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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

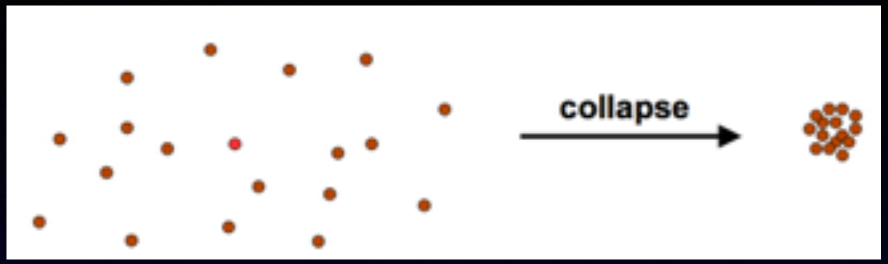
"Horses for courses"

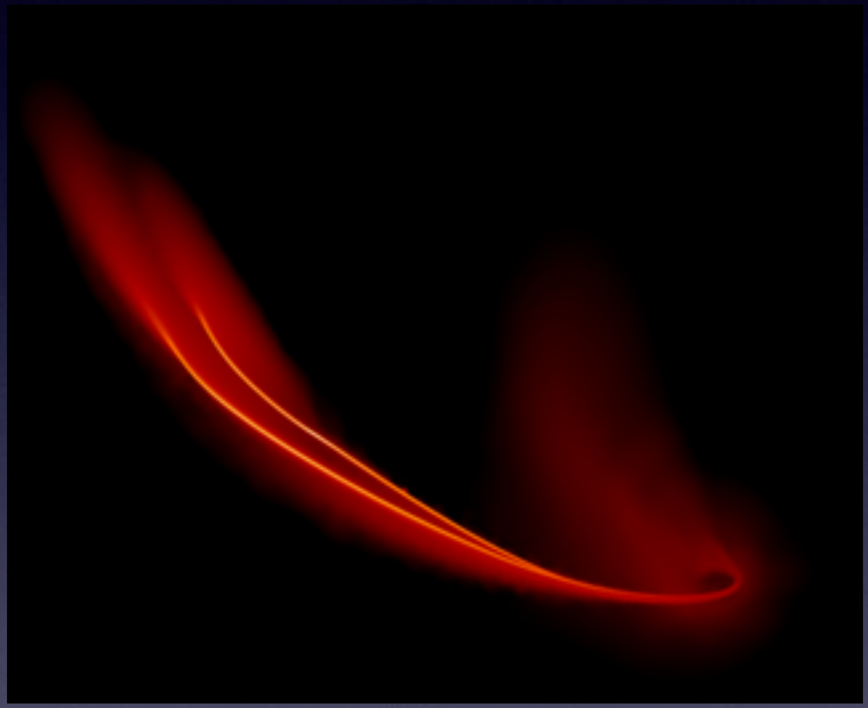
⇒ it IS important to choose the right method for the problem at hand

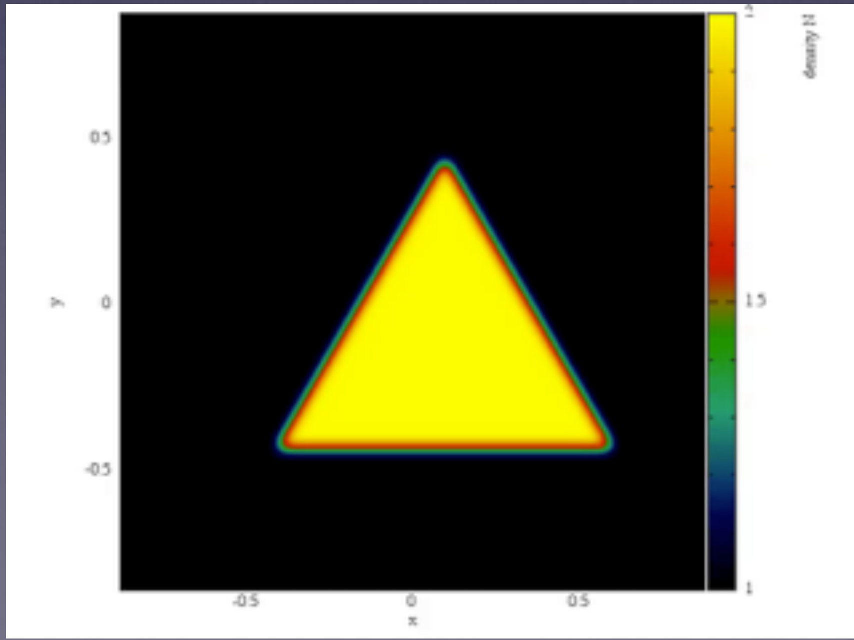
When /why use Lagrangian hydrodynamics?

