COMPUTATIONAL ASTROPHYSICS

- NUMERICAL MODELING OF ASTROPHYSICAL FLUIDS:

  - COLLISIONLESS FLUIDS (NO INTERNAL EOS)
    - GRAVITATIONAL INTERACTIONS (N-BODY METHODS)

  - COLLISIONAL FLUIDS (INTERNAL ENERGY, IDEAL GAS
    - GRAVITY (N-body)
    - FLUID DYNAMICS

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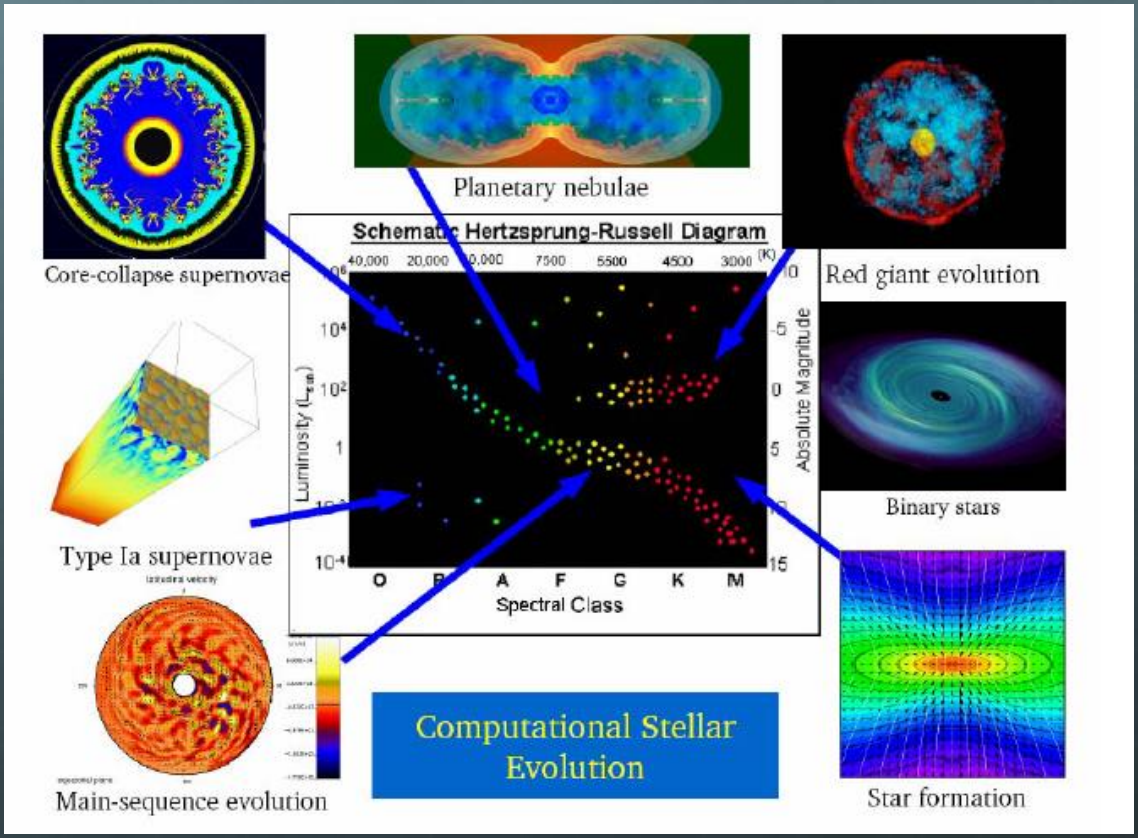
    - GRAVITY (N-body)
    - FLUID DYNAMICS
      - Lagrangian Methods (SPH)
      - Mesh based Eulerian Methods:
        - *Fixed grid*
        - *Adaptive grid (AMR)*
      - Unstructured Mesh

FLUID DYNAMICS IN ASTROPHYSICS AND COSMOLOGY

ASTROPHYSICAL FLUID PROBLEMS



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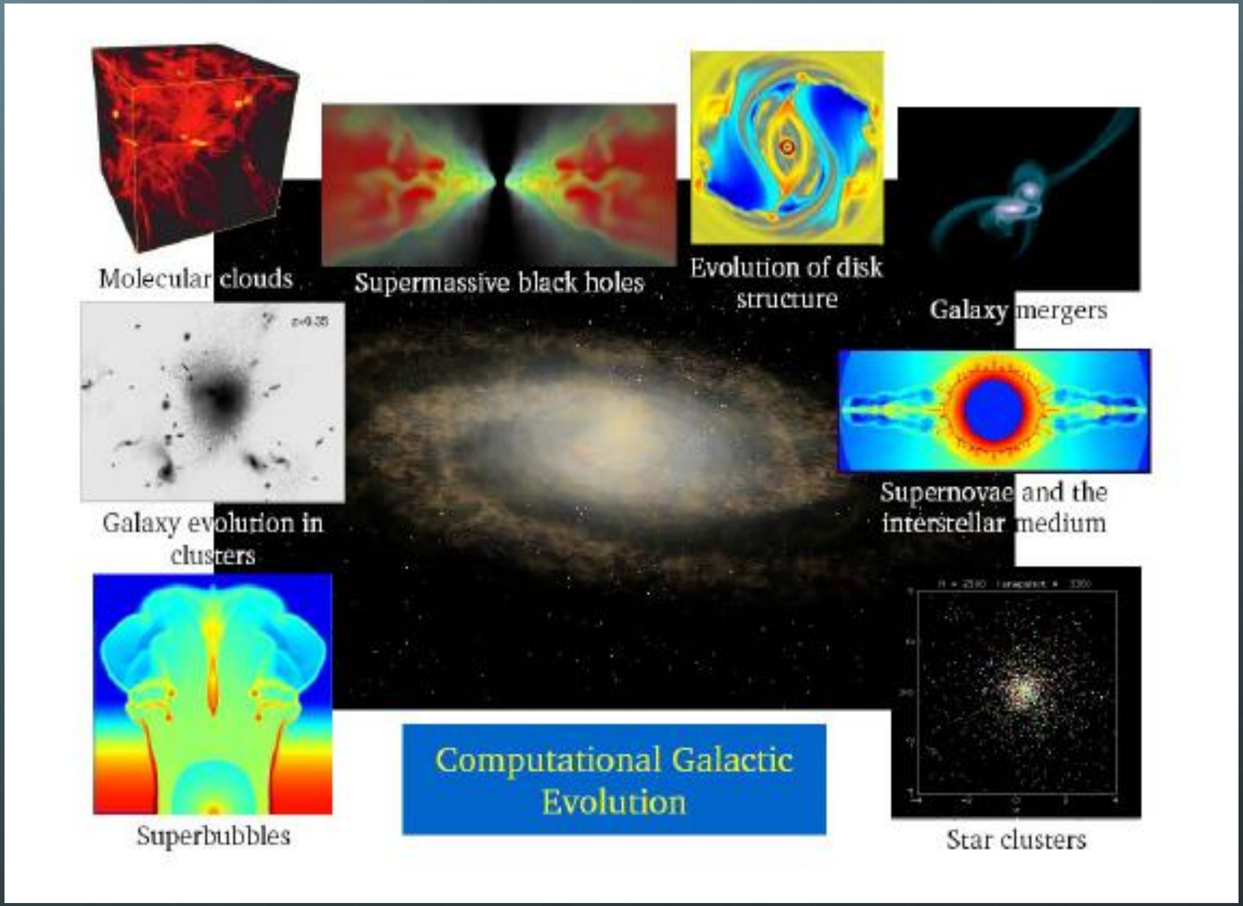

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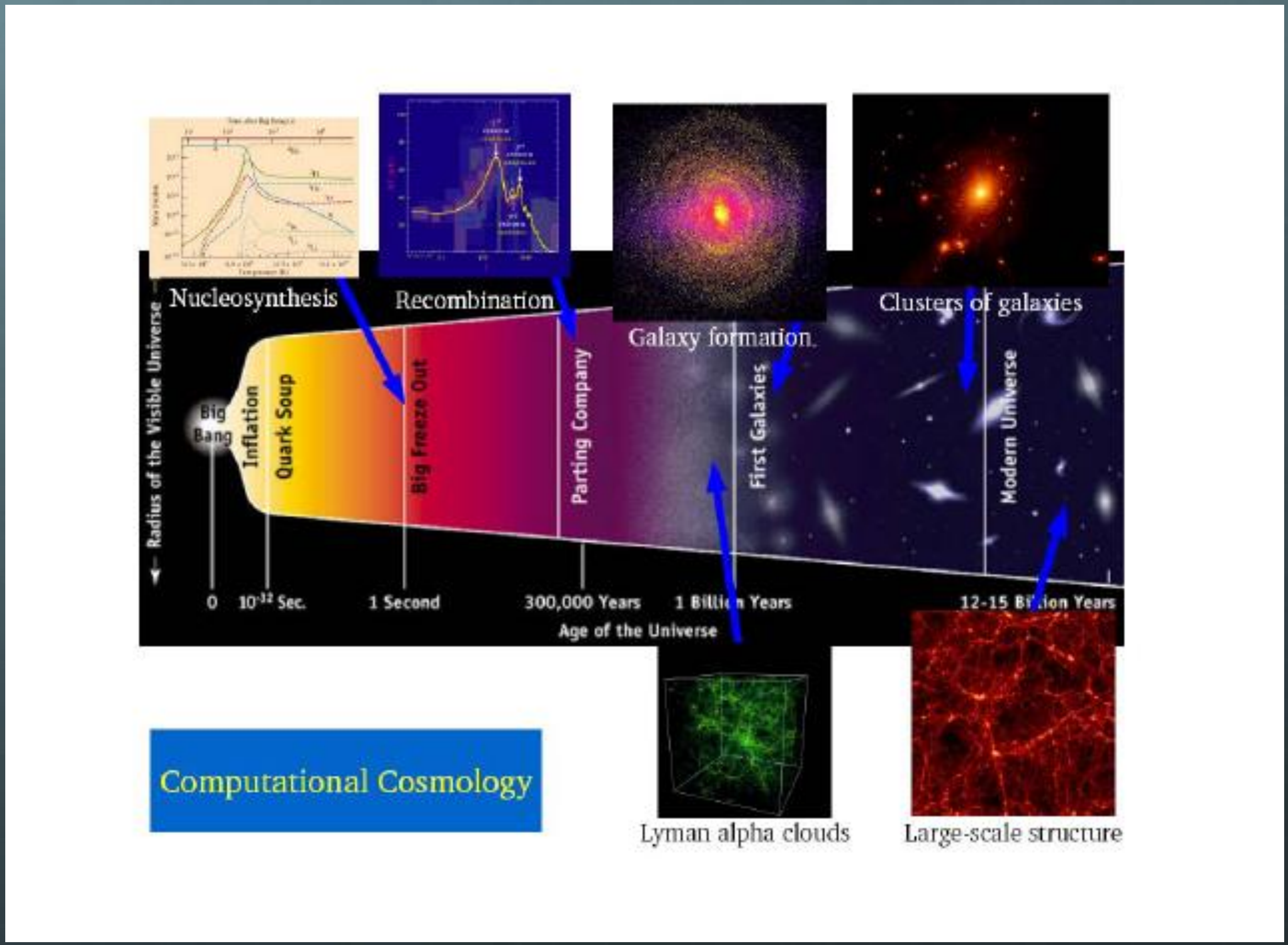
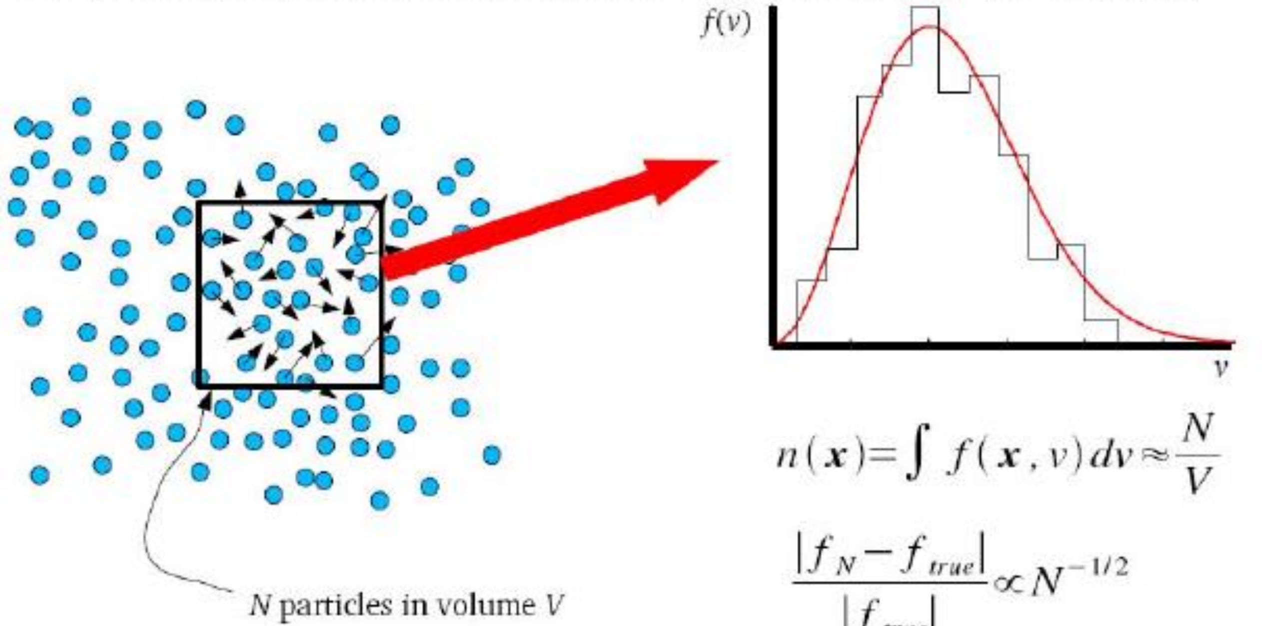


