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Lagrangian Numerical Hydrodynamics

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Plan

- Motivation:
  - What is special about "astrophysical" fluid dynamics?
  - Which method to choose?

- Basics of Lagrangian Fluid Dynamics

- Smooth Particle Hydrodynamics (SPH)
  - "Vanilla Ice"
  - derivation from variational principle
  - subtleties and recent developments
  - extension to Relativity

- "Hybrid"/"Adaptive Lagrangian Eulerian" approaches

mostly following: "Astrophysical Smooth Particle Hydrodynamics", SR (2009)

0. Motivation

- Deal here with *ideal* fluid dynamics, ignore effects such as viscosity, conductivity

- hydrodynamics equations historically among the first partial differential equations ever written down, yet surprisingly difficult to solve

- which method is "best" is often problem-dependent

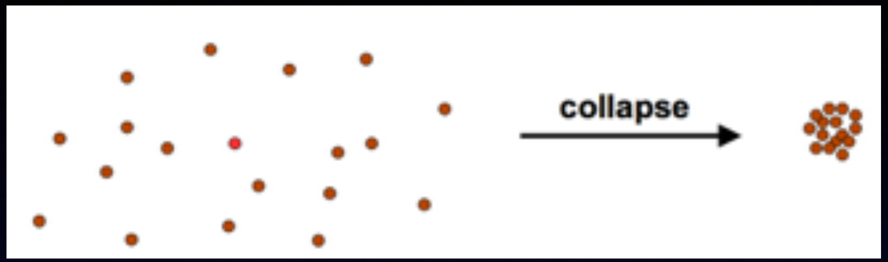
"Horses for courses"

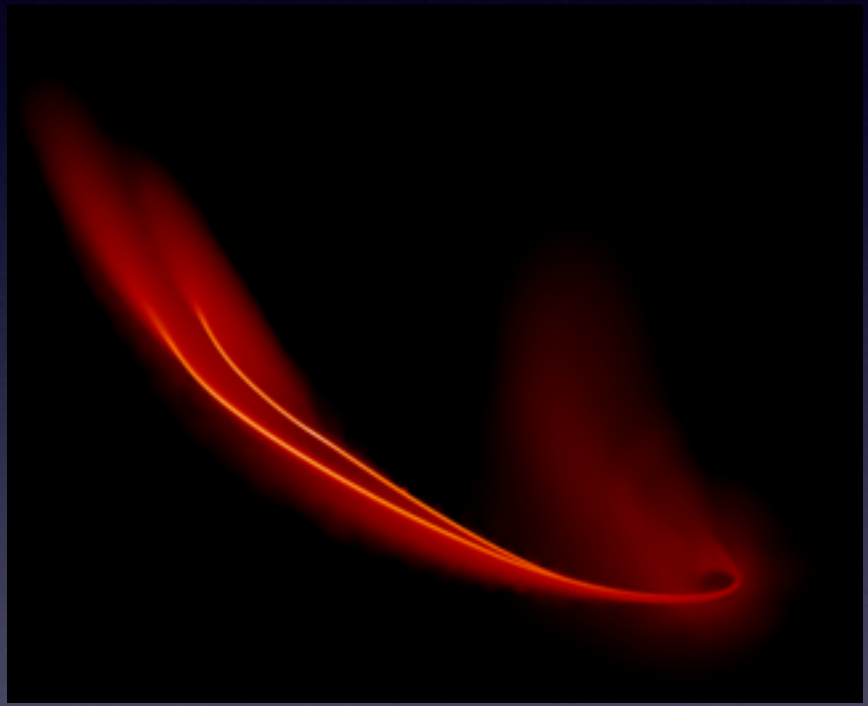
⇒ it IS important to choose the right method for the problem at hand

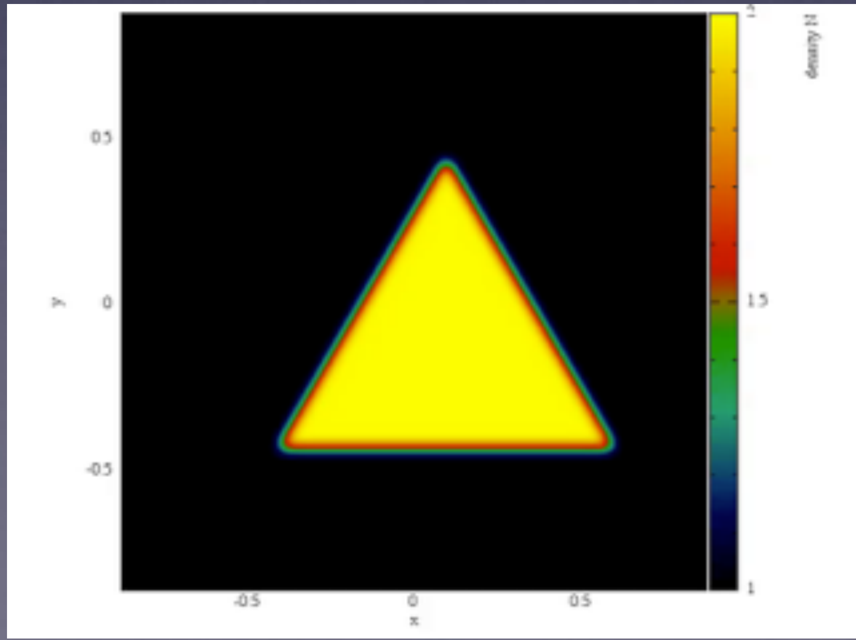
When /why use Lagrangian hydrodynamics?

Lagrangian hydrodynamics:

- automatic adaptation to complicated geometries
- no restriction to “computational domain”
- “vacuum is vacuum”
- exact conservation can be “hard-wired”
- advection exact
- easy coupling to n-body methods
- very accurate (Newtonian) self-gravity via trees

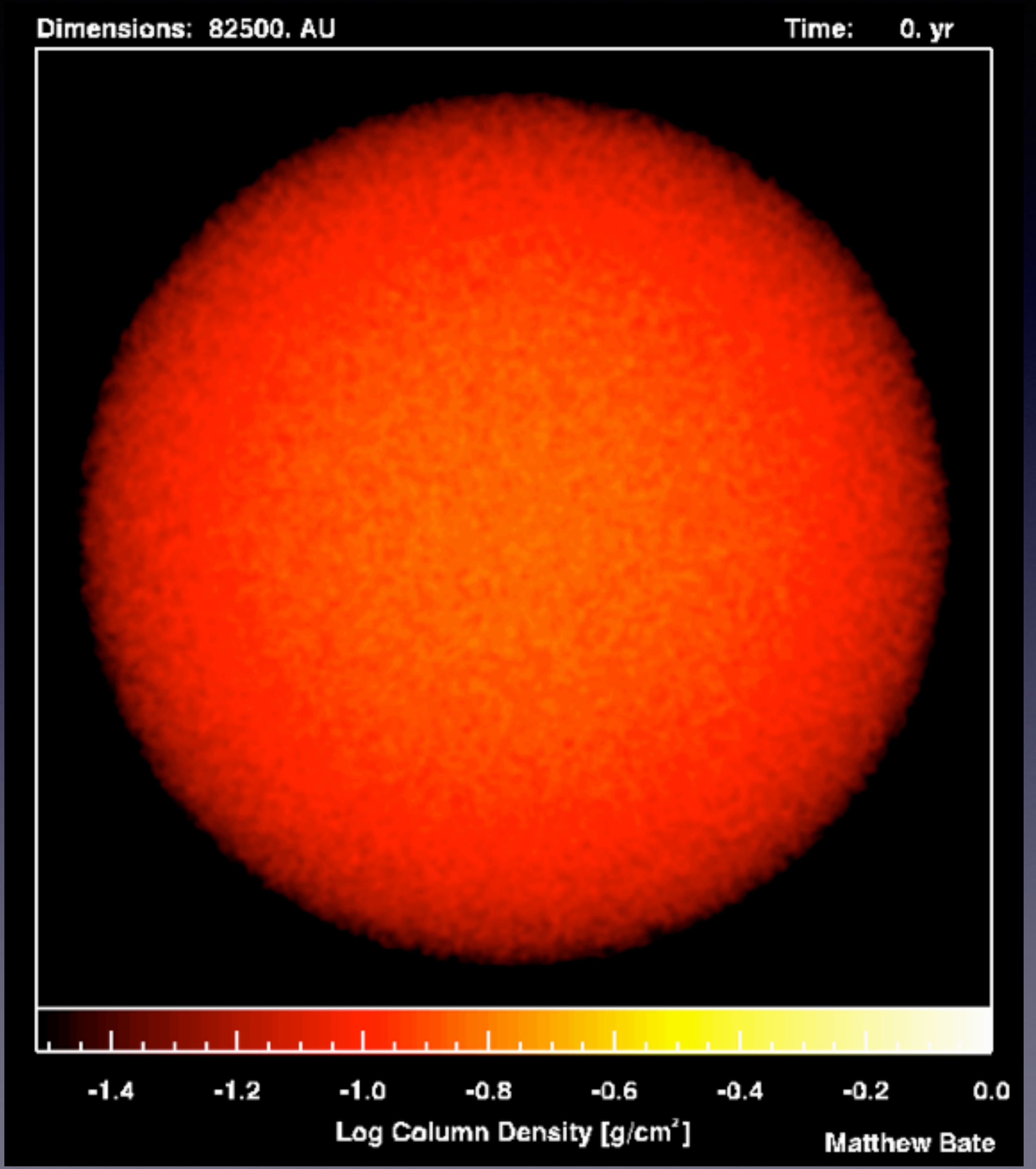






Some examples

- dynamical star formation calculation



<u>modeled physics:</u>
- self-gravity
- gas dynamics

(Simulation Matthew Bate)

- Tidal disruption of a white dwarf by an intermediate-mass black hole

<u>modeled physics:</u>

- self-gravity
- gravity black hole via pseudo-potential
- gas dynamics
- nuclear burning

<u>Astrophysical signatures:</u>

- thermonuclear Supernova
- X-ray flare

(Simulation S.R.)

WD−BH encounter

****

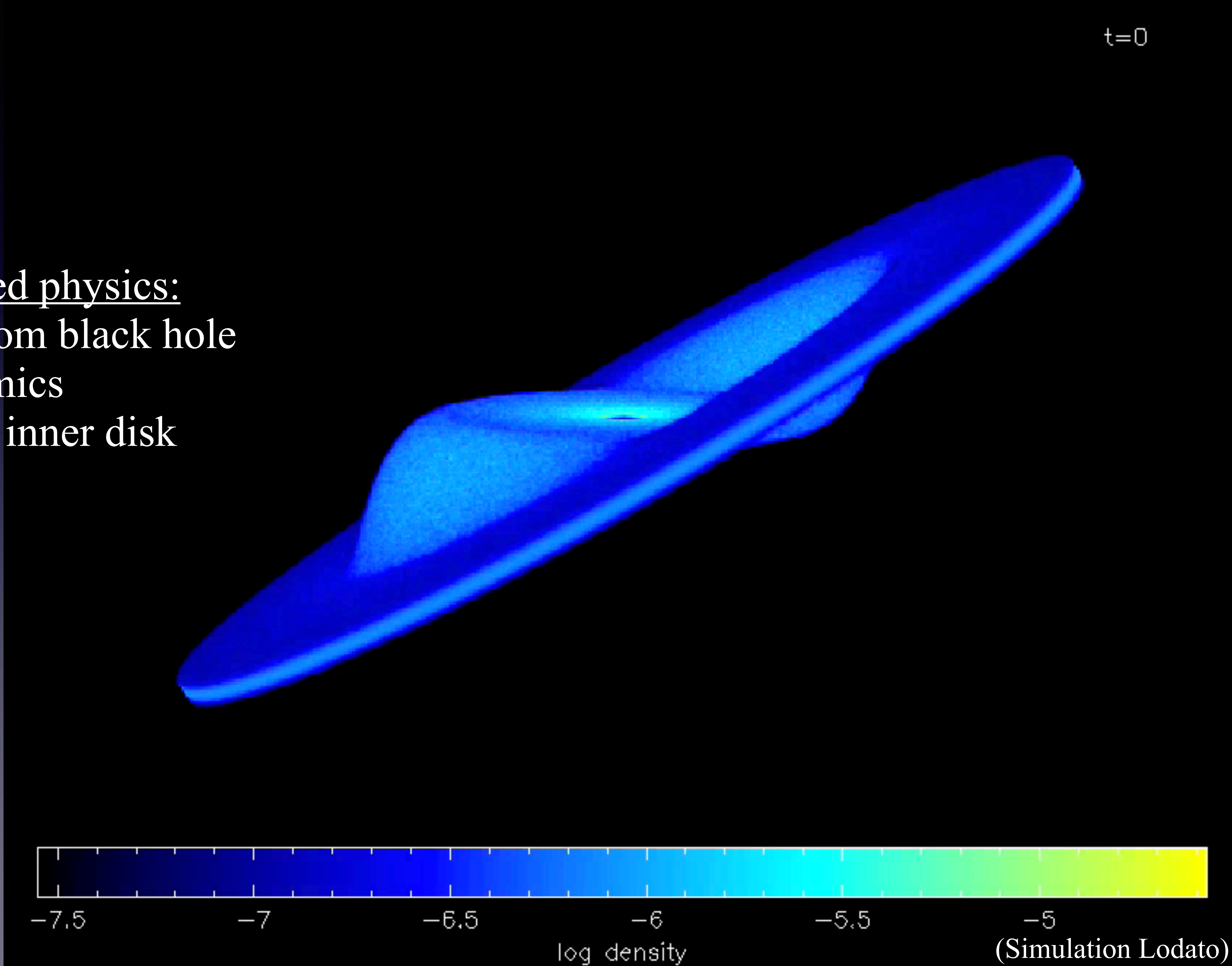
masses (sol.)	0.2 (WD) & 1000 (BH)
in. separation	50 (in 1.E9 cm)
hydrodynamics	SPH (4 030 000 particles)
EOS, gravity	Helmholtz, N
nucl. burning	red. QSE−network (Hix 98)
simul. time	5.4 min
color coded	column density
penet. factor	12

coding, simulation, visualisation: S. Rosswog

- Disk “warped” by a rotating central black hole

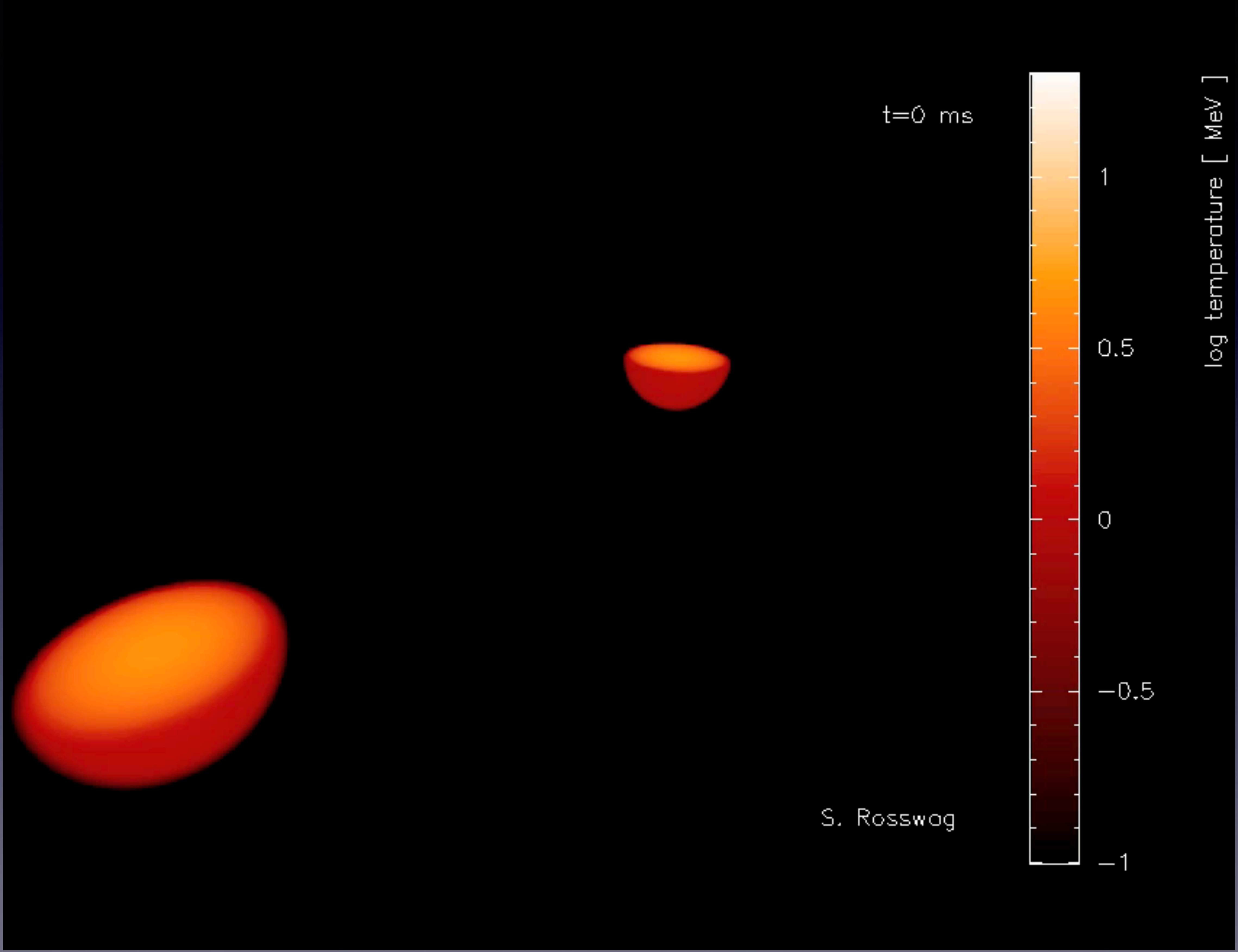
<u>modeled physics:</u>

- gravity from black hole
- gas dynamics
- torque on inner disk

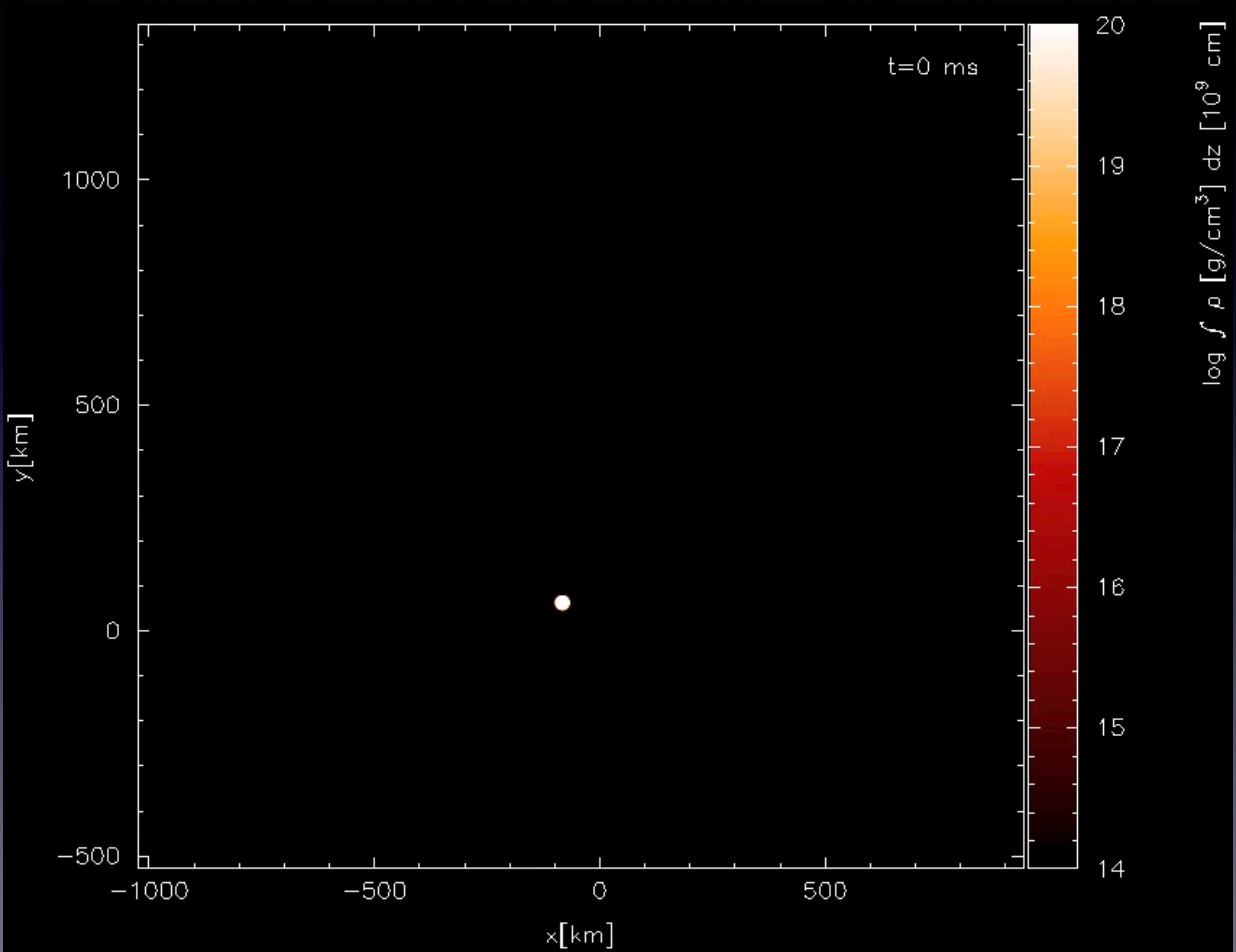


(Simulation Lodato)

- collision between two neutron stars (β=2)



- collision between a neutron star and a low-mass black hole (5M☉, β=1)



(Simulation S.R.)

