High performance computing and numerical modeling

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Plan for my lectures

Lecture 1:	Collisional and collisionless N-body dynamics
Lecture 2:	Gravitational force calculation
Lecture 3:	Basic gas dynamics
Lecture 4:	Smoothed particle hydrodynamics
Lecture 5:	Eulerian hydrodynamics
Lecture 6:	Moving-mesh techniques
Lecture 7:	Towards high dynamic range
Lecture 8:	Parallelization techniques and current computing trends

Heidelberg Institute for Theoretical Studies
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Universität Heidelberg

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Basics of SPH

The governing equations of an *ideal* gas can also be written in **Lagrangian form**

BASIC HYDRODYNAMICAL EQUATIONS

Euler equation:

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{\nabla P}{\rho} - \nabla\Phi$$

Continuity equation:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\nabla\cdot\mathbf{v} = 0$$

First law of thermodynamics:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{P}{\rho}\nabla\cdot\mathbf{v} - \frac{\Lambda(u,\rho)}{\rho}$$

Equation of state of an ideal monoatomic gas:

$$P = (\gamma - 1)\rho u\,, \qquad \gamma = 5/3$$

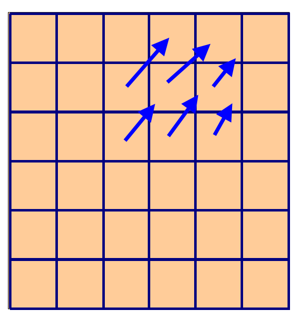
What is smoothed particle hydrodynamics?

DIFFERENT METHODS TO DISCRETIZE A FLUID

Eulerian

discretize space

representation on a mesh
(volume elements)



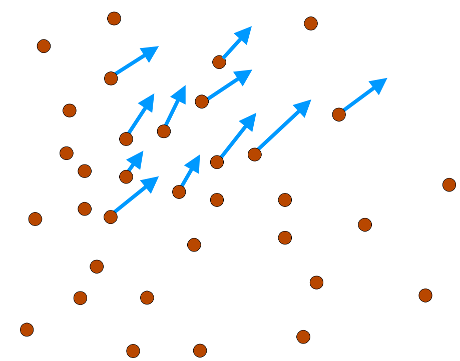
principle advantage:

high accuracy (shock capturing),
low numerical viscosity

Lagrangian

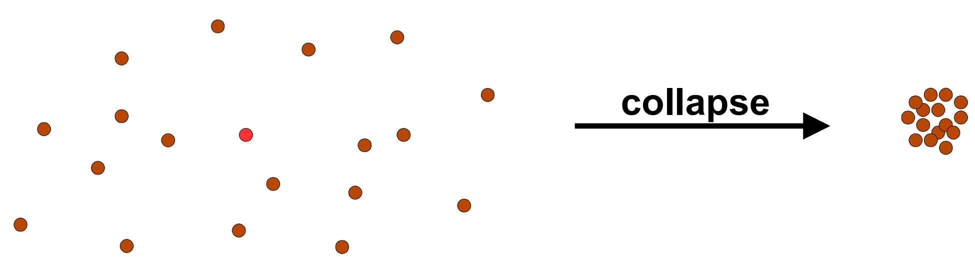
discretize mass

representation by fluid
elements (particles)



principle advantage:

resolutions adjusts
automatically to the flow

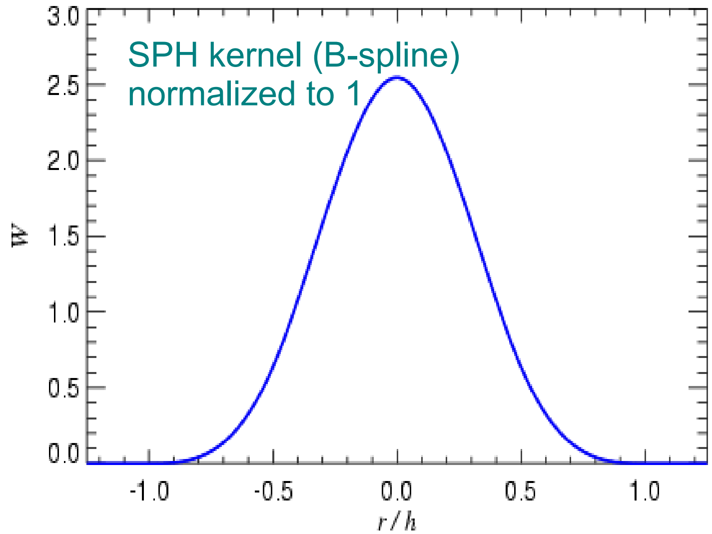


Kernel interpolation is used in smoothed particle hydrodynamics to build continuous fluid quantities from discrete tracer particles

DENSITY ESTIMATION IN SPH BY MEANS OF ADAPTIVE KERNEL ESTIMATION

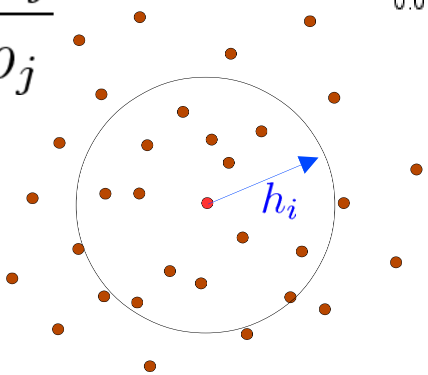
Kernel interpolant of an arbitrary function:

$$\langle A(\mathbf{r})\rangle = \int W(\mathbf{r}-\mathbf{r}', h)\, A(\mathbf{r}')\, \mathrm{d}^3 r'$$



If the function is only known at a set of discrete points, we approximate the integral as a sum, using the replacement:

$$\mathrm{d}^3 r' \mapsto \frac{m_j}{\rho_j}$$



$$\langle A_i\rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} A_j\, W(\mathbf{r}_{ij}; h_i)$$

This leads to the SPH density estimate, for $A_i = \rho_i$

$$\rho_i = \sum_{j=1}^{N} m_j W(|\mathbf{r}_{ij}|, h_i)$$

This can be differentiated !

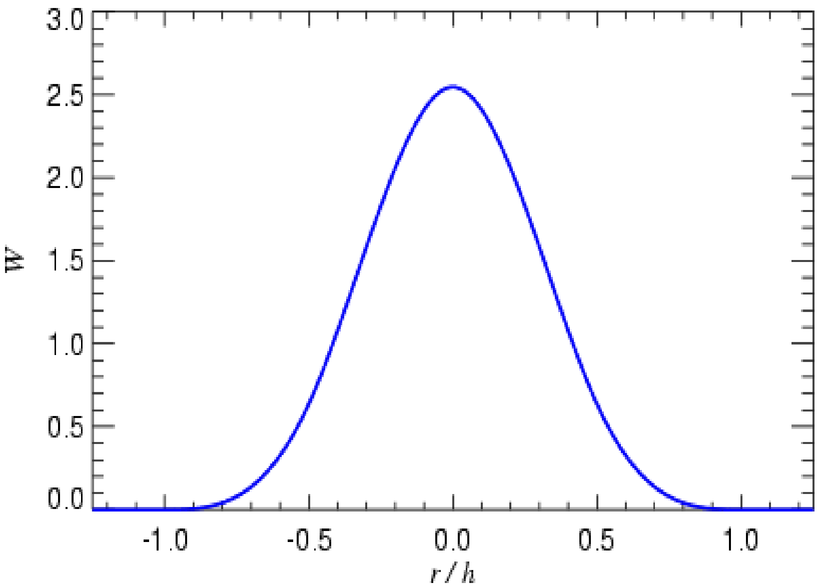
Good kernel shapes need to fulfill a number of constraints