Basic Equations: statistical mechanics

Particle representations

- Direct representation of objects (galaxies, stars, planets)
- Monte Carlo sampling of particle distribution function (gas, dust, dark matter)



$$n(\mathbf{x}) = \int f(\mathbf{x}, v)\, dv \approx \frac{N}{V}$$

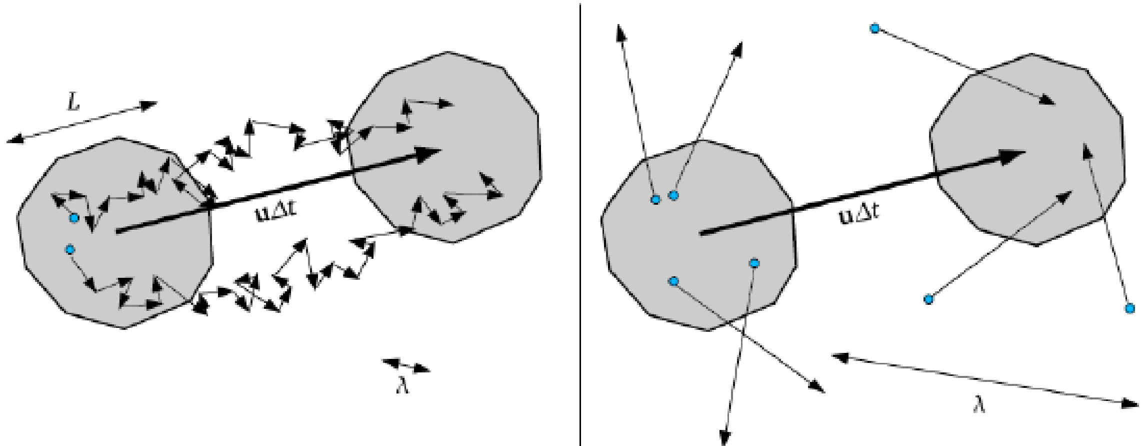
$$\frac{|f_N - f_{true}|}{|f_{true}|} \propto N^{-1/2}$$

Basic requirements:

- As $N \to \infty$, error ("shot noise") in approximate distribution function f_N goes to 0
- As $N \to \infty$, equation describing evolution of f_N becomes the Boltzmann equation

Basic Equations

Collisionality of a gas



Collisional gas (fluid): Kn → 0

- Mean free path $\lambda \ll$ typical scale L
- Random motions do not carry particles far from mean trajectory
- Solve moment equations for motion of fluid elements

Collisionless gas: Kn → ∞

- Mean free path $\lambda \gg$ typical scale L
- Random motions carry particles far from mean trajectory
- Solve kinetic equations for motion of particles (or distribution)

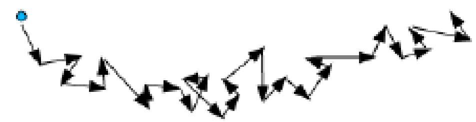
Knudsen number $\mathrm{Kn} \equiv \lambda / L$

Basic Equations

Boltzmann equation

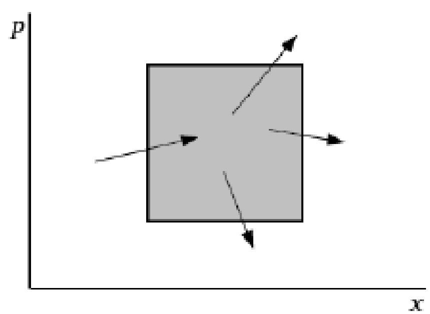
Write single-particle Hamiltonian as

$$H(\mathbf{x},\mathbf{p}) = H_{\text{smooth}}(\mathbf{x},\mathbf{p}) + H_{\text{irregular}}(\mathbf{x},\mathbf{p})$$



Use classical mechanics for H_{smooth}; treat $H_{\text{irregular}}$ statistically

Single-particle distribution function is $f(\mathbf{x},\mathbf{p},t)$
Number of particles in differential volume element is $f(\mathbf{x},\mathbf{p},t)\, d^3x\, d^3p$



Net flux in x-direction

$$f\,\dot{x} = f\,\frac{\partial H_{sm}}{\partial p}$$

Net flux in p-direction

$$f\,\dot{p} = -f\,\frac{\partial H_{sm}}{\partial x}$$

Basic Equations

The Boltzmann equation is then

$$\frac{\partial f}{\partial t} + \nabla_x f \cdot \nabla_p H_{sm} - \nabla_p f \cdot \nabla_x H_{sm} = \left(\frac{\delta f}{\delta t} \right)_c$$

or, for $H_{sm} = \frac{p^2}{2\mathrm{m}} + \Phi(\boldsymbol{x})$

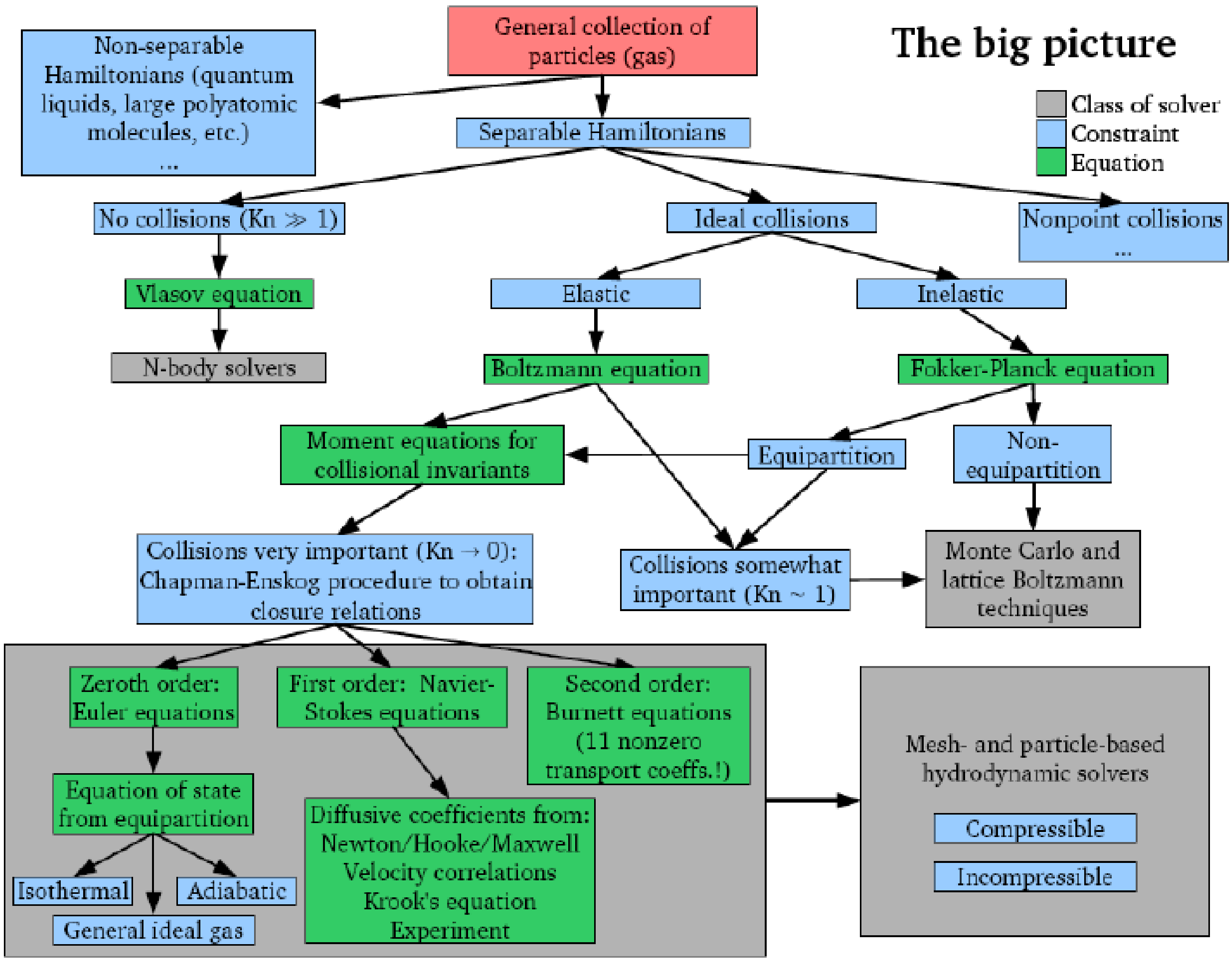
$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m} \cdot \nabla_x f - \nabla_x \Phi \cdot \nabla_p f = \left(\frac{\delta f}{\delta t} \right)_c$$

For self-gravity as a potential source we have

$$\nabla^2 \phi = 4 \pi G \rho$$

where ρ = space density.

The big picture



EULER FLUID EQUATIONS

Moment equations

Define

$$\langle Q \rangle \equiv \frac{1}{n} \int Q f_v d^3 v \qquad n \equiv \int f_v d^3 v$$

then

$$\frac{\partial}{\partial t}(n\langle \chi \rangle) + \nabla_x \cdot (n \langle \boldsymbol{v} \chi \rangle) + n \nabla_x \phi \cdot \langle \nabla_v \chi \rangle = 0$$

or, for $\chi = m$,

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

Continuity equation

Also written:

$$\rho^{-1} \frac{D\rho}{Dt} = -\nabla \cdot \boldsymbol{u}$$

The *convective derivative* is defined as

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \nabla$$

EULER FLUID EQUATIONS

Moment equations – 2

Now take moment of $\chi = mv_i$:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_k}(\rho \langle v_i v_k \rangle) + \rho \frac{\partial \Phi}{\partial x_i} = 0$$

Let $\mathbf{v} = \mathbf{u} + \mathbf{w}$; then

$$\langle v_i v_k \rangle = u_i u_k + \langle w_i w_k \rangle$$

Now write

$$\rho \langle w_i w_k \rangle = P\,\delta_{ik} - \pi_{ik}$$

$$P \equiv \frac{1}{3} \rho \langle |\mathbf{w}|^2 \rangle \qquad \textit{Gas pressure}$$

$$\pi_{ik} \equiv \rho \langle \frac{1}{3} |\mathbf{w}|^2 \delta_{ik} - w_i w_k \rangle \qquad \textit{Viscous stress tensor}$$

then:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_k}(\rho u_i u_k + P\,\delta_{ik} - \pi_{ik}) + \rho \frac{\partial \Phi}{\partial x_i} = 0$$

Momentum equation

EULER FLUID EQUATIONS

Moment equations – 3

Now take moment of $\chi = mv^2/2$:

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho\left(|\boldsymbol{u}|^2+\langle|\boldsymbol{w}|^2\rangle\right)\right]+\frac{\partial}{\partial x_k}\left[\frac{1}{2}\rho\langle(u_k+w_k)|u_i+w_i|^2\rangle\right]+\rho\frac{\partial\phi}{\partial x_k}u_k=0$$

now

$$\langle(u_k+w_k)|u_i+w_i|^2\rangle=|\boldsymbol{u}|^2u_k+2u_i\langle w_i w_k\rangle+u_k\langle|\boldsymbol{w}|^2\rangle+\langle w_k|\boldsymbol{w}|^2\rangle$$

define

$$\varepsilon\equiv\langle\frac{1}{2}|\boldsymbol{w}|^2\rangle=\frac{3}{2}\frac{P}{\rho} \quad \textit{Specific internal energy}$$

$$F_k\equiv\rho\langle w_k\frac{1}{2}|\boldsymbol{w}|^2\rangle \quad \textit{Conductive heat flux}$$

then

$$\frac{\partial}{\partial t}\left(\frac{\rho}{2}|\boldsymbol{u}|^2+\rho\,\varepsilon\right)+\frac{\partial}{\partial x_k}\left(\frac{\rho}{2}|\boldsymbol{u}|^2u_k+u_i\left(P\,\delta_{ik}-\pi_{ik}\right)+\rho\,\varepsilon\,u_k+F_k\right)+\rho\,u_k\frac{\partial\phi}{\partial x_k}=0$$

Total energy equation

EULER FLUID EQUATIONS

Lowest-order moment equations: ***Euler equations***

Letting f_v be Maxwellian, obtain

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \boldsymbol{u}$$

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\rho \nabla \phi - \nabla P$$

$$\rho \frac{D\varepsilon}{Dt} = -P \nabla \cdot \boldsymbol{u}$$

$$\rho \varepsilon = \frac{3}{2} P = \frac{3}{2} n k_B T$$

Because $f_v^{(0)}$ depends only on $|\mathbf{v} - \mathbf{u}|$, to lowest order

$$\pi_{ik} = 0, F_i = 0, \Psi = 0$$

ie. Euler equations neglect particle diffusive effects.

EULER FLUID EQUATIONS

Lowest-order moment equations: ***Euler equations***

Letting f_ν be Maxwellian, obtain

Convective Derivative

$$\frac{Dy}{Dt} = \frac{\partial y}{\partial t} + \boldsymbol{u}.\boldsymbol{\nabla} y$$

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \boldsymbol{u}$$

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\rho \nabla \phi - \nabla P$$

$$\rho \frac{D\varepsilon}{Dt} = -P \nabla \cdot \boldsymbol{u}$$

$$\rho \varepsilon = \frac{3}{2} P = \frac{3}{2} n k_B T$$

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EULER FLUID EQUATIONS

Equations of state (EOS) – ideal gases with inelastic collisions

- Nontranslational modes add degrees of freedom to collisions
- Equipartition assumption: energy equally distributed among modes *in the average*
- General EOS for ideal gases:

$$\rho\,\varepsilon = \frac{P}{\gamma - 1} = \frac{n\,k_B T}{\gamma - 1}$$

$$\rho\, s \equiv -k_B \int f \ln f\, d^3 p = \rho\, c_v \ln\left(P\, \rho^{-\gamma}\right)$$

where $\gamma \equiv c_v / c_p$ = ratio of specific heats

$s \equiv$ specific entropy

Barotropic equations of state (ie. P is a function of ρ only)

- Special case: isothermal gas ($\gamma = 1$)

$$P \propto \rho$$

- Special case: adiabatic gas ("polytropic EOS")

$$s = \text{constant} \quad \Rightarrow \quad P \propto \rho^{\gamma}$$

EULER FLUID EQUATIONS

Intuition regarding γ and the EOS

- For particles with d degrees of freedom, $\gamma = 1 + \frac{2}{d}$
- Large $\gamma \rightarrow$ "stiff" equation of state
  - Adiabatic compression yields large pressure increase
- Small $\gamma \rightarrow$ "soft" equation of state
  - Adiabatic compression yields small pressure increase
- Typical values:

$\gamma = 1.6667$	monatomic gas (no internal degrees of freedom)
$\gamma = 1.3333$	relativistic monatomic gas
$\gamma = 1.4$	diatomic gas (rotational d. o. f. only)
$\gamma = 1.3333$	diatomic gas (rotational + vibrational d. o. f.)
$\gamma = 1$	isothermal gas (compression cannot heat, $d = \infty$)
$\gamma \approx 1.4$	air (mostly N_2 and O_2)

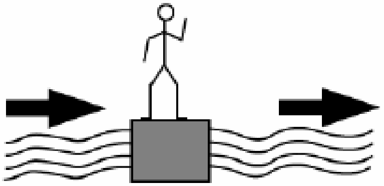
EULER FLUID EQUATIONS

Eulerian vs. Lagrangian viewpoints

Eulerian: stand still as fluid moves by

Fluid quantities functions of position **x** and time t

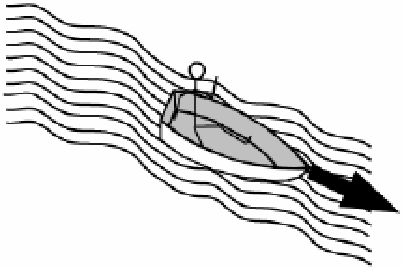
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{u})$$