Long-term evolution of NSNS-merger debris

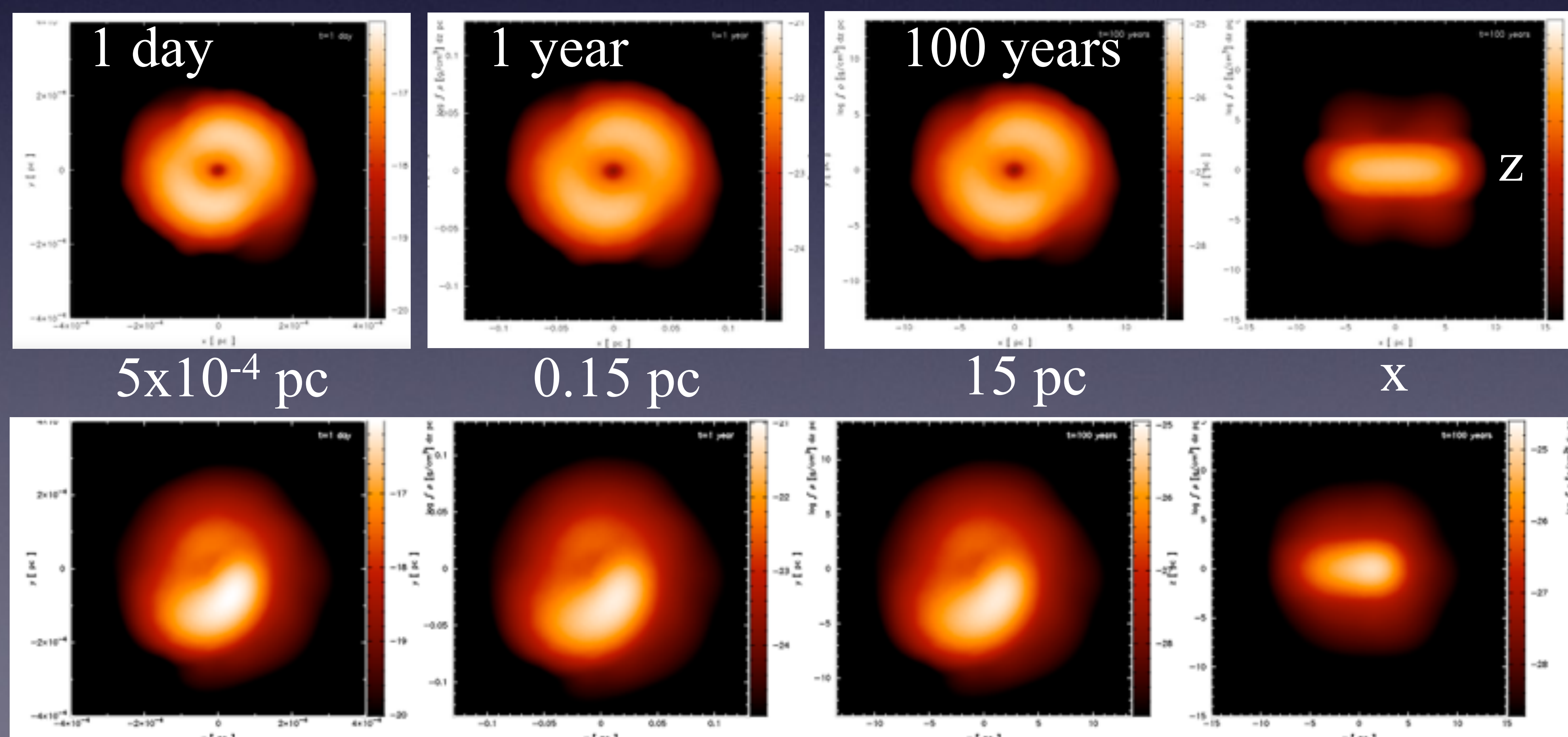
(Rosswog et al., 2014)

- typical merger simulations restricted to ≈ 20 ms, sound speed in neutron star ≈ 0.3c, CFL condition: $\Delta t < \Delta x / c_s \sim 10^{-7}$ s
- cut out central remnant, replace by potential, follow ejecta
- include heating by radioactive decays
- follow evolution up to 100 years

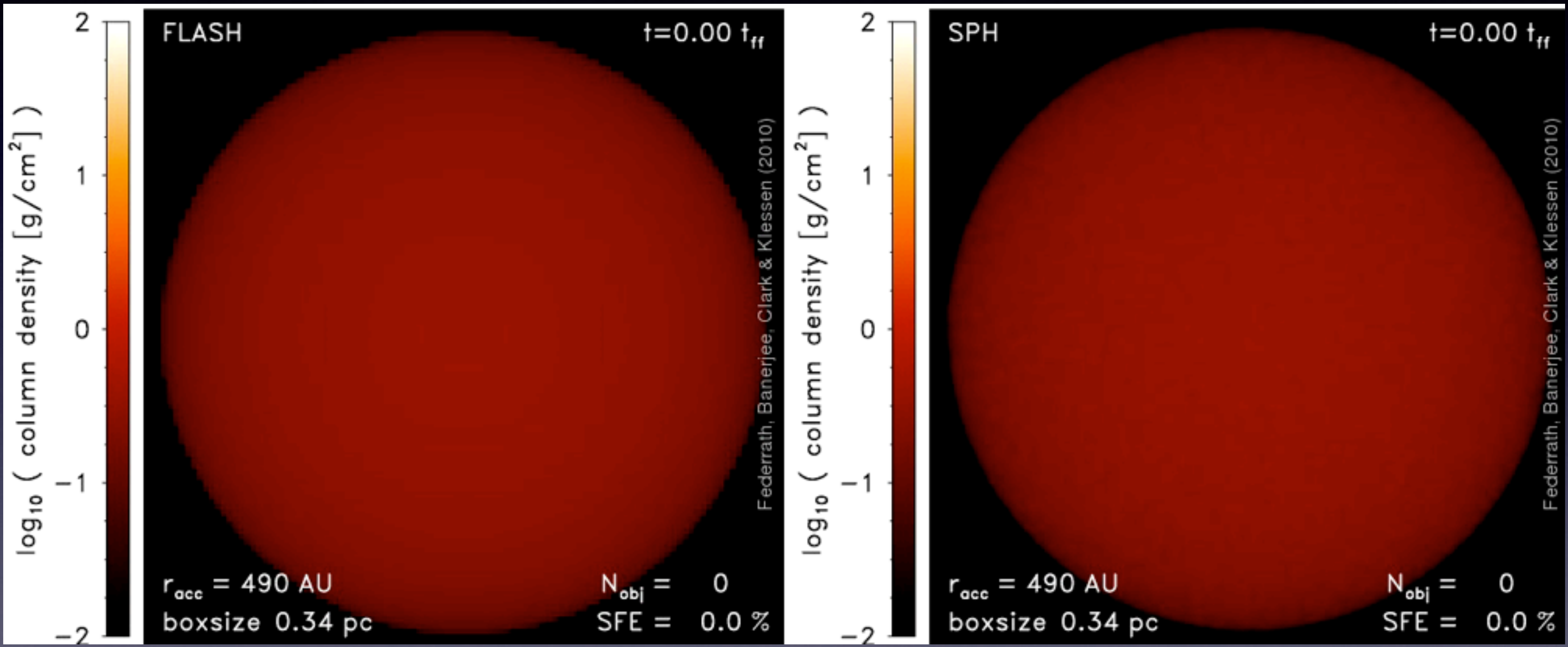
"100 years, but still in shape"

$2 \times 1.4 M_\odot$

1.3 & $1.4 M_\odot$



comparison Eulerian vs. Lagrangian



(Simulation Federrath)

1. Basics of Lagrangian fluid dynamics

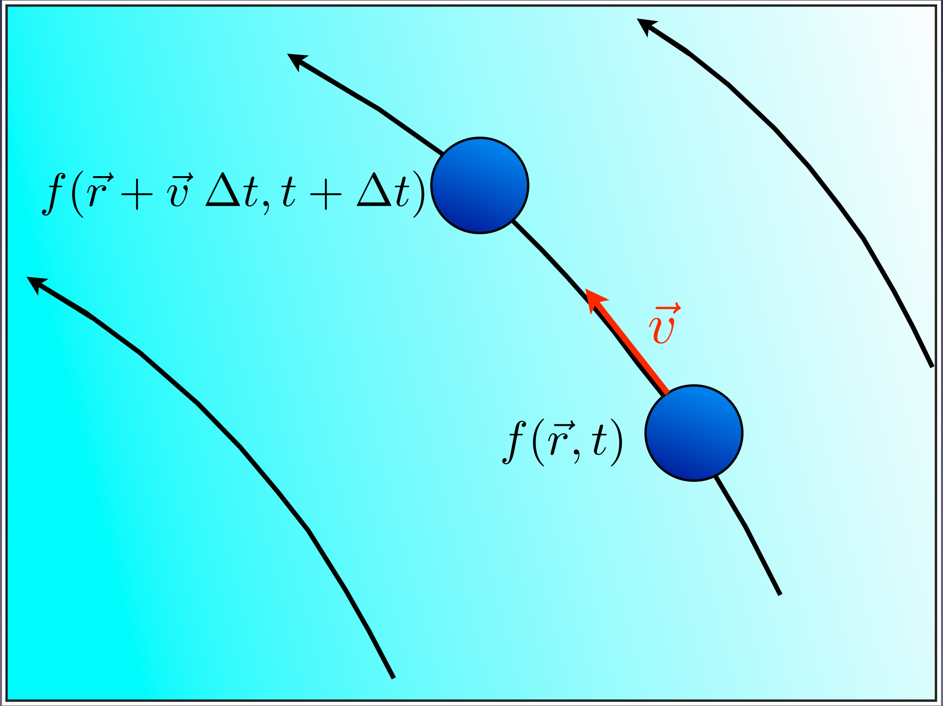
- in all of this lecture: restriction to ideal fluids (no viscosity, conductivity…)

- Lagrangian time derivative $\frac{d}{dt}$ or $\frac{D}{Dt}$

(other names: "Convective derivative", "material derivative", "substantial derivative", ...)

- $\frac{d}{dt} f(\vec{r},t) =$ "rate of change of quantity f of a fluid parcel traveling with velocity $\vec{v}$ "

$$\begin{aligned}\Delta f &= f(\vec{r}+\vec{v}\,\Delta t, t+\Delta t) - f(\vec{r},t)\\ &\simeq \left[f(\vec{r},t) + \Delta t\, \vec{v}\cdot\nabla f(\vec{r},t) + \Delta t\, \frac{\partial f}{\partial t}(\vec{r},t)\right] - f(\vec{r},t)\\ &= \Delta t \left(\vec{v}\cdot\nabla + \frac{\partial}{\partial t}\right) f(\vec{r},t)\end{aligned}$$



$$\frac{d}{dt} f \equiv \lim_{\Delta t \to 0} \frac{\Delta f}{\Delta t} = \left(\frac{\partial}{\partial t} + \vec{v}\cdot\nabla\right) f(\vec{r},t)$$

example: write (Eulerian) continuity equation in Lagrangian form

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

$$\boxed{\frac{d\rho}{dt} = -\rho \nabla \cdot \vec{v}}$$

continuity equation
Lagrangian form

- physical interpretation of $\nabla \cdot \vec{v}$:

$$\nabla \cdot \vec{v} = -\frac{d\rho/dt}{\rho}$$

"rate of relative volume expansion"

First law of thermodynamics (for our purposes)

- conservation of energy

- from thermodynamics: $$dU = \cancel{T\,ds} - P\,dV$$

"change of energy" ~~"change of entropy"~~ "work done via volume change"

- for our purposes: want quantities "per mass"

$$U \longrightarrow u$$ "energy per mass"

$$V \longrightarrow \frac{1}{\rho}$$ "volume per mass" = "1/density"

$$d\left(\frac{1}{\rho}\right) = -\frac{d\rho}{\rho^2}$$

$$\Rightarrow \boxed{du = +\frac{P}{\rho^2}\,d\rho}$$

- implications: a) evolution equation

$$\boxed{\frac{du}{dt} = \frac{P}{\rho^2}\frac{d\rho}{dt}}$$

b) for later use:

$$\boxed{\left(\frac{\partial u}{\partial \rho}\right)_s = \frac{P}{\rho^2}}$$

- side remark: for the relativistic cases we will express everything "per baryon"

$\rho \rightarrow n$ "baryon number density" (in local fluid rest frame)

$$\left(\frac{\partial u}{\partial n}\right)_s = \frac{P}{n^2}$$

Equations ideal, Lagrangian hydrodynamics

- conservation of mass:

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \vec{v}$$

- conservation of energy:

$$\frac{du}{dt} = \frac{P}{\rho^2}\frac{d\rho}{dt}$$

$$\frac{du}{dt} = -\frac{P}{\rho} \nabla \cdot \vec{v}$$

- conservation of momentum:

$$\frac{d\vec{v}}{dt} = -\frac{1}{\rho} \nabla P$$

- plus: appropriate equation of state (EOS)

e.g. polytropic EOS: $P = K \rho^{\Gamma}$

2. Numerical Lagrangian hydrodynamics

- task: "discretize" = replace continuous equations by a finite set of values so so that a computer can deal with them
  e.g. $\rho(\vec{x},t) \rightarrow \rho_a^n$ "density in comp.element a at time t^n "

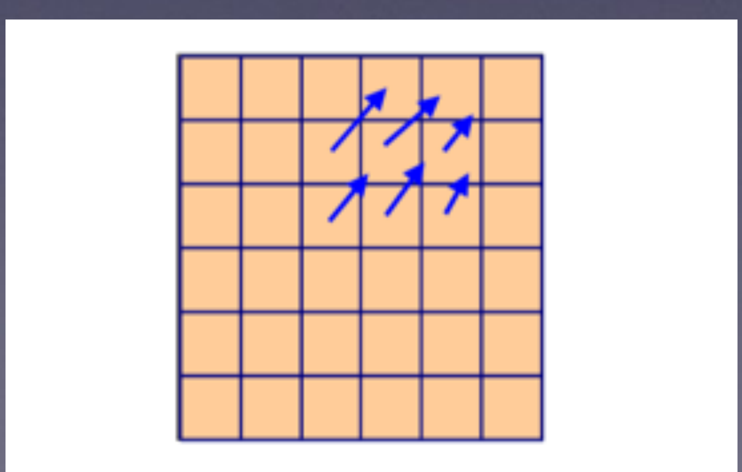
- many different possibilities

- long wish-list:
  - "accurate"
  - "simple": implement new physics
  - "Nature's conservation laws built in"
  - "fast"
  - "scalable"
  - "robust": no "crashes" for the problems that interest you
  - …

Types of numerical schemes

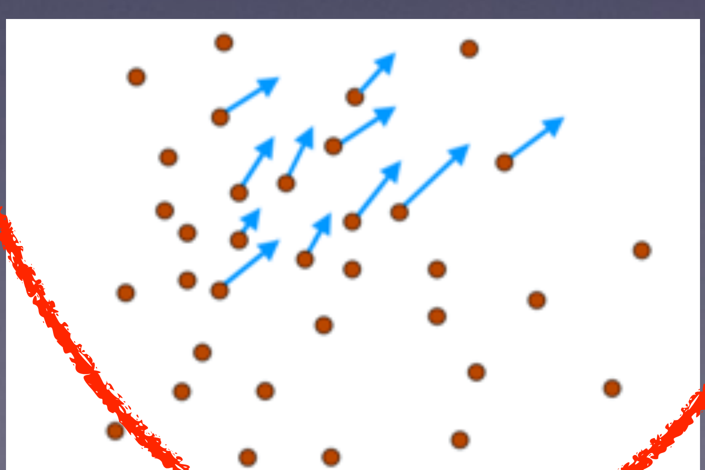
Eulerian

- usually on a (fixed) mesh
- calculate fluxes between cells



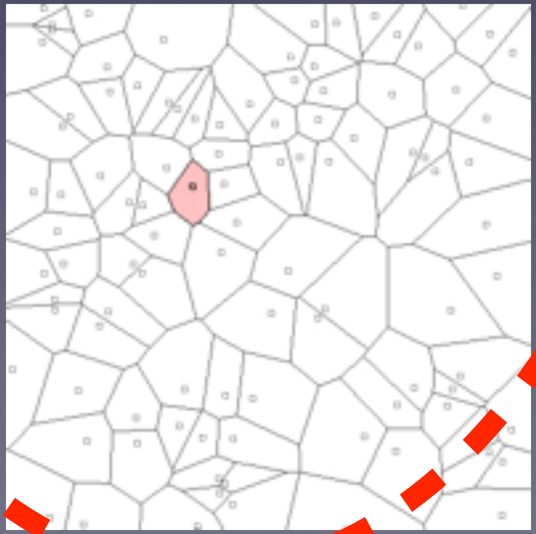
Lagrangian

- computational elements move with fluid velocity
- often with particles



ALE= Adaptive Lagrangian Eulerian

- computational elements move with velocity not necessarily = fluid velocity
- computational elements can be (e.g. Voronoi) cells, particles…



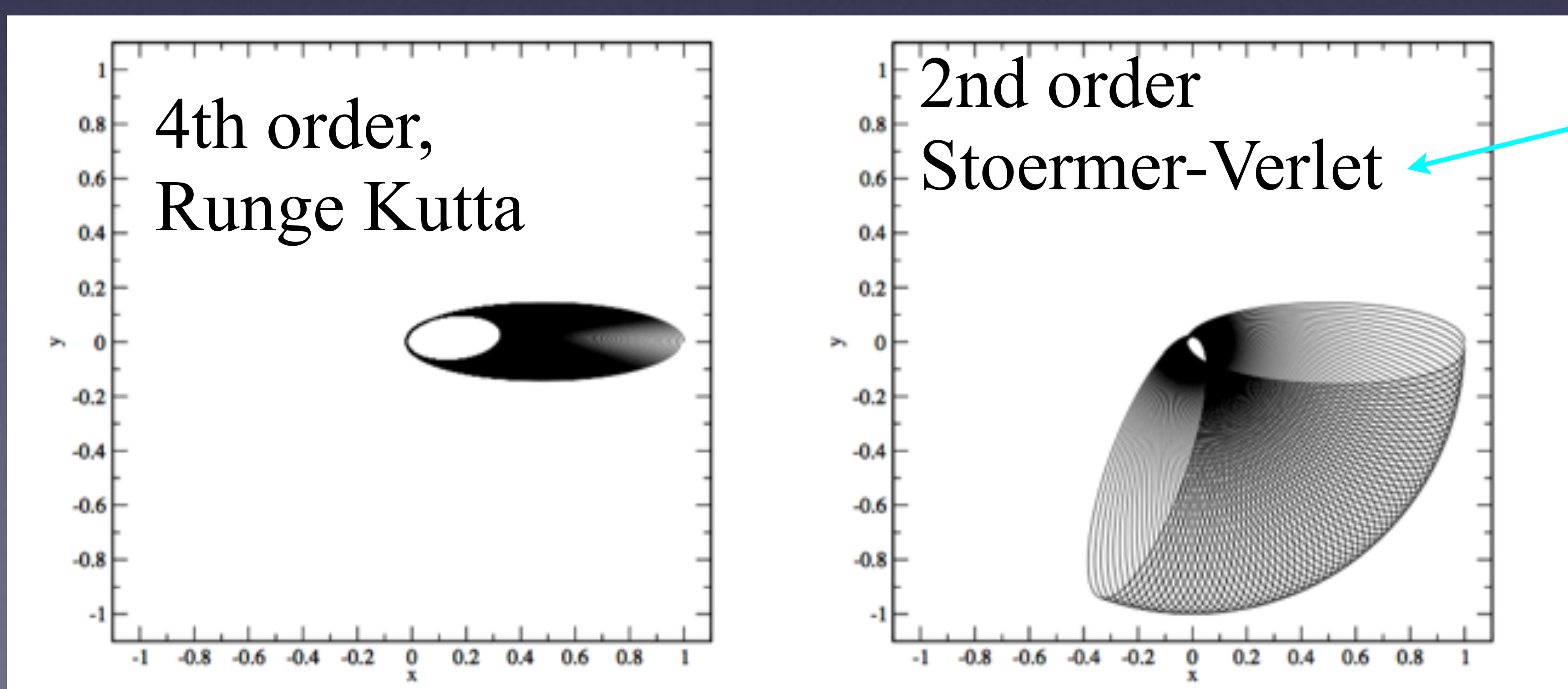
Importance of conservation

- keep in mind:
  - we rarely have all the numerical resolution we would want
  - we are solving “conservation laws”

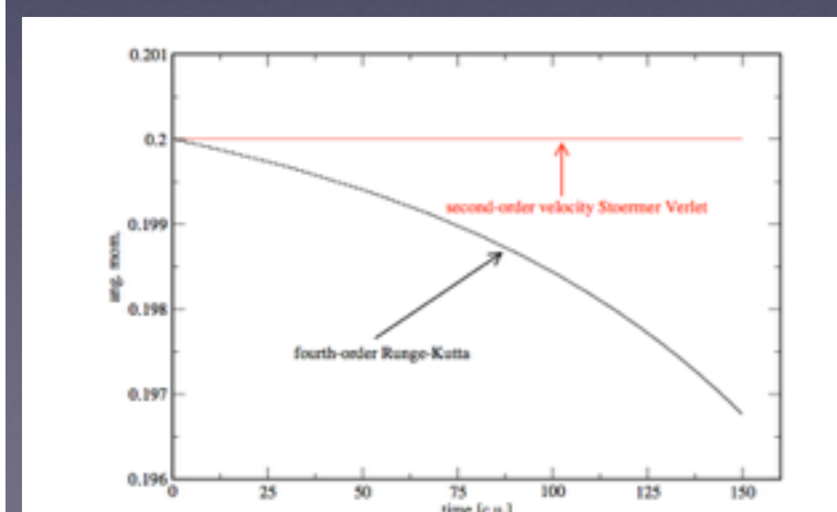
⇒ if conservation is “hardwired” (independent of resolution), we can hope to stay close to the real, physical solution

- Example 1: “Order vs. Conservation”

  ⇒ Kepler problem with too large a time step

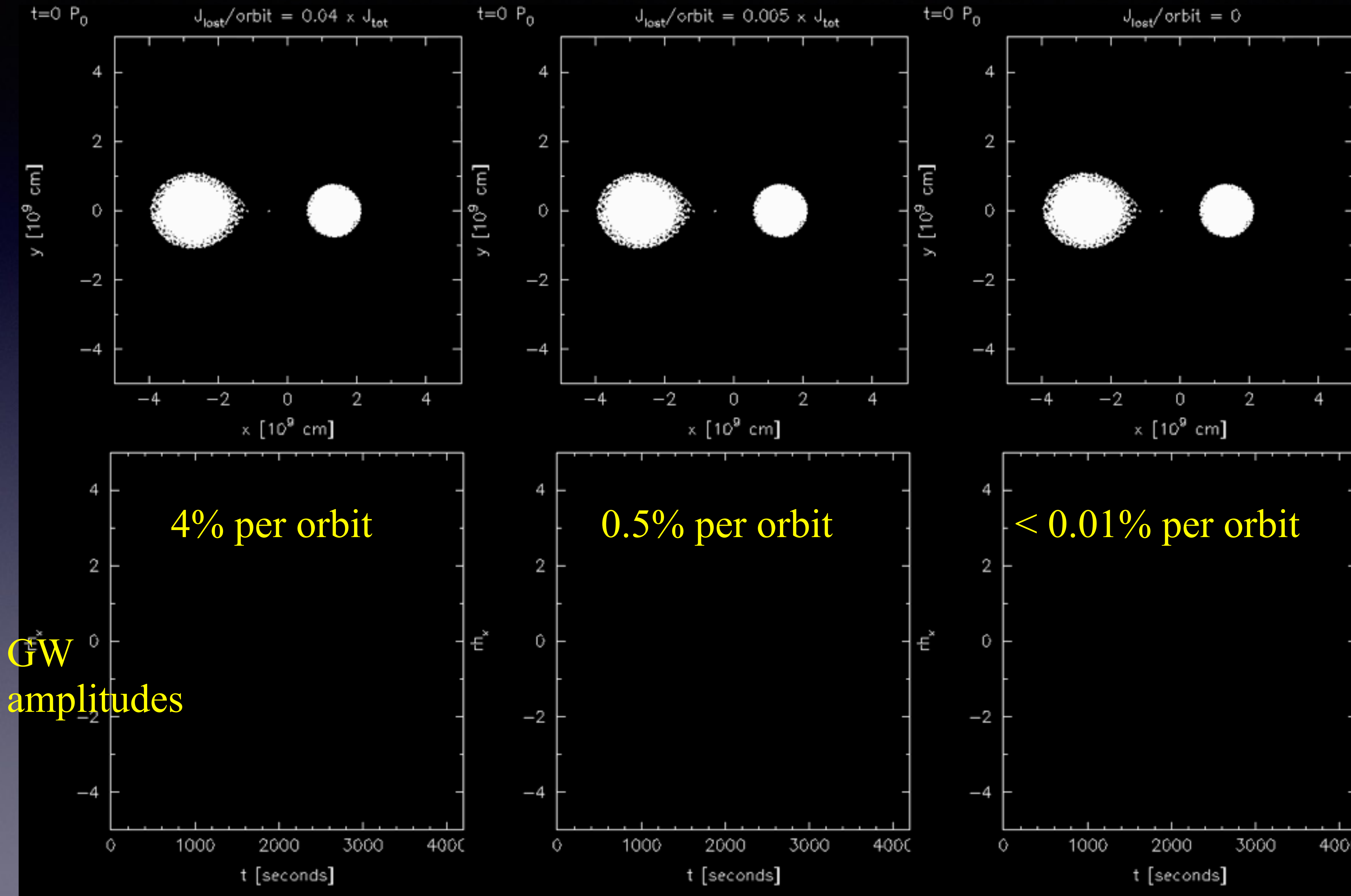


angular momentum conservation built-in!

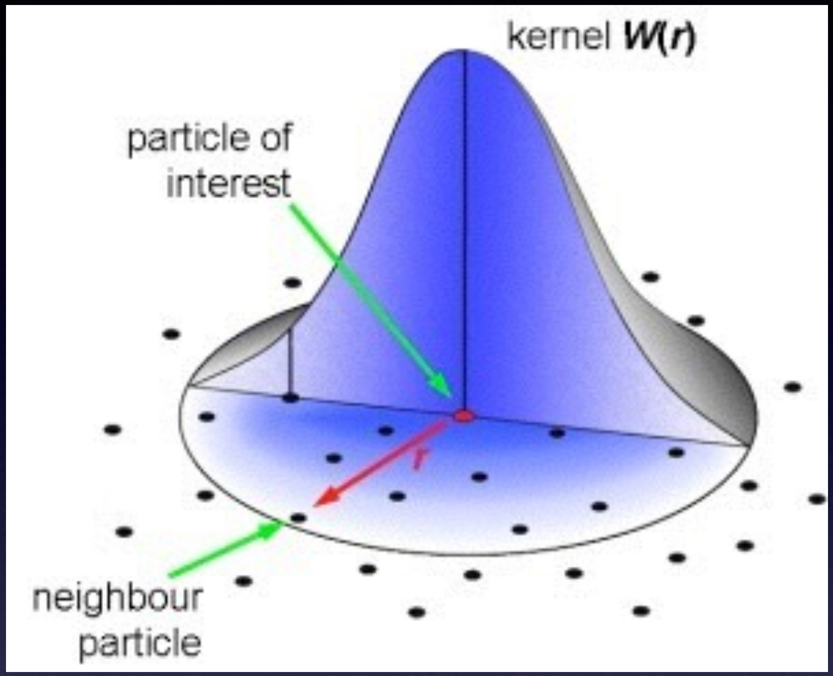


• Example 2: "How much non-conservation can we tolerate?"