CONDITIONS ON KERNELS

- Must be normalized to unity
- Compact support (otherwise N^2 bottleneck)
- High order of interpolation
- Spherical symmetry (for angular momentum conservation)

Nowadays, almost exclusively the cubic spline is used:

$$W(u) = \frac{8}{\pi} \begin{cases} 1 - 6u^2 + 6u^3, & 0 \le u \le \frac{1}{2}, \\ 2(1-u)^3, & \frac{1}{2} < u \le 1, \\ 0, & u > 1. \end{cases}$$



Kernel interpolants allow the construction of derivatives from a set of discrete tracer points

EXAMPLES FOR ESTIMATING THE VELOCITY DIVERGENCE

Smoothed estimate for the velocity field:

$$\langle \mathbf{v}_i \rangle = \sum_j \frac{m_j}{\rho_j} \mathbf{v}_j W(\mathbf{r}_i - \mathbf{r}_j)$$

Velocity divergence can now be readily estimated:

$$\nabla \cdot \mathbf{v} = \nabla \cdot \langle \mathbf{v}_i \rangle = \sum_j \frac{m_j}{\rho_j} \mathbf{v}_j \nabla_i W(\mathbf{r}_i - \mathbf{r}_j)$$

But alternative (and better) estimates are possible also:

Invoking the identity

$$\rho \nabla \cdot \mathbf{v} = \nabla \cdot (\rho \mathbf{v}) - \mathbf{v} \cdot \nabla \rho$$

one gets a “pair-wise” formula:

$$\rho_i (\nabla \cdot \mathbf{v})_i = \sum_j m_j (\mathbf{v}_j - \mathbf{v}_i) \nabla_i W(\mathbf{r}_i - \mathbf{r}_j)$$

Smoothed particle hydrodynamics is governed by a set of ordinary differential equations

BASIC EQUATIONS OF SMOOTHED PARTICLE HYDRODYNAMICS

Each particle carries either the energy or the entropy per unit mass as independent variable

Density estimate $\rho_i = \sum_{j=1}^{N} m_j W(|\mathbf{r}_{ij}|, h_i)$ → **Continuity equation automatically fulfilled.**

→ $P_i = (\gamma - 1)\rho_i u_i$

Euler equation

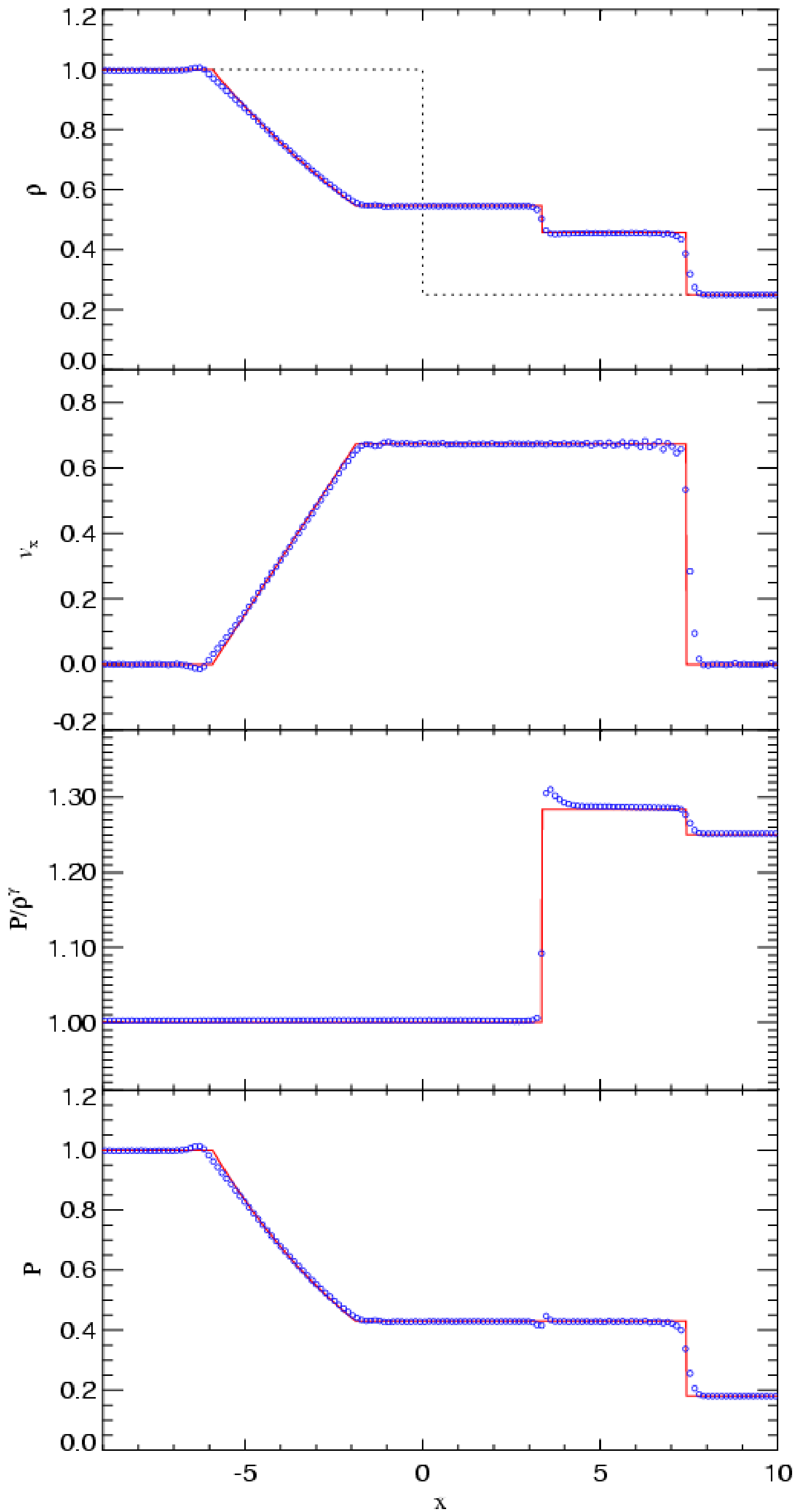
$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i \overline{W}_{ij}$$

Artificial viscosity: $+\Pi_{ij}$

First law of thermodynamics

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \frac{1}{2}\sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \mathbf{v}_{ij} \cdot \nabla_i \overline{W}_{ij}$$

Viscosity and shock capturing



An artificial viscosity needs to be introduced to capture shocks

SHOCK TUBE PROBLEM AND VISCOSITY

viscous force:

$$\left.\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t}\right|_{\mathrm{visc}} = -\sum_{j=1}^{N} m_j \Pi_{ij} \nabla_i \overline{W}_{ij}$$

parameterization of the artificial viscosity:

$$\Pi_{ij} = \begin{cases} -\frac{\alpha}{2}\frac{[c_i+c_j-3w_{ij}]w_{ij}}{\rho_{ij}} & \text{if } \mathbf{v}_{ij}\cdot\mathbf{r}_{ij} < 0 \\ 0 & \text{otherwise} \end{cases}$$