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

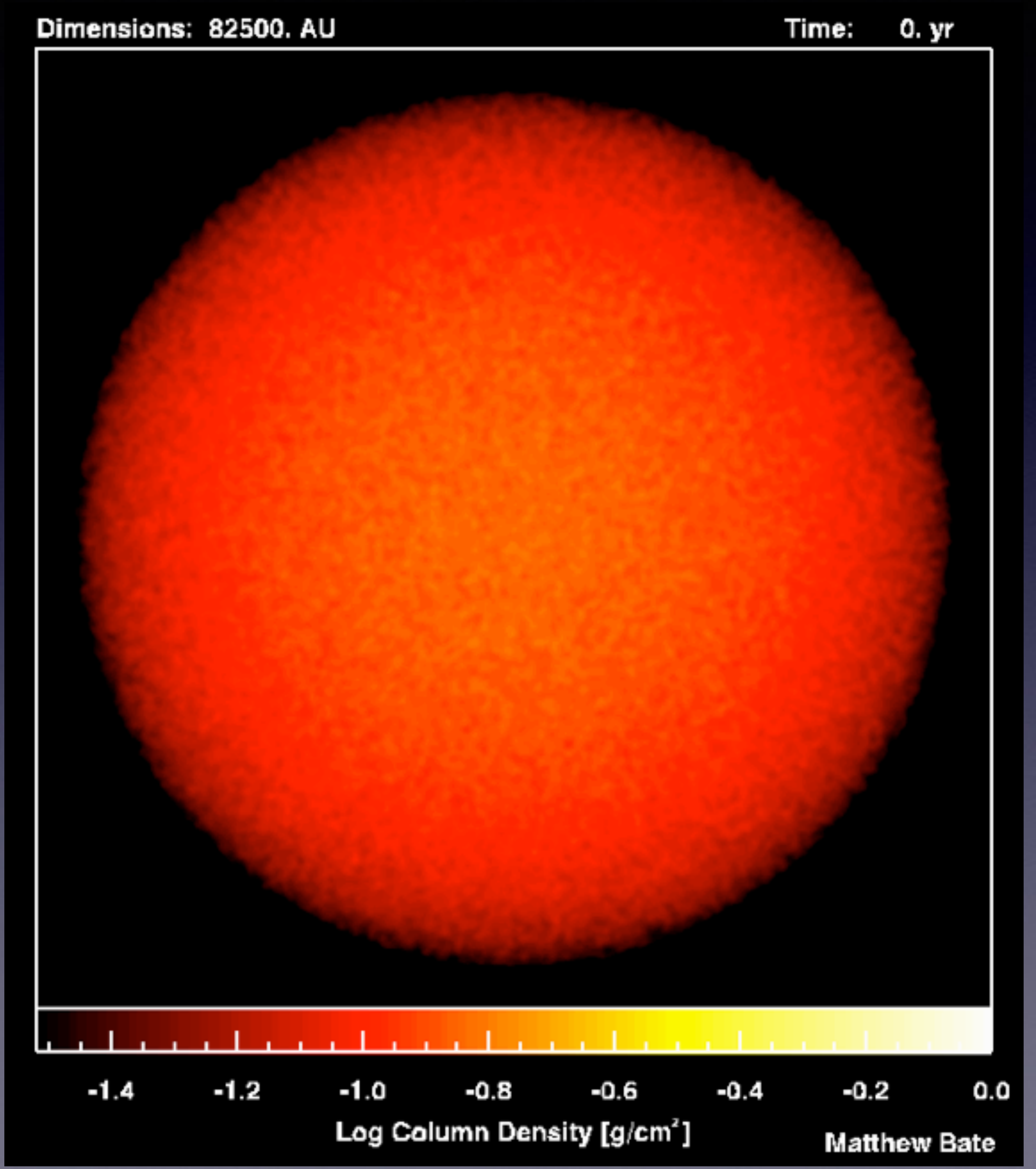






Some examples

- dynamical star formation calculation