Lagrangian: move with the fluid

Fluid quantities functions of initial position $\mathbf{x}(t_0)$ and time t

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \boldsymbol{u}$$



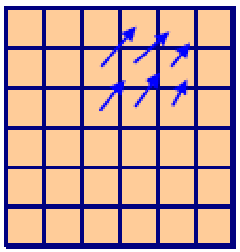
Euler equations in Lagrangian form

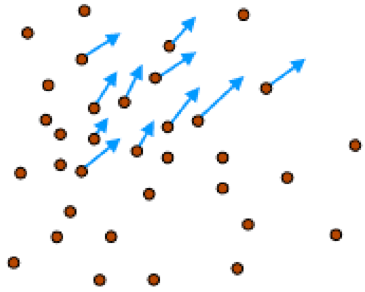
Euler equation:	$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{\nabla P}{\rho} - \nabla\Phi$$
Continuity equation:	$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\nabla\cdot\mathbf{v} = 0$$
First law of thermodynamics:	$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{P}{\rho}\nabla\cdot\mathbf{v} - \frac{\Lambda(u,\rho)}{\rho}$$
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	Lagrangian
discretize space	discretize mass
representation on a mesh (volume elements)	representation by fluid elements (particles)



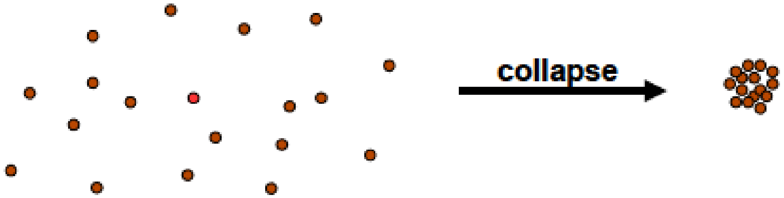


Eulerian — principle advantage:

high accuracy (shock capturing), low numerical viscosity

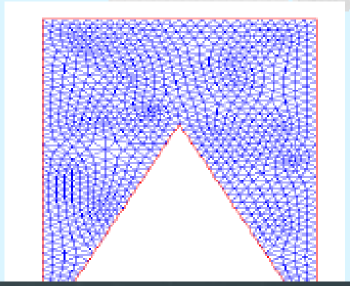
Lagrangian — principle advantage:

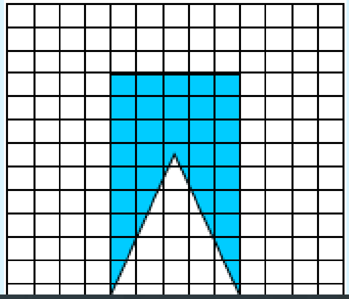
resolutions adjusts automatically to the flow



Eulerian vs Lagrangian descriptions

	Lagrangian methods	Eulerian methods
Grid	Attached on the moving material	Fixed in the space
Track	Movement of any point on materials	Mass, momentum, and energy flux across grid nodes and mesh cell boundary
Time history	Easy to obtain time-history data at a point attached on materials	Difficult to obtain time-history data at a point attached on materials
Moving boundary and interface	Easy to track	Difficult to track
Irregular geometry	Easy to model	Difficult to model with good accuracy
Large deformation	Difficult to handle	Easy to handle





Lagrangian Method for CFD

- One of the most often used is :

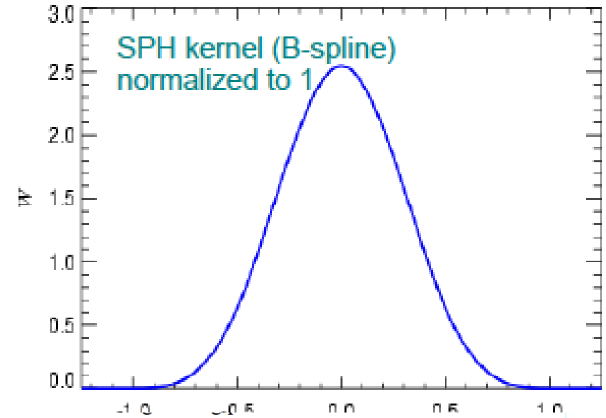
- SMOOTHED PARTICLE HYDRODYNAMICS (SPH)
  - Introduced by Lucy (1972) and Gingold and Monaghan (1977) in the context of Astrophysical Fluids

Basic Concepts of SPH

- Discretization using a set of arbitrarily distributed particles.
- Integral function approximation: kernel approximation
- Particle approximation of field functions.
  - Summation to replace integration
  - Field function and its derivatives
- PDEs are represented directly in particle approximation
- No connectivity is defined between particles: large deformation.
- The ODE's are solved using explicit integration algorithm

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



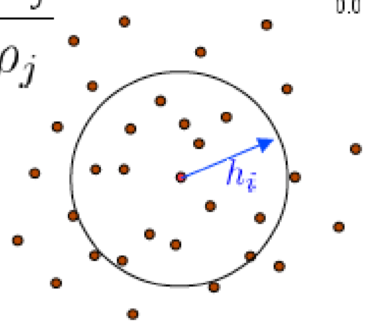
Kernel interpolant of an arbitrary function:

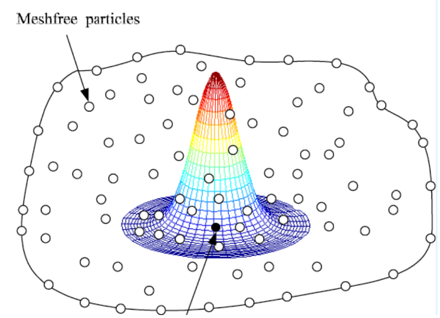
$$\langle A(\mathbf{r})\rangle = \int W(\mathbf{r}-\mathbf{r}', h)\, A(\mathbf{r}')\, \mathrm{d}^3 r'$$

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 !**

Basic properties of the Kernel function

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

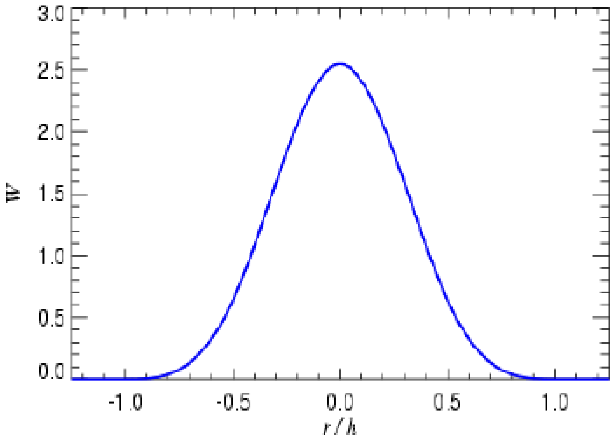
$$\int W(\mathbf{x}-\mathbf{x}', h)\, d\mathbf{x} = 1$$

$$\lim_{h\to 0} W(\mathbf{x}-\mathbf{x}', h) = \delta(\mathbf{x}-\mathbf{x}')$$

Nowadays, almost exclusively the cubic spline is used:

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

$u = |x-x_i|/h_i$



Derivative of a Function

- Any fluid quantity can be estimated as

$$A_S(\mathbf{r}) = \sum_b m_b \frac{A_b}{\rho_b} W(\mathbf{r} - \mathbf{r}_b, h),$$

- The spatial derivative can simply be computed:

$$\nabla A(\mathbf{r}) = \sum_b m_b \frac{A_b}{\rho_b} \nabla W(\mathbf{r} - \mathbf{r}_b, h),$$

- Or better using this relation

$$\rho \nabla A = \nabla(\rho A) - A \nabla \rho,$$

SPH Fluid Equations

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:

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

SPH Fluid Equations

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

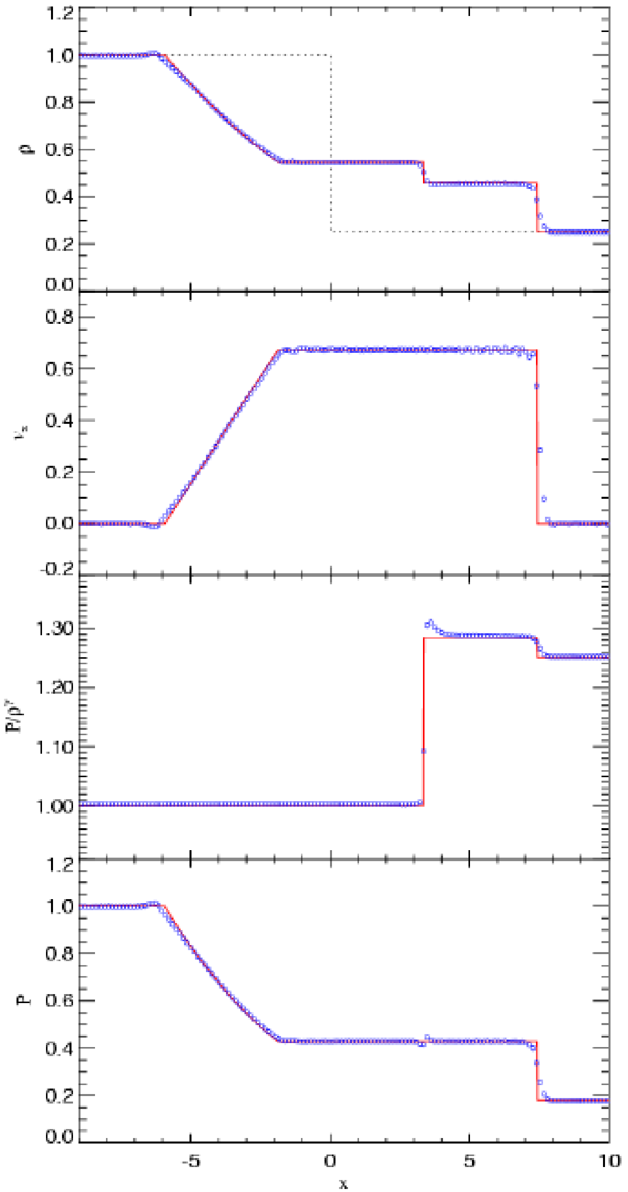
$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i \overline{W}_{ij}$$

Artificial viscosity: $+\Pi_{ij}$

$$\overline{W}_{ij} = \frac{1}{2}[W_{ij}(h_i) + W_{ij}(h_j)]$$

First law of thermodynamics

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



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:

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

Varying smoothing kernels

Efficiency and usefulness of SPH are maximized when each particle is allowed to have its own smoothing kernel size h_p.

Typically h_p is chosen so that the number of particles within h_p stays roughly constant (as with adaptive particle-mesh) – so it gets smaller in high-density regions.

Typically h_p is taken to satisfy

$$\frac{dh_p}{dt} = -\frac{h_p}{\rho_p d}\frac{d\rho_p}{dt}, \quad d = \#\ of\ dimensions$$

The SPH equations then must use symmetrized kernels to ensure conservation of mass, momentum, and energy:

$$W_{pq} \to \frac{1}{2}\left[W(\boldsymbol{x}_p - \boldsymbol{x}_q, h_p) + W(\boldsymbol{x}_p - \boldsymbol{x}_q, h_q)\right]$$

or

$$W_{pq} \to W\left(\boldsymbol{x}_p - \boldsymbol{x}_q, \frac{1}{2}(h_p + h_q)\right)$$

Symmetrization of the Pressure term

- Arithmetic mean

$$\frac{\nabla P}{\rho} = \nabla\left(\frac{P}{\rho}\right) + \frac{P}{\rho^2}\nabla\rho.$$

$$\Rightarrow \quad \frac{1}{2}\left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right)$$

- Geometric mean

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

$$\Rightarrow \quad \sqrt{\frac{P_i\, P_j}{\rho_i^2\, \rho_j^2}}$$

SPH entropy formulation

An alternative formulation is the entropy formulation (Hernquist 1993):

$$P = A(s)\,\rho^{\gamma}$$

In adiabatic flow we have $dA/dt = 0$; the specific internal energy is inferred from

$$\varepsilon = \frac{A(s)}{\gamma - 1}\rho^{\gamma-1}$$

With artificial viscosity added, we have

$$\frac{dA_p}{dt} = \frac{1}{2}\frac{\gamma-1}{\rho_p^{\gamma-1}}\sum_q m_q \Pi_{pq}(\mathbf{v}_p - \mathbf{v}_q)\cdot\nabla_p W_{pq}$$

showing that entropy is generated *only* in shocks.

In general:

- Energy formulation does poor job of conserving entropy
- Entropy formulation does poor job of conserving energy

In continuum limit both formulations give the correct answers, but for finite numbers of particles the two approaches are not equivalent.

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

Variational derivation of SPH equations

SPH equations – conservative formulation

Springel & Hernquist (2002) find that standard formulations' treatment of entropy is poor enough that when radiative cooling is included, SPH significantly overestimates amount of cooled gas:

- Excessive broadening of shock fronts allows gas to cool more than it would otherwise (since $\Lambda(T)$ increases with decreasing T at low temperatures)
- Density estimates for hot gas in contact with cool, dense gas will be biased high, again increasing cooling rate

They propose an alternative formulation that explicitly conserves both energy and entropy (in adiabatic flow): start with Lagrangian

$$L(\boldsymbol{q},\dot{\boldsymbol{q}})=\frac{1}{2}\sum_{p=1}^{N} m_p \dot{\boldsymbol{x}}_p^2-\frac{1}{\gamma-1}\sum_{p=1}^{N} m_p A_p \rho_p^{\gamma-1}$$

The independent variables are

$$\boldsymbol{q}\equiv(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N,h_1,\ldots,h_N)$$

So thermal energy is treated as a “potential,” and smoothing length is a dynamical variable.