$$v_{ij}^{\mathrm{sig}} = c_i + c_j - 3w_{ij},$$

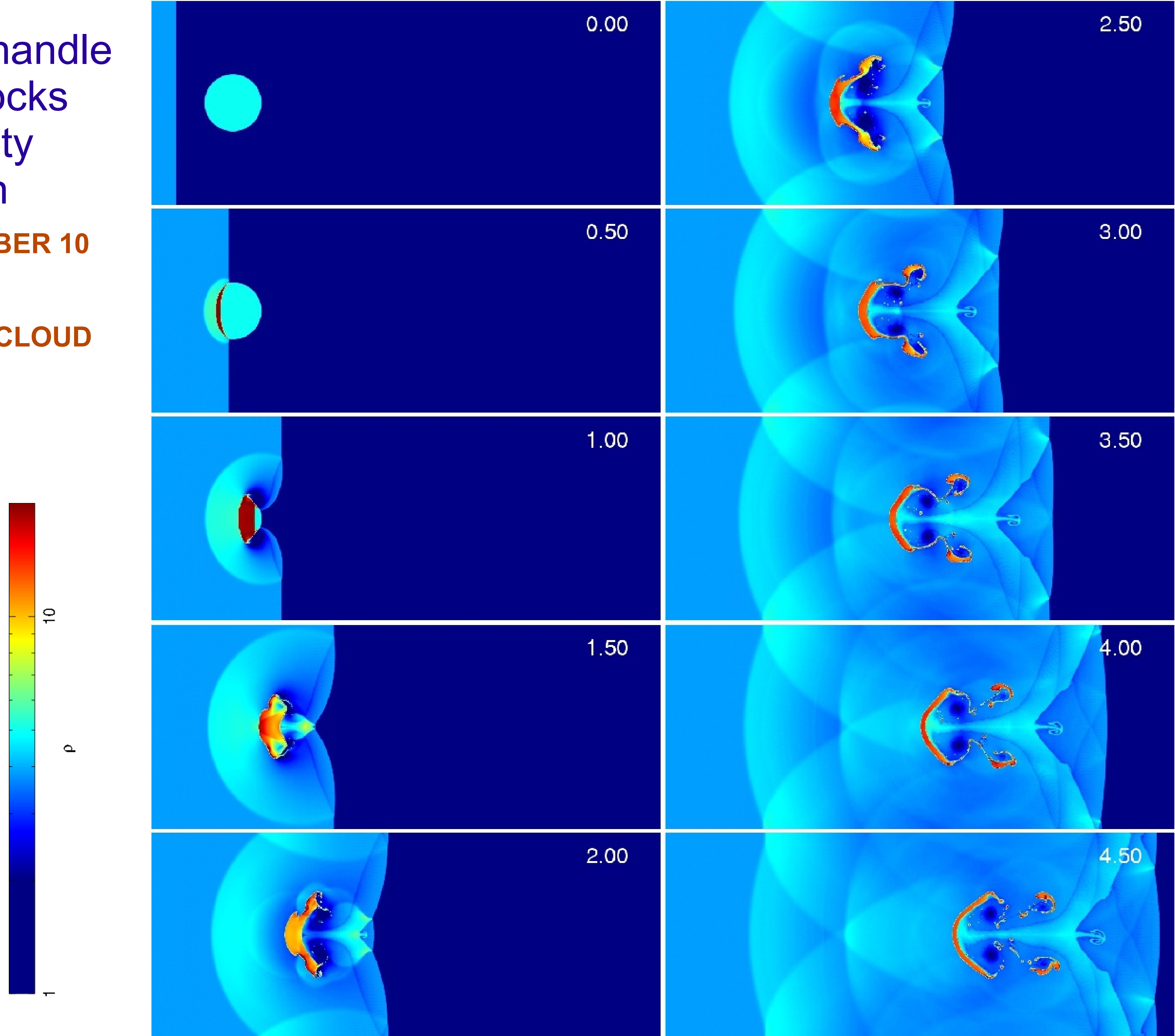
$$w_{ij} = \mathbf{v}_{ij}\cdot\mathbf{r}_{ij}/|\mathbf{r}_{ij}|$$

heat production rate:

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \frac{1}{2}\sum_{j=1}^{N} m_j \Pi_{ij} \mathbf{v}_{ij}\cdot\nabla_i \overline{W}_{ij}$$

SPH can handle strong shocks and vorticity generation

A MACH NUMBER 10 SHOCK THAT STRIKES AN OVERDENSE CLOUD



Variational derivation of SPH

The traditional way to derive the SPH equations leaves room for many different formulations

SYMMETRIZATION CHOICES

Symmetrized kernel:

$$\overline{W}_{ij} = W(|\mathbf{r}_{ij}|, [h_i + h_j]/2)$$

$$\overline{W}_{ij} = \frac{1}{2}\left[W(|\mathbf{r}_{ij}|, h_i) + W(|\mathbf{r}_{ij}|, h_j)\right]$$

Symmetrization of pressure terms:

Using $\nabla P = 2\sqrt{P}\nabla\sqrt{P}$

$$\frac{1}{2}\left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right) \iff \sqrt{\frac{P_i\, P_j}{\rho_i^2\, \rho_j^2}}$$

Is there a best choice?

For an adiabatic flow, temperature can be derived from the specific entropy

ENTROPY FORMALISM

Definition of an **entropic function**:

$$P_i = A_i \, \rho_i^{\gamma}$$

for an adiabtic flow:

$$A_i = A_i(s_i) = \mathrm{const.}$$

don't integrate the temperature, but infer it from:

$$u_i = \frac{A_i}{\gamma - 1} \rho^{\gamma - 1}$$

Use an artificial viscosity to generate entropy in shocks:

$$\frac{\mathrm{d}A_i}{\mathrm{d}t} = \frac{1}{2} \frac{\gamma - 1}{\rho_i^{\gamma-1}} \sum_{j=1}^{N} m_j \Pi_{ij} \mathbf{v}_{ij} \cdot \nabla_i \overline{W}_{ij}$$

None of the adaptive classic SPH schemes conserves energy and entropy simultaneously

CONSERVATION LAW TROUBLES

Hernquist (1993):

> If the **thermal energy** is **integrated**, **entropy** conservation can be **violated**...
>
> If the **entropy** is **integrated**, total **energy** is **not** necessarily **conserved**...

The trouble is caused by varying smoothing lengths... ∇h -terms

Do we have to worry about this? **YES**

Can we do better? **YES**

A fully conservative formulation of SPH

DERIVATION

Springel & Hernquist (2002)

Lagrangian:

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}\sum_{i=1}^{N} m_i \dot{\mathbf{r}}_i^2 - \frac{1}{\gamma - 1}\sum_{i=1}^{N} m_i A_i \rho_i^{\gamma-1}$$

$$\mathbf{q} = (\mathbf{r}_1, \ldots, \mathbf{r}_N, h_1, \ldots, h_N)$$

Constraints:

$$\phi_i(\mathbf{q}) \equiv \frac{4\pi}{3} h_i^3 \rho_i - M_{\rm sph} = 0$$

Equations of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = \sum_{j=1}^{N} \lambda_j \frac{\partial \phi_j}{\partial q_i}$$