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

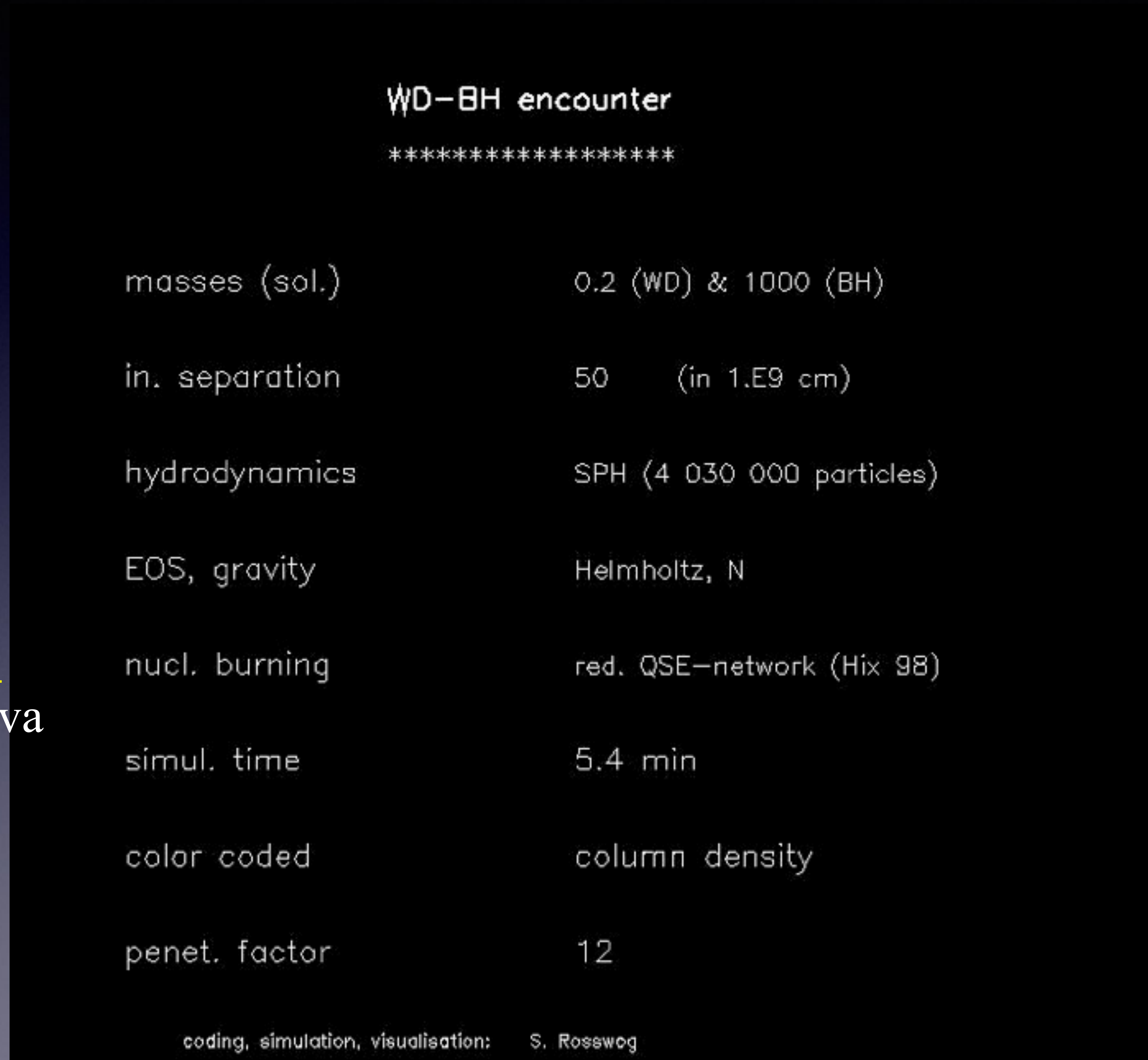
(Simulation Matthew Bate)