⇒ mass transfer in white dwarf binary



2.1 Smooth Particle Hydrodynamics (SPH)



- basic ideas:
  - replace fluid by finite set of particles
  - particles move with local fluid velocities
  - each particle carries a smooth “kernel function”; used to recover smooth fields and calculate gradients
  - aim: particles should move in a way so that mass, energy, momentum and angular momentum are conserved “by construction”

2.1.1 Kernel interpolation

Integral approximation

- idea similar to δ-distribution: $$f(\vec{r}) = \int f(\vec{r}')\delta(\vec{r}' - \vec{r})\, dV$$

- smooth approximation: $$\tilde{f}_h(\vec{r}) = \int f(\vec{r'})W(\vec{r} - \vec{r'}, h)\, d^3r'$$

"smoothed approximation" "original function" "smoothing kernel" "smoothing length"

- obviously required kernel properties:

  - W has dimension "1/volume"

  - normalization $$\int W(\vec{r} - \vec{r'}, h)\, d^3r' = 1$$

  - "delta-property" $$\lim_{h\to 0} \tilde{f}_h(\vec{r}) = f(\vec{r})$$

particle approximation

- write integral approximation as $\tilde{f}_h(\vec{r}) = \int \frac{f(\vec{r'})}{\rho(\vec{r'})} W(\vec{r} - \vec{r'}, h)\ \rho(\vec{r'}) d^3 r'$

approximate as

"particle mass"

$$f(\vec{r}) = \sum_b \frac{m_b}{\rho_b} f_b W(\vec{r} - \vec{r}_b, h)$$

"mass density"

"SPH approximant"

"at position of particle b"

- check dimensions:

[f]= volume * [f] * 1/volume

- approximant can be applied to find density estimate

$$\rho(\vec{r}) = \sum_b m_b W(|\vec{r} - \vec{r}_b|, h)$$

gradient approximation

- several possibilities
- easiest: take straight-forward gradient of approximant

$$A(\vec{r}) = \sum_a \frac{m_a}{\rho_a} A_a W(|\vec{r} - \vec{r}_a|, h)$$

$$\Downarrow$$

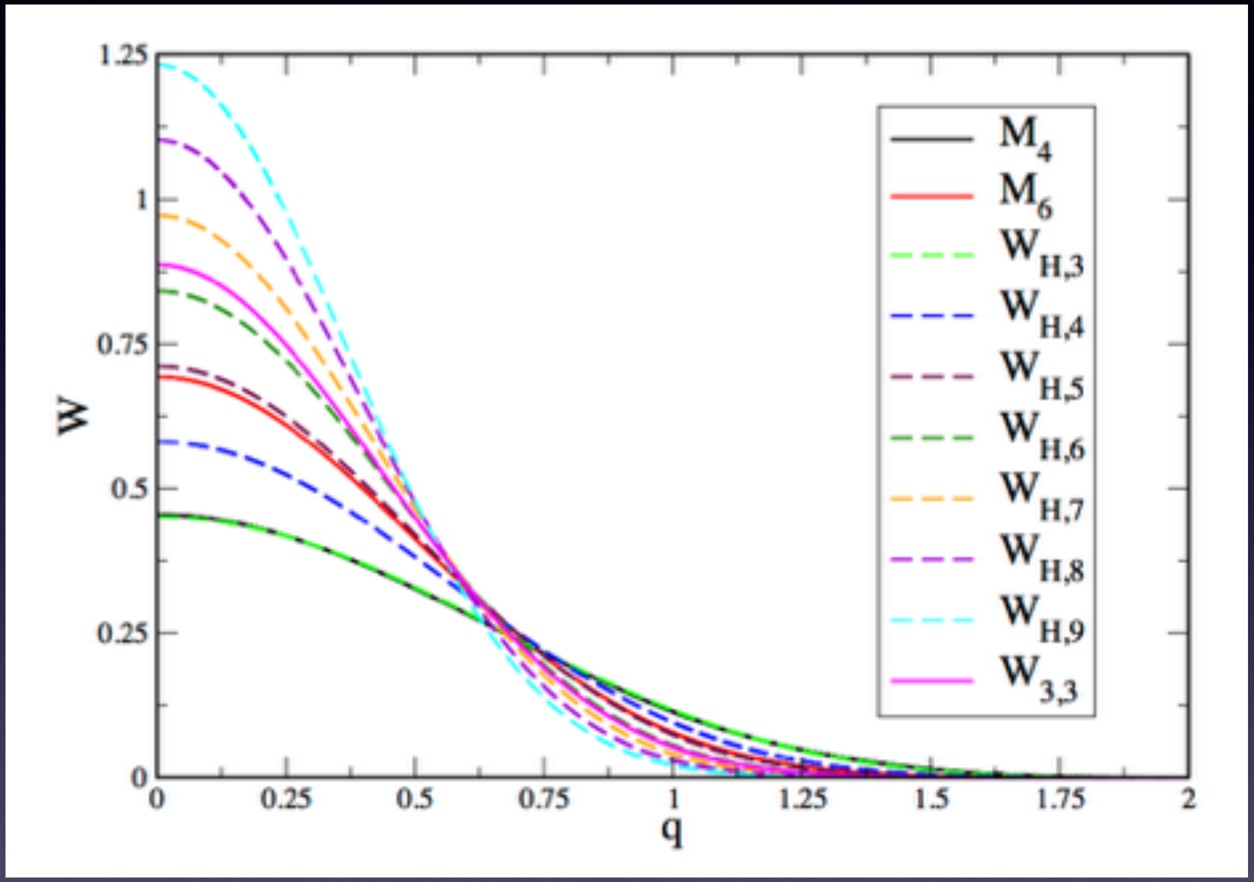
$$\boxed{\nabla A(\vec{r}) = \sum_a \frac{m_a}{\rho_a} A_a \nabla W(|\vec{r} - \vec{r}_a|, h)}$$

- there are more sophisticated/accurate/expensive ways to calculate gradients on particles
- usually tension: accurate gradient $\Longleftrightarrow$ exact conservation
- more on gradients later

Which kernels?

- for now just:

(a) "compact support"
$\Rightarrow$ zero outside of given radius
$\Rightarrow$ determined by "smoothing length" h
$\Rightarrow$ sum over local neighbours
(avoid N^2-behaviour)



(b) "bell-shaped"

(c) "radial":

$$W(\vec{r}_a - \vec{r}_b, h) = W(|\vec{r}_a - \vec{r}_b|, h)$$

$\Rightarrow$ crucial for exact angular momentum conservation

Kernel derivatives

We collect here a few relations that are often used throughout the text. We use the notation $\vec{r}_{bk} = \vec{r}_b - \vec{r}_k$, $r_{bk} = |\vec{r}_{bk}|$ and $\vec{v}_{bk} = \vec{v}_b - \vec{v}_k$. For the kernels we ignore for a moment derivatives coming from the smoothing lengths. We will address this topic later separately. By straight-forward component wise differentiation one finds

$$\frac{\partial}{\partial \vec{r}_a}|\vec{r}_b - \vec{r}_k| = \frac{(\vec{r}_b - \vec{r}_k)(\delta_{ba} - \delta_{ka})}{|\vec{r}_b - \vec{r}_k|} = \hat{e}_{bk}(\delta_{ba} - \delta_{ka}) \tag{3.20}$$

where $\hat{e}_{bk}$ is the unit vector from particle k to particle b.

$$\frac{\partial}{\partial \vec{r}_a}\frac{1}{|\vec{r}_b - \vec{r}_k|} = -\frac{\hat{e}_{bk}(\delta_{ba} - \delta_{ka})}{|\vec{r}_b - \vec{r}_k|^2}. \tag{3.21}$$

We will also need

$$\begin{aligned}
\frac{dr_{ab}}{dt} &= \frac{\partial r_{ab}}{\partial x_a}\frac{dx_a}{dt} + \frac{\partial r_{ab}}{\partial y_a}\frac{dy_a}{dt} + \frac{\partial r_{ab}}{\partial z_a}\frac{dz_a}{dt} \\
&\quad + \frac{\partial r_{ab}}{\partial x_b}\frac{dx_b}{dt} + \frac{\partial r_{ab}}{\partial y_b}\frac{dy_b}{dt} + \frac{\partial r_{ab}}{\partial z_b}\frac{dz_b}{dt} \\
&= \nabla_a r_{ab} \cdot \vec{v}_a + \nabla_b r_{ab} \cdot \vec{v}_b = \nabla_a r_{ab} \cdot \vec{v}_a - \nabla_a r_{ab} \cdot \vec{v}_b \\
&= \nabla_a r_{ab} \cdot \vec{v}_{ab} = \hat{e}_{ab} \cdot \vec{v}_{ab},
\end{aligned} \tag{3.22}$$

where we have used $\partial r_{ab}/\partial x_b = -\partial r_{ab}/\partial x_a$ etc.
For kernels that only depend on the magnitude of the separation, $W(\vec{r}_b - \vec{r}_k) = W(|\vec{r}_b - \vec{r}_k|) \equiv W_{bk}$ the derivative with respect to the coordinate of an arbitrary particle a is

$$\nabla_a W_{bk} = \frac{\partial}{\partial \vec{r}_a} W_{bk} = \frac{\partial W_{bk}}{\partial r_{bk}}\frac{\partial r_{bk}}{\partial \vec{r}_a} = \frac{\partial W_{bk}}{\partial r_{bk}}\hat{e}_{bk}(\delta_{ba} - \delta_{ka}) = \nabla_b W_{kb}(\delta_{ba} - \delta_{ka}), \tag{3.23}$$

where we have use Eq. (3.20). This yields in particular

$$\nabla_a W_{ab} = \frac{\partial}{\partial \vec{r}_a} W_{ab} = \frac{\partial W_{ab}}{\partial r_{ab}}\frac{\partial r_{ab}}{\partial \vec{r}_a} = \frac{\partial W_{ab}}{\partial r_{ab}}\hat{e}_{ab} = -\frac{\partial W_{ab}}{\partial r_{ab}}\frac{\partial r_{ab}}{\partial \vec{r}_b} = -\frac{\partial}{\partial \vec{r}_b} W_{ab} = -\nabla_b W_{ab} \tag{3.24}$$

important for
exact conservation

For the time derivative of the kernel we have

$$\frac{dW_{ab}}{dt} = \frac{\partial W_{ab}}{\partial r_{ab}}\frac{dr_{ab}}{dt} = \frac{\partial W_{ab}}{\partial r_{ab}}\frac{(\vec{r}_a - \vec{r}_b)\cdot(\vec{v}_a - \vec{v}_b)}{r_{ab}} = \frac{\partial W_{ab}}{\partial r_{ab}}\hat{e}_{ab}\vec{v}_{ab} = \vec{v}_{ab} \cdot \nabla_a W_{ab} \tag{3.25}$$

energy equation

with $\vec{r}_{ab} \equiv \vec{r}_a - \vec{r}_b$

and $\hat{e}_{ab} \equiv \dfrac{\vec{r}_{ab}}{|\vec{r}_{ab}|}$

$W_{ab} = W(|\vec{r}_a - \vec{r}_b|, h)$

2.1.2 "Vanilla ice SPH"

"Discretize-and-hope-approach"

a) Momentum equation

- try a "brute-force discretization" of $\frac{d\vec{v}}{dt} = -\frac{1}{\rho}\nabla P$

  using $\nabla f(\vec{r}) = \sum_b \frac{m_b}{\rho_b} f_b \nabla W(\vec{r}-\vec{r}_b, h)$

  yields $\frac{d\vec{v}_a}{dt} = -\frac{1}{\rho_a}\sum_b \frac{m_b}{\rho_b} P_b \nabla_a W_{ab}$

is momentum conserved?

force from b on a: $\vec{F}_{ba} = \left(m_a \frac{d\vec{v}_a}{dt}\right)_b = -\frac{m_a}{\rho_a}\frac{m_b}{\rho_b} P_b \nabla_a W_{ab}$ $\quad \nabla_a W_{ab} = -\nabla_b W_{ab}$

force from a on b: $\vec{F}_{ab} = \left(m_b \frac{d\vec{v}_b}{dt}\right)_a = -\frac{m_b}{\rho_b}\frac{m_a}{\rho_a} P_a \nabla_b W_{ba} = \frac{m_a}{\rho_a}\frac{m_b}{\rho_b} P_a \nabla_a W_{ab}$

$\Longrightarrow$ (unless $P_a = P_b$) momentum NOT conserved, "actio $\neq$ reactio"

Exercise:

try to find a discretization of the momentum equation
that ensures exact momentum conservation

can this be fixed? Yes, easily…

- but now start from: $$\nabla\left(\frac{P}{\rho}\right) = \frac{\nabla P}{\rho} - P\frac{\nabla\rho}{\rho^2}$$

  i.e. $$\boxed{\frac{d\vec{v}_a}{dt} =} -\frac{\nabla P}{\rho} = -\frac{P}{\rho^2}\nabla\rho - \nabla\left(\frac{P}{\rho}\right)$$
  $$= -\frac{P_a}{\rho_a^2}\sum_b m_b \nabla_a W_{ab} - \sum_b \frac{m_b}{\rho_b}\frac{P_b}{\rho_b}\nabla_a W_{ab}$$
  $$\boxed{= -\sum_b m_b\left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right)\nabla_a W_{ab}}$$

- pressure part symmetric in a and b, with $\nabla_a W_{ab} = -\nabla_b W_{ab}$

  force from b on a= $\vec{F}_{ba} = -\vec{F}_{ba}$ = -force from a on b

→ forces opposite and equal, “actio = reactio”

momentum conserved by construction

b) Energy equation

- straight-forward translation of first law of thermodynamics:

$$\boxed{\frac{du}{dt} = \frac{P}{\rho^2}\frac{d\rho}{dt}}$$

$$\boxed{\frac{du_a}{dt}} = \frac{P_a}{\rho_a^2}\frac{d\rho_a}{dt} = \frac{P_a}{\rho_a^2}\frac{d}{dt}\left(\sum_b m_b W_{ab}\right) = \boxed{\frac{P_a}{\rho_a^2}\sum_b m_b \vec{v}_{ab}\cdot\nabla_a W_{ab}}$$

- this straight-forward translation comes with some subtleties/implications for initial conditions… see later

c) Continuity equation

- most common approach: keep particle masses fix, m_b= const
  $\Rightarrow$ no need to solve momentum equation!
  exact mass conservation!

- but if wanted…

$$\boxed{\frac{d\rho_a}{dt}} = \frac{d}{dt}\left(\sum_b m_b W_{ab}\right) = \boxed{\sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab},}$$

- since $\boxed{\frac{d\rho}{dt} = -\rho \nabla \cdot \vec{v}}$ this can be used to find an expression

  for the velocity divergence:

$$\boxed{(\nabla \cdot \vec{v})_a = -\frac{1}{\rho_a} \sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab}}$$

- so far: momentum and mass conservation;

$\Longrightarrow$ What about angular momentum conservation?

- torque on particle a: $$\vec{M}_a = \vec{r}_a \times \vec{F}_a = \vec{r}_a \times \left(m_a \frac{d\vec{v}_a}{dt} \right) = \vec{r}_a \times \sum_b \vec{F}_{ba}$$

- total torque:

$$\frac{d\vec{L}}{dt} = \sum_a \vec{M}_a = \sum_{a,b} \vec{r}_a \times \vec{F}_{ba} = \frac{1}{2} \left(\sum_{a,b} \vec{r}_a \times \vec{F}_{ba} + \sum_{\boxed{a,b}} \vec{r}_a \times \vec{F}_{\boxed{ba}} \right)$$

$$= \frac{1}{2} \left(\sum_{a,b} \vec{r}_a \times \vec{F}_{ba} + \sum_{\boxed{b,a}} \vec{r}_b \times \vec{F}_{\boxed{ab}} \right) = \frac{1}{2} \left(\sum_{a,b} (\vec{r}_a - \vec{r}_b) \times \vec{F}_{ba} \right) = 0$$

$$\vec{F}_{ba} = -\vec{F}_{ba}$$

force along line joining particles $\quad \vec{F}_{ab} \propto \nabla_a W_{ab} \propto \hat{e}_{ab} \propto (\vec{r}_a - \vec{r}_b)$

$\Longrightarrow$ angular momentum conserved by construction (for radial kernels!)

- What about energy conservation?
  - change in total energy:

$$\frac{dE}{dt} = \frac{d}{dt}\sum_a \left(m_a u_a + \frac{1}{2} m_a v_a^2 \right) \quad = \quad \sum_a m_a \left(\frac{du_a}{dt} + \vec{v}_a \cdot \frac{d\vec{v}_a}{dt} \right)$$

$$\boxed{\frac{du_a}{dt} = \sum_b m_b \left(\frac{P_a}{\rho_a^2} \right) \vec{v}_{ab} \cdot \nabla_a W_{ab}} \qquad \boxed{\frac{d\vec{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla_a W_{ab}}$$

$$\begin{aligned}
\frac{dE}{dt} &= \sum_a m_a \left[\frac{P_a}{\rho_a^2} \sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab} - \vec{v}_a \cdot \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla_a W_{ab} \right] \\
&= \sum_{a,b} m_a m_b \frac{P_a}{\rho_a^2} \vec{v}_a \cdot \nabla_a W_{ab} - \sum_{a,b} m_a m_b \frac{P_a}{\rho_a^2} \vec{v}_b \cdot \nabla_a W_{ab} \\
&\quad - \sum_{a,b} m_a m_b \frac{P_a}{\rho_a^2} \vec{v}_a \cdot \nabla_a W_{ab} - \sum_{a,b} m_a m_b \frac{P_b}{\rho_b^2} \vec{v}_a \cdot \nabla_a W_{ab} \\
&= -\sum_{a,b} m_a m_b \left(\frac{P_a \vec{v}_b}{\rho_a^2} + \frac{P_b \vec{v}_a}{\rho_b^2} \right) \nabla_a W_{ab} = 0
\end{aligned}$$

symmetric / antisymmetric

w.r. a $\Leftrightarrow$ b

$\Rightarrow$ same “tricks” as before,

energy conserved by construction

Adaptive resolution

• desired: - small smoothing length h in high density regions
- large smoothing length in low density regions

• options: a) “keep neighbour number fix”

b) based on density $$h_a = \eta \left(\frac{m_a}{\rho_a} \right)^{1/D} \qquad \eta = 1.2...1.5$$

but : $$\rho_a = \sum_b m_b W(|\vec{r}_a - \vec{r}_b|, h_a)$$

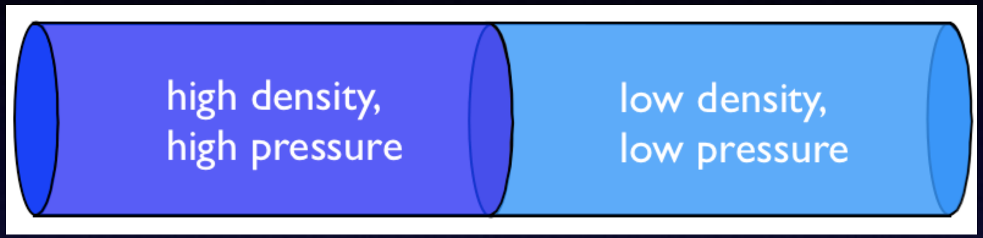
$\Rightarrow$ needs iteration for consistency

• Attention: careless h-update can introduce noise!

- by now we have equations for
  - mass
  - momentum
  - energy

Can we do shocks?

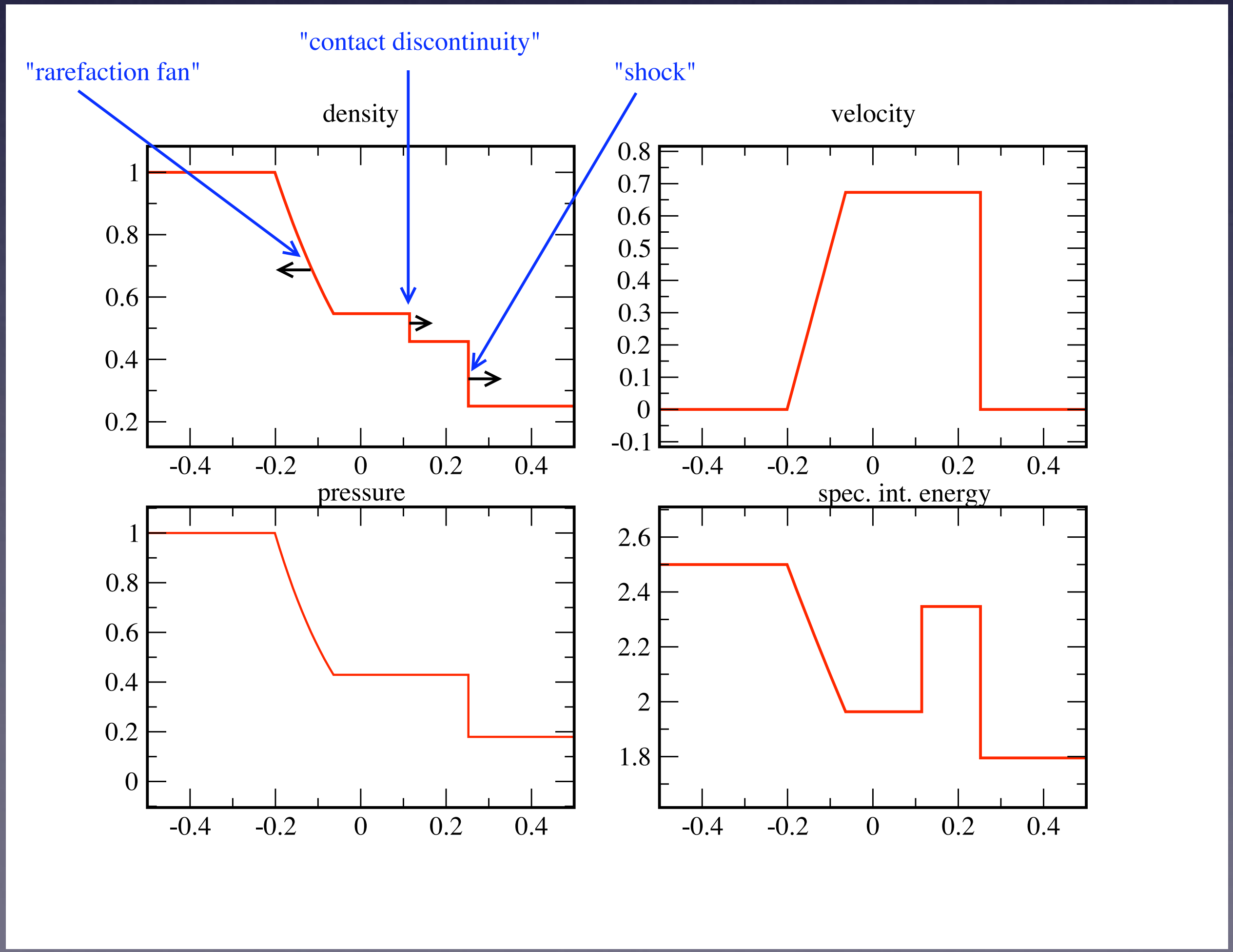
"Shock tube"



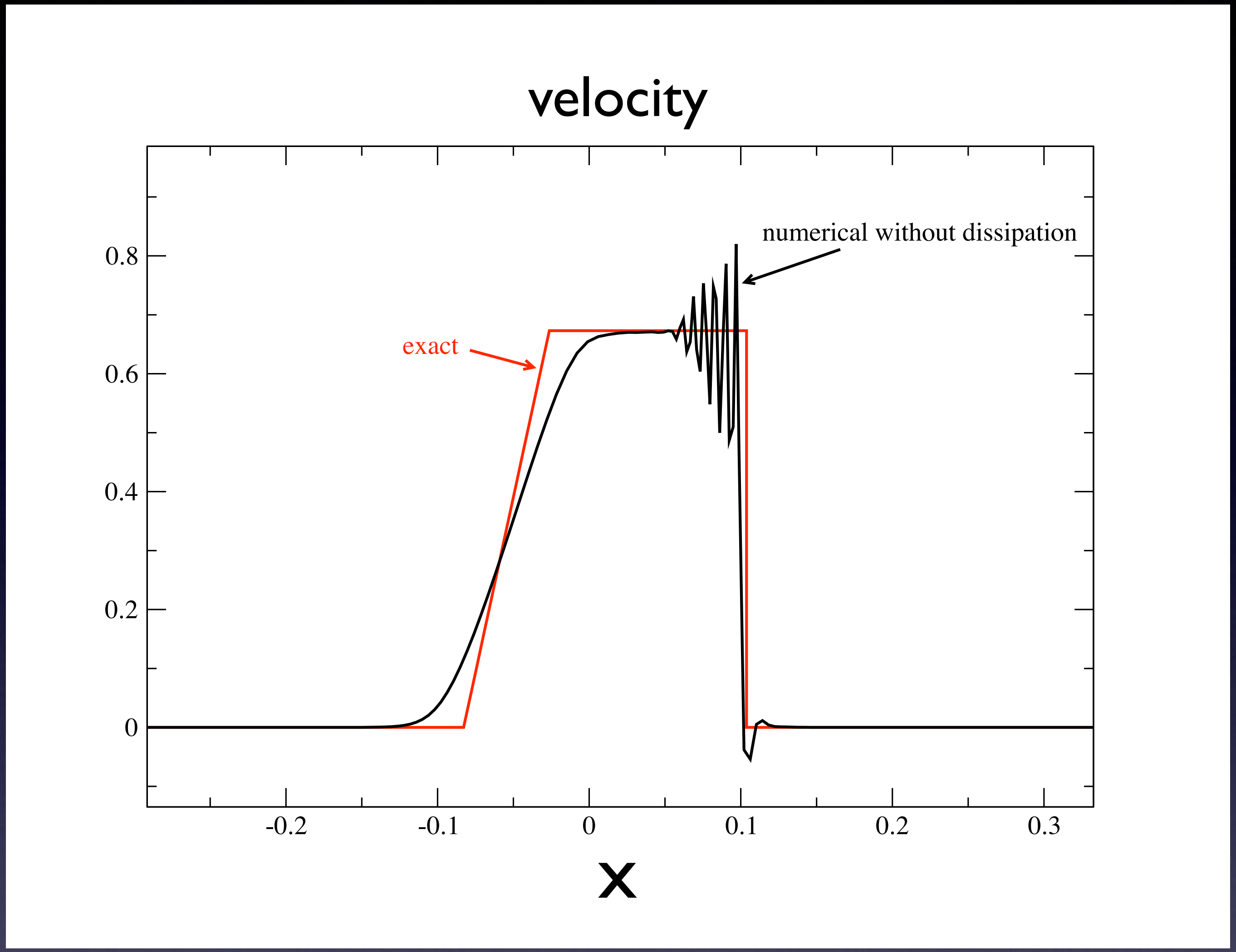
- mathematically: "Riemann problem"

how do physical quantities evolve as a function of time once the separating wall is removed?

can be solved exactly...



just apply our derived SPH formalism to shock tube problem:



- unphysical post-shock oscillations, kinetic energy not transformed properly into heat
- so far no dissipation/entropy production

dissipation needed at shocks → "artificial viscosity"

Artificial Viscosity (AV)

- keep in mind: even perfectly smooth initial conditions can evolve into shocks!