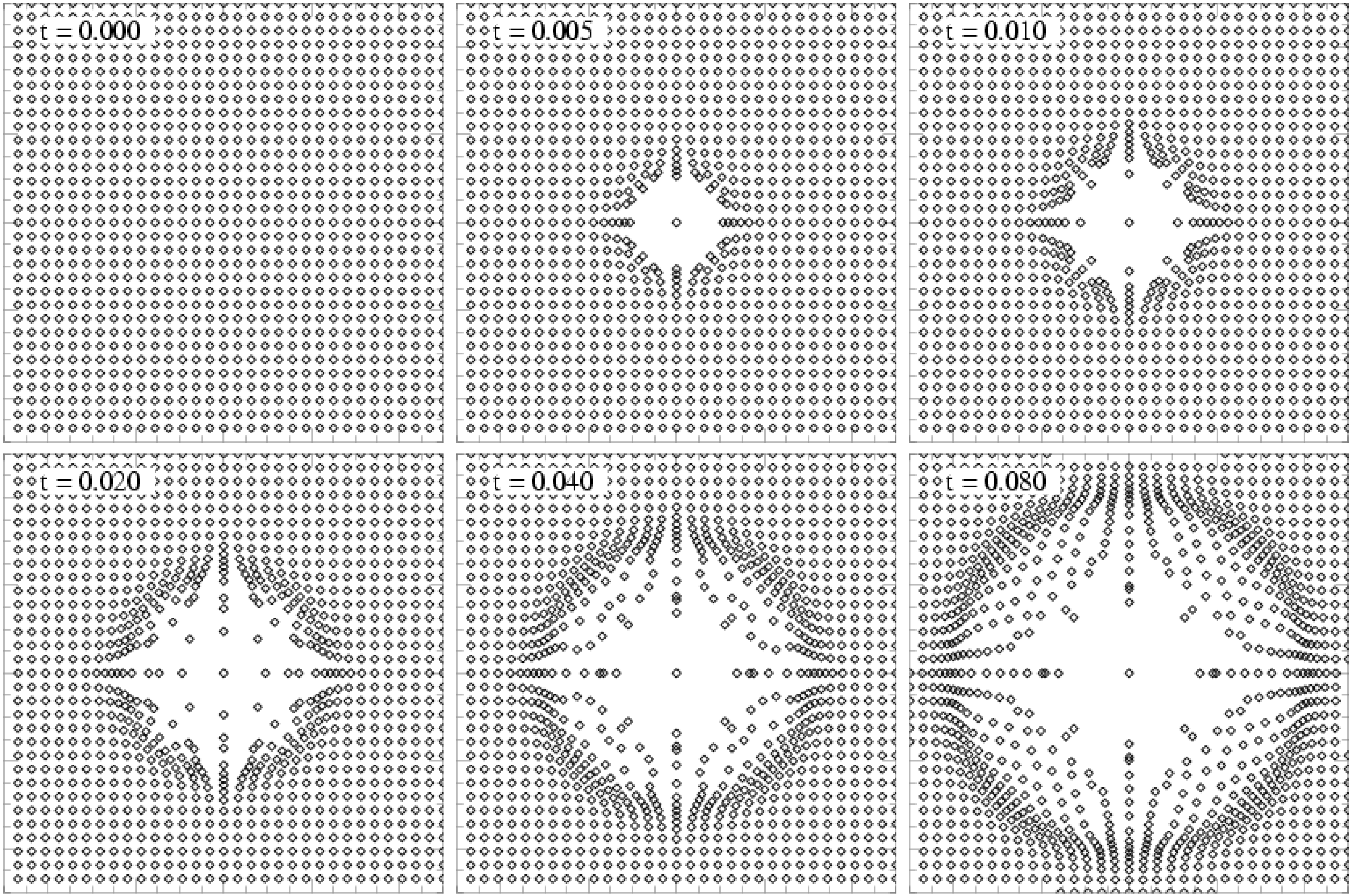
$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_{j=1}^{N} m_j \left[f_i \frac{P_i}{\rho_i^2} \nabla_i W_{ij}(h_i) + f_j \frac{P_j}{\rho_j^2} \nabla_i W_{ij}(h_j) \right]$$

$$f_i = \left[1 + \frac{h_i}{3\rho_i} \frac{\partial \rho_i}{\partial h_i} \right]^{-1}$$

Does the entropy formulation give better results?

A point-explosion in three-dimensional SPH

TAYLOR-SEDOV BLAST

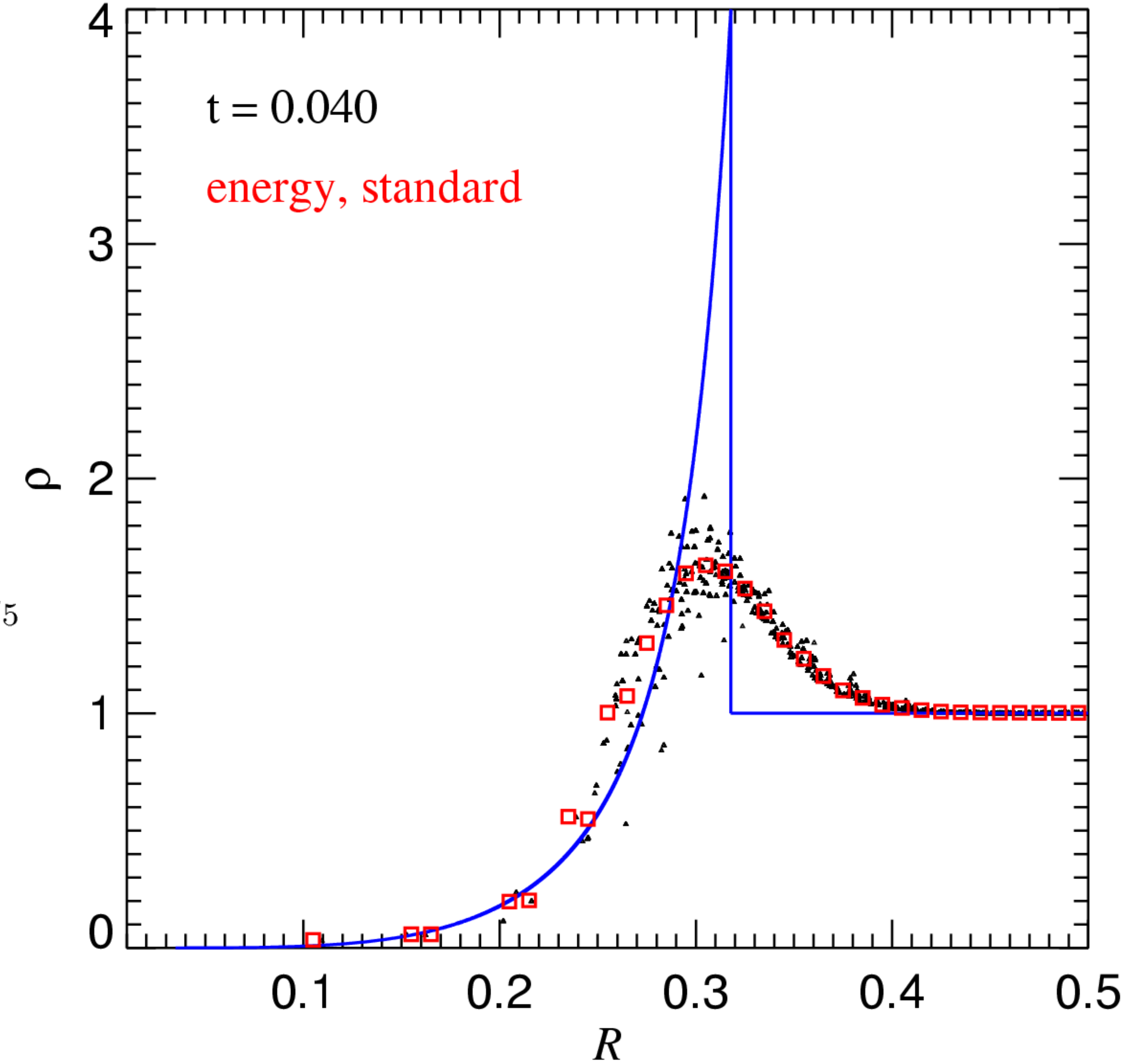


- Geometric formulation gives completely unphysical result (no explosion at all)
- Standard energy formulation produces severe error in total energy, but asymmetric form ok
- Standard entropy formulation ok, but energy fluctuates by several percent