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

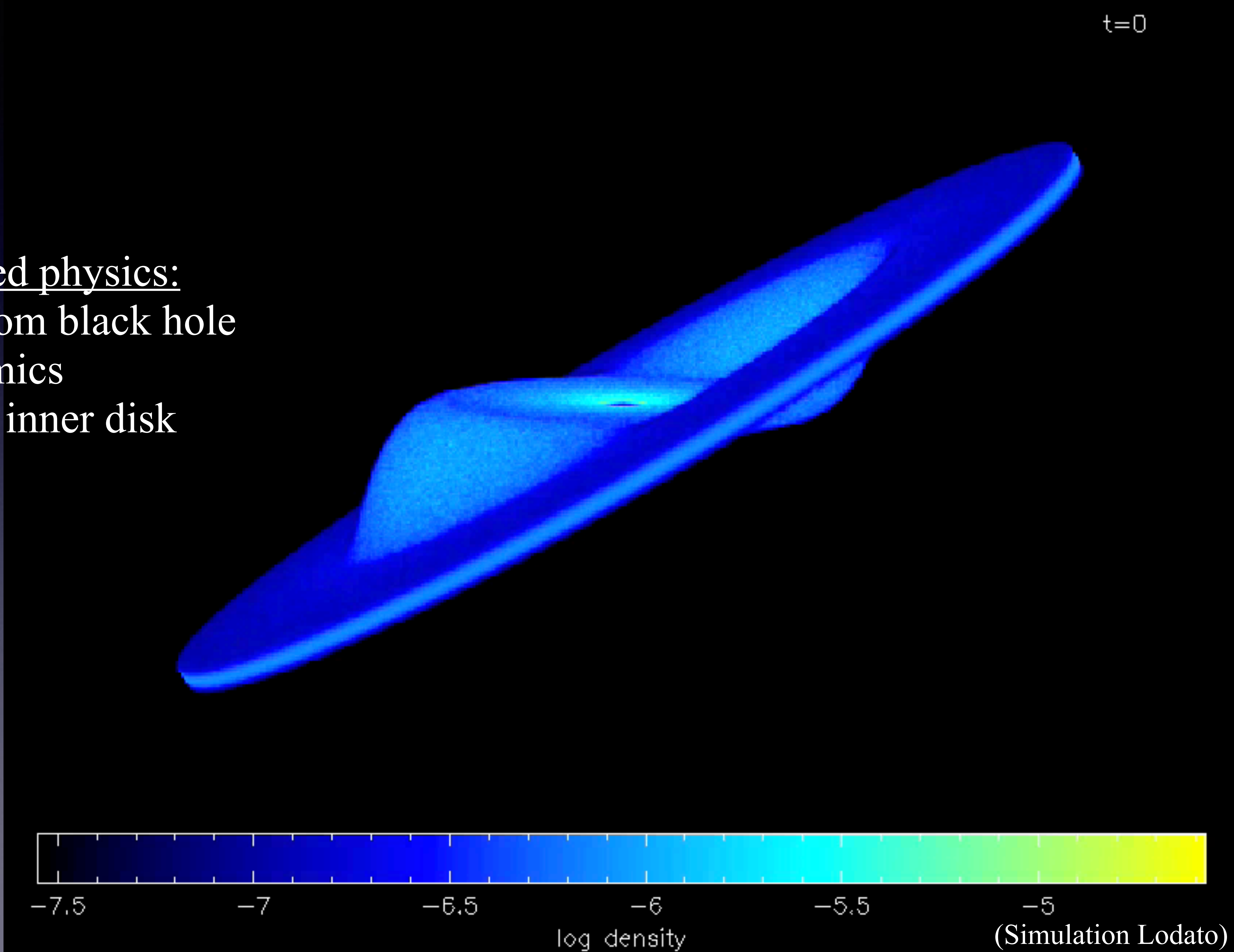
<u>modeled physics:</u>
- self-gravity
- gravity black hole via pseudo-potential
- gas dynamics
- nuclear burning