Variational derivation of SPH equations

Smoothing lengths h_p are chosen by requiring a fixed amount of *mass* M_{sph} (not number of neighbors) within a smoothing volume: leads to the N constraints

$$\phi_p(\boldsymbol{q}) \equiv \frac{4\pi}{3} h_p^3 \rho_p - M_{sph} = 0$$

The equations of motion are then

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_p} - \frac{\partial L}{\partial q_p} = \sum_{r=1}^{N} \lambda_r \frac{\partial \phi_r}{\partial q_p}$$

where the Lagrange multipliers are

$$\lambda_p = \frac{3}{4\pi}\frac{m_p}{h_p^3}\frac{P_p}{\rho_p^2}\left[1 + \frac{3\rho_p}{h_p}\left(\frac{\partial \rho_p}{\partial h_p}\right)^{-1}\right]^{-1}$$

Thus

$$m_p \frac{d\boldsymbol{v}_p}{dt} = -\sum_{r=1}^{N} m_r \frac{P_r}{\rho_r^2}\left[1 + \frac{h_r}{3\rho_r}\frac{\partial \rho_r}{\partial h_r}\right]^{-1} \nabla_p \rho_r$$

Variational derivation of SPH equations

The density gradient can be written

$$\nabla_p \rho_r = m_p \nabla_p W_{pr}(h_r) + \delta_{pr} \sum_{s=1}^{N} m_s \nabla_p W_{sp}(h_p)$$

so the velocity update equation finally becomes

$$\frac{d\boldsymbol{v}_p}{dt} = -\sum_{r=1}^{N} m_r \left[f_p \frac{P_p}{\rho_p^2} \nabla_p W_{pr}(h_p) + f_r \frac{P_r}{\rho_r^2} \nabla_p W_{pr}(h_r) \right]$$

$$f_p \equiv \left[1 + \frac{h_p}{3\rho_p} \frac{\partial \rho_p}{\partial h_p} \right]^{-1}$$

Together with the entropy formulation, this velocity update method gives automatic conservation of linear and angular momentum, energy, and entropy.

Artificial viscosity in the standard form is subtracted from the velocity update and added to the entropy update to allow for shocks.

SPH PERFORMACE: Sedov Solution

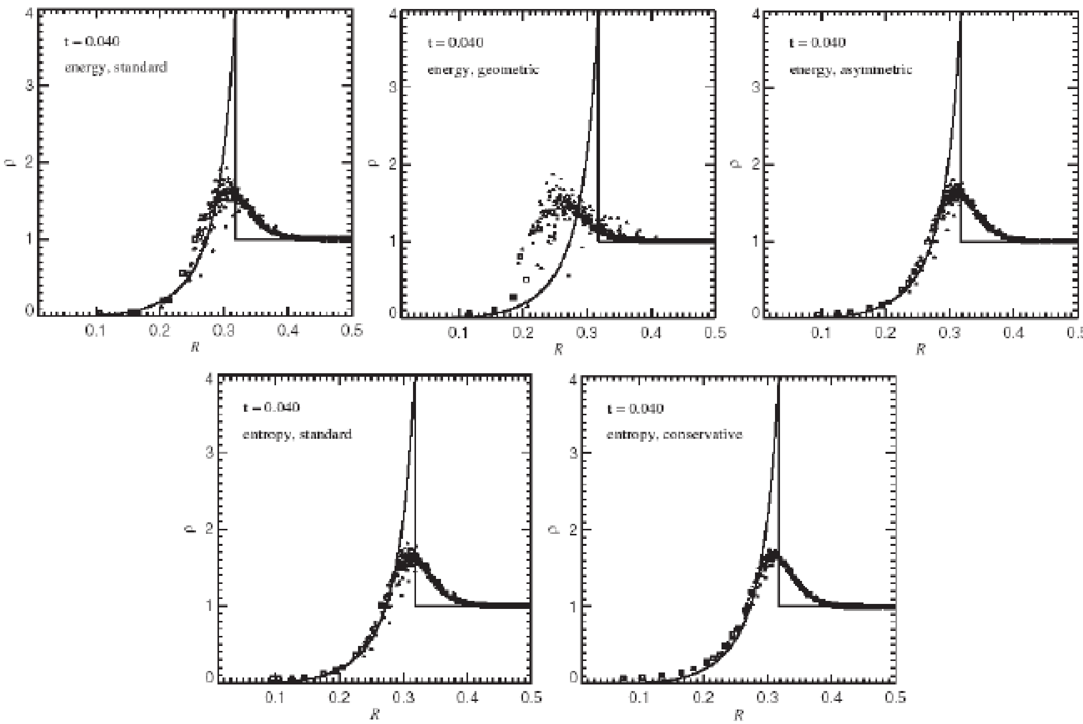


Figure 3. Radial density distribution at a time $t = 0.04$ after the triggering of an explosion in a 32^3 particle distribution, with the initial explosion energy smoothed by the SPH kernel. Results for different formulations of SPH are shown. Top: Integration of the thermal energy, from left to right: in its standard form, with geometric mean symmetrization, and with the asymmetric form of the energy equation. Bottom: Integration of the entropy equation in the standard form (left) and with the new conservative formulation (right). Small points indicate distances and densities measured from individual particles, while boxes denote spherically averaged values. Solid lines show the analytical Sedov solution (adiabatic index $\gamma = 5/3$).

Springel & Hernquist (2002)

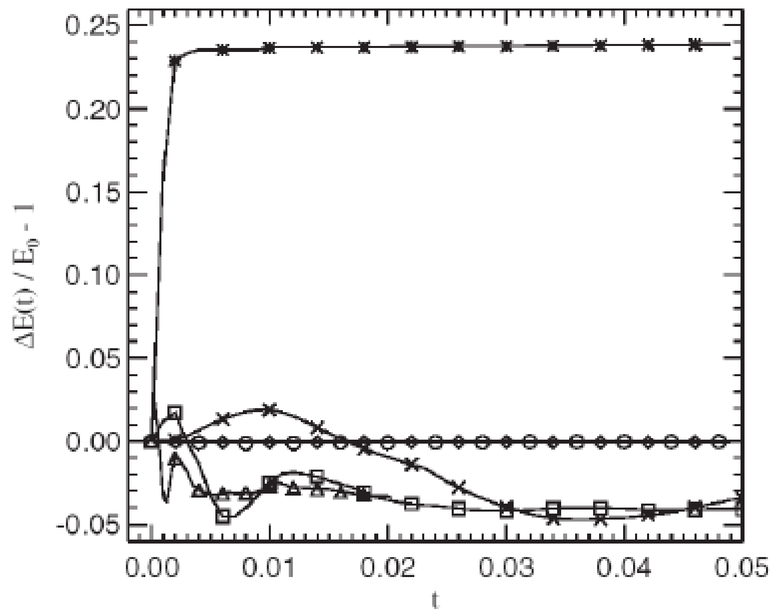
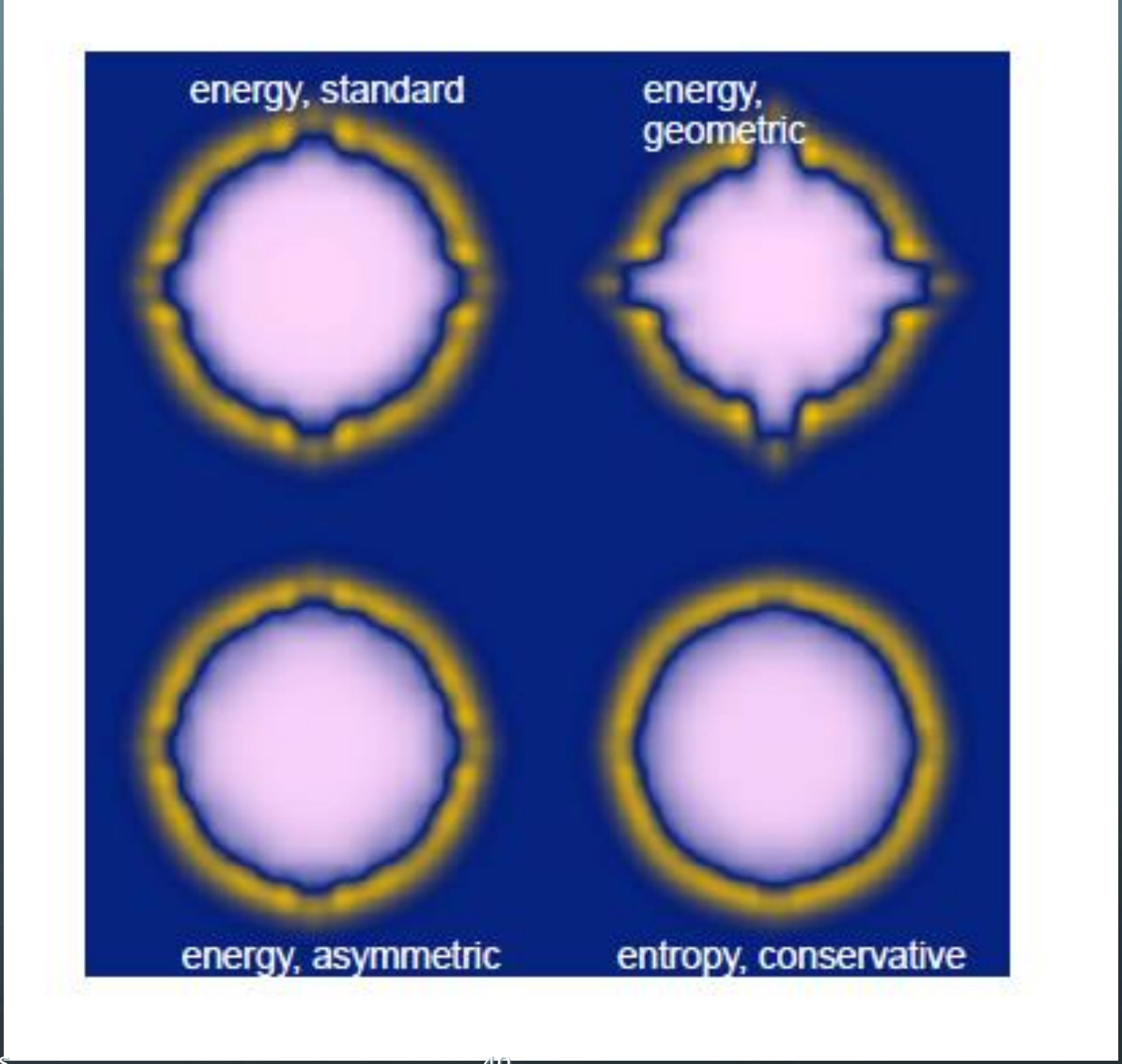


Figure 1. Deviation of the total energy from the initial explosion energy as a function of time for a number of different simulations. The large positive deviation that reaches a maximum error of ~24 per cent is for a 32^3 run where the initial energy is added to a single particle and the thermal energy equation is integrated in the standard form. In this case, energy conservation is violated, because the code prevents the occurrence of unphysical negative temperatures in the early phase of the evolution. When the initial energy is deposited smoothly instead, this is prevented, and energy is well conserved (diamonds). Crosses, boxes, and triangles indicate results for 16^3, 32^3 and 64^3 single point explosions where the code instead integrates the entropy equation and the equations of motion in a standard form. Initially, a fluctuation with a characteristic pattern is observed. The maximum error is about ~4 per cent, but at later times, energy conservation is reasonable. However, when our new conservative entropy formulation is employed, energy is again well conserved (circles).

Springel & Hernquist (2002)

EXPLOSION 3D



ADIABATIC COLLAPSE

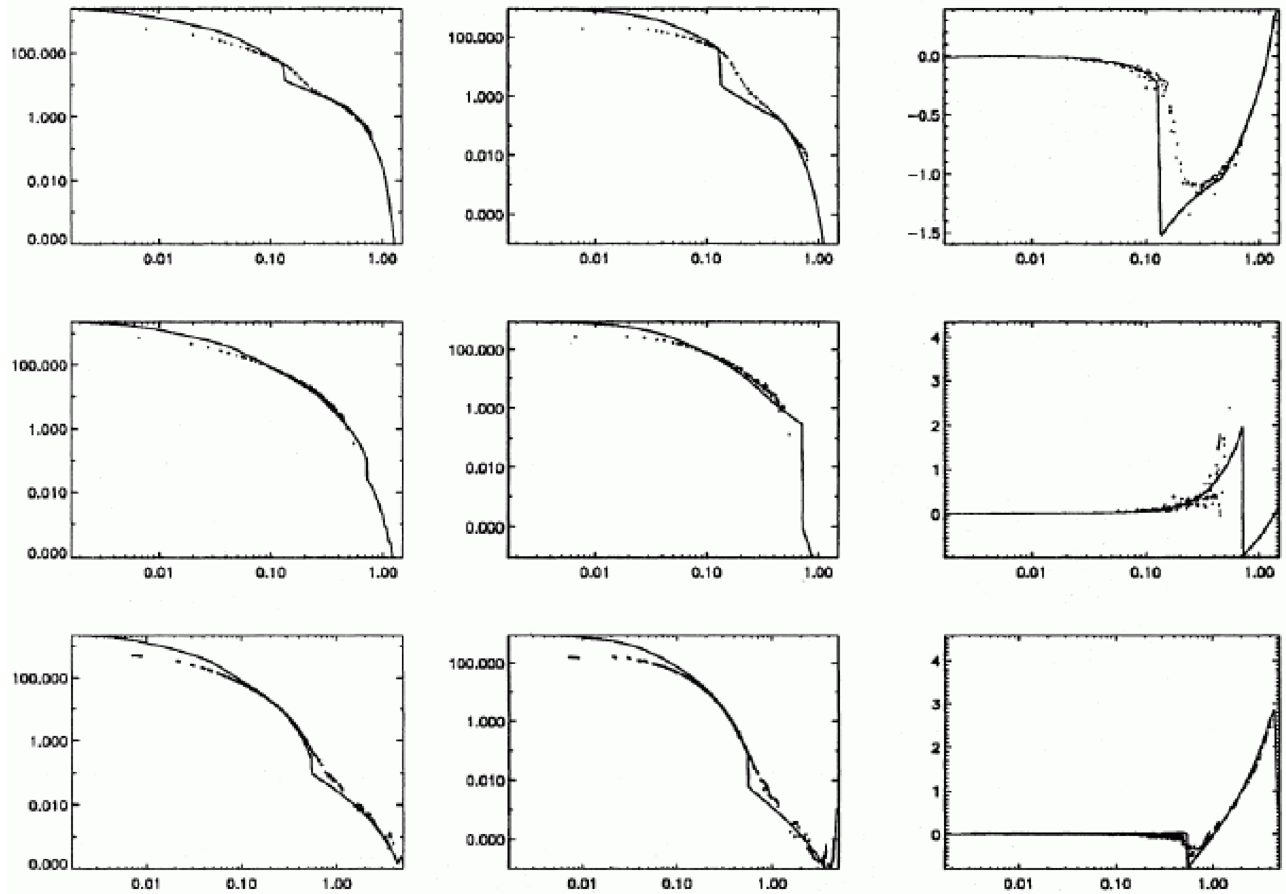


Fig. 7. Snapshots of density (left), pressure (middle), and velocity (right) for an adiabatic spherical collapse of an initially isothermal gas cloud obtained with a SPH calculation with $N = 4224$ particles (dots), and with a PPM calculation with 350 zones (solid lines). The snapshots are taken at t=0.77, t=1.29, and t=2.58, respectively. Dimensionless units are used.