- in nature: shock has finite width, because of dissipative processes on microscopic scales (i.e. on some level ideal fluid dynamics NOT applicable)

- basic idea behind: do the same on the numerical resolution scale

- John von Neumann (1950):

  The "idea is to introduce (artificial) dissipative terms into the equations so as to give the shocks a thickness comparable to (but preferentially larger than) the spacing ... [of the grid points]. Then the differential equations (more accurately, the corresponding difference equations) may be used for the entire calculation, just as though there were no shocks at all."

John von Neumann
(1903-1957)

- in practice: $P_{\rm phys} \rightarrow P_{\rm phys} + P_{\rm AV}$

  with $P_{\rm AV} = -c_1 \rho c_s l (\nabla \cdot \vec{v}) + c_2 \rho l^2 (\nabla \cdot \vec{v})^2$

- Artificial Viscosity should:

- always be dissipative: kinetic $\rightarrow$ thermal (NOT the other way)

- be absent:
  - if there is no shock
  - in rigid rotation
  - (shockless) differential rotation
  - expansion
  - …

- “intelligent enough” to distinguish uniform compression from a shock

- fulfil Rankine-Hugoniot conditions

- be properly symmetrized to ensure exact conservation

- a number of different forms for Π_{ab} can be used

- most common (detailed reasoning → Sec. 2.7 in "Astrophysical SPH"):

$$\Pi_{ab} = \Pi_{ab,\mathrm{bulk}} + \Pi_{ab,\mathrm{NR}} = \begin{cases} \frac{-\alpha \bar{c}_{ab} \mu_{ab} + \beta \mu_{ab}^2}{\bar{\rho}_{ab}} & \text{for } \vec{r}_{ab} \cdot \vec{v}_{ab} < 0 \\ 0 & \text{otherwise} \end{cases},$$

where

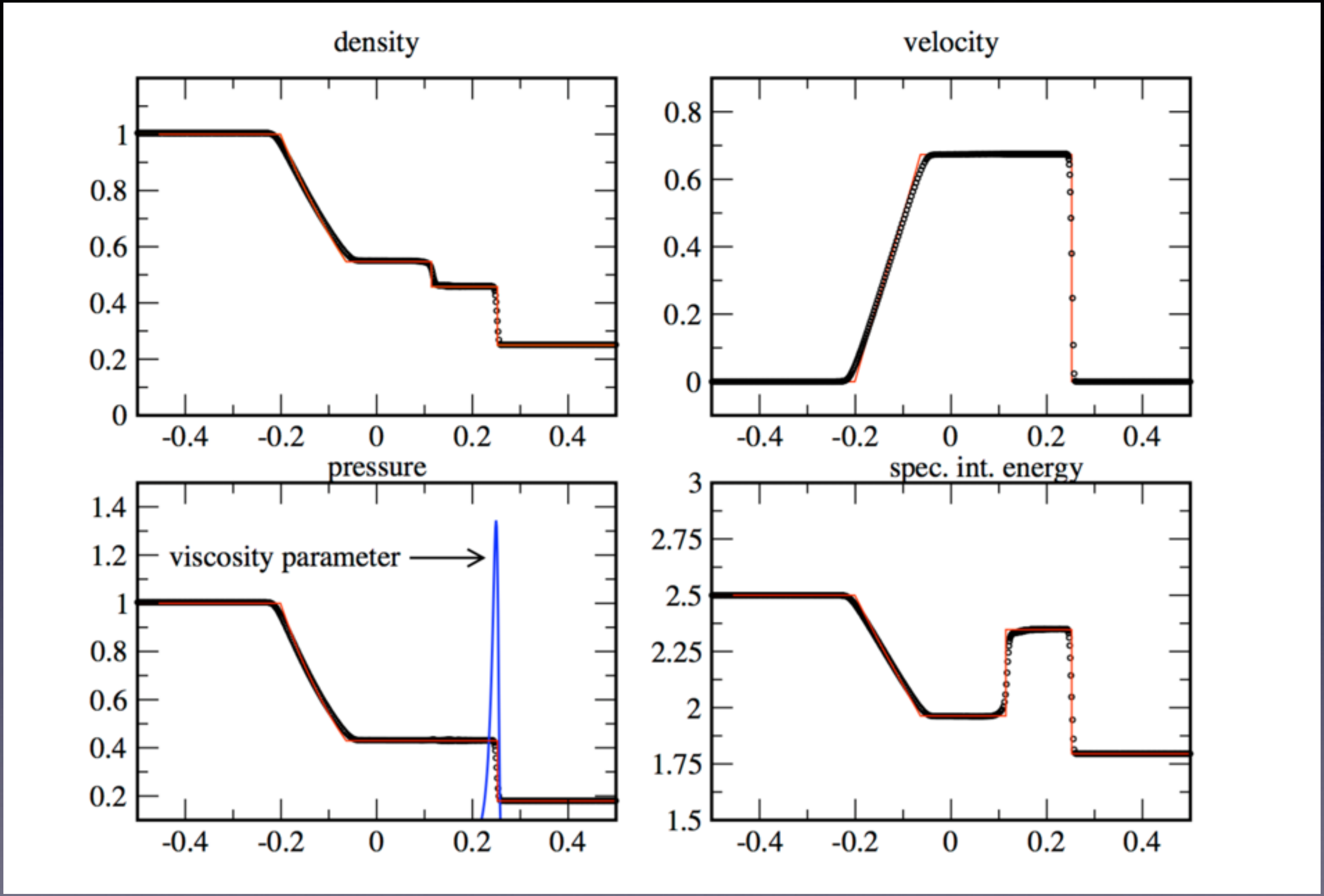
$$\mu_{ab} = \frac{\bar{h}_{ab} \vec{r}_{ab} \cdot \vec{v}_{ab}}{r_{ab}^2 + \epsilon \bar{h}_{ab}^2}.$$

- all forms reasonably good in shocks, the challenge is to avoid artifacts when AV is not needed

- $\alpha \approx 1$, $\beta \approx 2$ in shocks

- keeping α and β constant is a bad idea!
  ⇒ Intelligent "steering" of α and β required! (→ e.g. Cullen & Dehnen 2010, SR 2015a, 2015b)

• example: shock tube with dissipation steering



(from SR+ 2008)

Summary "Vanilla ice SPH"

- "continuity"

$$\rho(\vec{r}) = \sum_b m_b W(|\vec{r} - \vec{r}_b|, h)$$

or

$$\frac{d\rho_a}{dt} = \sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab}$$

artificial dissipation

- "momentum"

$$\frac{d\vec{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \nabla_a W_{ab}$$

- "energy"

$$\frac{du_a}{dt} = \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{1}{2}\Pi_{ab} \right) \vec{v}_{ab} \cdot \nabla_a W_{ab}$$

$\Rightarrow$ works well with good AV-steering, but symmetrization was "by hand"

$\Rightarrow$ much more elegant: derivation from variational principle

2.1.3 SPH from a Variational Principle

Classical Mechanics:

- Lagrange function: $$L(q, \dot{q}, t) = T - V$$

  “coordinates” “velocities” “kinetic energy” “potential energy”

- canonical momentum: $$p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$$

- canonical energy: $$E \equiv \sum_i p_i \dot{q}_i - L$$

- evolution determined by "Principle of least action", via

$$\delta \int_{t_1}^{t_2} L(q(t), \dot{q}(t), t) dt = 0$$

Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$$

- Invariance of Lagrangian under — conservation of
  - spatial shift → momentum
  - rotation → angular momentum
  - temporal shift → energy

- Lagrangian of ideal fluid (Eckhart 1960):

$$L = \int \left(\frac{v^2}{2} - u(\rho, s) \right) \rho \, dV$$

"specific energy takes over role of potential"

- SPH discretization:

$$L_{\rm SPH} = \sum_b m_b \left(\frac{v_b^2}{2} - u_b \right)$$

$$L_{\rm SPH} = \sum_b m_b \left(\frac{v_b^2}{2} - u_b \right)$$

- now apply:

a) Euler-Lagrange equations
$$\frac{d}{dt}\left(\frac{\partial L_{\rm SPH}}{\partial \vec{v}_a}\right) - \frac{\partial L_{\rm SPH}}{\partial \vec{r}_a} = 0$$

b) 1. law of thermodynamics
$$\frac{du}{dt} = \frac{P}{\rho^2}\frac{d\rho}{dt}$$

$\Rightarrow$ discrete fluid equations with “hardwired” conservation

- so we need:

a) $\frac{\partial L_{\rm SPH}}{\partial \vec{v}_a}$ easy : $\rightarrow m_a \vec{v}_a$ as usual: keep masses fixed!

b) $\frac{\partial L_{\rm SPH}}{\partial \vec{r}_a}$

c) $\frac{d\rho_a}{dt}$

b) $$\frac{\partial L_{\mathrm{SPH}}}{\partial \vec{r}_a} = \frac{\partial}{\partial \vec{r}_a}\left[\sum_b m_b \left(\frac{v_b^2}{2} - u_b\right)\right] = -\sum_b m_b \left(\frac{\partial u_b}{\partial \rho_b}\right)_s \frac{\partial \rho_b}{\partial \vec{r}_a}$$

1st law of thermodynamics:

$$m_a \frac{d\vec{v}_a}{dt} = -\sum_b m_b \frac{P_b}{\rho_b^2} \frac{\partial \rho_b}{\partial \vec{r}_a}$$

c) for energy equation $$\frac{du}{dt} = \frac{P}{\rho^2}\frac{d\rho}{dt}$$

$\Rightarrow$ need density derivatives $\dfrac{\partial \rho_b}{\partial \vec{r}_a}$ and $\dfrac{d\rho_a}{dt}$

- so far: never specified WHICH smoothing length to use

say, one could use: $$\rho_a = \sum_b m_b W(r_{ab}, h_a)$$

or $$\rho_a = \sum_b m_b W(r_{ab}, h_b)$$

or $$\rho_a = \sum_b m_b W(r_{ab}, \bar{h}_{ab}), \bar{h}_{ab} = \frac{h_a + h_b}{2}$$

- similar: $\nabla_a W_{ab}$ should be symmetric in h_a/h_b

could be achieved as $\nabla_a W_{ab}(\bar{h}_{ab})$

or $\frac{1}{2}(\nabla_a W_{ab}(h_a) + \nabla_a W_{ab}(h_b))$

or ...

- from now on use: $\rho_a = \sum_b m_b W(r_{ab}, h_a)$ $\qquad h_a = \eta \left(\frac{m_a}{\rho_a}\right)^{1/D}$

$$\frac{d\rho_a}{dt} = \frac{d}{dt}\left(\sum_b m_b W_{ab}(h_a)\right) = \sum_b m_b \left\{ \frac{\partial W_{ab}(h_a)}{\partial r_{ab}} \frac{dr_{ab}}{dt} + \frac{\partial W_{ab}(h_a)}{\partial h_a} \frac{dh_a}{dt} \right\}$$

$$= \sum_b m_b \frac{\partial W_{ab}(h_a)}{\partial r_{ab}} \hat{e}_{ab} \cdot \vec{v}_{ab} + \sum_b m_b \frac{\partial W_{ab}(h_a)}{\partial h_a} \cdot \frac{\partial h_a}{\partial \rho_a} \frac{d\rho_a}{dt}$$

$$= \sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab}(h_a) + \frac{\partial h_a}{\partial \rho_a} \frac{d\rho_a}{dt} \sum_b m_b \frac{\partial W_{ab}(h_a)}{\partial h_a}$$

collect

$$\Rightarrow \quad \boxed{\frac{d\rho_a}{dt} = \frac{1}{\Omega_a} \sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab}(h_a)}$$

with $\boxed{\Omega_a \equiv \left(1 - \frac{\partial h_a}{\partial \rho_a} \sum_b m_b \frac{\partial W_{ab}(h_a)}{\partial h_a}\right)}$ "grad-h term"

- similar to time derivative

$$\boxed{\frac{\partial \rho_b}{\partial \vec{r}_a}} = \sum_k m_k \left\{ \nabla_a W_{bk}(h_b) + \frac{\partial W_{bk}(h_b)}{\partial h_b} \frac{\partial h_b}{\partial \rho_b} \frac{\partial \rho_b}{\partial \vec{r}_a} \right\}$$

$$\boxed{= \frac{1}{\Omega_b} \sum_k m_k \nabla_a W_{bk}(h_b)}$$

- then the energy equation reads:

$$\left.\begin{aligned} \frac{du}{dt} &= \frac{P}{\rho^2}\frac{d\rho}{dt} \\ \frac{d\rho_a}{dt} &= \frac{1}{\Omega_a}\sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab}(h_a) \end{aligned}\right\} \boxed{\frac{du_a}{dt} = \frac{1}{\Omega_a}\frac{P_a}{\rho_a^2}\sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab}(h_a)}$$

- from

$$m_a \frac{d\vec{v}_a}{dt} = -\sum_b m_b \frac{P_b}{\rho_b^2} \frac{\partial \rho_b}{\partial \vec{r}_a} \quad \& \quad \frac{\partial \rho_b}{\partial \vec{r}_a} = \frac{1}{\Omega_b} \sum_k m_k \nabla_a W_{bk}(h_b)$$

$$m_a \frac{d\vec{v}_a}{dt} = -\sum_b m_b \frac{P_b}{\rho_b^2} \left(\frac{1}{\Omega_b} \sum_k m_k \nabla_a W_{bk}(h_b) \right)$$

$$\nabla_a W_{bk} = \nabla_b W_{kb} (\delta_{ba} - \delta_{ka})$$

$$= -\sum_b m_b \frac{P_b}{\rho_b^2} \frac{1}{\Omega_b} \sum_k m_k \nabla_b W_{kb}(h_b) \, (\delta_{ba} - \delta_{ka})$$

$$= \quad -m_a \frac{P_a}{\rho_a^2} \frac{1}{\Omega_a} \sum_k m_k \nabla_a W_{ka}(h_a) + \sum_b m_b \frac{P_b}{\rho_b^2} \frac{1}{\Omega_b} m_a \nabla_b W_{ab}(h_b)$$

$$= \quad -m_a \frac{P_a}{\rho_a^2} \frac{1}{\Omega_a} \sum_b m_b \nabla_a W_{ba}(h_a) - m_a \sum_b m_b \frac{P_b}{\rho_b^2} \frac{1}{\Omega_b} \nabla_a W_{ab}(h_b)$$

$$= -m_a \sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2} \nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} \nabla_a W_{ab}(h_b) \right)$$

$$\boxed{\frac{d\vec{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2} \nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} \nabla_a W_{ab}(h_b) \right)}$$

- comments:

i) similar to “vanilla ice version”

ii) but gradients augmented by “grad-h-terms”

iii) no more ambiguities in symmetrization, stringent consequence from variational procedure

Summary SPH from Variational Principle:

“vanilla ice version”

- mass:

$$\rho_a = \sum_b m_b W_{ab}(h_a)$$

$$\frac{du_a}{dt} = \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{1}{2}\Pi_{ab} \right) \vec{v}_{ab} \cdot \nabla_a W_{ab}$$

- energy:

$$\frac{du_a}{dt} = \frac{1}{\Omega_a} \frac{P_a}{\rho_a^2} \sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab}(h_a)$$

$$\frac{d\vec{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \nabla_a W_{ab}$$

- momentum:

$$\frac{d\vec{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2} \nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} \nabla_a W_{ab}(h_b) \right)$$

2.1.4 Subtleties and recent developments

Subtleties

- two points, both related to “initial conditions”
  - setting up contact discontinuities ⇒ Kelvin Helmholtz instabilities
  - built-in remeshing mechanism ⇒ initial particle distribution

Recent developments

- one has choices in the discretization process, e.g.
  - kernel function
  - volume elements
  - dissipation steering
  - gradient estimates

⇒ substantial impact on accuracy (some with higher computational effort)

Two important (but not so obvious) implications:

- I. "density is smooth, internal energy not"
    - for a careless setup of contact discontinuities this can lead to surface tension effects
      $\Rightarrow$ (for such a setup) weak instabilities may be suppressed

- II. built-in "re-meshing mechanism"
    - drives particles towards optimal distribution
    - in simulations that start from non-optimal distributions, this can cause substantial particle motion
      $\Rightarrow$ "noise"

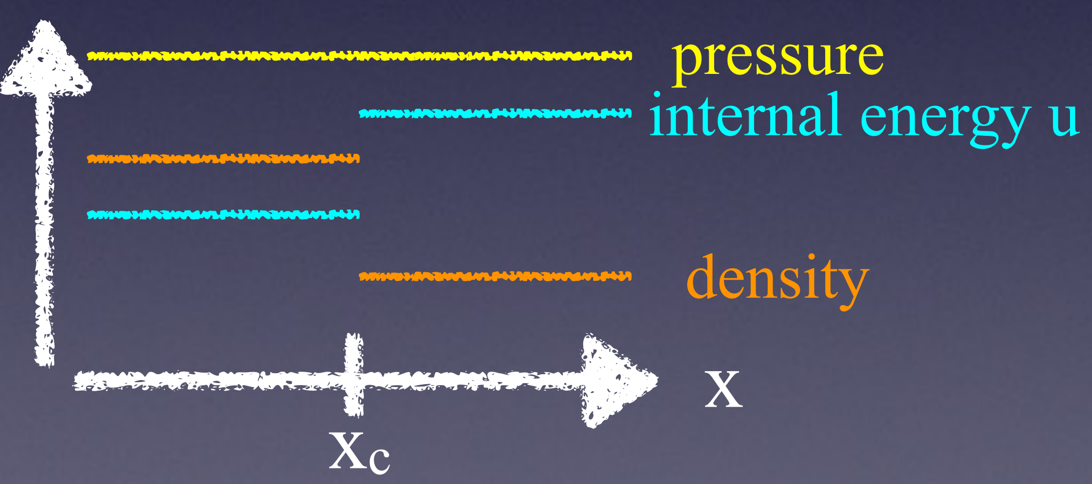
$\Rightarrow$ Good initial conditions crucial!

Implication I: density ρ comes from kernel smoothing process, internal energy not!