<u>Astrophysical signatures:</u>
- thermonuclear Supernova
- X-ray flare

(Simulation S.R.)



- Disk “warped” by a rotating central black hole

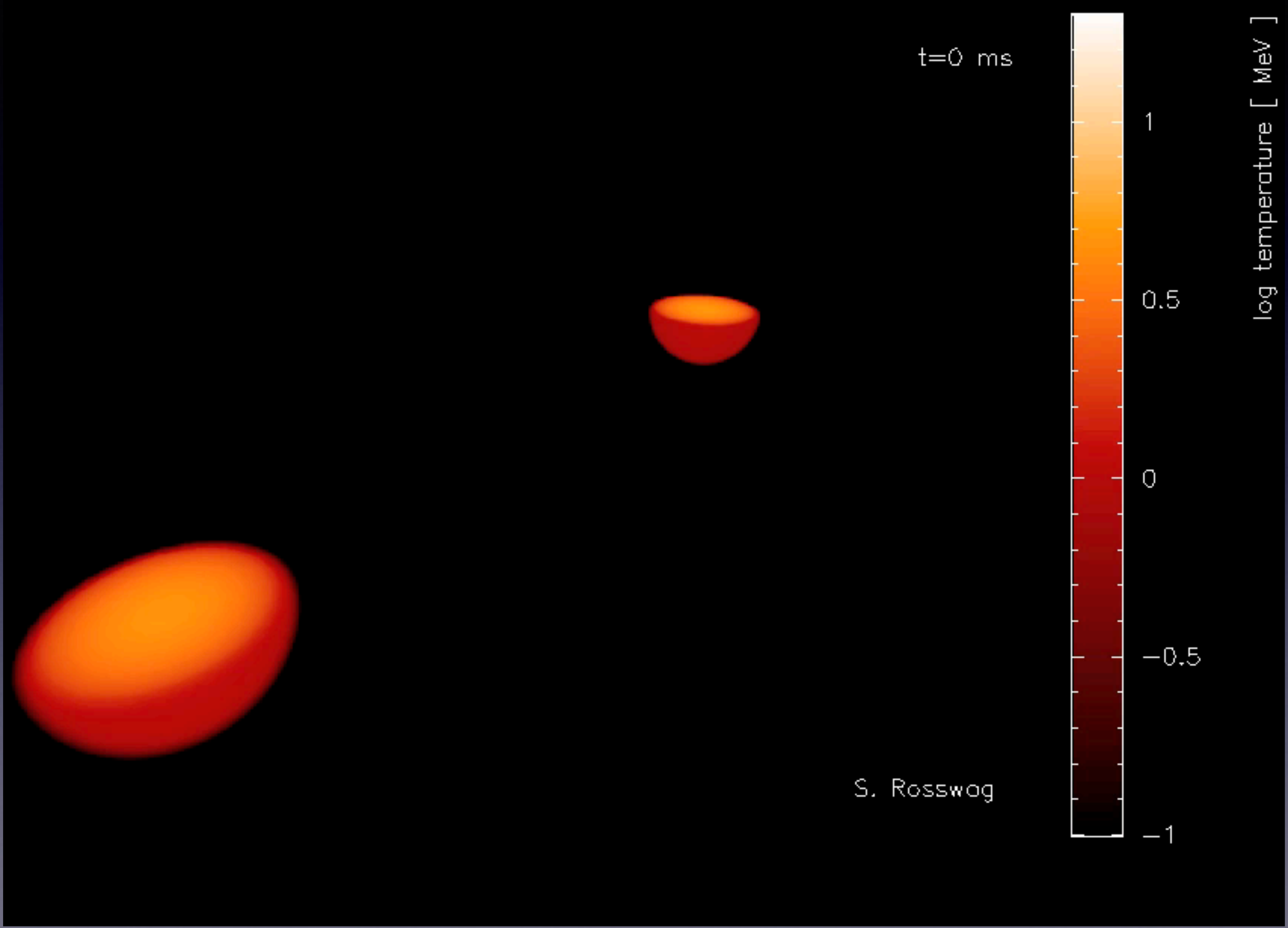


(Simulation Lodato)