There is a well-known similarity solution for strong point-like explosions

SEDOV-TAYLOR SOLUTIONS FOR **SMOOTHED** EXPLOSION ENERGY

$$R(t) = \beta \left(\frac{Et^2}{\rho} \right)^{1/5}$$



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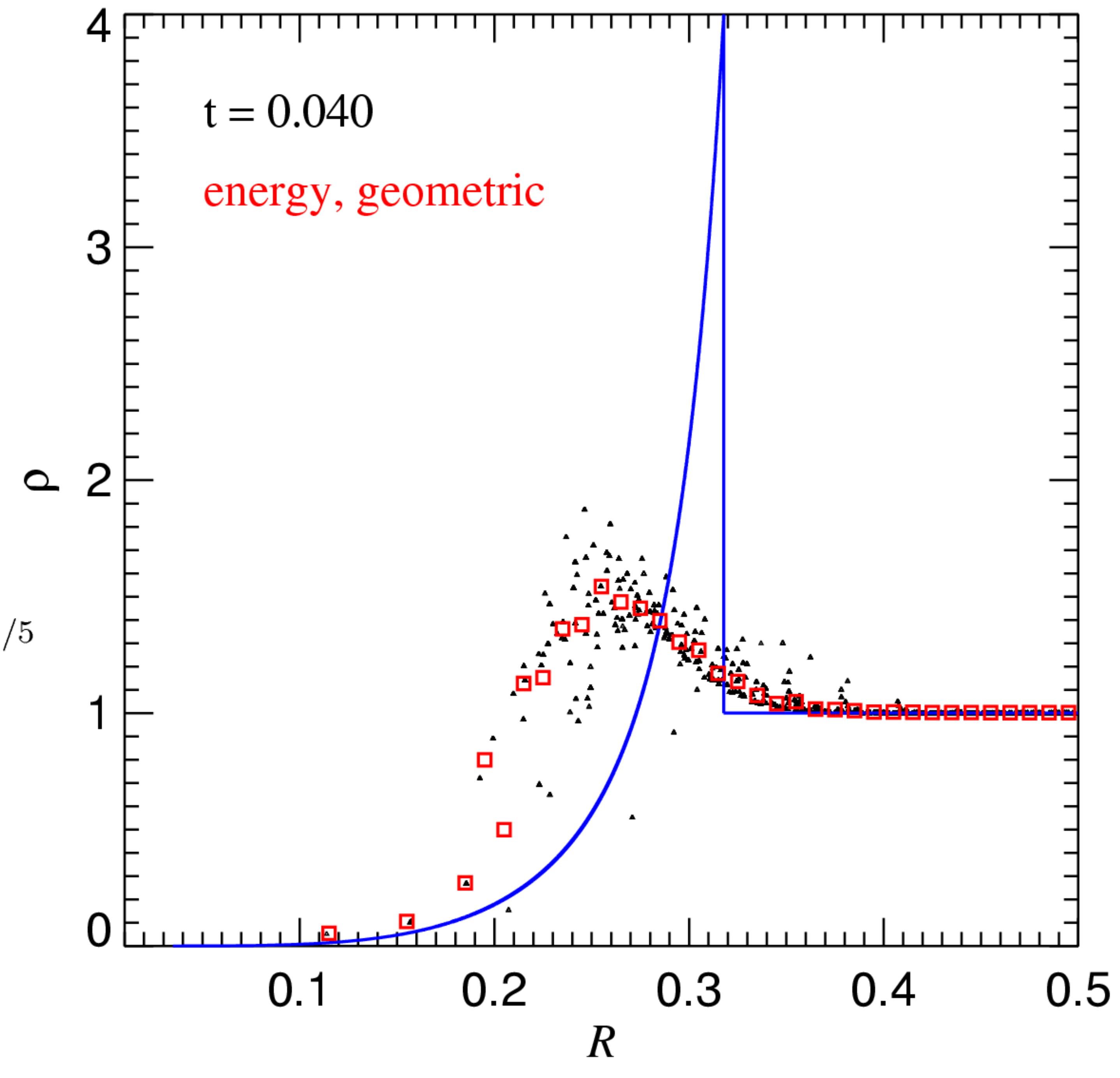