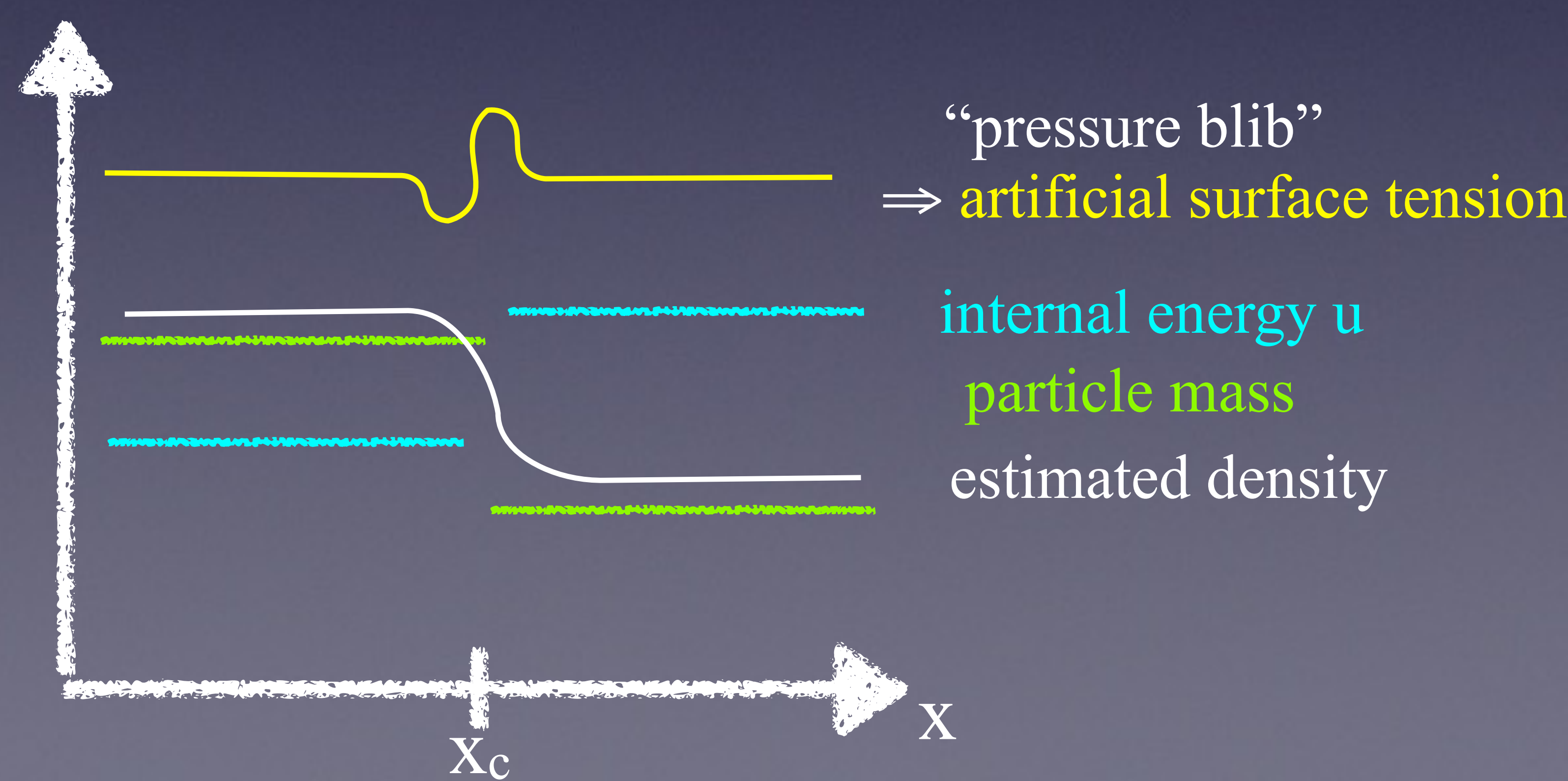
$\Rightarrow$ care needed when setting up initial conditions!

example: set up contact discontinuity:
- density has a jump
- $P_1 = P_2$
- polytropic EOS $P = (\Gamma - 1)\,\rho\, u$

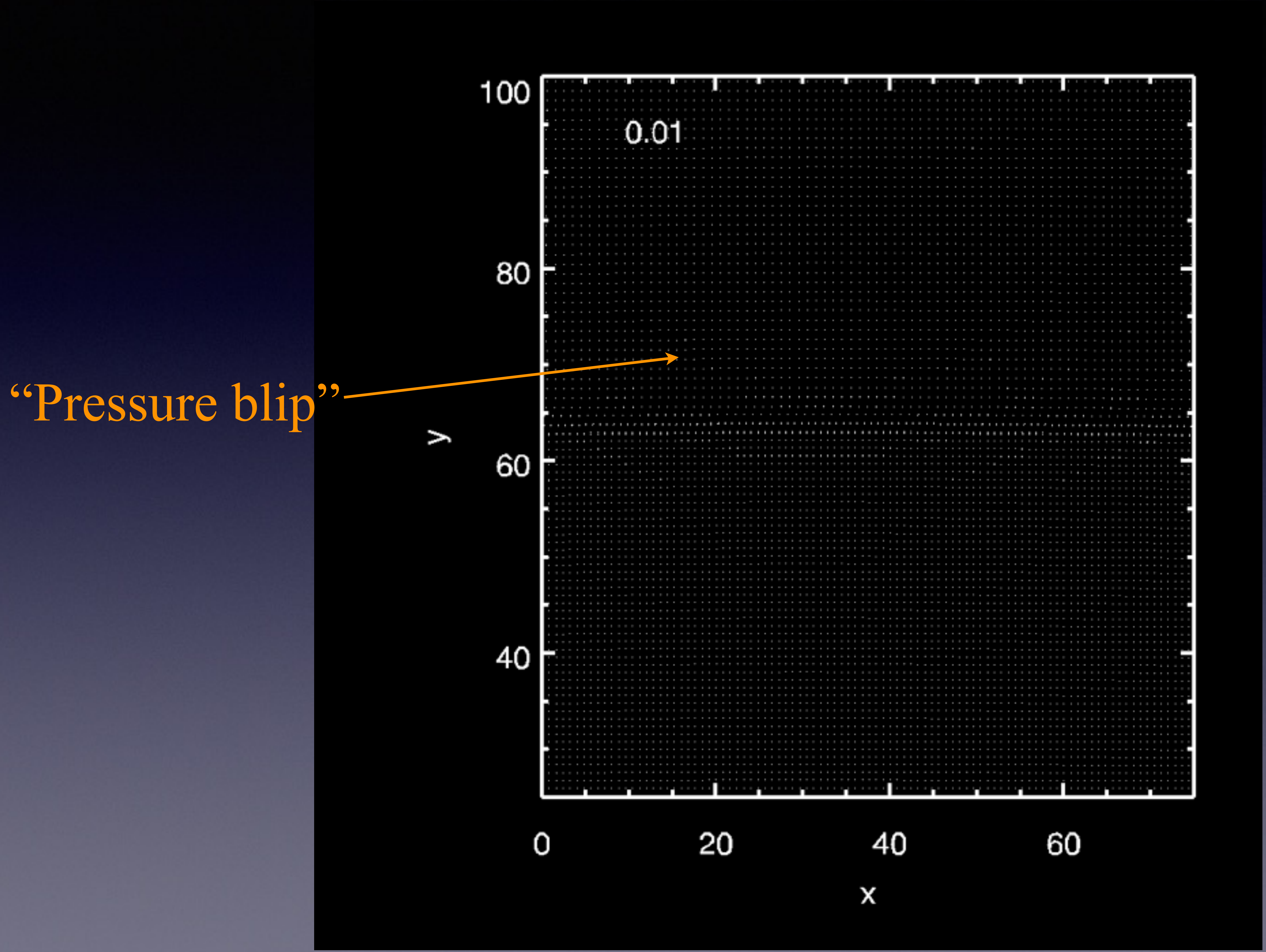
wanted:



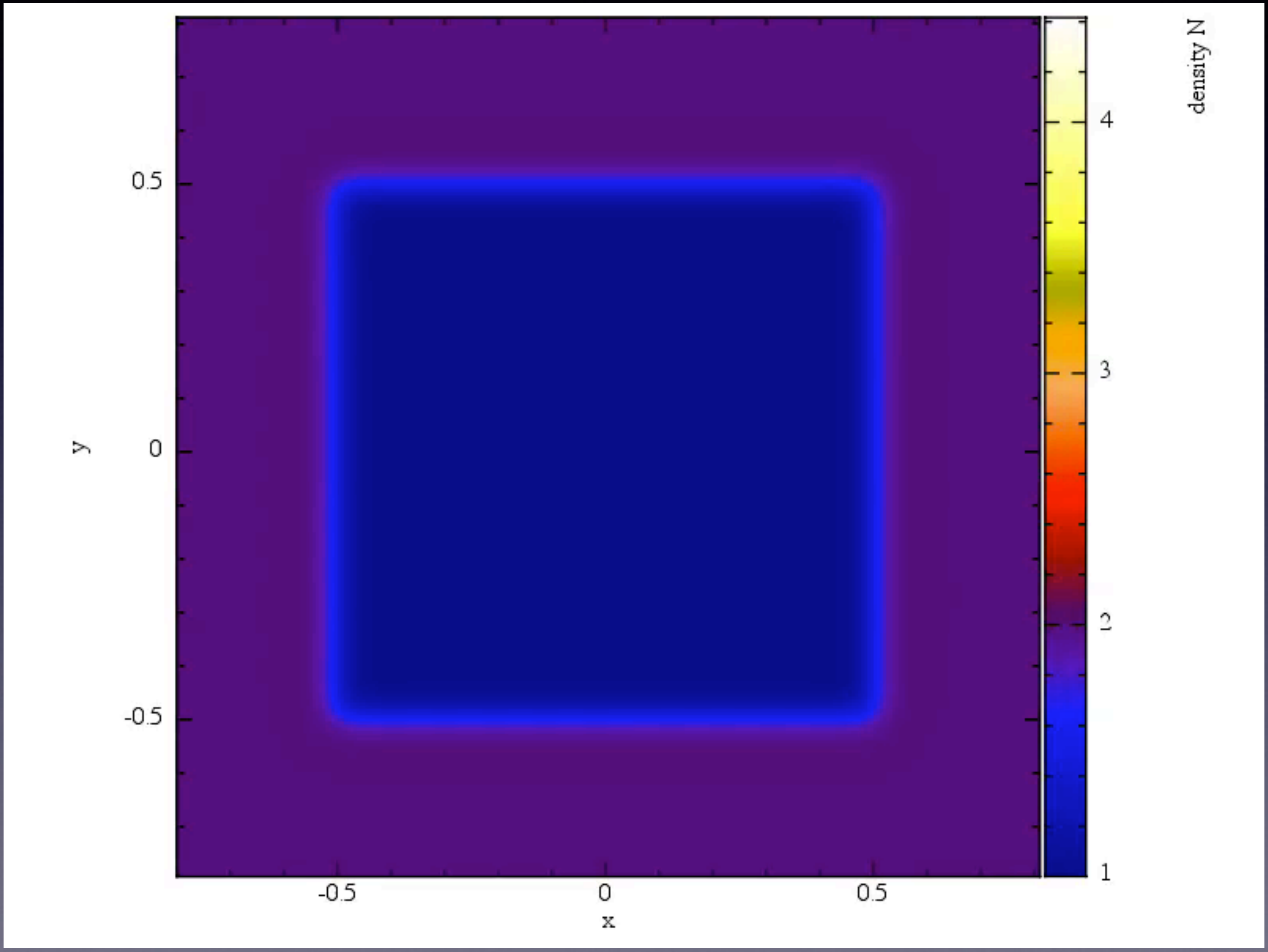
"straight forward setup"



Bad initial conditions I:



Bad initial conditions II:



Implication II: SPH has a built-in "re-meshing mechanism"

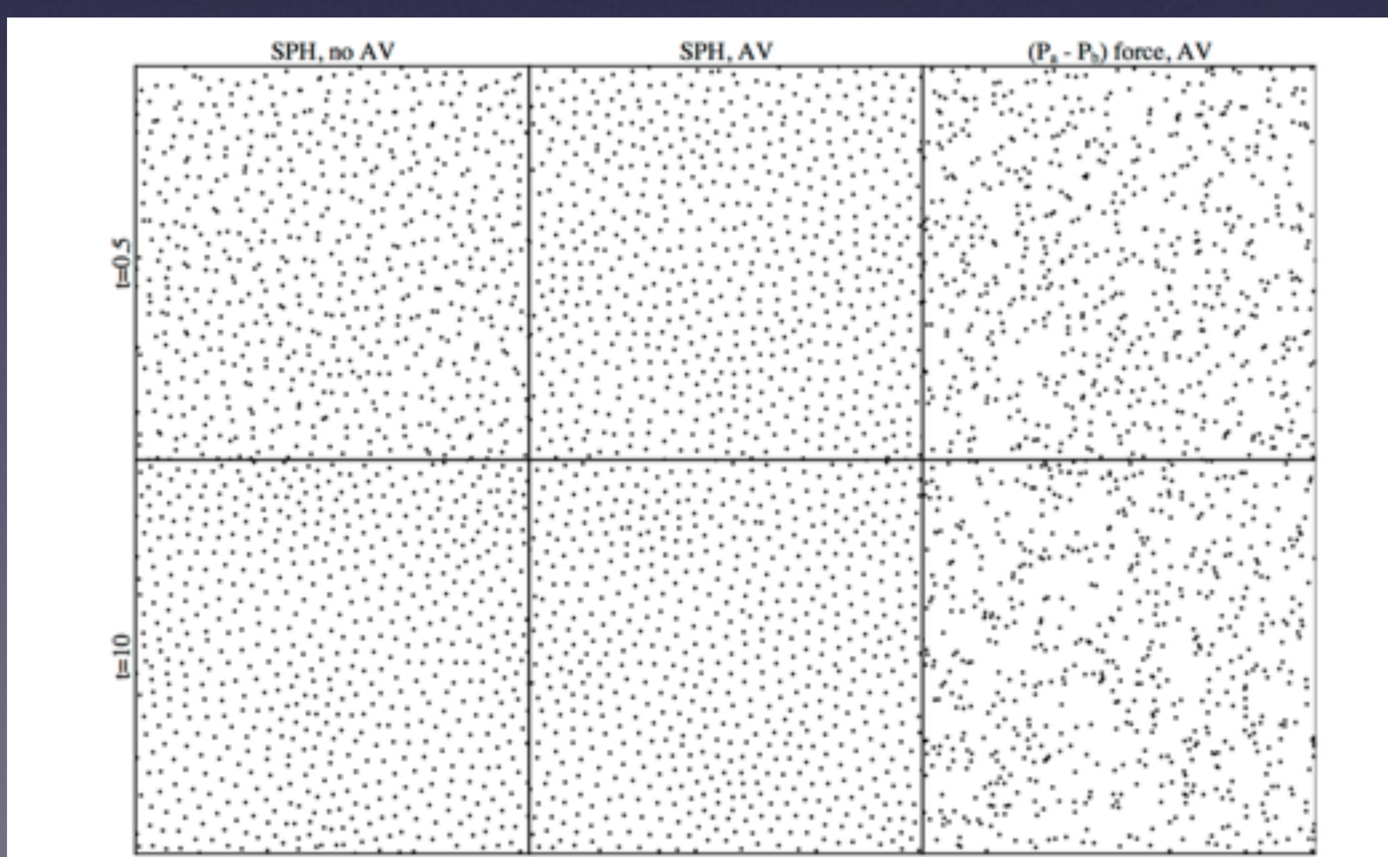
(e.g. SR Liv. Rev. Comp. Astr. 2015)

- momentum equation from Lagrangian: $$\frac{d\vec{v}_a}{dt} = \frac{1}{m_a} \sum_b P_b \frac{\partial V_b}{\partial \vec{r}_a}$$
- Taylor expansion around $\vec{r}_a$ shows: $$\frac{d\vec{v}_a}{dt} = \vec{f}_{\rm Euler} + \vec{f}_{\rm regul.}$$

- "regularization force"
- "volume maximizing"
- vanishes for "perfect particle distribution"

SPH

without regularization force



(Price 2012)

⇒ for non-perfect initial setup particles start to move

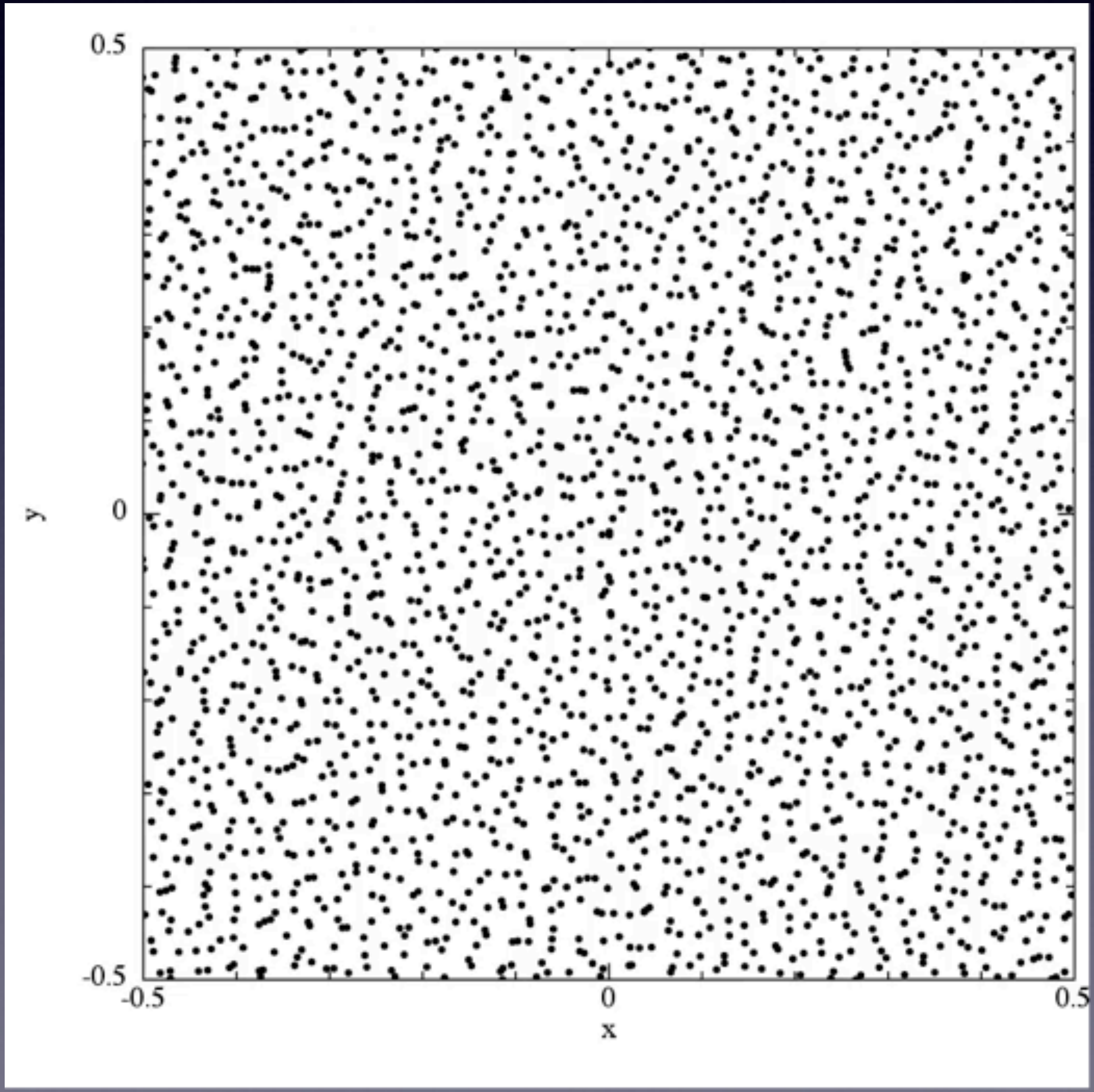
⇒ "noise"

Producing a “glass-like” particle distribution

Steps: a) hexagonal lattice

b) heavy perturbation ~ particle spacing

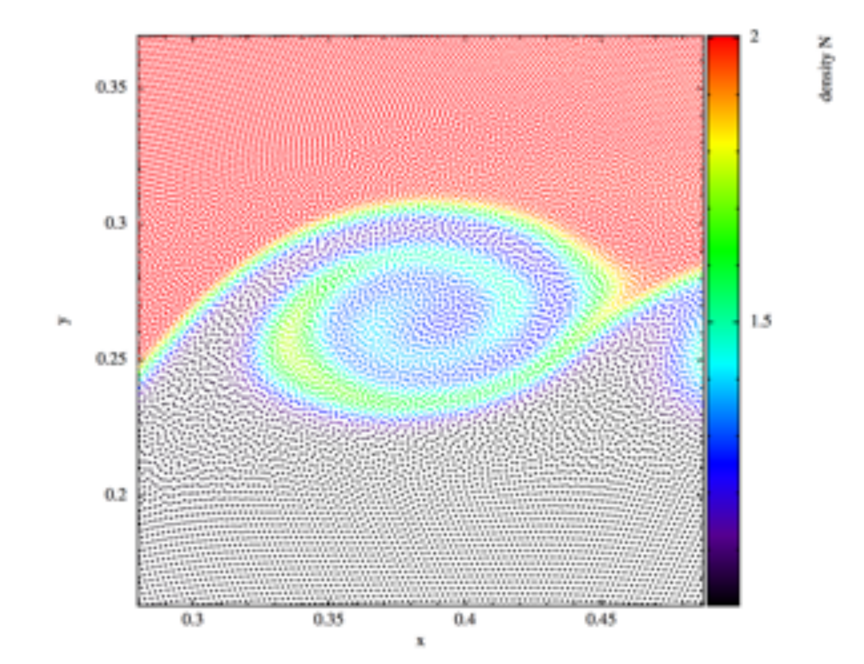
c) apply a pseudo-force $\vec{f}_a \propto -\sum_b \nabla_a W_{ab}(h_a)$



Recent developments

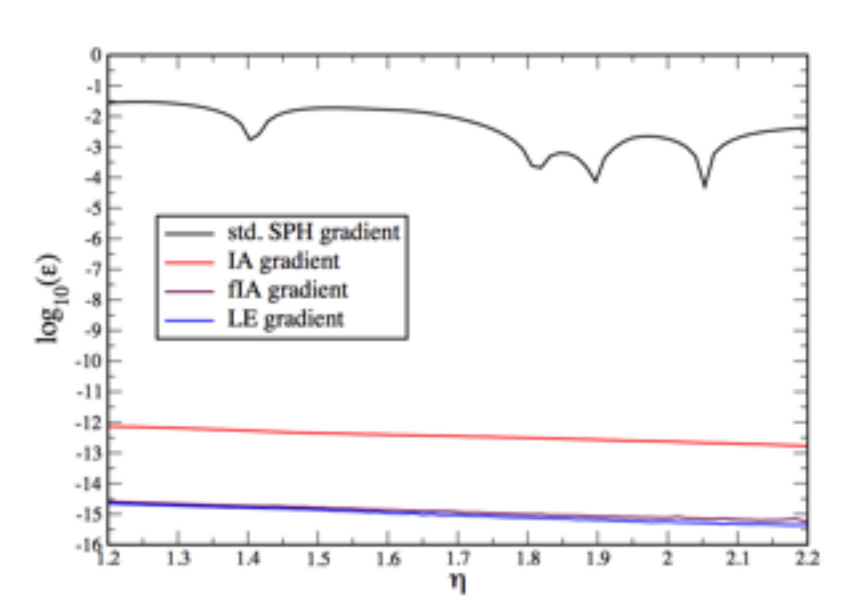
(SR, MNRAS, 2015: "Boosting the accuracy of SPH methods: Newtonian and special-relativistic tests")

- type of kernel function: Wendland kernels produce practically noise free particle distributions



- volume elements: include pressure in volume element
  $\Rightarrow$ much better at fluid instabilities

- dissipation steering: ONLY where necessary

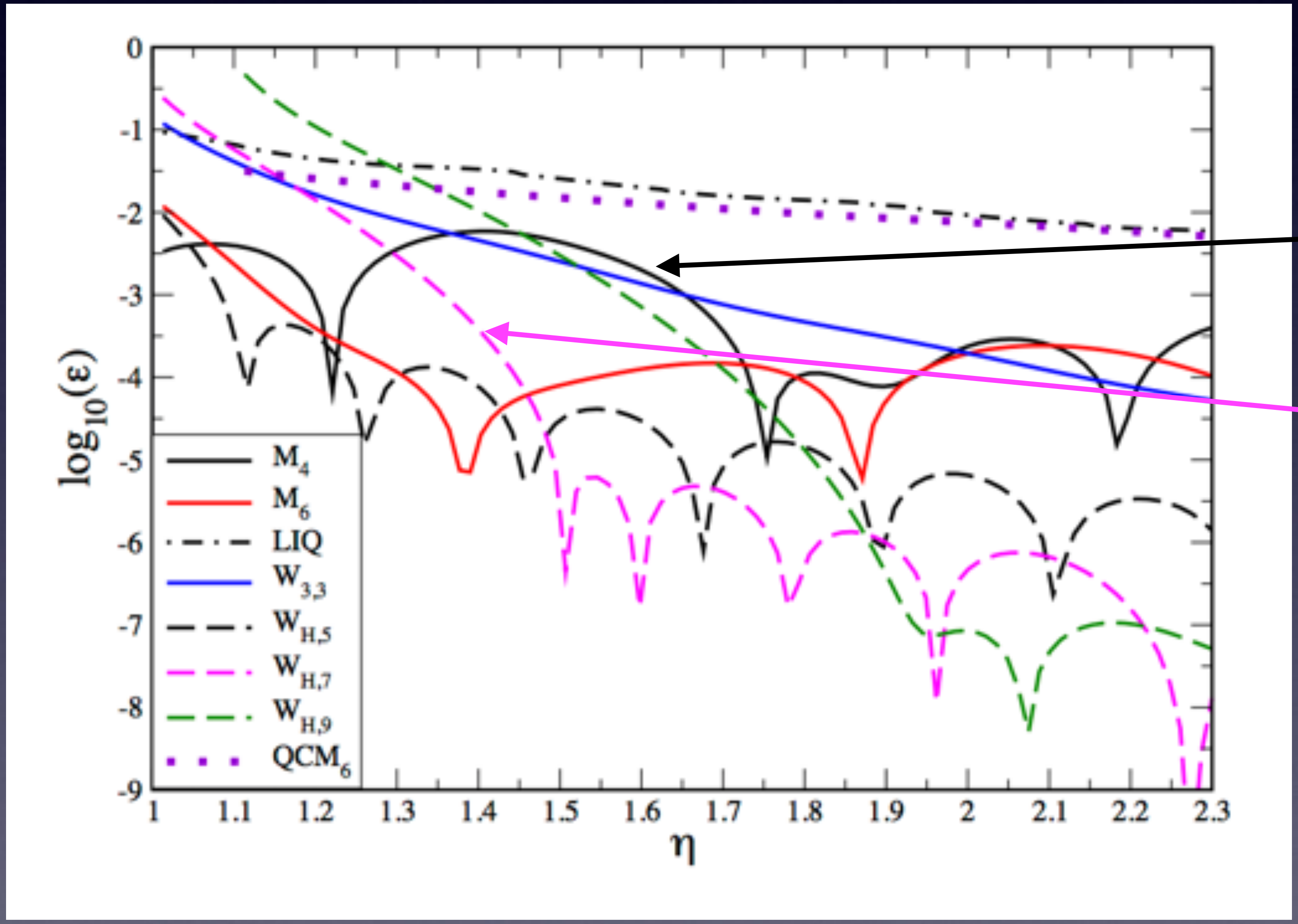


- accurate gradients: more elaborate scheme (with matrix inversion)

$\Rightarrow$ accuracy improvement by orders of magnitude!