ADIABATIC COLLAPSE

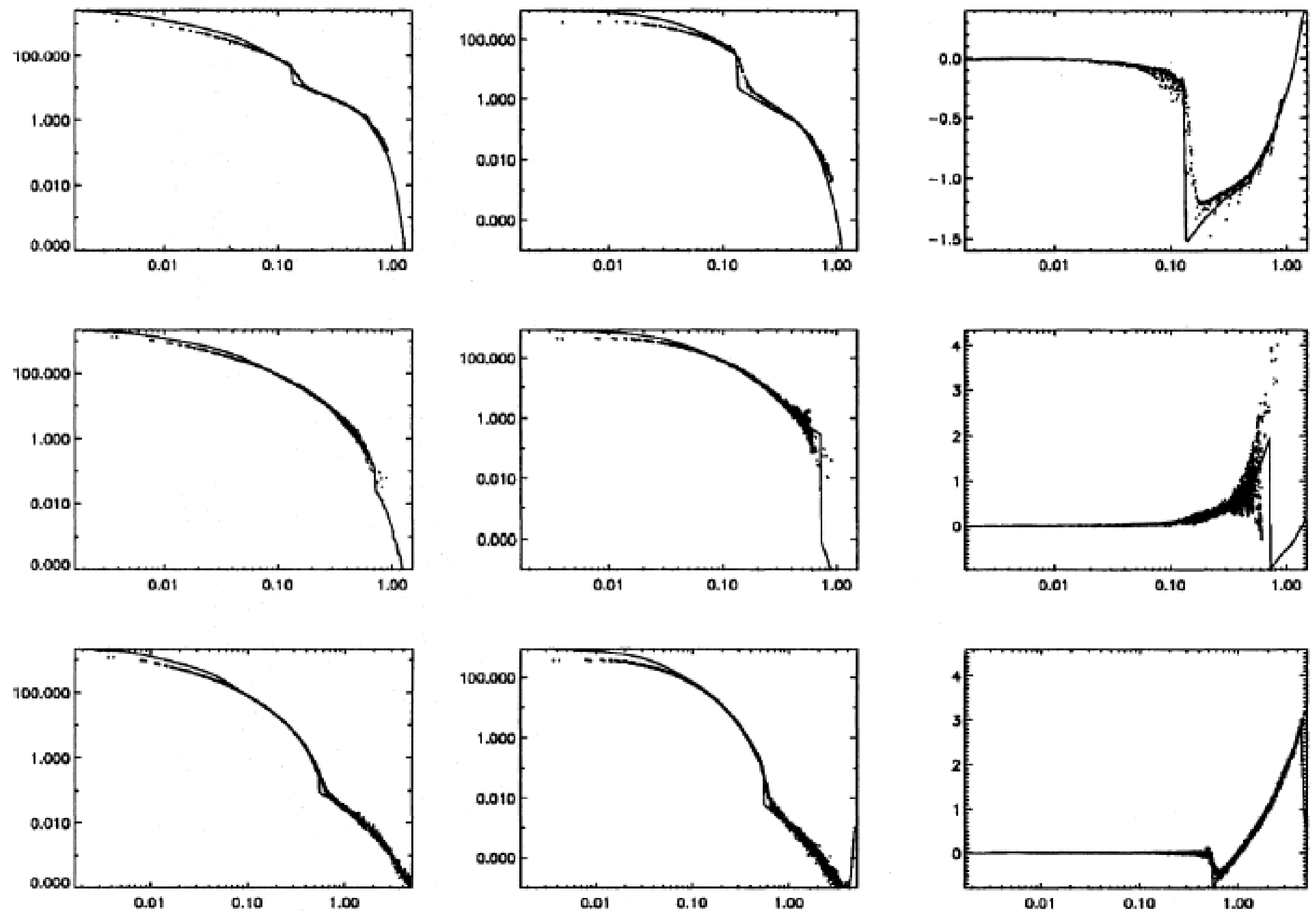


Fig. 8. Same as Fig. 7 but for the SPH run with N=28768 particles.

Steinmetz & Müller (1993) concluded:

1. SPH can get accurate results for problems including strong shocks.
2. In 3D SPH requires at least ~ several x 10^4 particles to get reasonable results on shock problems (comparable to finite-difference methods).
3. Using tree data structures for gravity solver and for finding nearest neighbors makes SPH much more complicated than original SPH method, and of comparable complexity to Godunov-based Eulerian schemes, but not as complex as AMR.
4. From shot noise arguments we might expect resolution of SPH to be no better than $N^{1/2}$ per dimension. But results in 3D are better than one would expect from this argument.

SPH AND SELF-GRAVITY

- In a self-gravitating SPH gas there is a minimum mass resolution (minimum number of particles) needed to resolve the Jeans Mass for a gas of constant density and T.

$$M_J = \left(\frac{5R_g T}{2G\mu}\right)^{3/2} \left(\frac{4\pi\rho}{3}\right)^{-1/2}$$

$$R_g = k_B/m_u$$

- In SPH the minimum resolved gas mass MUST be small than M_J at all times and locatons. This can be formulated in terms of the Jeans length:
  - R_J>(1.5-2)h
  - M_{min} (h)

$$R_J \approx \left(\frac{3M_J}{4\pi\rho}\right)^{1/3} = \left(\frac{5R_g T}{2\mu}\right)^{1/2} \left(\frac{3}{4\pi G\rho}\right)^{1/2}$$

$$M_{\mathrm{min}} \approx (1.5-2)mN_{\mathrm{target}} \approx (75-100)m,$$

SPH AND SELF-GRAVITY

- It is also assumed that gravitational smoothing ε is similar to the SPH smoothing scale, h.
- If $\varepsilon < h$ then if $M_{lim} < M_J$ artificial fragmentation of gas cloud can be produced because pressure forces are poorly resolved
- If $\varepsilon > h$ and $M_{lim} < M_J$, gravitational fragmentation can be avoided even if the gas cloud is gravitationally unstable (M>MJ)
- For regions that are marginally unstable (M~MJ) and $\varepsilon \sim h$ but Mlim <MJ , the gas will collapse but the collapse will be slower as the graviy and P forces are poorly resolved on the small scales..
- CONCLUSION: Use as many particles as possible to minimize these resolution effects.

time stepping

- Time integration of the equations of motion by Leap frog scheme.

$$
\begin{cases}
t = t + \Delta t \\
\rho_i(t + \Delta t/2) = \rho_i(t - \Delta t/2) + \Delta t \cdot D\rho_i(t) \\
e_i(t + \Delta t/2) = e_i(t - \Delta t/2) + \Delta t \cdot De_i(t) \\
v_i(t + \Delta t/2) = v_i(t - \Delta t/2) + \Delta t \cdot Dv_i(t) \\
x_i(t + \Delta t) = x_i(t) + \Delta t \cdot v_i(t + \Delta t/2)
\end{cases}
$$

- Δt is restricted by the CFL stability conditions due to the characteristic adiabatic sound velocity $c_s = \delta p/\delta\rho$
  - Min (Δt_i = CFL h_i/c_s). CFL = 0.1-0.3
  - or a more detailed estimate taking into account the artificial viscosity (Monaghan 92)

Adaptive kernels

Adaptive SPH (Shapiro et al. 1996; Owen et al. 1998)

Uses an anisotropic smoothing kernel to capture quasi-1D flows (such as cosmological pancakes)

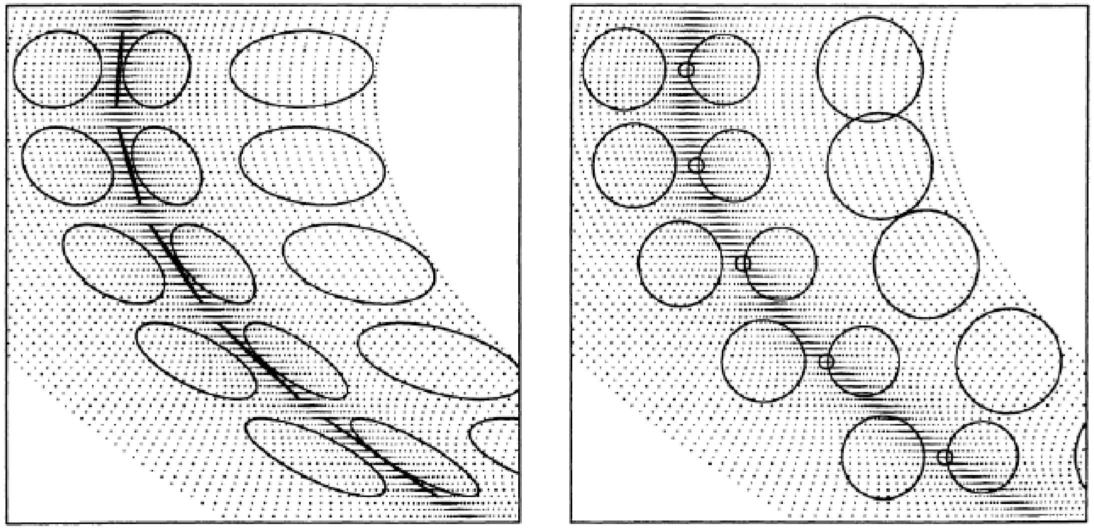


FIG. 8.—Two-dimensional kinematical test: warped planar collapse with vorticity, for time slice $a = 0.975a_c$. Limits of displayed area are $-0.5 \le x \le 0.5$, $-0.5 \le y \le 0.5$. Points are Lagrangian fluid elements (i.e., like SPH particles). Smoothing kernels for ASPH (*left*) and SPH (*right*) for the same selected set of particles are shown (i.e., ASPH **H** ellipsoids and SPH h circles, with **H** and h scaled by a factor 3; these are the "zones of influence" which contain the nearest neighbors).

Smoothing length scalar h becomes a smoothing tensor ***H*** – local velocity field determines orientation of principal axes and smoothing lengths along them

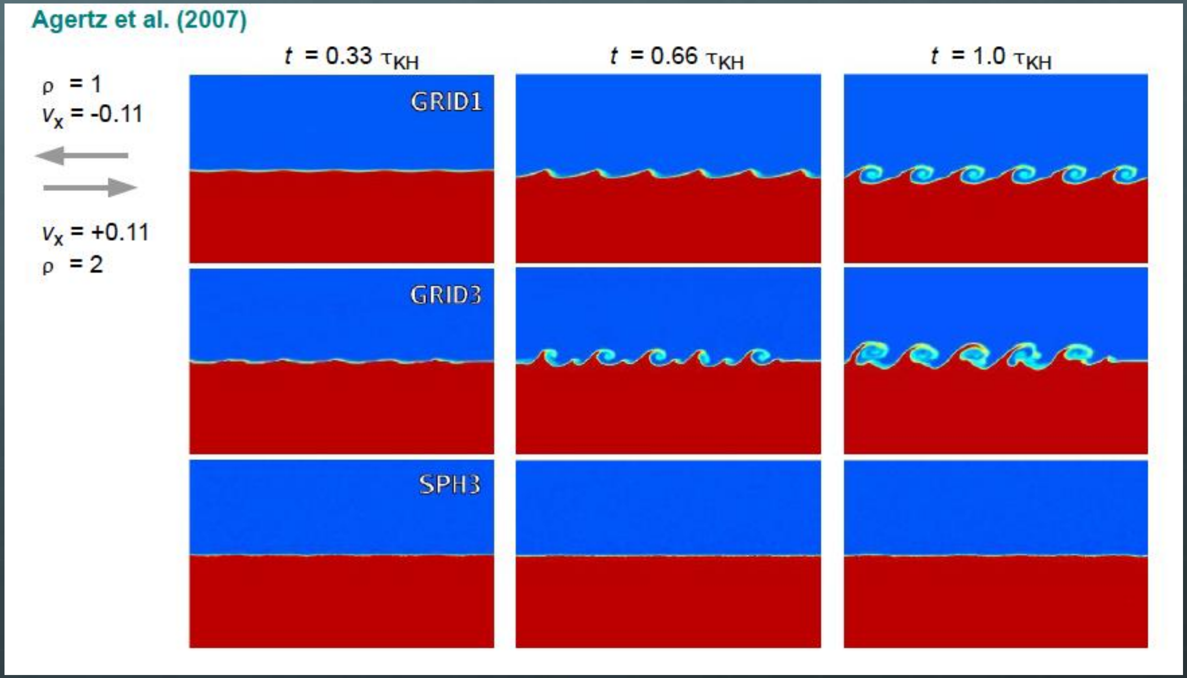
Works best in irrotational flow ($\nabla \times \mathbf{v} = 0$)

PROS AND CONS OF SPH

- ADVANTAGES OF SPH METHOD:
  - MASS, TOTAL AND ANGULAR MOMENTUM AND TOTAL ENERGY CONSERVED EVEN IN THE PRESENCE OF SELF-GRAVITY.
  - TOTAL ENERGY IS REASONABLY CONSERVED
  - ENTROPY IS CONSERVED AND IS ONLY PRODUCED BY ARTIFICIAL VISCOSITY.
  - HIGH FLEXIBILITY TO PROBLEMS WITH COMPLEX GEOMETRY
  - EASY TO INCORPORATE VACUUM BOUNDARY CONDITIONS
  - GOOD TREATMENT OF PROBLEMS WITH HIGH MACH NUMBERS.
  - CONSERVE GALILEAN INVARIANCE.