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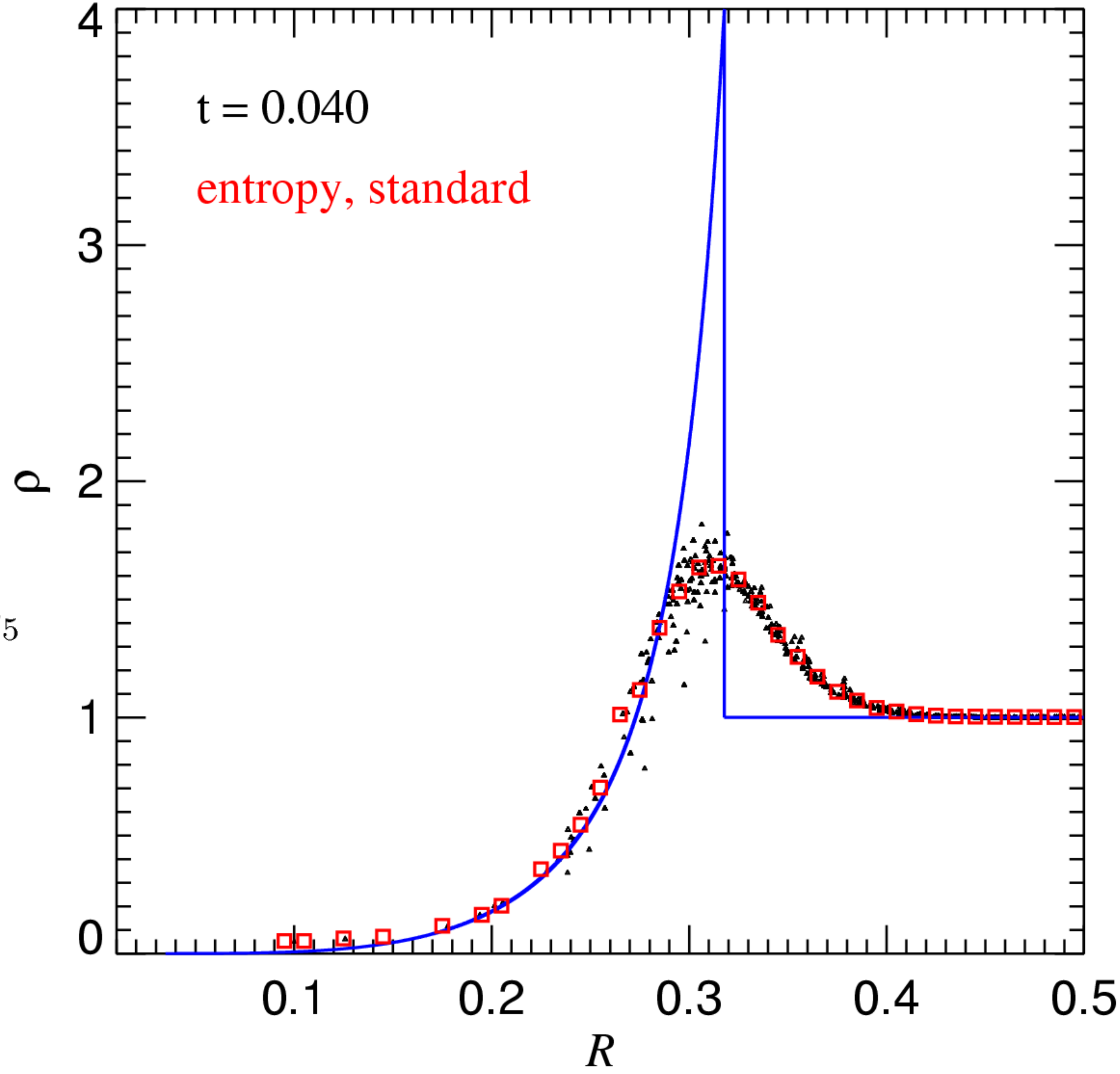
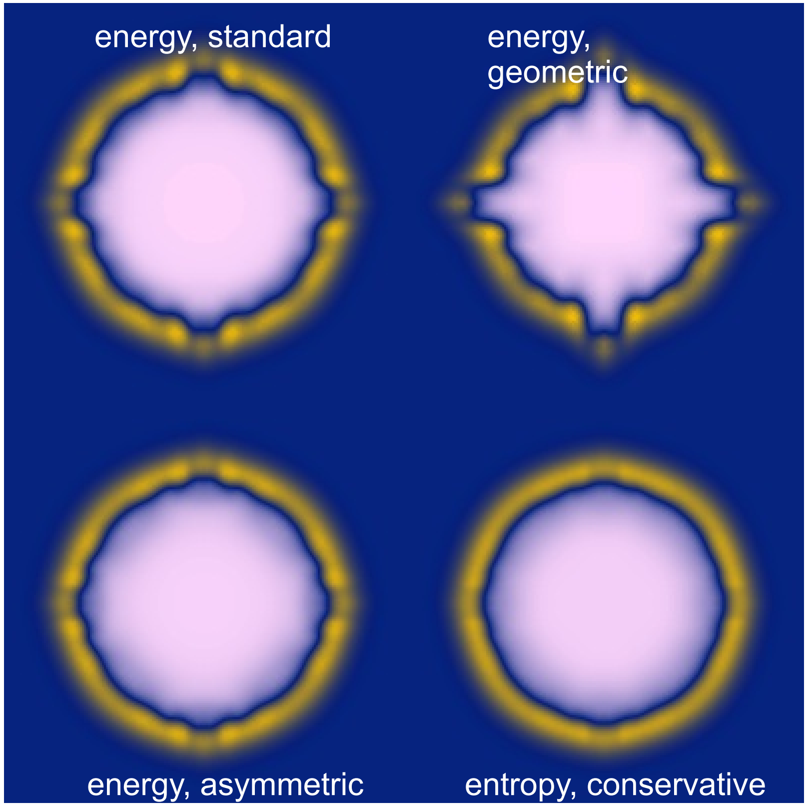
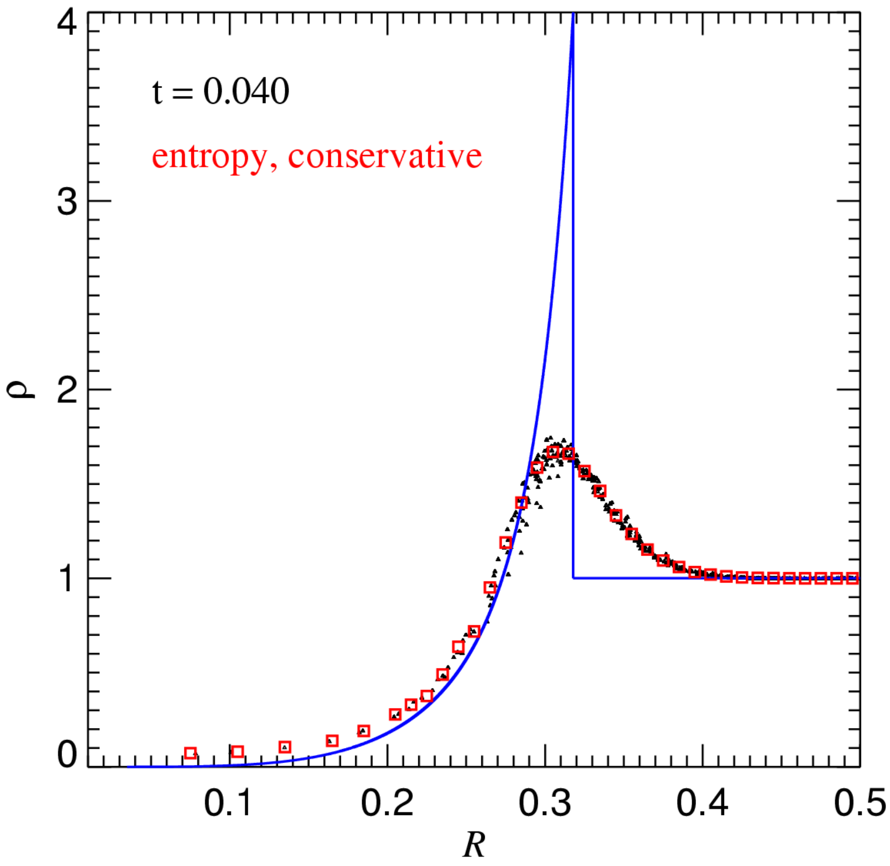


The new conservative formulation gives better results for adiabtic flows

EXPLOSION PROBLEM





Neighbor search in SPH

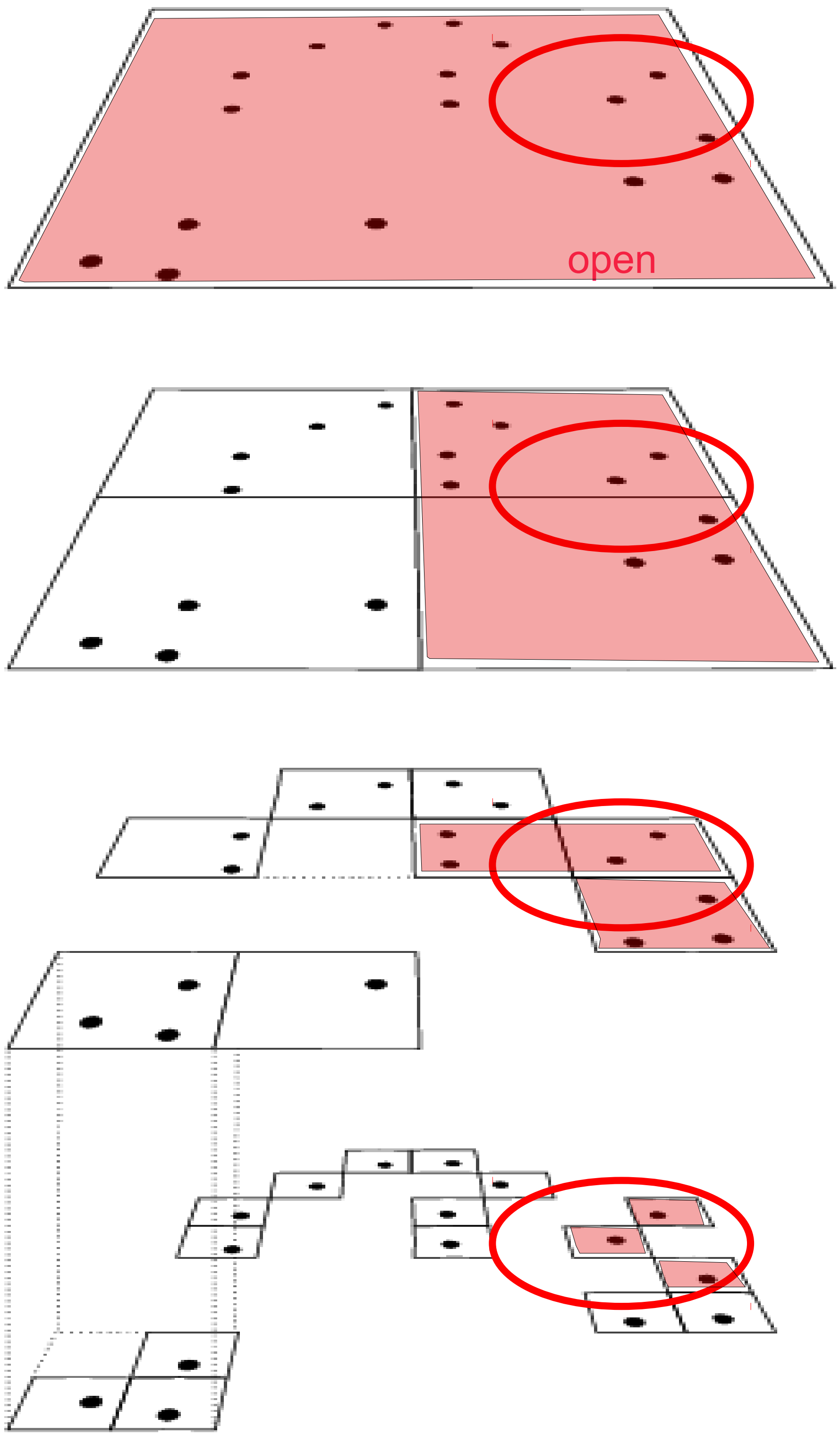
RANGE SEARCHING WITH THE TREE

An efficient neighbor search is the most important factor that determines the speed of an SPH code

<u>But:</u> A simple search radius is not always sufficient, since for the hydro force we need to find all particles with

$$|\mathbf{r}_i - \mathbf{r}_j| < \max(h_i, h_j)$$

Solution: Store in each tree node the maximum h of all particles in the node.