Are all kernels equally good?
How does the accuracy depend on the smoothing length?

- experiment:
  - place particles on lattice (know volumes!)
  - give them equal masses ⇒ theoretical density
  - measure density



$$h_a = \eta \left(\frac{m_a}{\rho_a}\right)^{1/D}$$

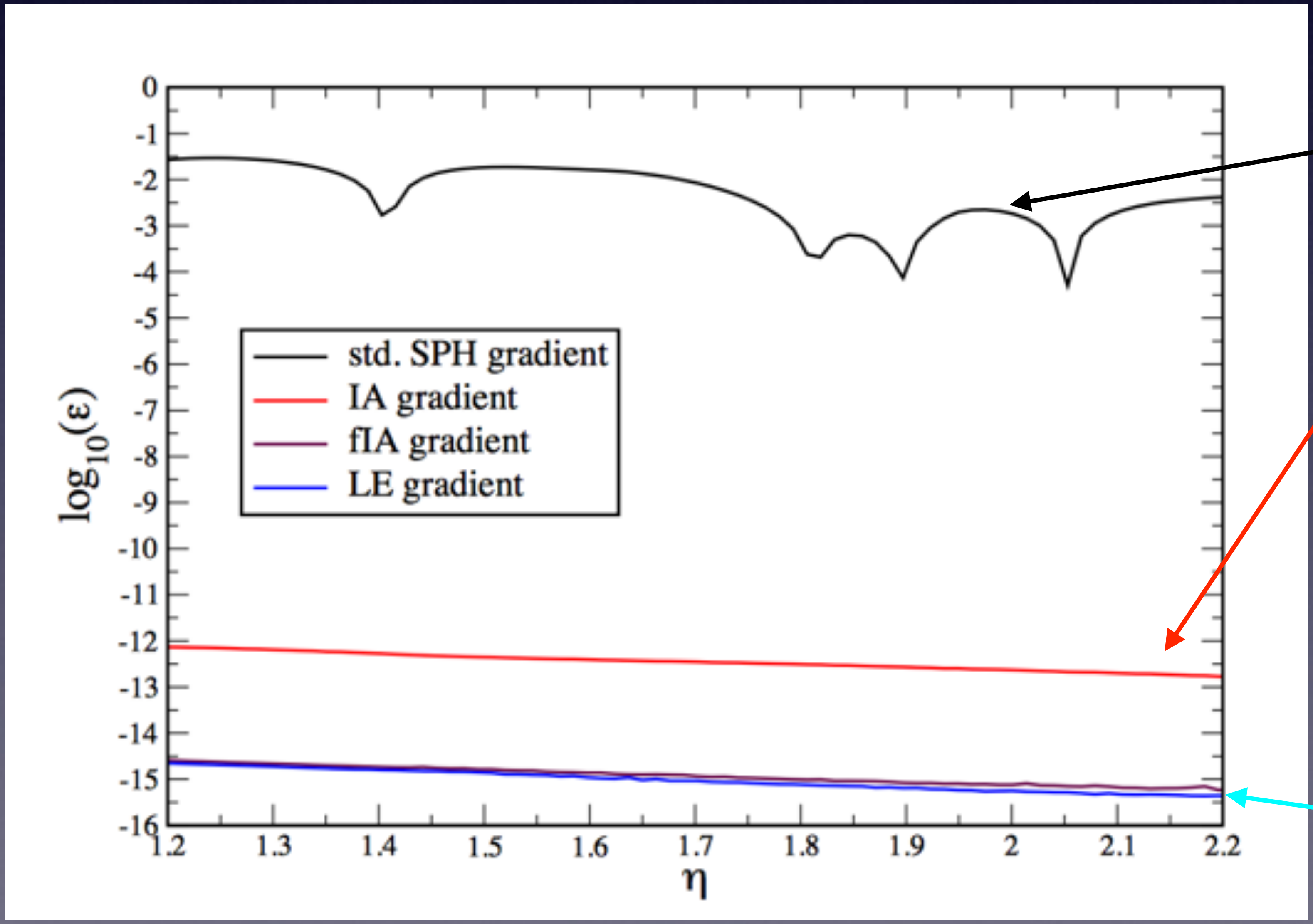
- "std. SPH kernel" is pretty bad
- smoother kernels are worse for small neighbour numbers, but *much* better for higher neighbour numbers

⇒ similar for gradients…

Gradient calculations can be (much) improved!

- you can calculate gradients much more accurate: small (3x3) matrix inversion
  (see e.g. Garcia-Senz+ 2012, SR 2015a, SR 2015b)

- similar experiment:
  - place particles on lattice (know volumes!)
  - set up linearly rising pressure
  - measure pressure

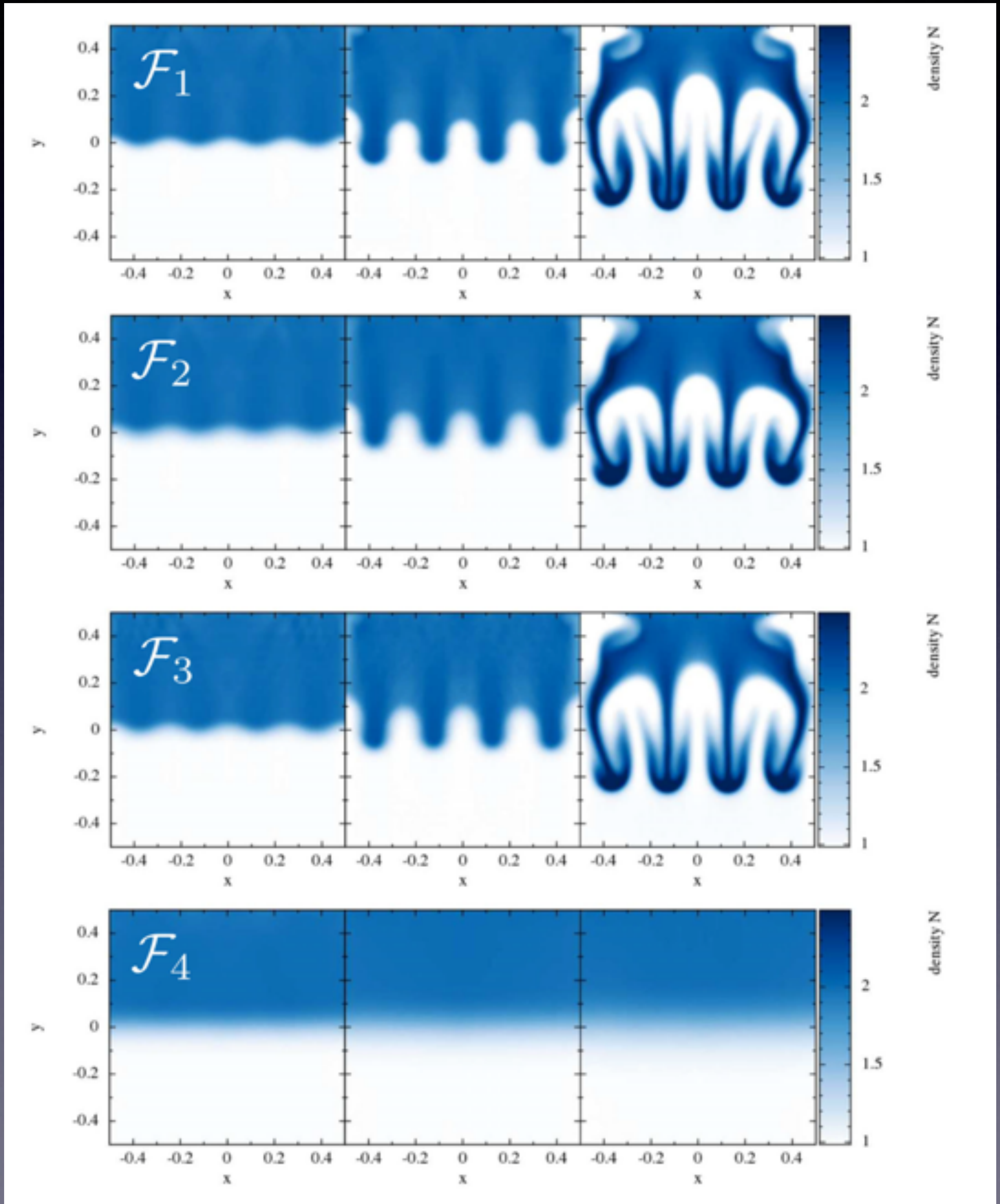


standard gradient

symmetry as standard SPH:
a $\Leftrightarrow$ b $\Rightarrow$ gradient changes sign
$\Rightarrow$ exact conservation

no particular symmetry

“Rayleigh-Taylor”



“best”

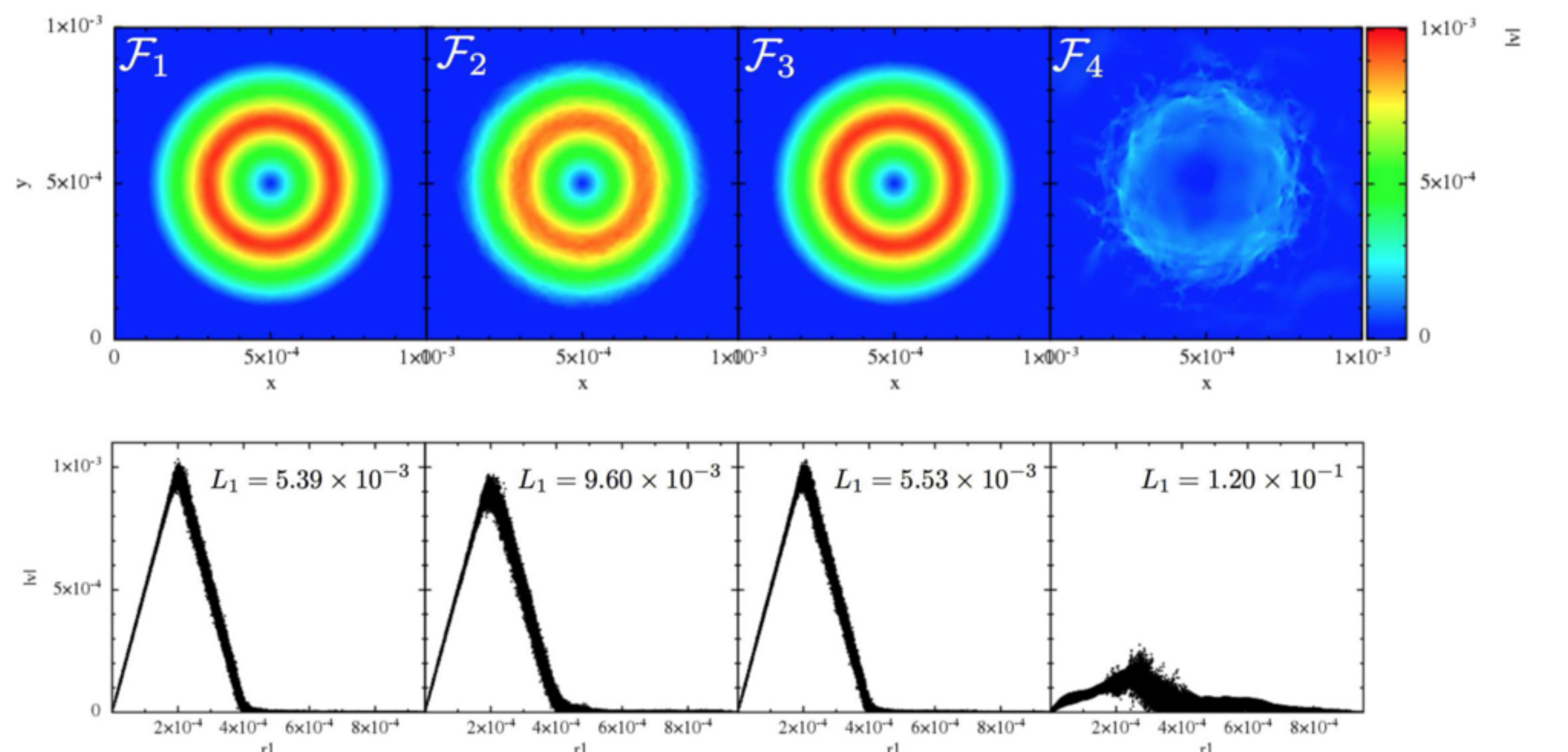
“best, but std. gradient”

“best, but std. volume”

“worst = std. approach”

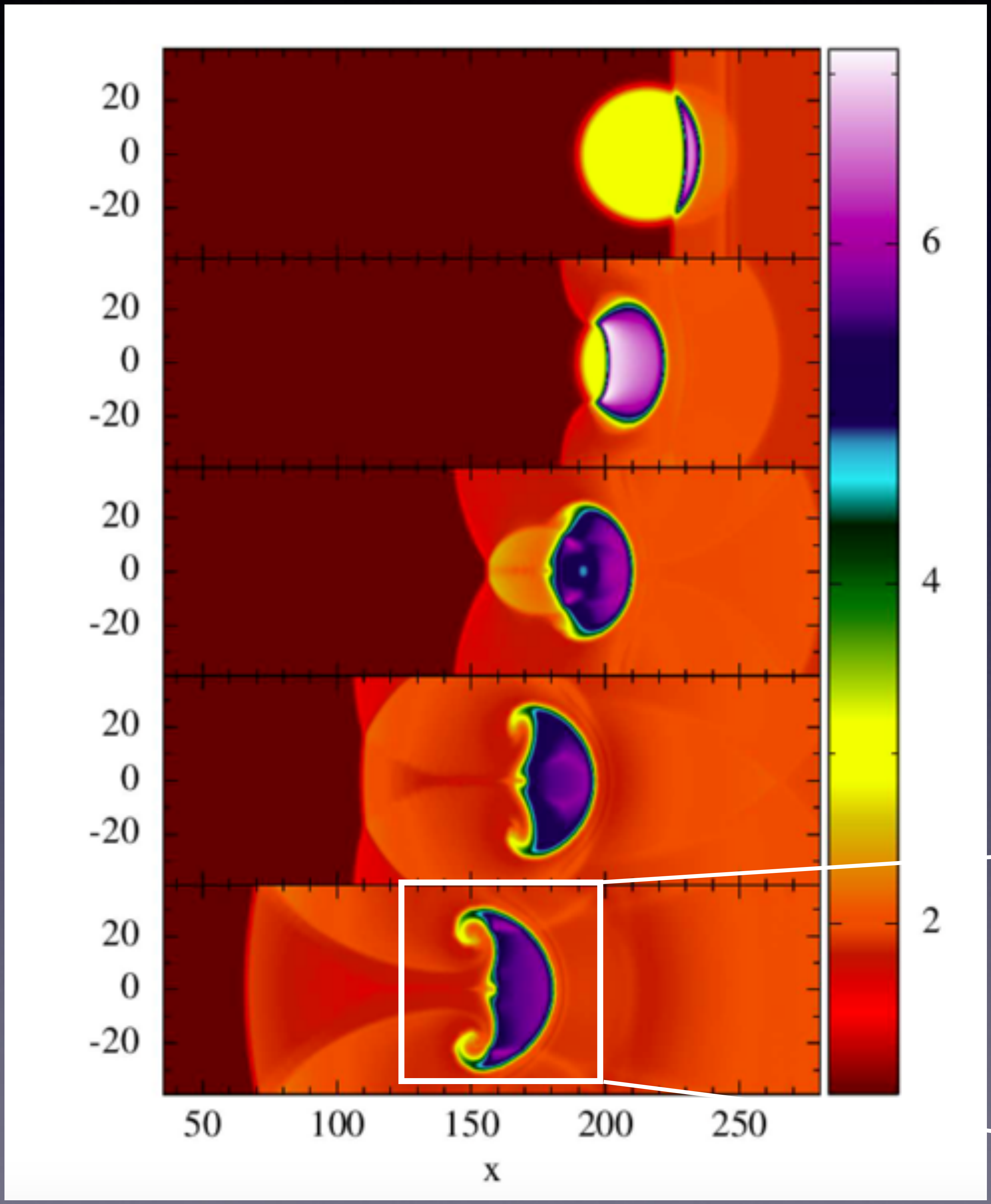
“Gresho-Chan vortex”

“best” | “best, but std. gradient” | “best, but std. volume” | “worst = std. approach”

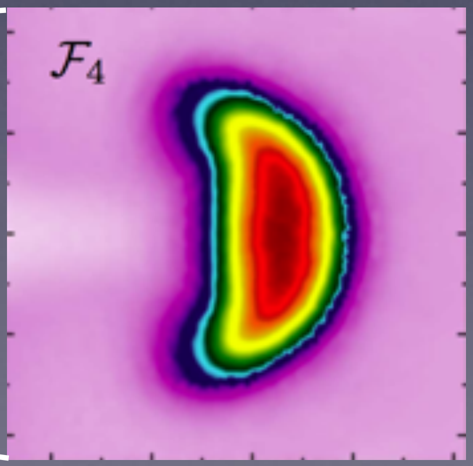


Blast-wave impacting on high-density bubble

"new"

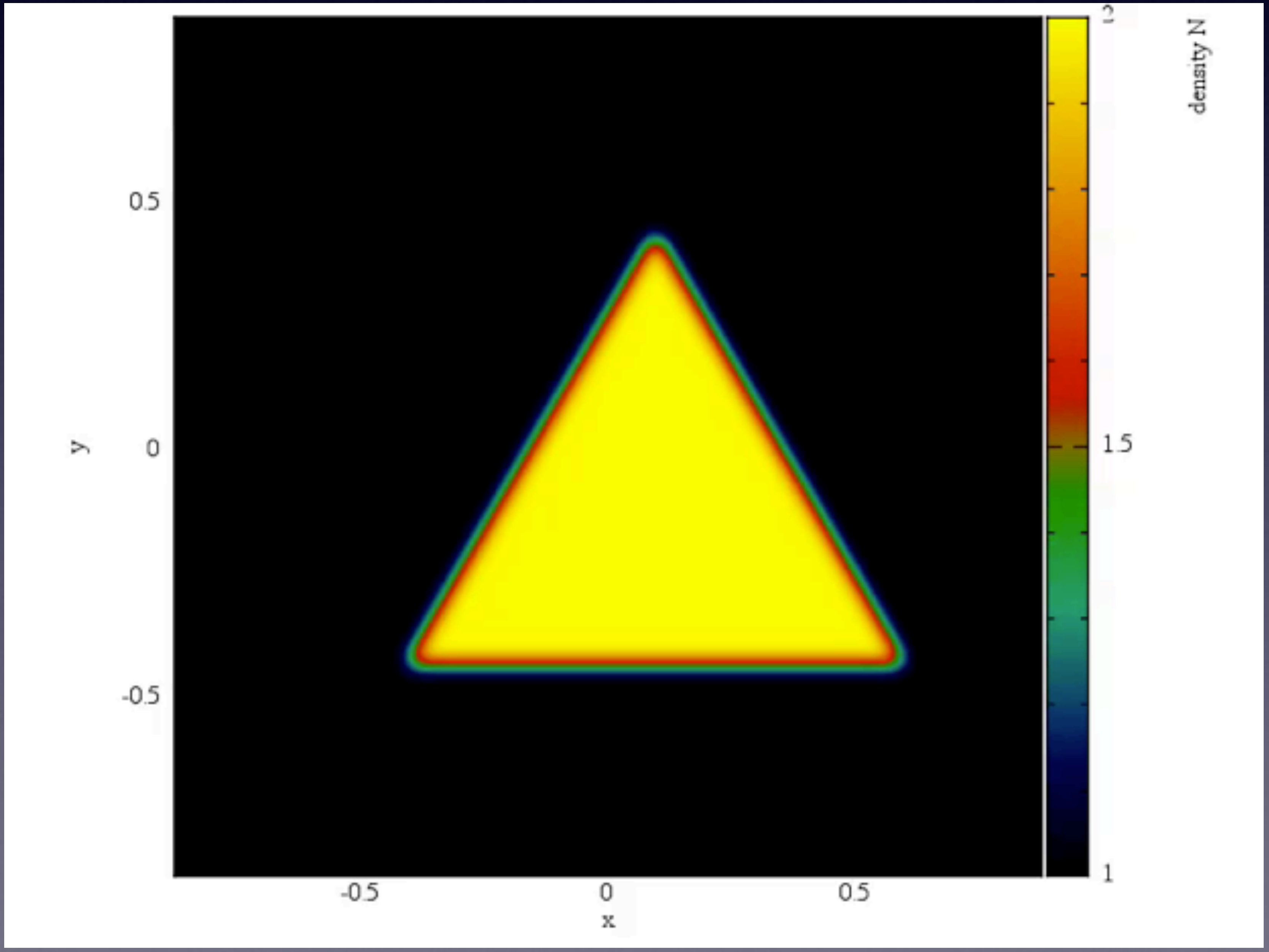


"standard"



Advection through periodic box

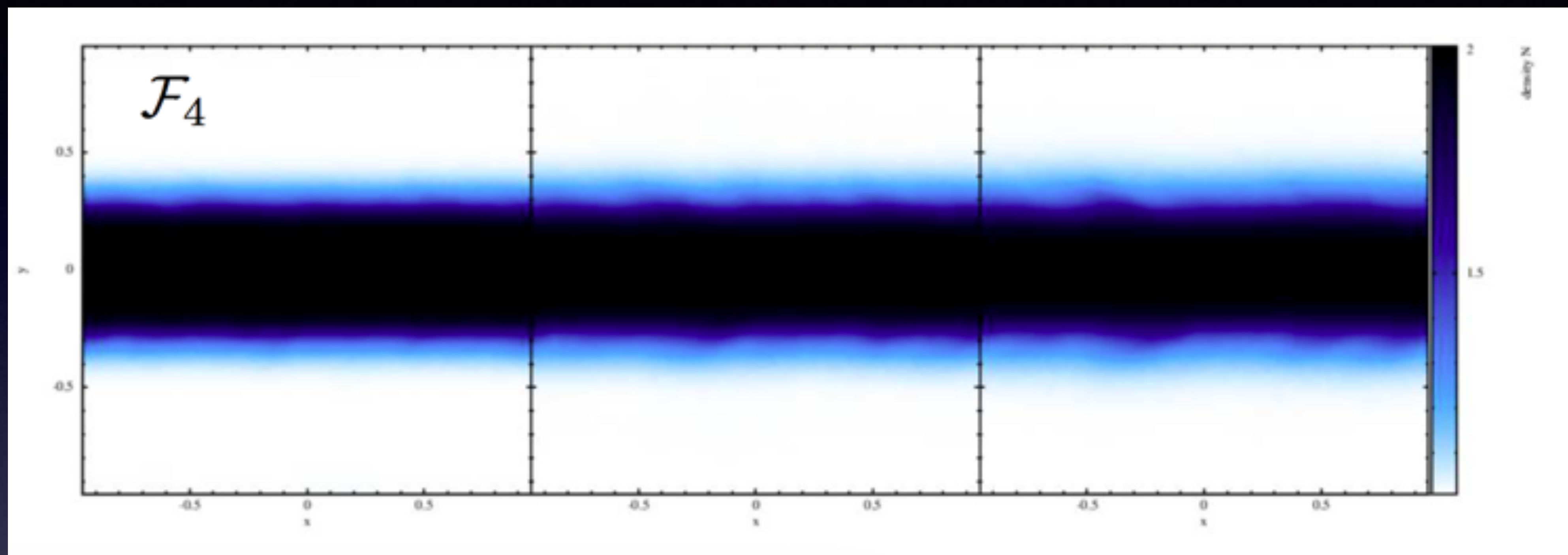
pattern:	triangle
density:	=2 (inside), =1 (outside)
pressure:	$P = P_0 = 2.5$ everywhere
advection speed:	$0.9999c \Rightarrow \Gamma = 70.7$
numer. parameters:	20 K particles, close-packed, equal mass



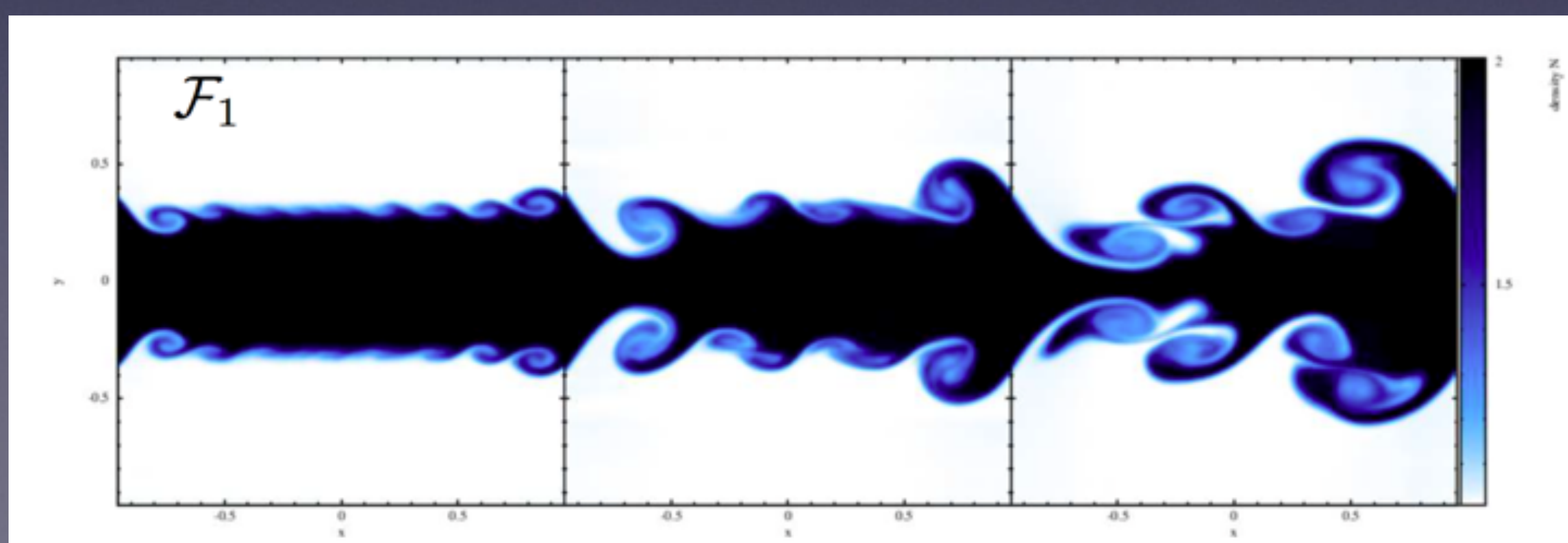
perfect advection!