PROS AND CONS OF SPH

- PROBLEMS OF SPH METHOD:
  - FLUID INSTABILITIES AND DISCONTINUITIES WITH LARGE DENSITY JUMPS TEND TO BE SUPPRESSED DUE TO NUMERICAL SURFACE TENSION EFFECTS:



GAS MIXING PROBLEM

Fundamental differences between SPH and grid methods

Oscar Agertz,[1★] Ben Moore,[1] Joachim Stadel,[1] Doug Potter,[1] Francesco Miniati,[2] Justin Read,[1] Lucio Mayer,[2] Artur Gawryszczak,[3] Andrey Kravtsov,[4] Åke Nordlund,[5] Frazer Pearce,[6] Vicent Quilis,[7] Douglas Rudd,[4] Volker Springel,[8] James Stone,[9] Elizabeth Tasker,[10] Romain Teyssier,[11] James Wadsley[12] and Rolf Walder[13]

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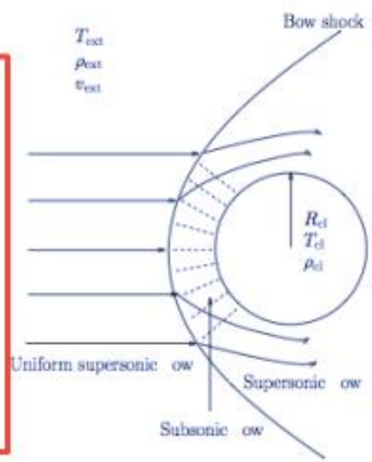
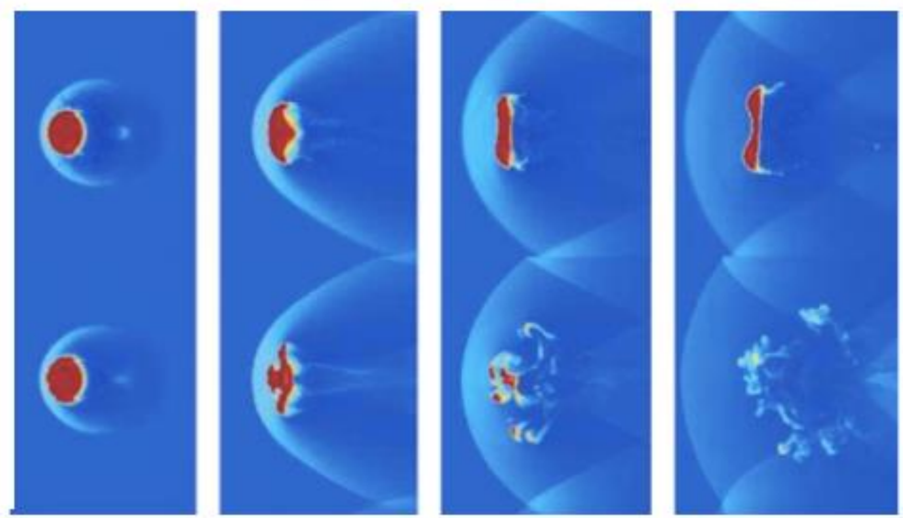
Infalling cloud of gas onto hot halo; ablates with grid codes, but survives with SPH codes.

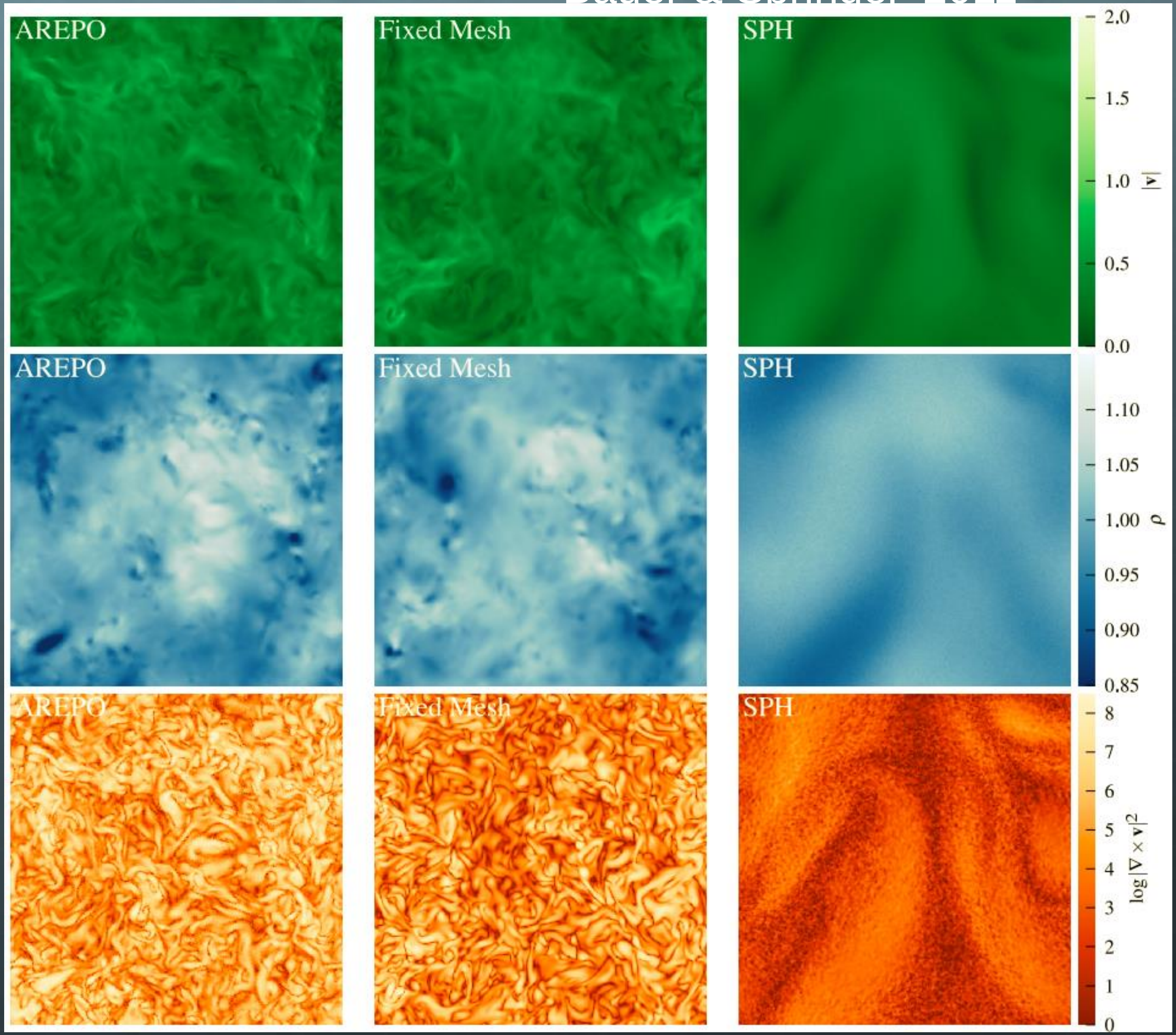




Subsonic turbulence

Bauer & Springel 2011

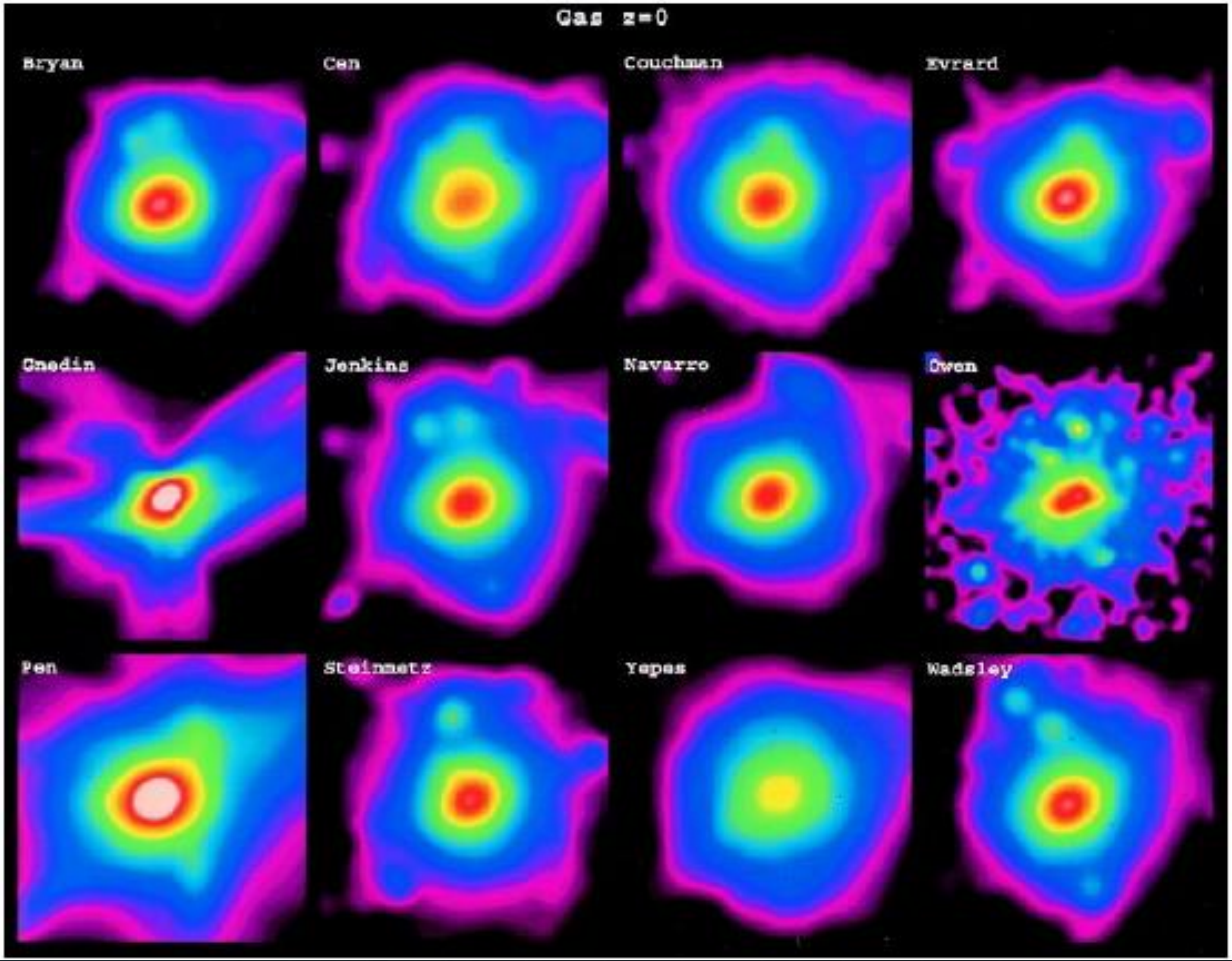
SPH does not resolve the small scale motions in the gas in subsonic regime



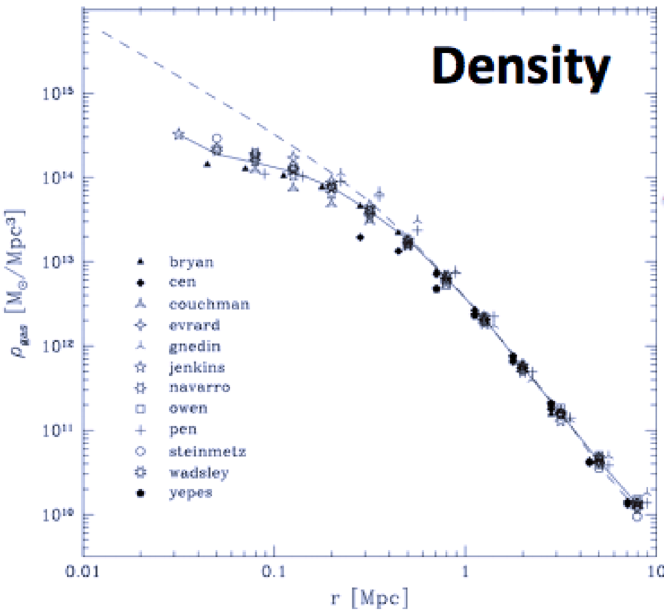
Different hydrodynamical simulation codes are broadly in agreement, albeit with substantial scatter and differences in detail

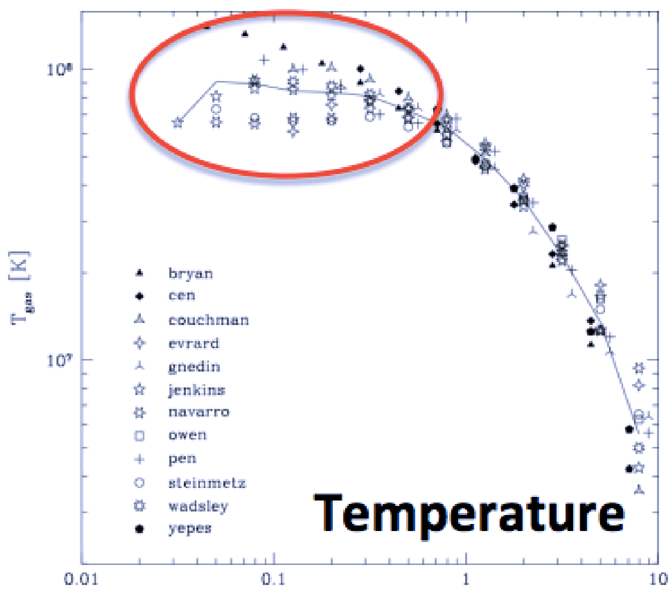
THE SANTA BARBARA CLUSTER COMPARISON PROJECT

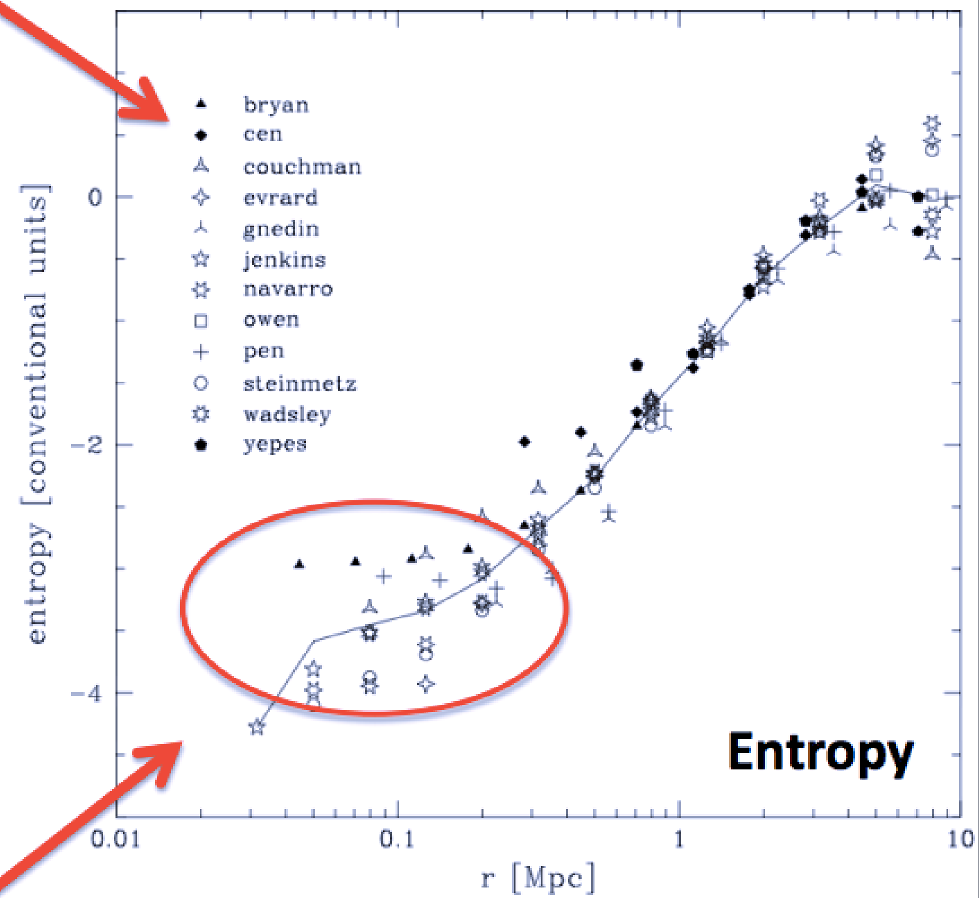
Frenk, White & 23 co-authors (1999)



Differences evident between grid codes and SPH codes – encapsulated neatly in entropy profile.







$$S(R) = \log\left[T_{\rm gas}(R)/\rho_{\rm gas}(R)^{2/3}\right]$$

MODERN SPH METODS

- Modificantions to the standard SPH implentation have been proposed to try to solve the problems of SPH with mixing and contact discontinuities
- Two approaches:
  - Artificial heating terms (Price08, Wadsley+08,Beck15)
  - New kernel functions optimized to avoid contact discontinuities (Read+09)

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.