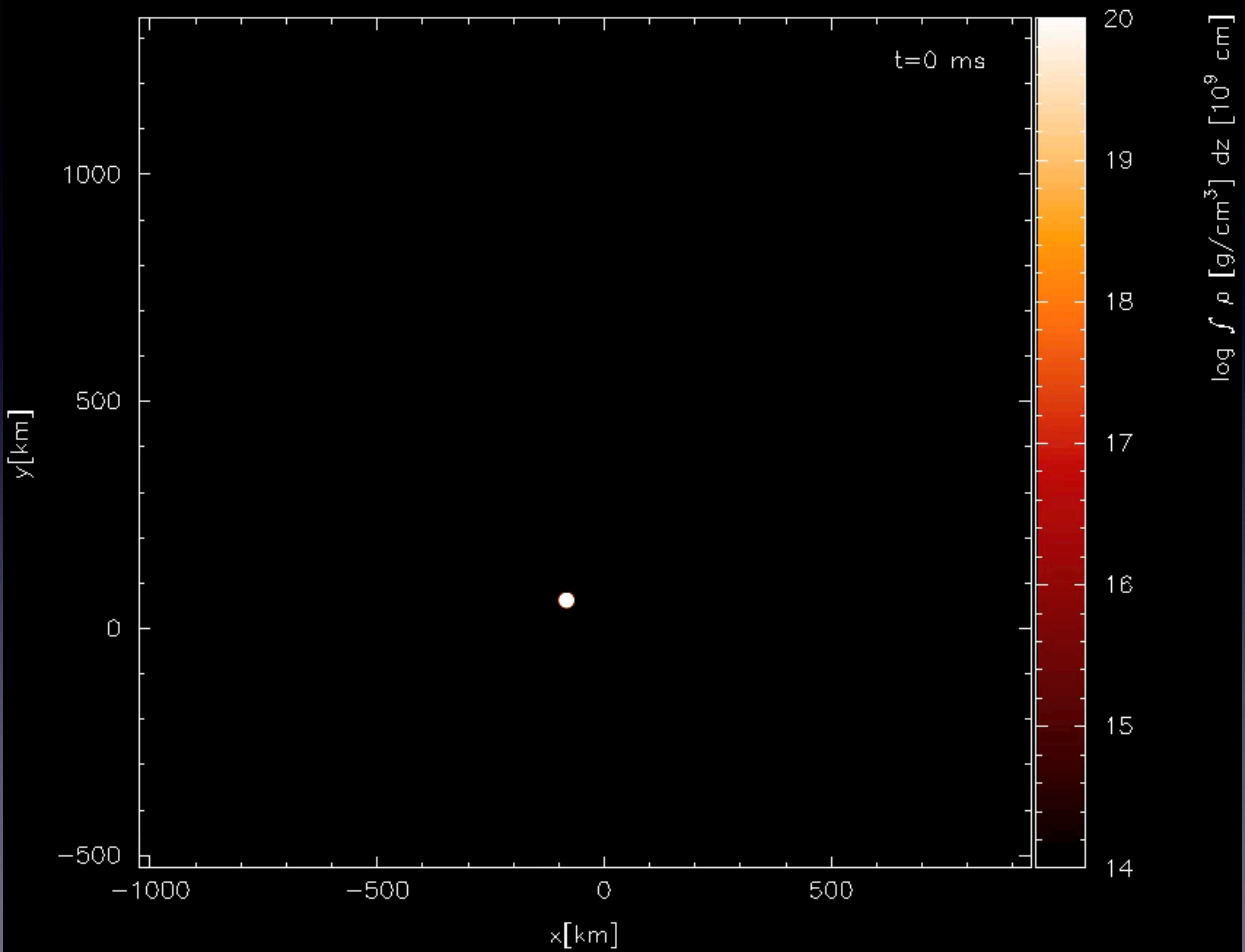
<u>modeled physics:</u>

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

- collision between two neutron stars (β=2)



- collision between a neutron star and a low-mass black hole ($5M_\odot$, $\beta=1$)