Un-triggered Kelvin-Helmholtz instability

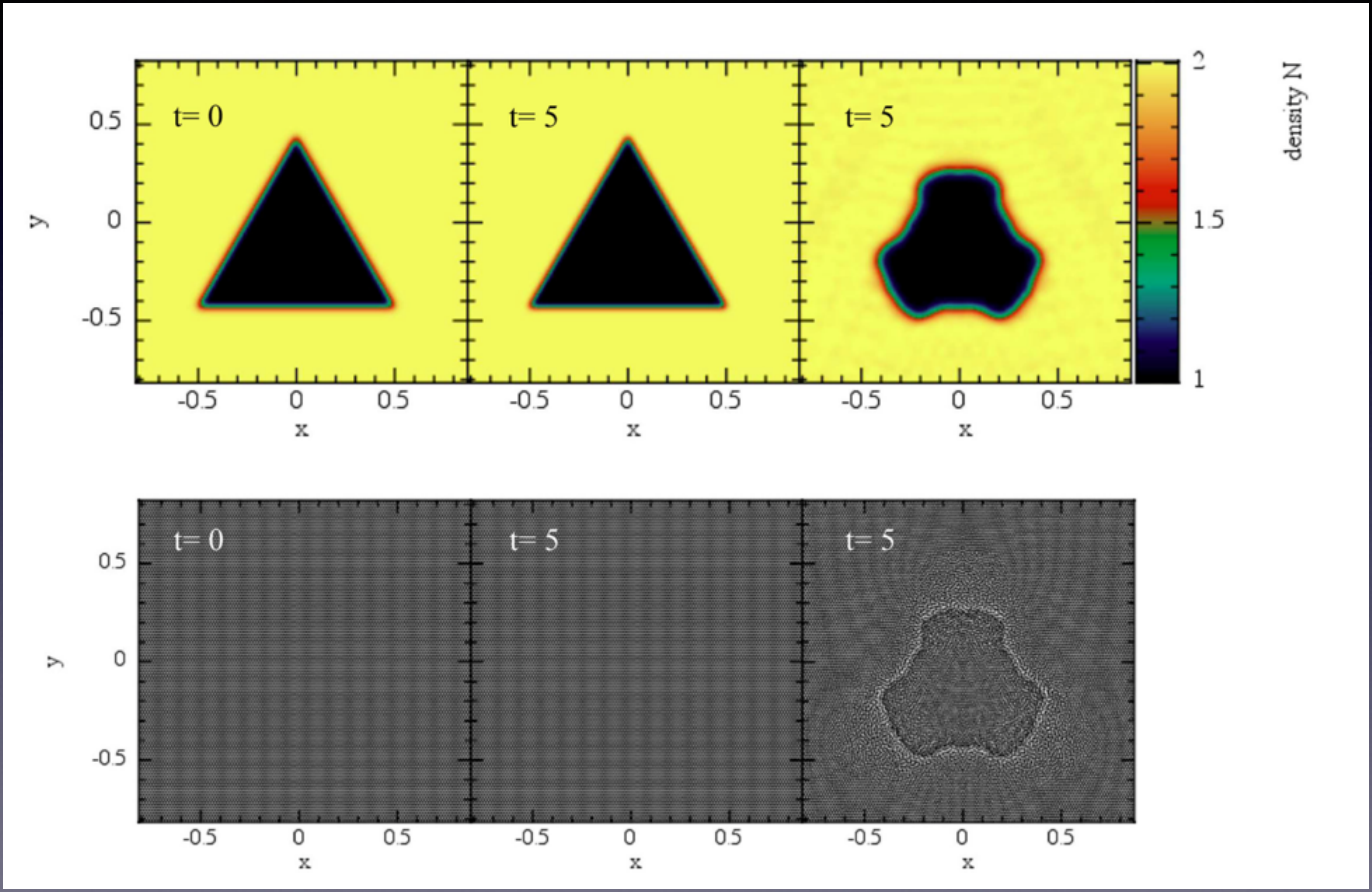
"standard"



"new"

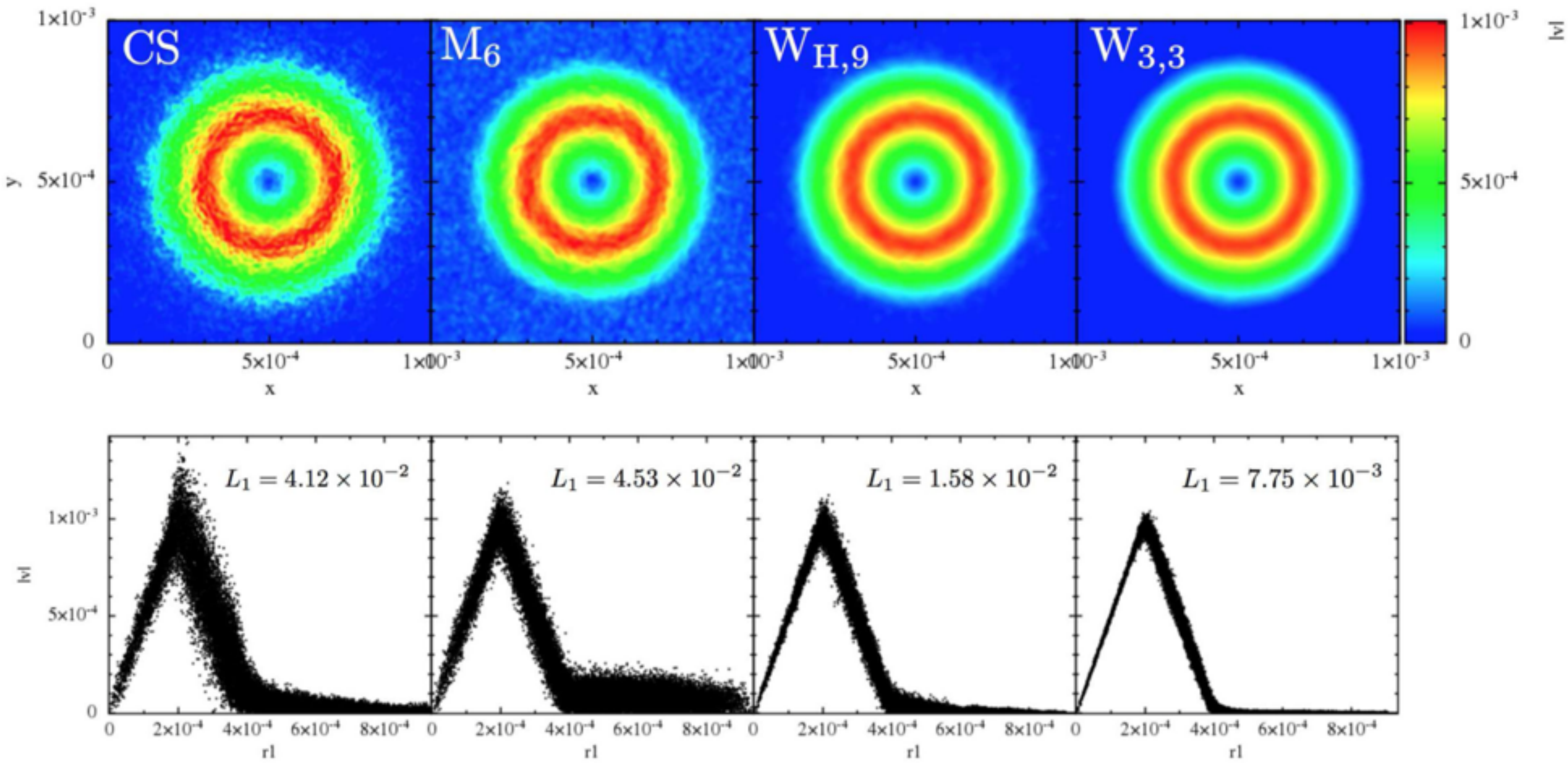


“surface tension with standard volume element”



"Gresho-Chan vortex: impact of kernel function"

"best", but different kernel functions



Special-Relativistic SPH

- general strategy:
  - similar to Newtonian SPH from variational principle, use:
    - Lagrangian for perfect fluid
    - 1st law of thermodynamics

- resulting equations:
  - use canonical energy & canonical momentum as numerical variables
  - similar to Newtonian SPH from variational principle

- differences:
  - Lagrangian: $L = \int \left(\frac{v^2}{2} - u(\rho, s) \right) \rho \, dV \quad \Rightarrow$

$$L_{\rm SR} = - \int T^{\mu\nu} U_\mu U_\nu \, dV$$

$$L_{\rm GR} = - \int T^{\mu\nu} U_\mu U_\nu \sqrt{-g} \, dV$$

with Energy-Momentum Tensor $\quad T^{\mu\nu} = (e + P) U^\mu U^\nu + P g^{\mu\nu}$

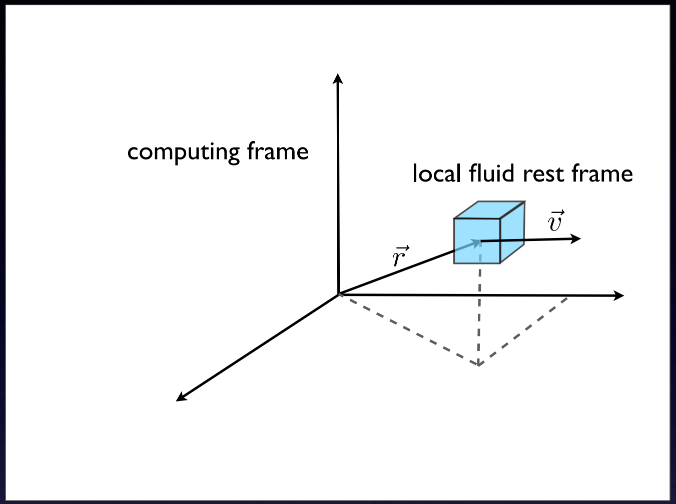
energy density in comoving frame

pressure

4-velocity $\quad U^\mu = \frac{dx^\mu}{d\tau}$

- still differences…

  - perform simulations in computing frame (CV) $\Longleftrightarrow$ local rest frame of fluid (lrf)



  - in CF: fluid parcels are moving $\Rightarrow$ Lorentz contraction $\Rightarrow$ volumes/densities related via Lorentz factor

$$V_{\mathrm{CF}} = \frac{V_{\mathrm{lrf}}}{\gamma}$$

  - lrf density:

$$e = e_{\mathrm{rest}} + e_{\mathrm{therm}} = \rho_{\mathrm{rest}} c^2 + u\rho_{\mathrm{rest}} = n m_0 c^2 (1 + u/c^2)$$

  - convention (!): if we measure energies in m_0c^2 and use c=1, Lagrangian simplifies to

$$L_{\mathrm{pf,sr}} = -\int n(1+u)\, dV$$

- from here, like before:
  - CF density by summation

$$N_a = \sum_b \nu_b W_{ab}(h_a) \; (= \gamma_a n_a)$$

baryon number carried by particle

  - discretize Lagrangian:

$$L_{\mathrm{SPH,SR}} = -\sum_b \frac{\nu_b}{\gamma_b}(1 + u_b)$$

  - from $\dfrac{\partial L_{\mathrm{SPH,SR}}}{\partial \vec{v}_a}$ and the first law of thermodynamics

$$\left(\frac{\partial u}{\partial n}\right)_s = \frac{P}{n^2}$$

we find the canonical momentum per baryon

$$\vec{S}_a = \gamma_a \vec{v}_a \left(1 + u_a + \frac{P_a}{n_a}\right)$$

  - similarly: canonical energy per baryon

$$\hat{\epsilon}_a = \vec{v}_a \cdot \vec{S}_a + \frac{1 + u_a}{\gamma_a}$$

$\Rightarrow$ these are our new numerical variables

- applying Euler-Lagrange equations yields:

$$\frac{d\vec{S}_a}{dt} = -\sum_b \nu_b \left\{ \frac{P_a}{\tilde{\Omega}_a N_a^2} \nabla_a W_{ab}(h_a) + \frac{P_b}{\tilde{\Omega}_b N_b^2} \nabla_a W_{ab}(h_b) \right\}$$

momentum equation

- direct derivatives of canonical energy gives:

$$\frac{d\hat{\epsilon}_a}{dt} = -\sum_b \nu_b \left(\frac{P_a \vec{v}_b}{\tilde{\Omega}_a N_a^2} \cdot \nabla_a W_{ab}(h_a) + \frac{P_b \vec{v}_a}{\tilde{\Omega}_b N_b^2} \cdot \nabla_a W_{ab}(h_b) \right)$$

energy equation

$\Rightarrow$ (like in Eulerian hydro): conversion primitive $\Leftrightarrow$ conservative variables

- comparison with Newtonian equations:

$$\frac{d\vec{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\Omega_a \rho_a^2} \nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} \nabla_a W_{ab}(h_b) \right)$$

$$\frac{d\hat{e}_a}{dt} = -\sum_b m_b \left(\frac{P_a \vec{v}_b}{\rho_a^2} + \frac{P_b \vec{v}_a}{\rho_b^2} \right) \cdot \nabla_a W_{ab}$$

thermokinetic energy:

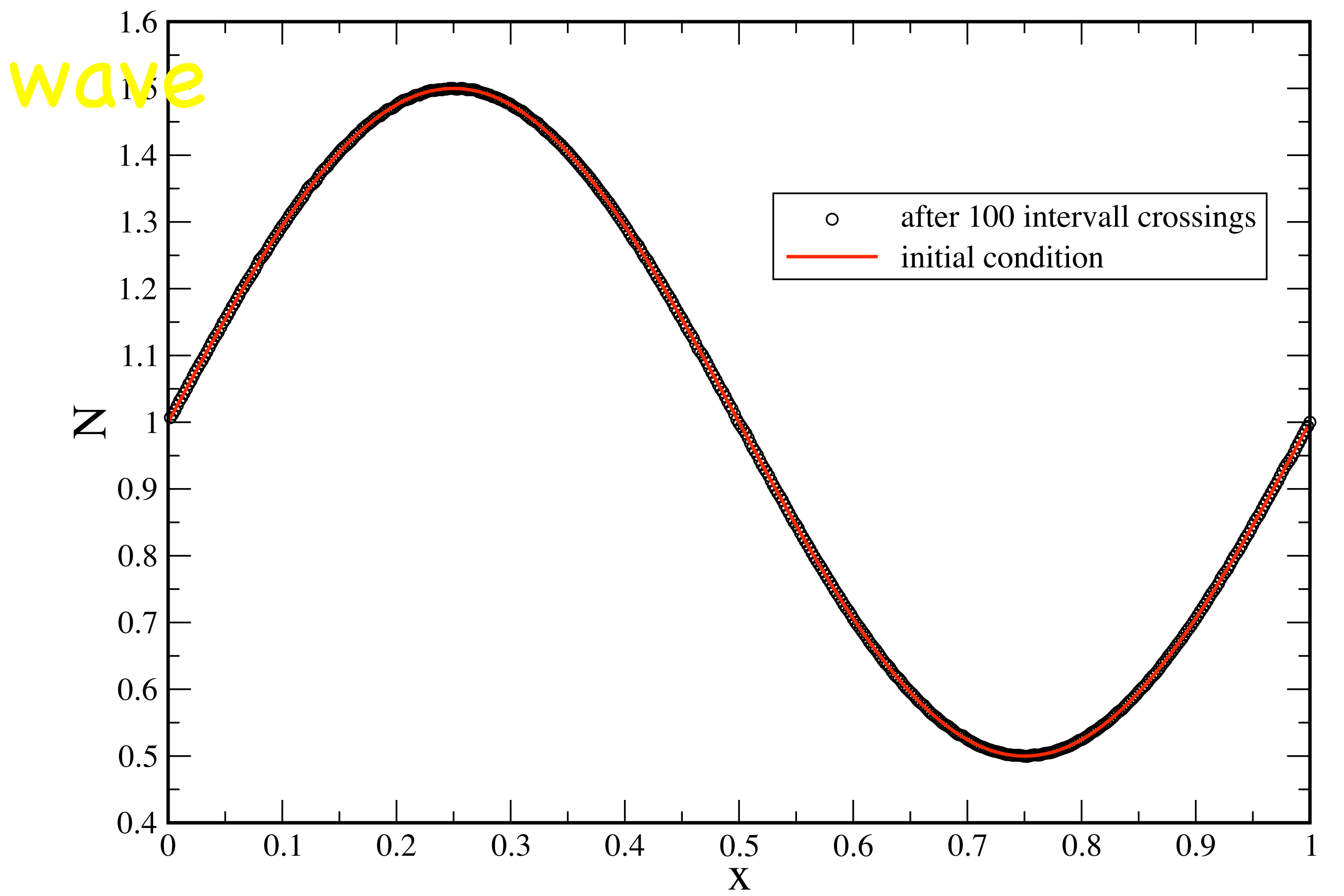
$$\hat{e} = u + \frac{1}{2} v^2$$

A slew of benchmark tests

I "Advection tests"

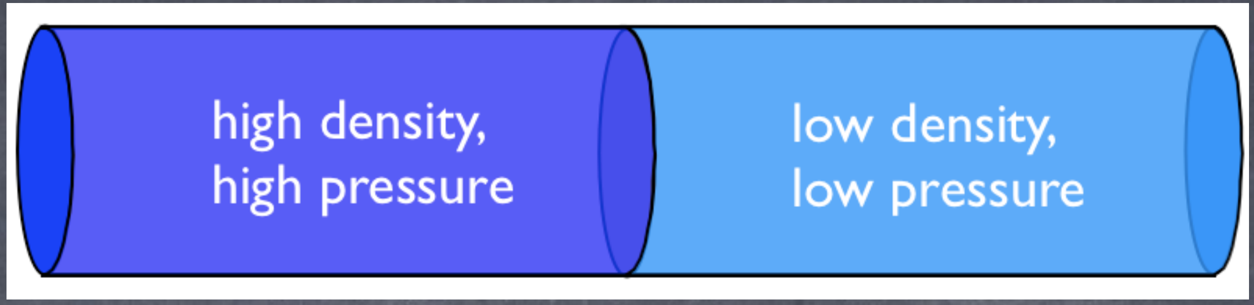
- "set up a situation where a geometrical shape (in density) should just be advected with the fluid. Test on which time scale unwanted effects deteriorate the numerical solution"

- Test 1: Advection of sine wave
  - set up density sine wave in periodic box, so that pressure is the same everywhere
  - give pattern a boost with v= 0.997 (γ=12.92)

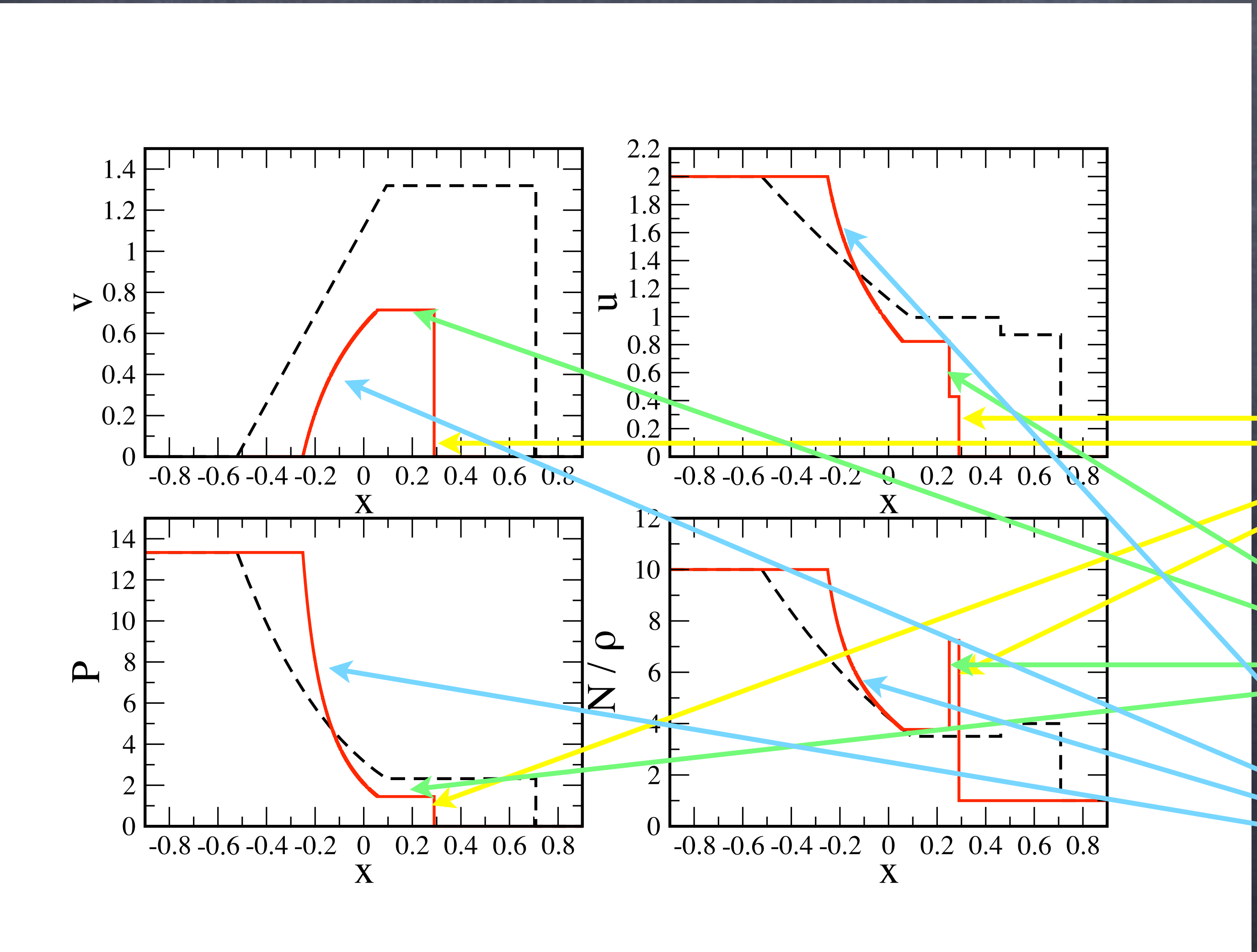


500 particles

II "Shock tests"



- Test 3: mildly relativistic shock tube
  - left: $(P,N,v) = (40/3, 10, 0)$; right: $(P,N,v) = (10^{-6}, 1, 0)$
  - How important are relativistic effects?