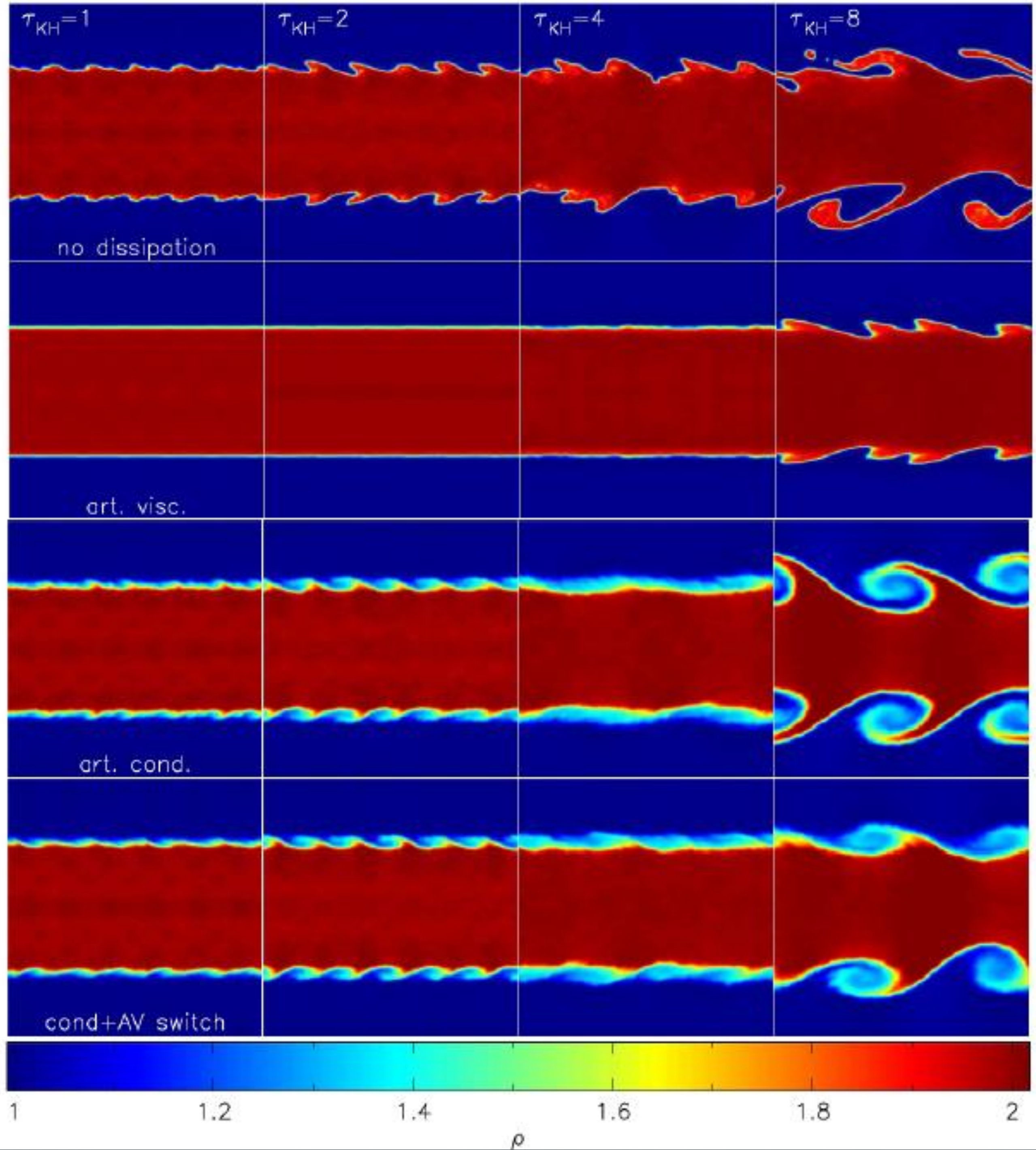
This is the discretized form of a diffusion problem:

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

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

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

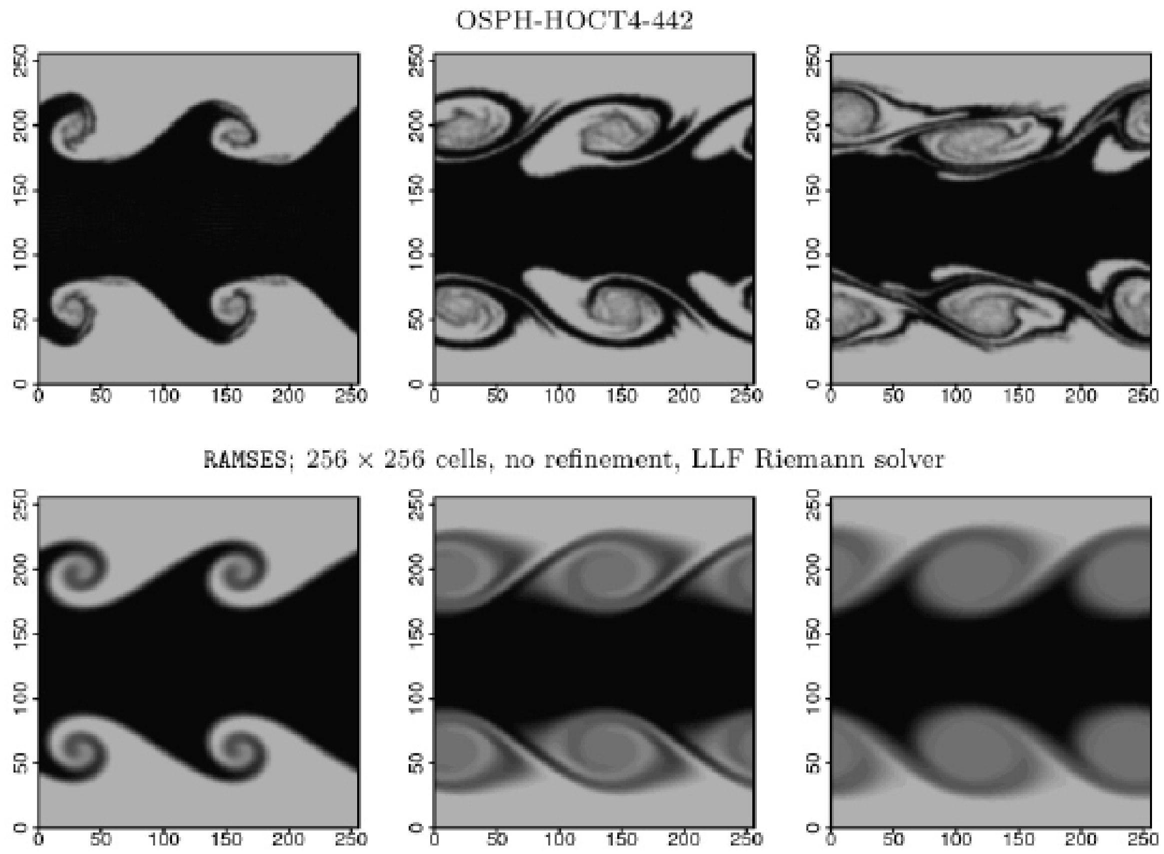
AN ALTERNATIVE SPH FORMULATION

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

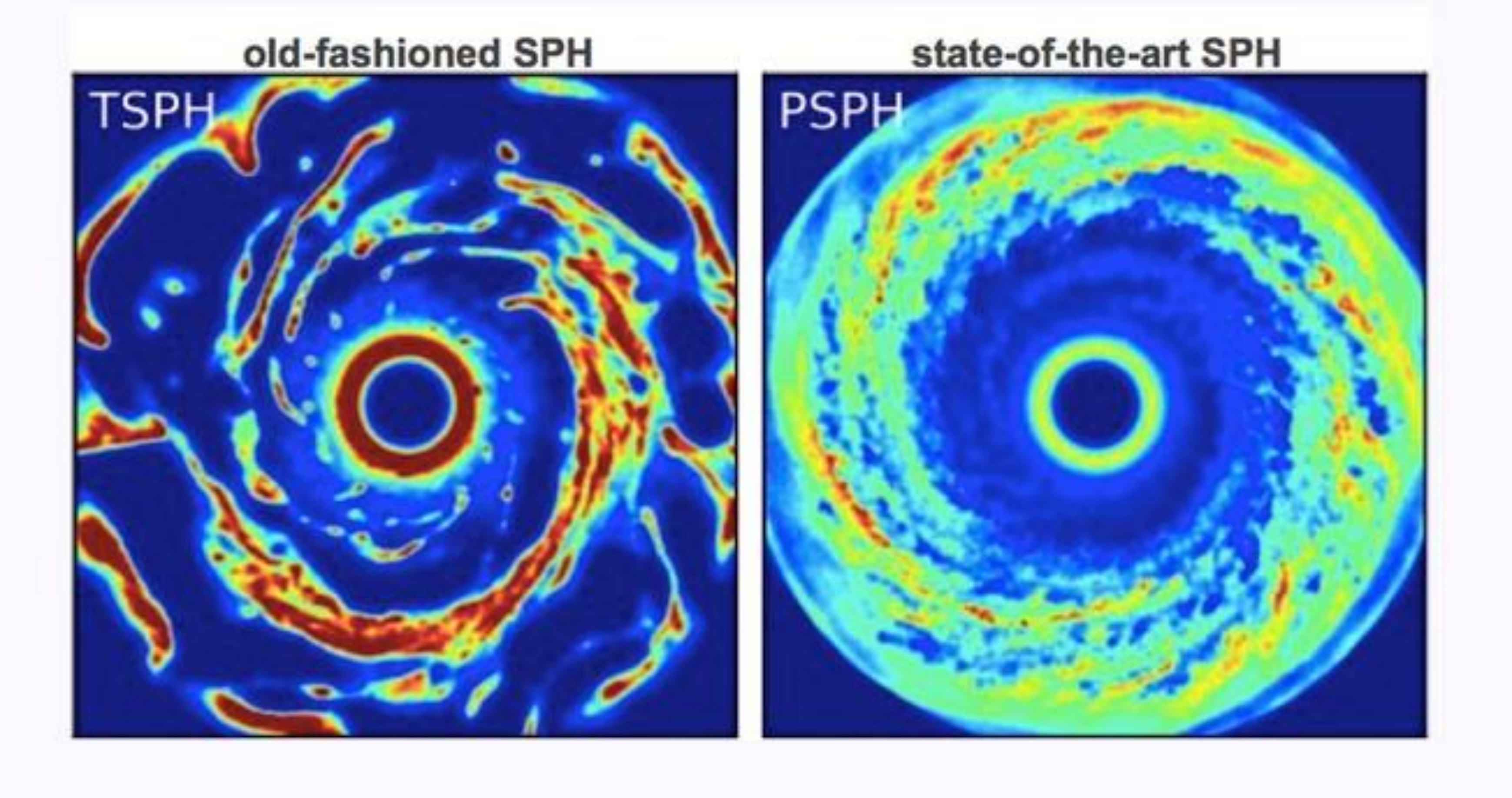
- Density estimate like Ritchie & Thomas (2001):

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

- 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.



Tensile instability



Santa Barbara Cluster Comparison Project
15 years later

nIFTy Cosmology: NUMERICAL SIMULATIONS FOR LARGE SURVEYS

SOC:
Alexander Knebe (UAM)
Frazer Pearce (Nottingham)
Juan Garcia-Bellido (UAM/IFT-CSIC)
Chris Power (Western Australia)
Richard Bower (Durham)

Arthur et al, 2017, MNRAS, 464, 2627
Sembolini et al, 2016, MNRAS, 459, 2973
Cui et al, 2016, MNRAS, 458, 4052
Elahi et al., 2016, MNRAS, 458, 1096
Sembolini et al., 2016, MNRAS, 457, 4063

