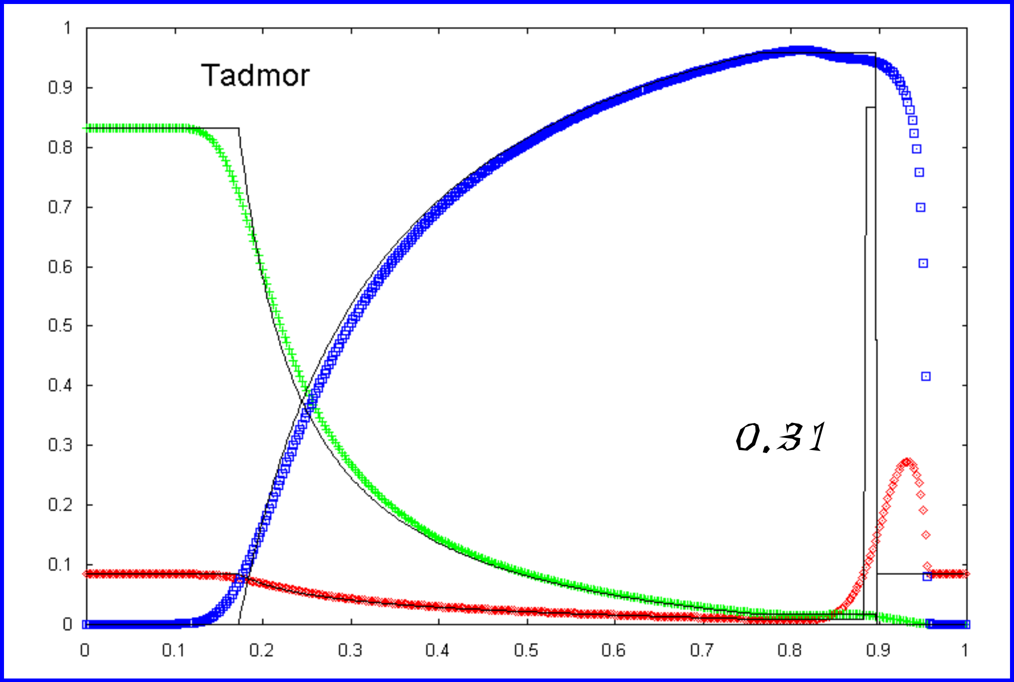
generic problems:

- long term numerical stability
  (hyperbolic vs constraint formulation)
- choice of optimal gauge and coordinates
  (to avoid too small timesteps)
- excision of singularities
- gw extraction (null cone formulation, compactified grids)

Relativistic blast wave (N=400, CFL=0.3)



Tadmor central scheme:
- waves badly resolved
- unphysical shock speed (v>1)



Roe approximate Riemann solver:

- structures quite well resolved
- correct shock speed

Magneto-Hydrodynamics

Ideal (R)MHD: The physical viewpoint

Equations describe flow of an infinitely well conducting fluid in the presence of a magnetic field

neglected:

- displacement currents
- electrostatic forces
- viscosity
- resistivity
- heat conduction

Equations of ideal MHD

$$\rho_t + \nabla(\rho\vec{v}) = 0$$

$$(\rho\vec{v})_t + \nabla(\rho\vec{v}\vec{v} + \underline{\underline{I}}\,P^{tot} - \vec{B}\vec{B}) = 0$$

$$E_t + \nabla[(E + P^{tot})\vec{v} - \vec{B}(\vec{B}\vec{v})] = 0$$

$$\vec{B}_t + \nabla(\vec{v}\vec{B} - \vec{B}\vec{v}) = 0$$

$$\nabla\vec{B} = 0$$

$$P^{tot} = P + \vec{B}^2/2$$

$$E = \rho\vec{v}^2/2 + P/(\gamma - 1) + \vec{B}^2/2$$

(units where 4 and c disappear)

Ideal (R)MHD: The mathematical viewpoint

Non-linear system of conservation laws (7 waves; 10 if covariant)

- non-strictly hyperbolic (not all of the real eigenvalues may be distinct)

--> Riemann solver complicated (many cases)

- non-convex (characteristic fields which are neither linearly degenerate nor genuinely nonlinear)

--> complicated wave structure (compound waves)

+ additional constraint equation (div$\underline{B}$ = 0)

Ideal (R)MHD: The numerical viewpoint

- CPU requirements considerably larger than in (R)HD
  (more equations, more waves, degeneracies, ...)

- calculation of eigenvalues involves solving a quartic

  * no simple analytic solution in closed form
  * eigenvalues must be obtained numerically
  * eigenvectors depend nonlinearly on eigenvalues

  --> serious numerical complications

- pressure positivity more difficult to maintain than in (R)HD

- numerical problems in RMHD even worse

constraint equation: div$\underline{B}$ = 0

- shock-capturing MHD codes

  base scheme (well established HD algorithm) to evolve mass, momentum, energy & (similarly) B-field

  & modification/addition for $\underline{B}$ evolution to maintain div$\underline{B}$=0

- constrained transport (Evans & Hawley 1988)

  applies staggered grid: $\underline{B}$ components defined at cell interfaces are updated by finite differencing the electric field at cell corners

  --> maintains div$\underline{B}$=0 to machine round off error

Some references:

Laney, C.B., 1998, “Computational Gasdynamics”, CUP, Cambridge, UK

LeVeque, R.J., 1998, in “Computational Methods for Astrophysical Fluid Flow”, SaasFee Advanced Course 27, eds. O.Steiner & A.Gautschy, Springer, Berlin

Marti, J.M. & Müller, E., 2003, “Numerical Hydrodynamics in Special Relativity”, Living Reviews in Relativity, http://www.livingreviews.org/Articles/lrr-2003-7

Potter, D., 1973, “Computational Physics”, Wiley, New York

Toro, E.F., 1997, “Riemann Solvers and Numerical Methods for Fluid Dynamics”, Springer, Berlin