red: special-relativistic

black: Newtonian

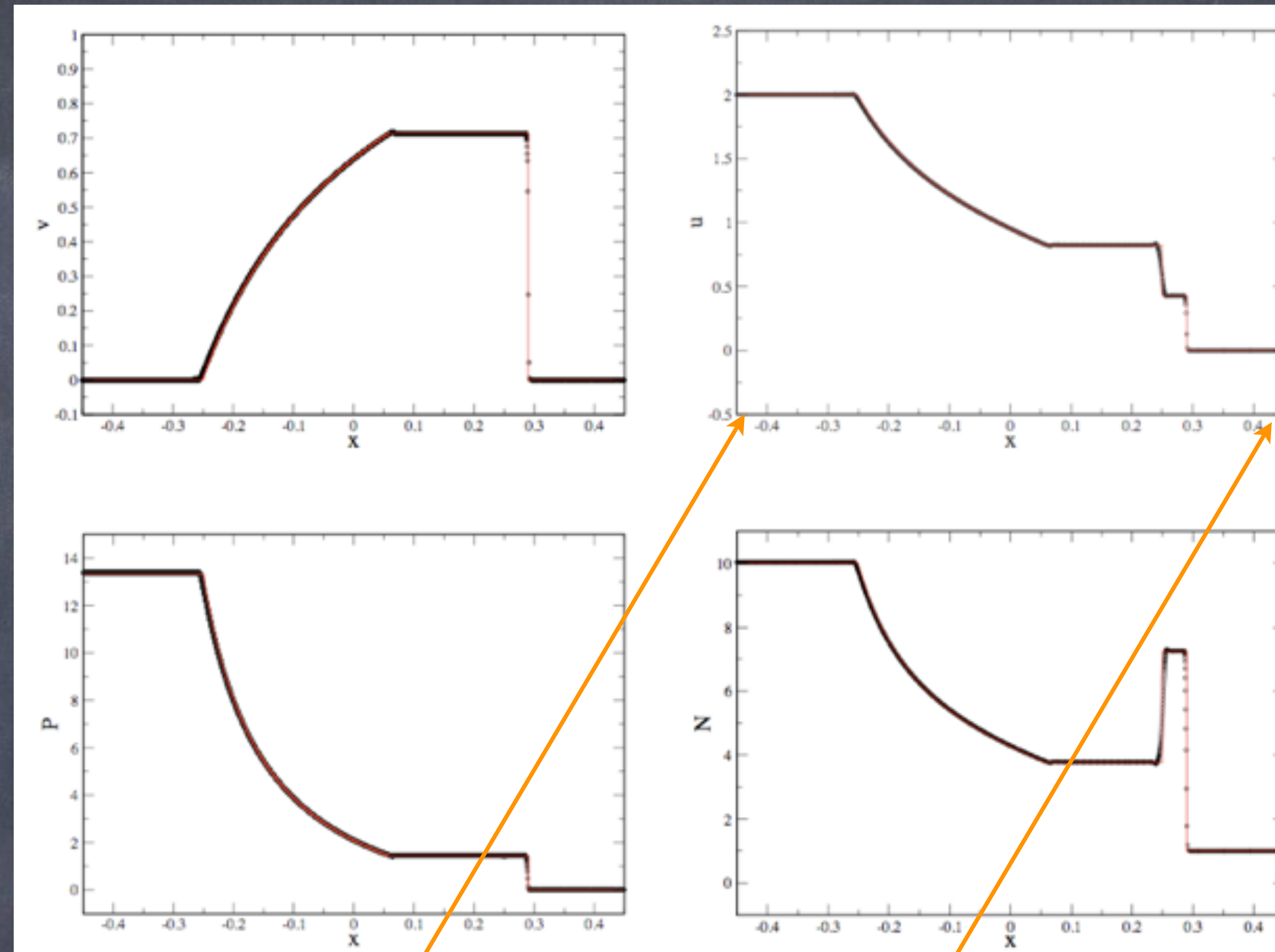
shock

contact discontinuity

rarefaction fan

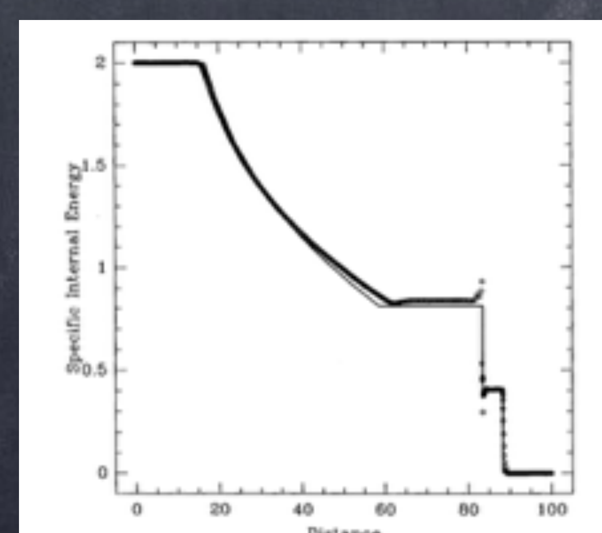
- numerical result:

  (from SR 2010)

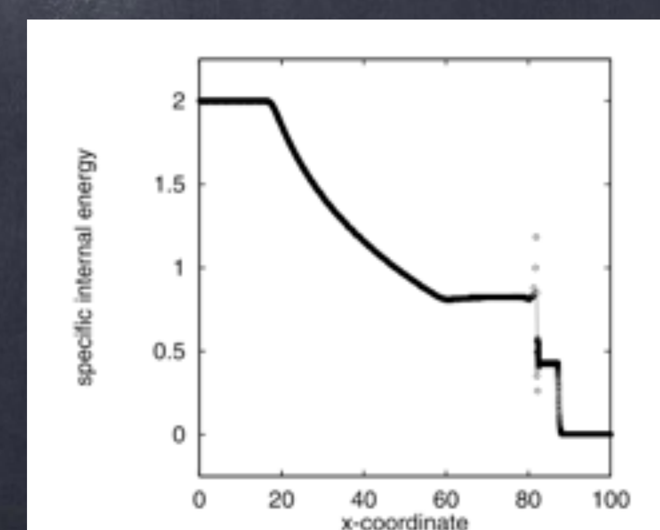


- for comparison:

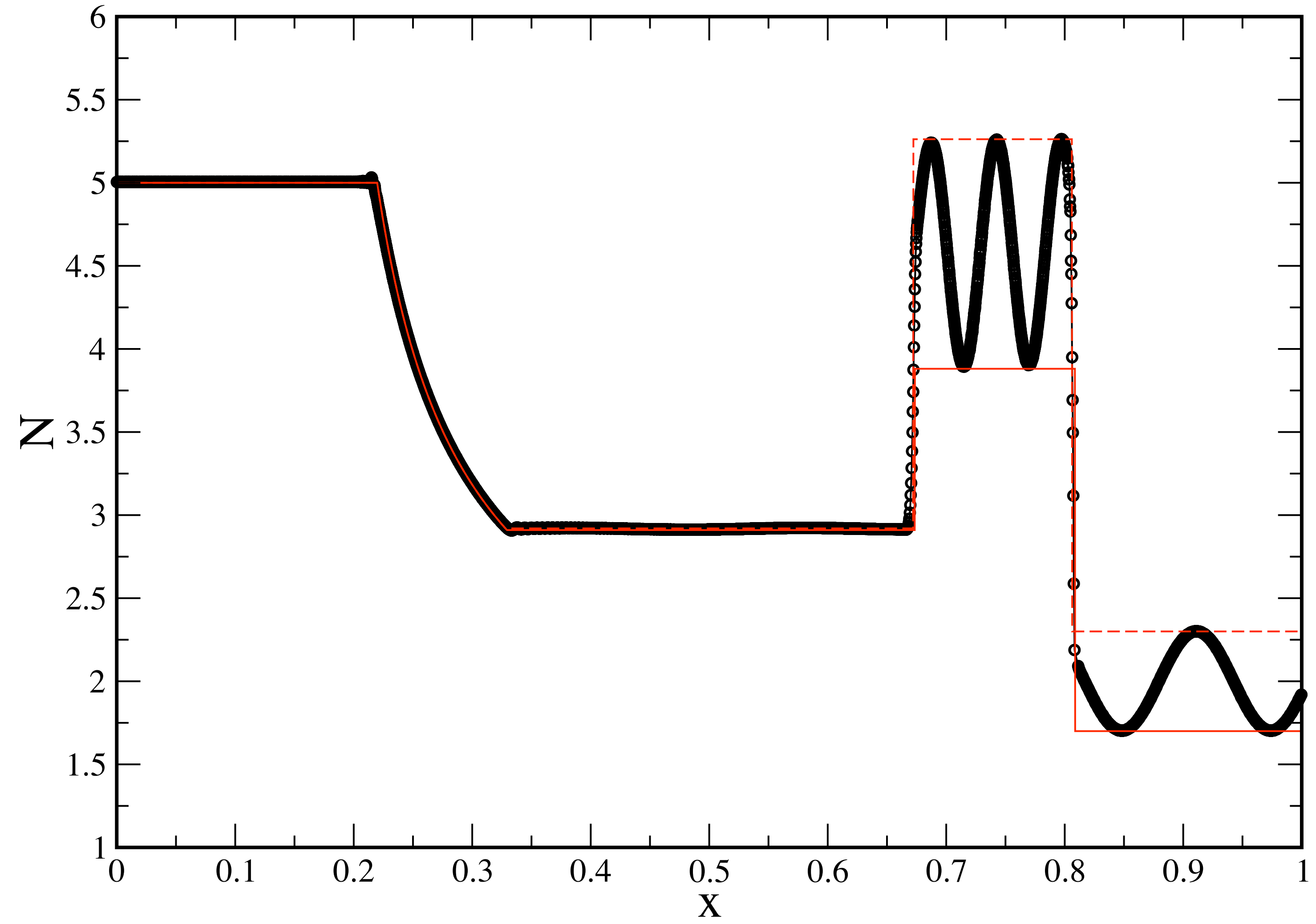
Laguna et al. (1993)



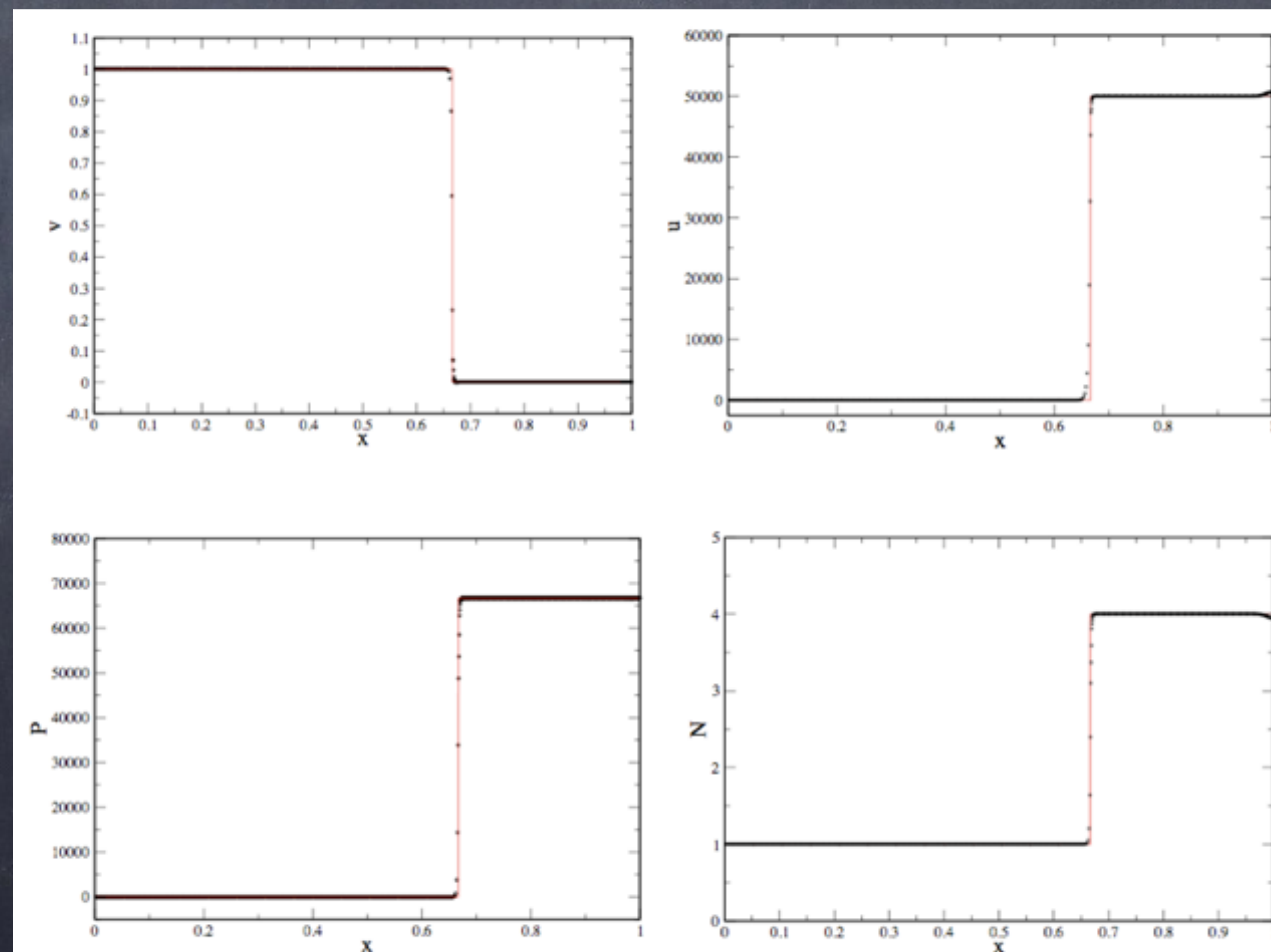
Siegler & Riffert (2000)



- Test 5: sinusoidally perturbed shock tube
- left: (P,N,v)= (50, 5, 0); right: (P,N,v)= (5,2+0.3 sin(50x), 0)
- challenge: transport smooth structure across shock
- numerical result:



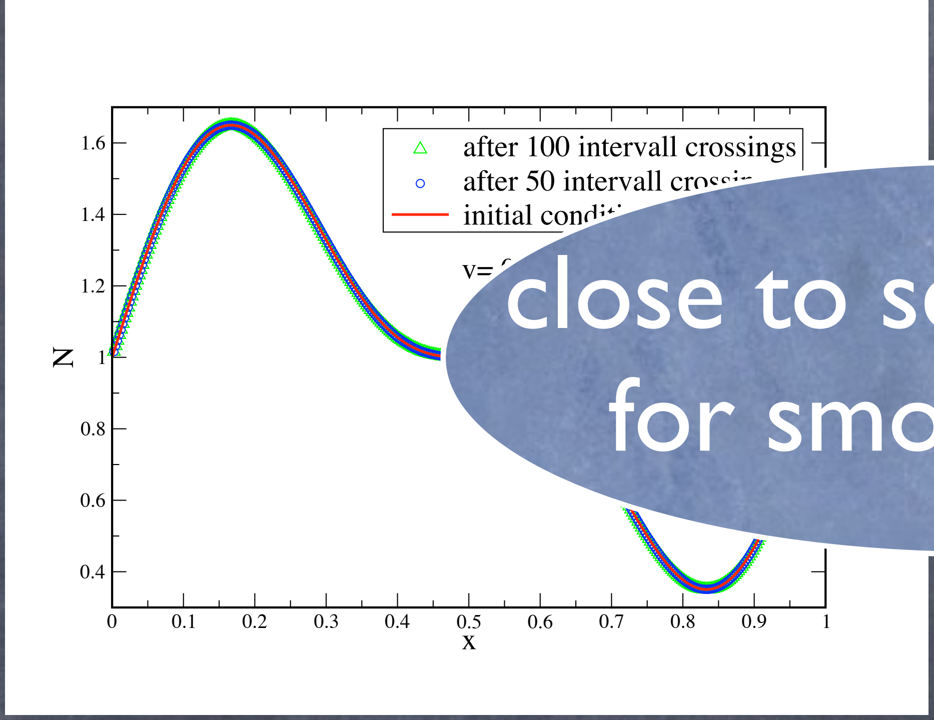
- Test 6: ultra-relativistic wall shock test
  - reflecting boundary (“wall”) at x= 1
  - cold gas streams towards wall with v= 0.9999999998, i.e. γ = 50 000 !
  - numerical result:

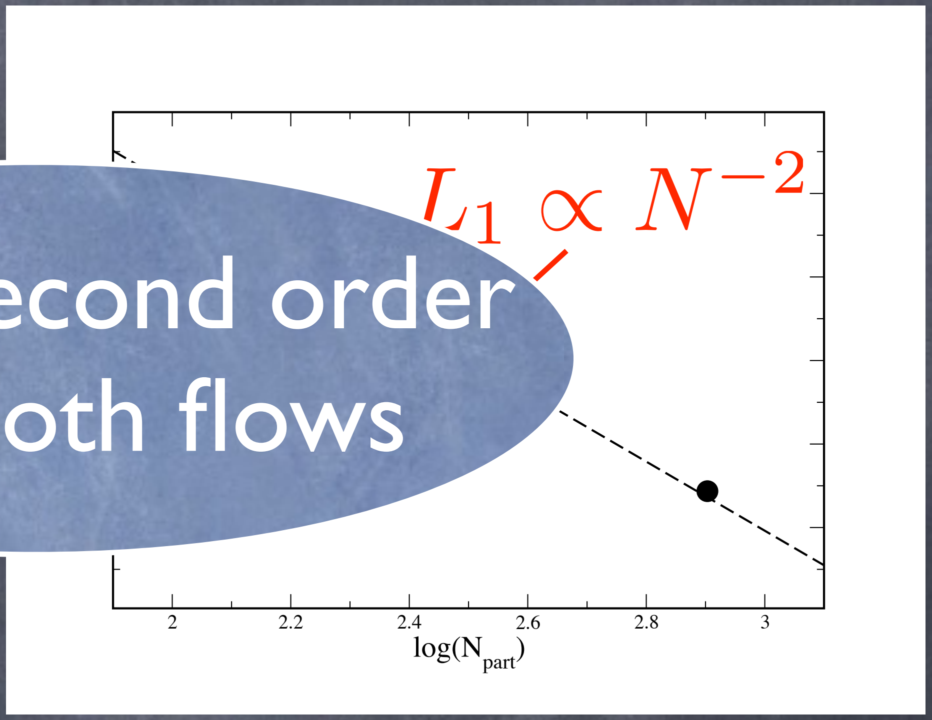


So what is the order of this scheme?

- numerical experiments (Rosswog 2010):

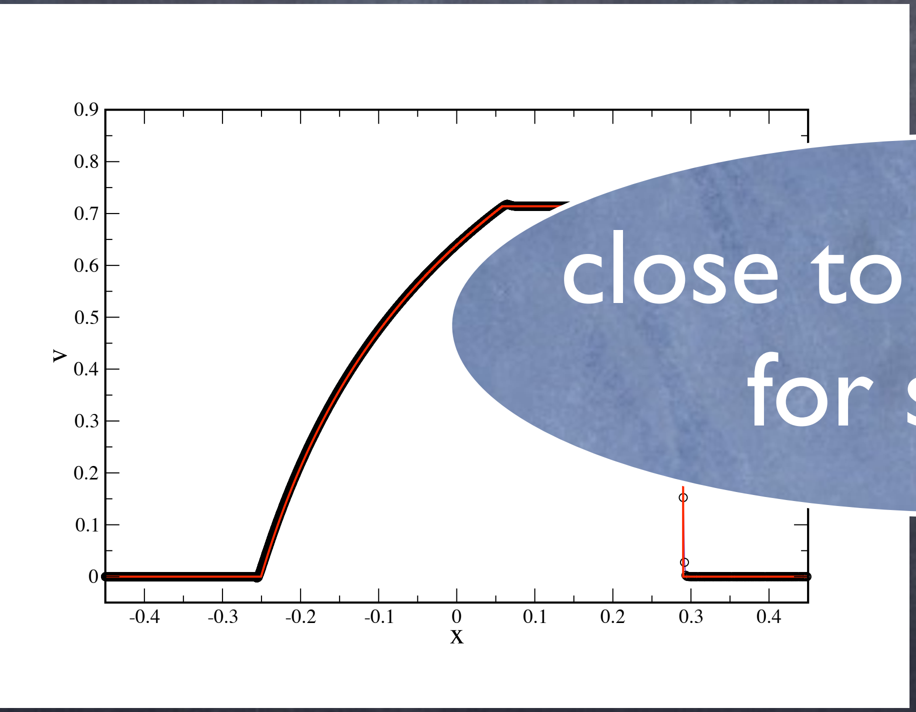
smooth advection:

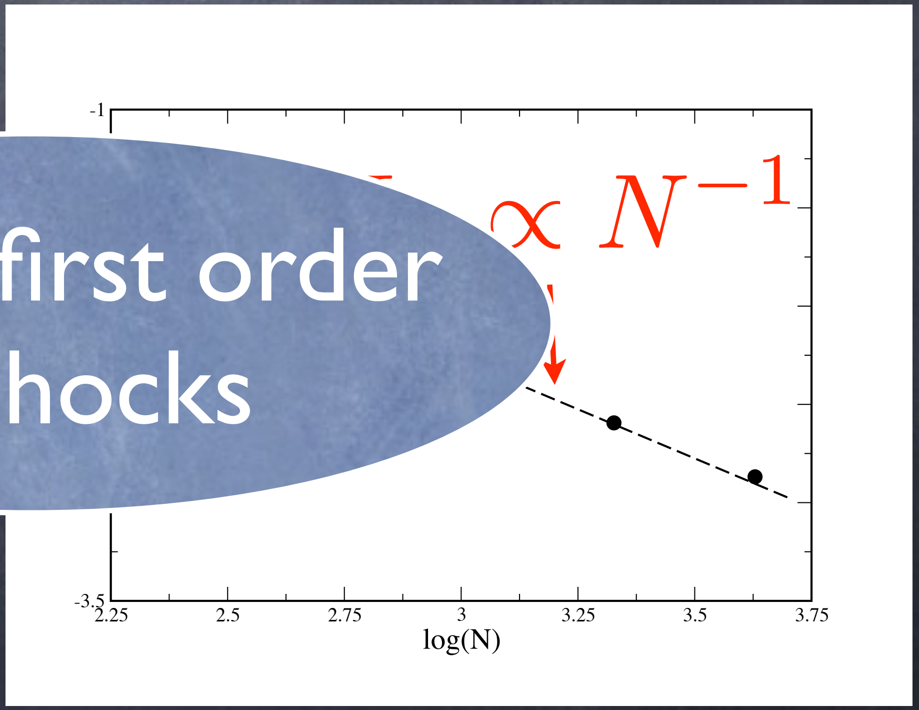




close to second order for smooth flows

shocks:





close to first order for shocks

General-relativistic SPH

- very similar "program" to special-relativity, but more involved algebra

Summary of the general-relativistic SPH equations on a fixed background metric

Ignoring derivatives from the smoothing lengths, the momentum equation reads

$$\frac{dS_{i,a}}{dt} = -\sum_b \nu_b \left(\frac{\sqrt{-g_a} P_a}{N_a^{*2}} + \frac{\sqrt{-g_b} P_b}{N_b^{*2}} \right) \frac{\partial W_{ab}}{\partial x_a^i} + \frac{\sqrt{-g_a}}{2N_a^*} \left(T^{\mu\nu} \frac{\partial g_{\mu\nu}}{\partial x^i} \right)_a \quad (226)$$

where

$$S_{i,a} = \Theta_a \left(1 + u_a + \frac{P_a}{n_a} \right) (g_{i\mu} v^\mu)_a \quad (227)$$

is the canonical momentum per baryon and

$$\Theta_a = (-g_{\mu\nu} v^\mu v^\nu)_a^{-\frac{1}{2}} \quad (228)$$

the generalized Lorentz factor. The energy equation reads

$$\frac{d\hat{\epsilon}_a}{dt} = -\sum_b \nu_b \left(\frac{\sqrt{-g_a} P_a}{N_a^{*2}} \vec{v}_b + \frac{\sqrt{-g_b} P_b}{N_b^{*2}} \vec{v}_a \right) \cdot \nabla_a W_{ab} - \frac{\sqrt{-g_a}}{2N_a^*} \left(T^{\mu\nu} \frac{\partial g_{\mu\nu}}{\partial t} \right)_a , \quad (229)$$

where

$$\hat{\epsilon}_a = S_{i,a} v_a^i + \frac{1 + u_a}{\Theta_a} \quad (230)$$

is the canonical energy per nucleon. The number density can again be calculated via summation,

$$N_a^* = \sum_b \nu_b W_{ab}(h_a). \quad (231)$$