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EXCELENCIA SEVERO OCHOA

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THE UNIVERSITY OF WESTERN AUSTRALIA
CAASTRO

nIFTy galaxy cluster simulations I: dark matter & non-radiative models

2016, MNRAS, 457, 4063

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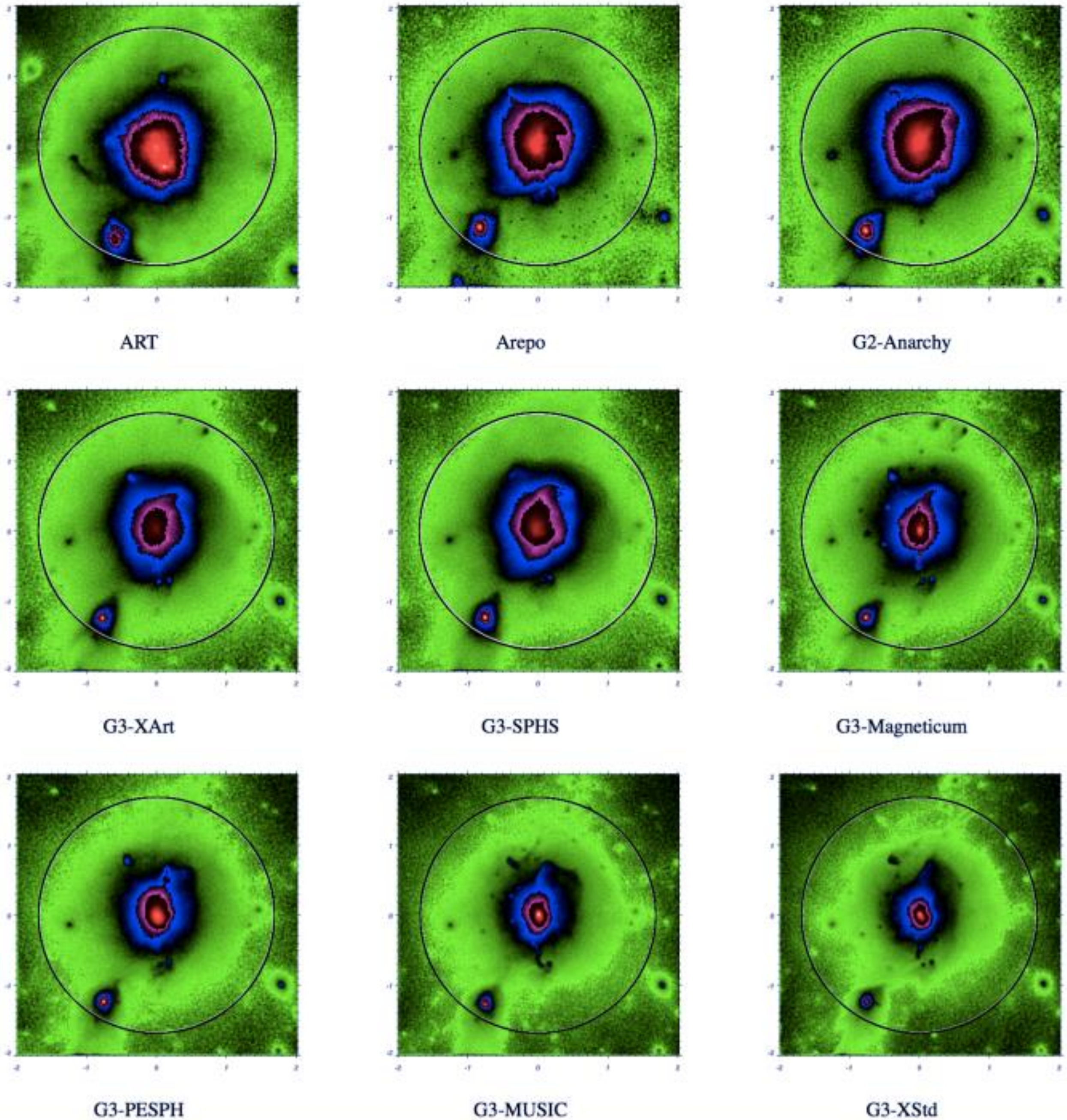
Claudio Dalla Vecchia,[12,13] Romeel Davé,[14,15,16] Pascal Jahan Elahi,[17] Sean February,[18]
Shuiyao Huang[27] Alex Hobbs,[19] Neal Katz[19] Erwin Lau,[20,21] Ian G. McCarthy,[22]
Guiseppe Murante,[9] Daisuke Nagai,[20,21,23] Kaylea Nelson,[21,23] Richard D. A. Newton,[5,6]
Ewald Puchwein,[24] Justin I. Read,[25] Alexandro Saro,[14] Joop Schaye, [27] Robert J. Thacker[28]

Table 1. List of all the simulation codes participating in the nIFTy cluster comparison project.

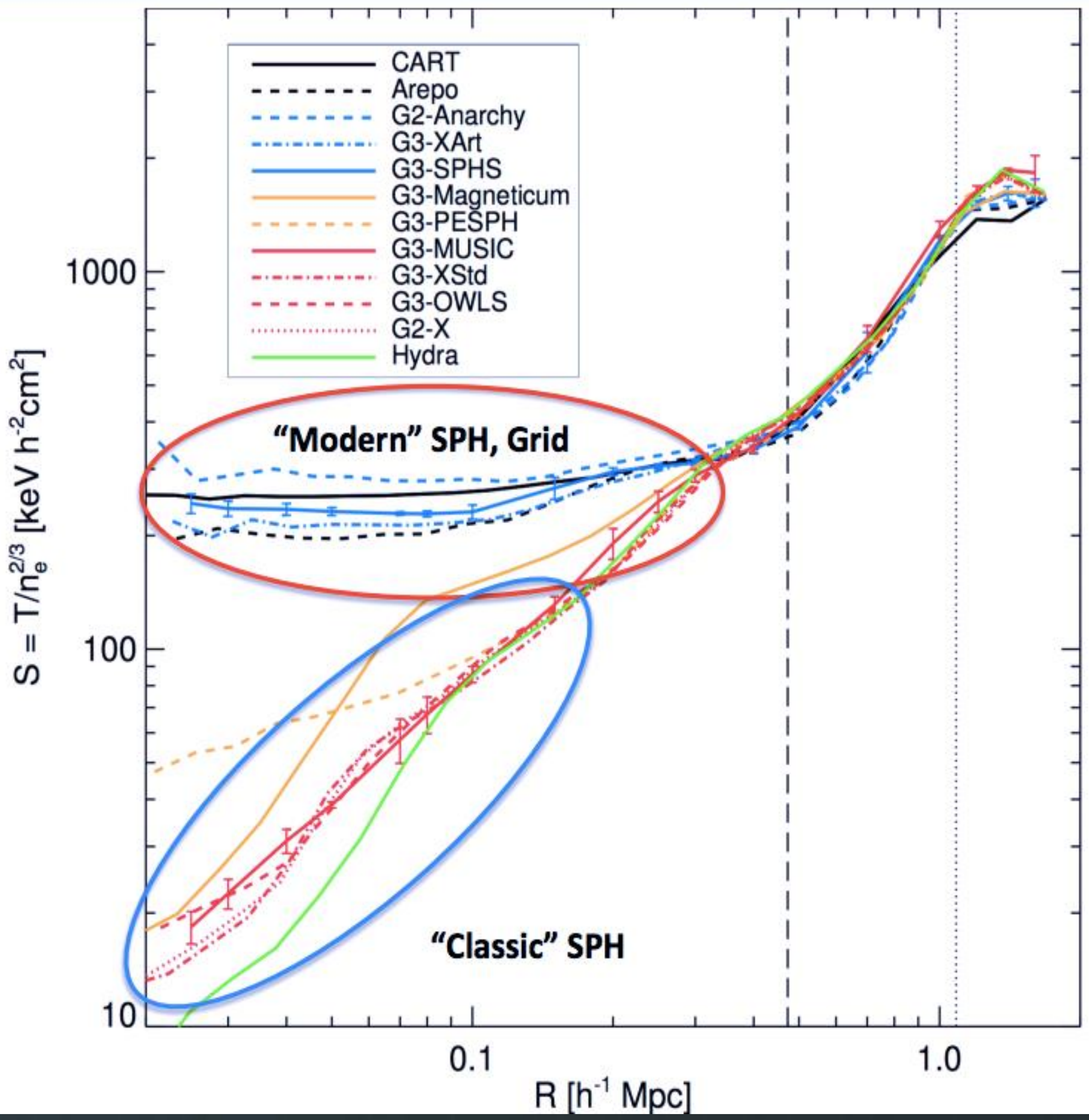
Code name	Reference
CART	Rudd, Zentner & Kravtsov (2008)
AREPO	Springel (2010)
HYDRA	Couchman, Thomas & Pearce (1995)
GADGET:	Springel (2005)
G2-Anarchy	Dalla Vecchia et al. in prep.
G3-X	Beck et al. (2015)
G3-SPHS	Read & Hayfield (2012a)
G3-Magneticum	Hirschmann et al. (2014)
G3-PESPH	Huang et al. in prep.
G3-MUSIC	Sembolini et al. (2013)
G3-OWLS	Schaye et al. (2010)
G2-X	Pike et al. (2014)

"Classic" SPH
vs
"Modern" SPH
vs
Grid

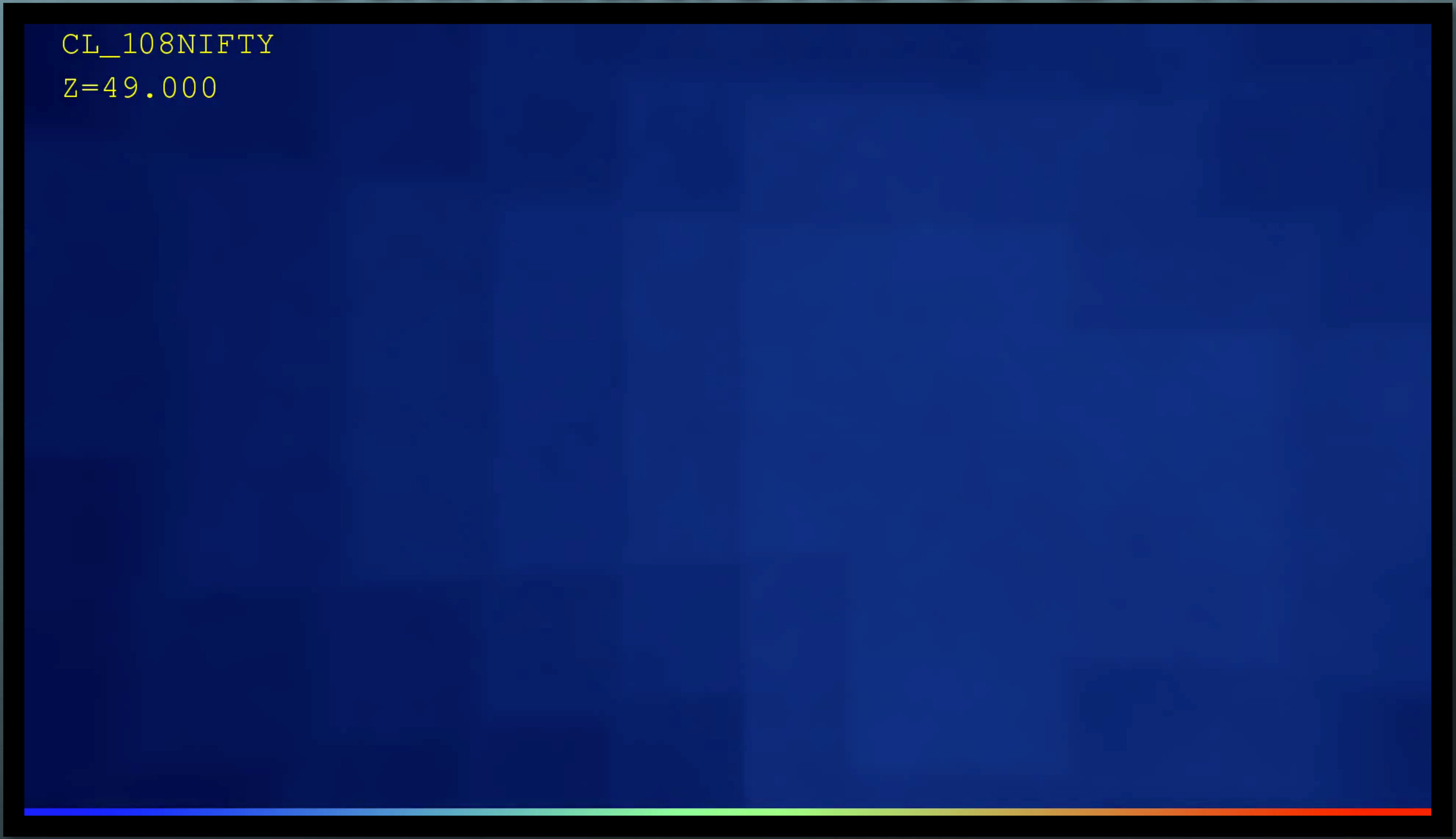
Non-Radiative



Radial Entropy Profile

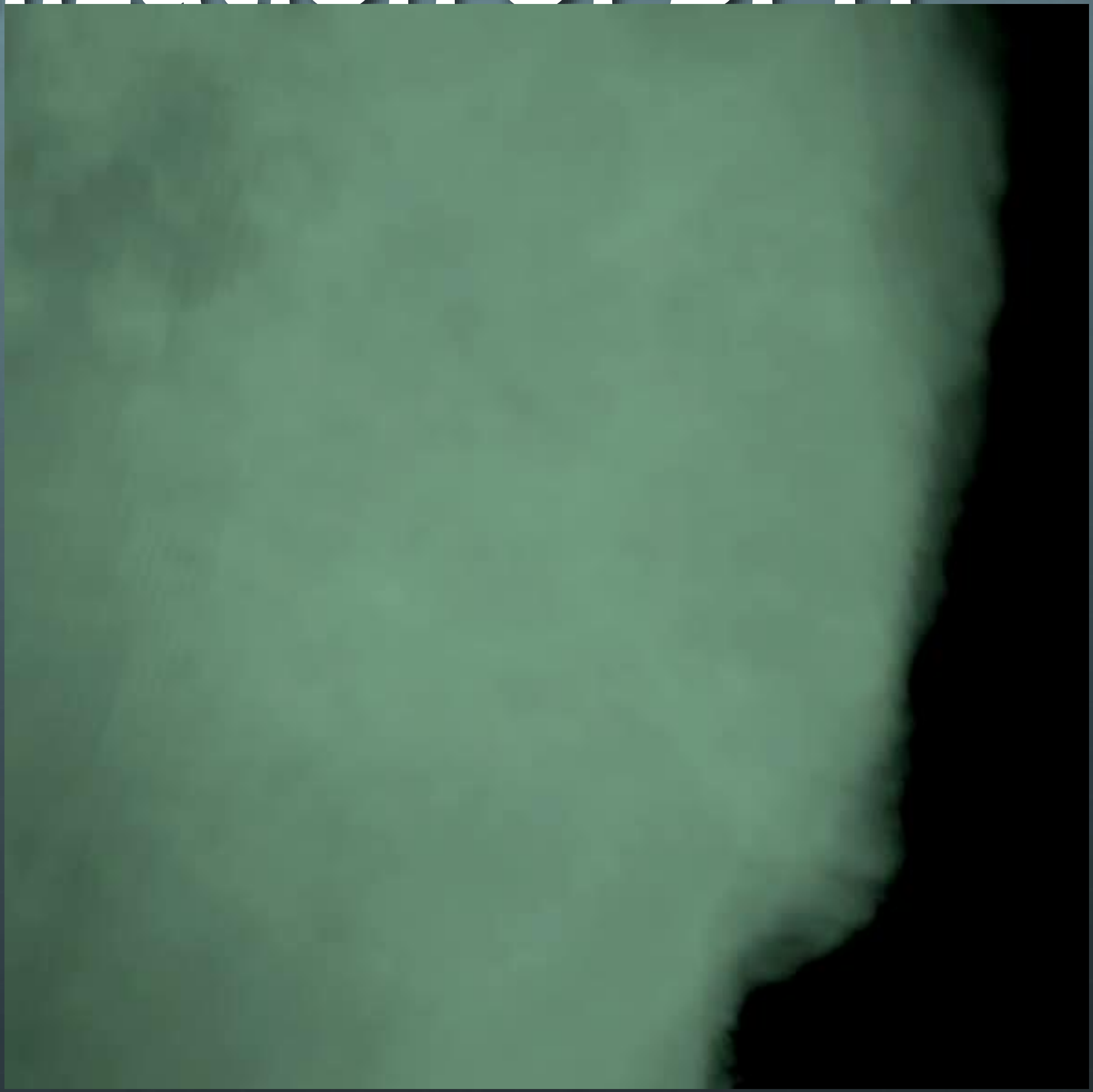


Visualizations of SPH



Visualization of SPH

GASOLINE (standard SPH+TREE)
Cosmological simulation of the Formation of disk galaxy



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