(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

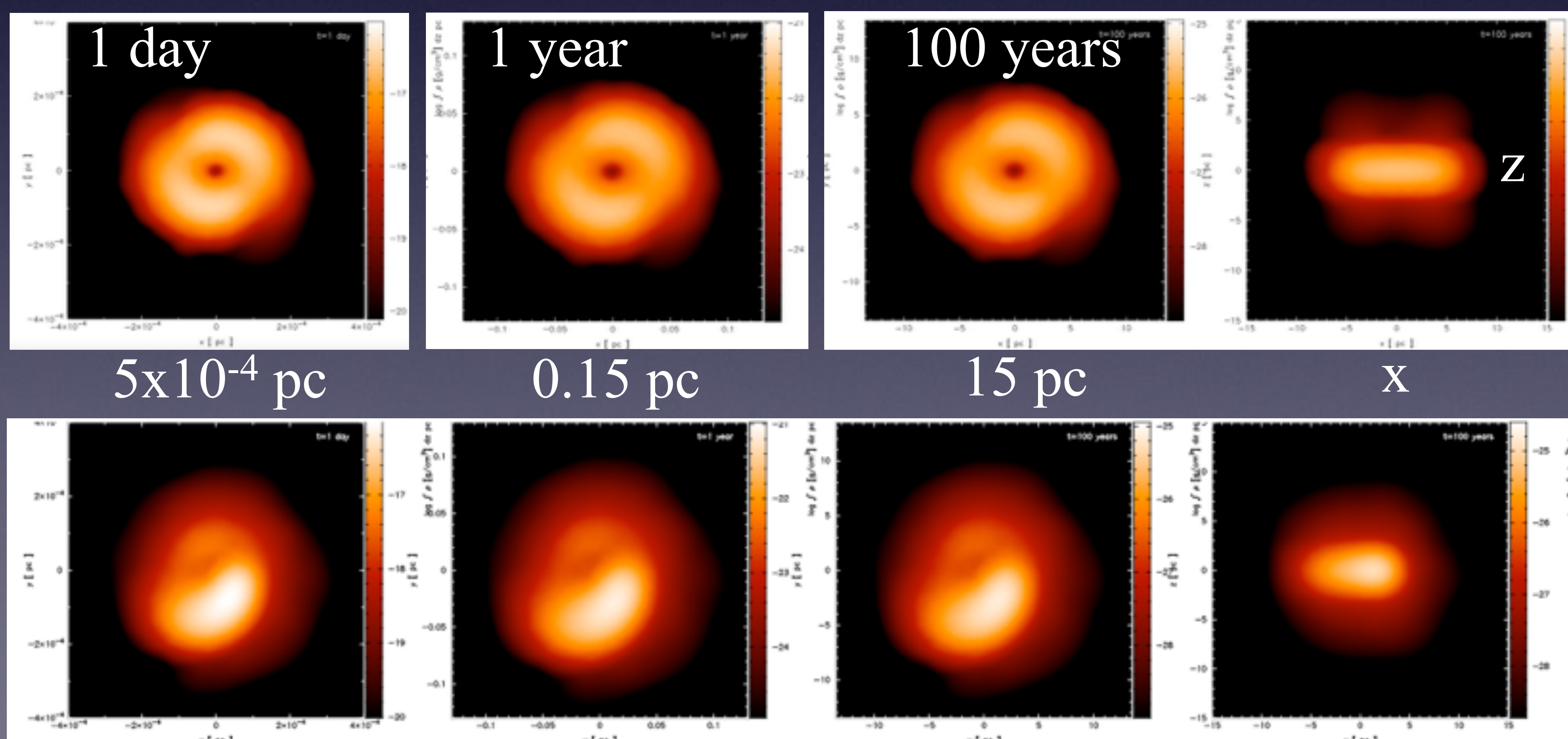
- include heating by radioactive decays