SPH accurately conserves all relevant conserved quantities in self-gravitating flows

SOME NICE PROPERTIES OF SPH

- ★ **Mass is conserved**
- ★ **Momentum is conserved**
- ★ **Total energy is conserved – also in the presence of self-gravity !**
- ★ **Angular momentum is conserved**
- ★ **Entropy is conserved – only produced by artificial viscosity, no entropy production due to mixing or advection**

Furthermore:

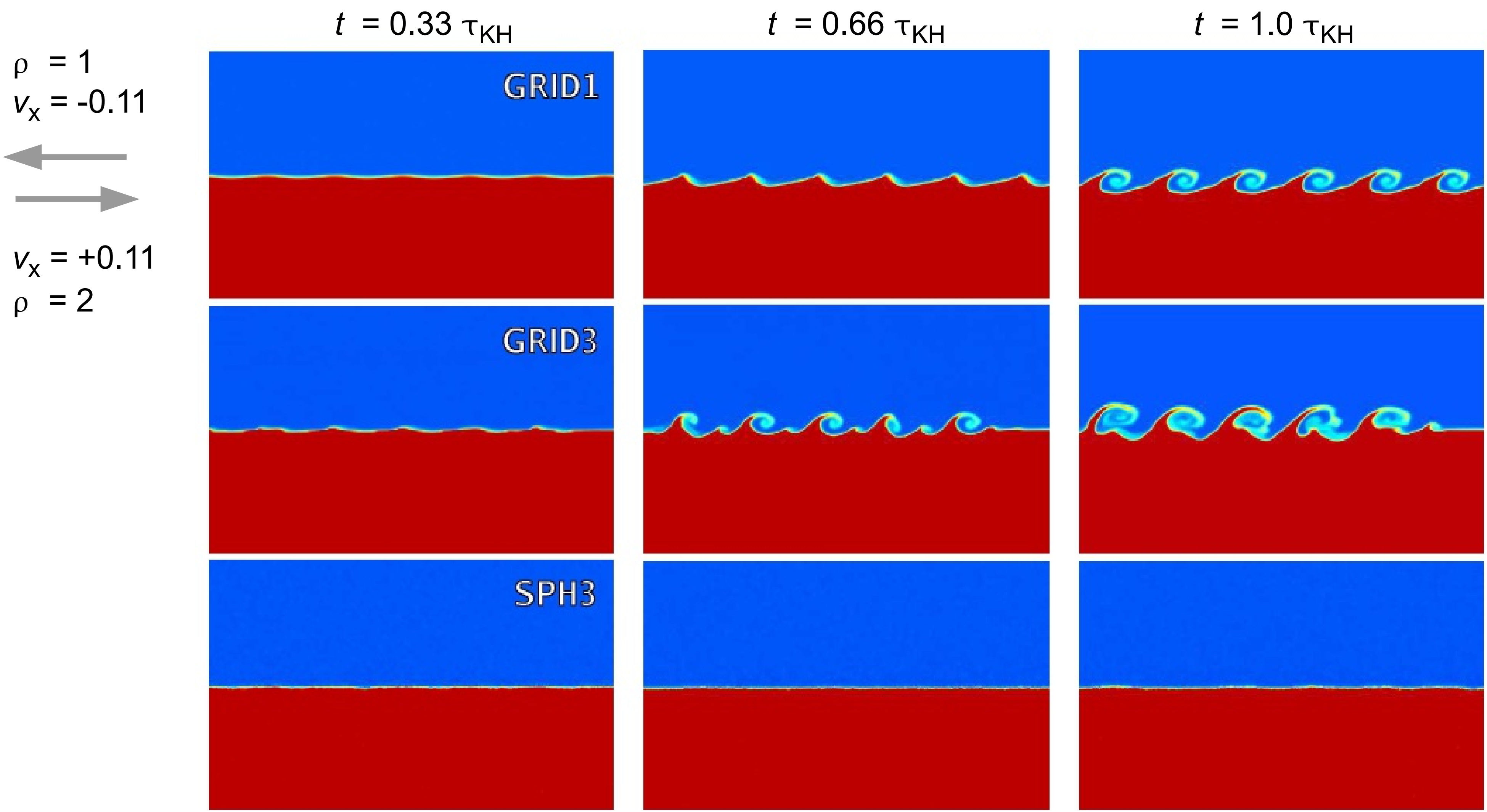
- ★ **High geometric flexibility**
- ★ **Easy incorporation of vacuum boundary conditions**
- ★ **No high Mach number problem**

Fluid instabilities and mixing in SPH

In SPH, fluid instabilities at contact discontinuities with large density jumps tend to be suppressed by a spurious numerical surface tension

KELVIN-HELMHOLTZ INSTABILITIES IN SPH

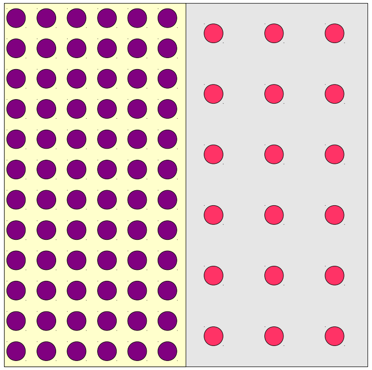
Agertz et al. (2007)



A simple *Gedankenexperiment* about mixing in SPH

$\rho_1 = 8$

$u_1 = \frac{1}{8}$



$\rho_2 = 1$

$u_2 = 1$

$V_1 = \frac{1}{2}$ $\quad V_2 = \frac{1}{2}$

The pressure is constant:

$$P_1 = (\gamma - 1)\rho_1 u_1 = \frac{2}{3} \qquad P_2 = P_1$$

The specific entropies are:

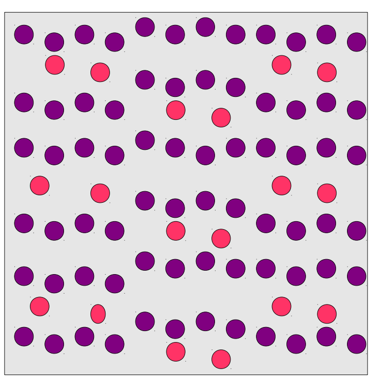
$$A_i = \frac{P_i}{\rho_i^\gamma} \qquad A_1 = \frac{1}{48} \qquad A_2 = \frac{2}{3}$$

Let's calculate the total thermal energy of the system:

$$E_{\rm therm} = \int \frac{A\rho^{\gamma-1}}{\gamma - 1}\,{\rm d}m$$

$$E_{\rm therm} = 1$$

We now mix the particles, keeping their specific entropies fixed:



All particles estimate the same mean density: $\quad M_{\rm tot} = \frac{9}{2} \qquad \overline{\rho} = \frac{9}{2}$

The thermal energy thus becomes:

$$E_{\rm therm} = \frac{M_1 A_1 \overline{\rho}^{2/3}}{2/3} + \frac{M_2 A_2 \overline{\rho}^{2/3}}{2/3}$$

$$E_{\rm therm} = \frac{5}{8}\left(\frac{9}{2}\right)^{2/3} \simeq 1.7$$

⇨ **This mixing process is energetically forbidden!**

What happened to the entropy in our *Gedankenexperiment* ?

In slowly mixing the two phases, we preserve the total thermal energy:

Expect: $\overline{u} = \frac{2}{9}$ $\overline{A} = \frac{2}{3}\frac{\overline{u}}{\overline{\rho}^{2/3}}$ $\overline{A} = \frac{2^{8/3}}{3^{13/3}} \simeq 0.054$

The Sackur-Tetrode equation for the entropy of an ideal gas can be written as:

$$S = \frac{3}{2}\frac{k_{\rm B}}{\mu}M\left[\ln\left(\frac{P}{\rho^{\gamma}}\right) + \ln\left(\frac{2\pi\mu^{8/3}}{h^2}\right) + \frac{5}{3}\right]$$

If the mass in a system is conserved, it is sufficient to consider the simplified entropy:

$$\tilde{S} = M \ln A$$

When the system is mixed, the change of the entropy is:

$$\Delta\tilde{S} = M_{\rm tot} \ln \overline{A} - (M_1 \ln A_1 + M_2 \ln A_2)$$

$$\Delta\tilde{S} \simeq 2.55 \quad \geq \quad 0$$

→ **Unless this entropy is generated somehow, SPH will have problems to mix different phases of a flow.**

(Aside: Mesh codes can generate entropy outside of shocks – this allows them to treat mixing.)

New developments in SPH that try to address mixing

Artificial heat conduction at contact discontinuities has been proposed as a solution for the suppressed fluid instabilities

ARTIFICIAL HEAT MIXING TERMS

Price (2008) **Wadsley, Veeravalli & Couchman (2008)**

Price argues that in SPH every conservation law requires dissipative terms to capture discontinuities.

The normal artificial viscosity applies to the momentum equation, but discontinuities in the (thermal) energy equation should also be treated with a dissipative term.

For every conserved quantity *A*

$$\sum_j m_j \mathrm{d}A_j/\mathrm{d}t = 0$$

a dissipative term is postulated

$$\left(\frac{\mathrm{d}A_i}{\mathrm{d}t}\right)_{\mathrm{diss}} = \sum_j m_j \frac{\alpha_A v_{\mathrm{sig}}}{\bar{\rho}_{ij}} (A_i - A_j) \hat{\mathbf{r}}_{ij} \cdot \nabla W_{ij}$$

that is designed to capture discontinuities.

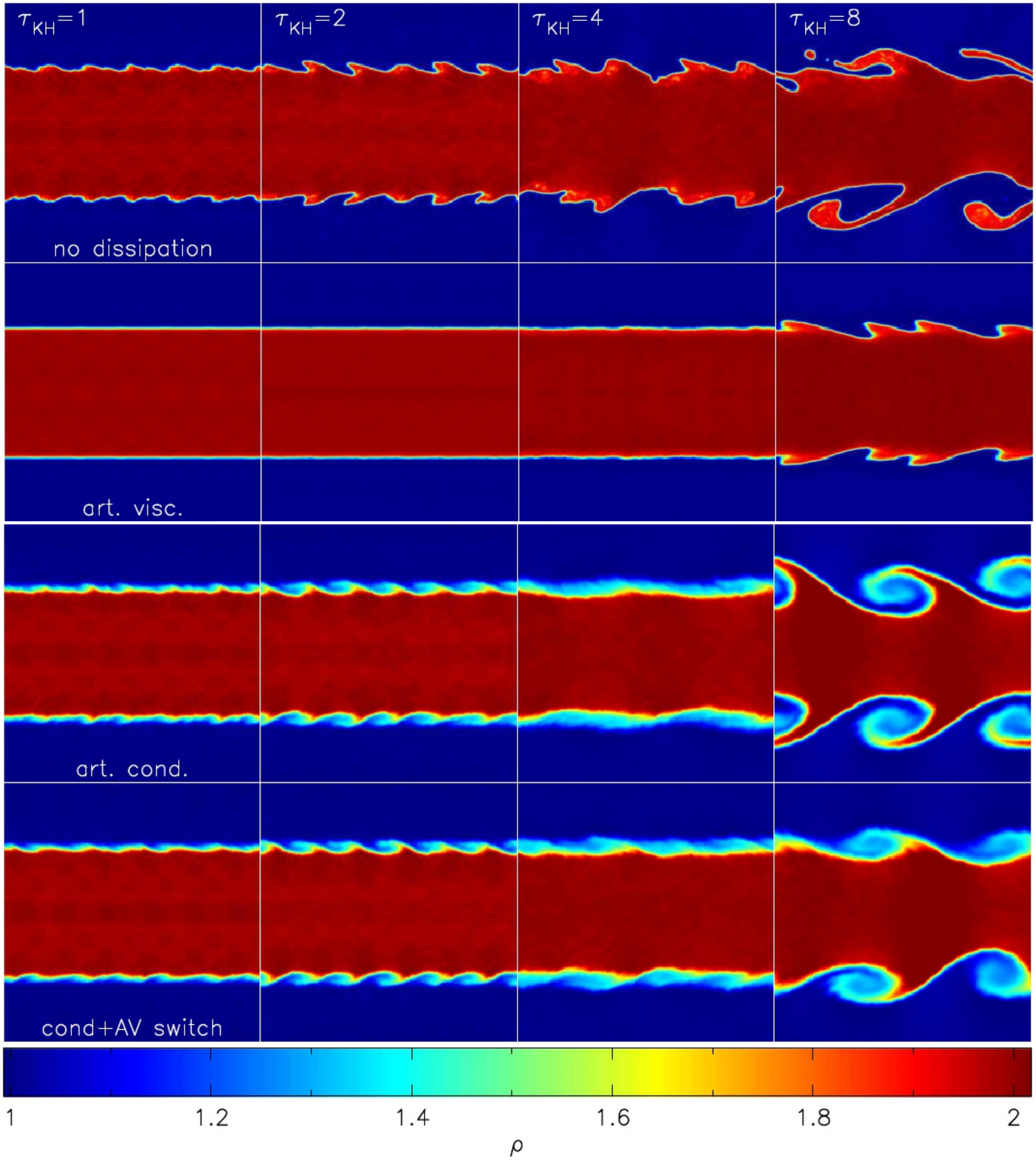
This is the discretized form of a diffusion problem:

$$\left(\frac{\mathrm{d}A}{\mathrm{d}t}\right)_{\mathrm{diss}} \approx \eta \nabla^2 A$$

$$\eta \propto \alpha v_{\mathrm{sig}} |r_{ij}|$$

Artificial heat conduction drastically improves SPH's ability to account for fluid instabilities and mixing

COMPARISON OF KH TESTS FOR DIFFERENT TREATMENTS OF THE DISSIPATIVE TERMS



Price (2008)

Another route to better SPH may lie in different ways to estimate the density

AN ALTERNATIVE SPH FORMULATION

"Optimized SPH" (OSPH) of **Read, Hayfield, Agertz (2009)**

- Density estimate like Ritchie & Thomas (2001):

$$\rho_i = \sum_j^N \left(\frac{A_j}{A_i}\right)^{\frac{1}{\gamma}} m_j \overline{W}_{ij}$$

- Very large number of neighbors (442 !) to beat down noise
- Needs peaked kernel to suppress clumping instability
- This in turn reduces the order of the density estimate, so that a large number of neighbors is required.