- follow evolution up to 100 years

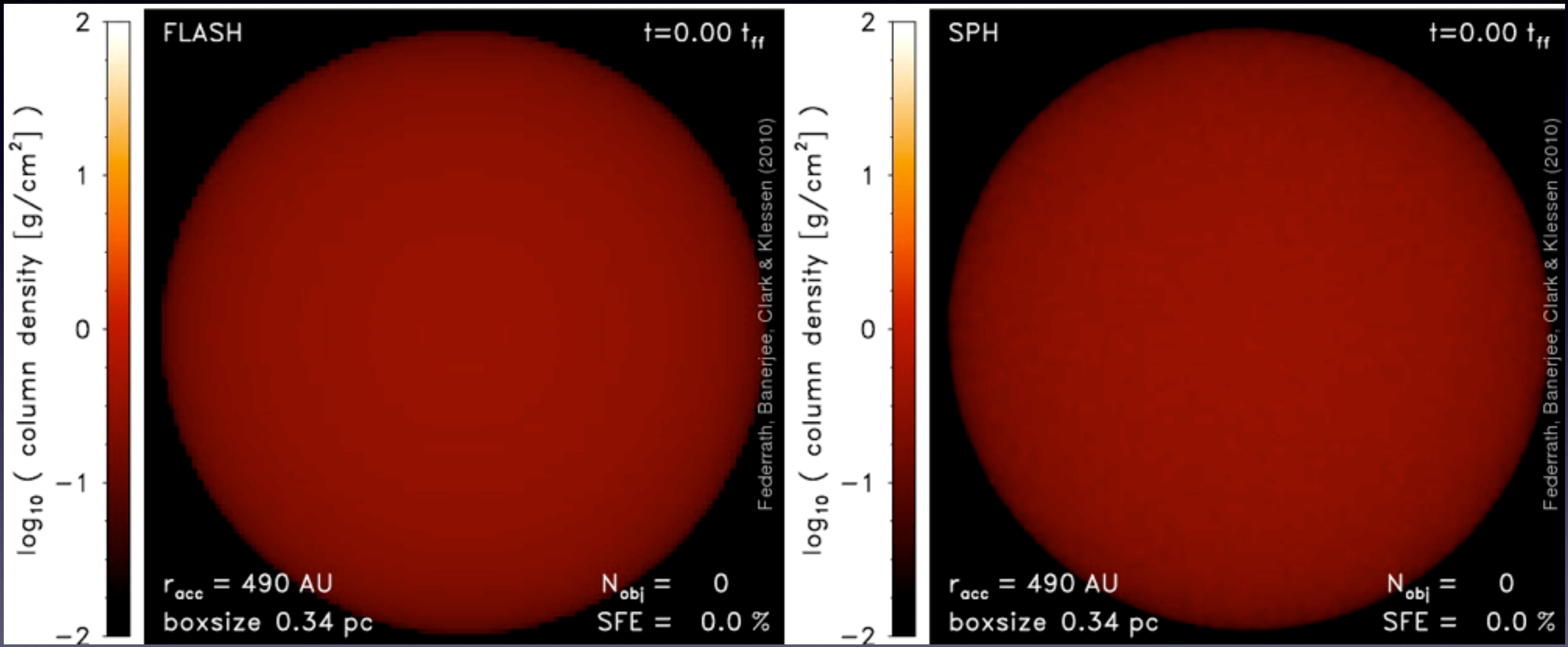
"100 years, but still in shape"

$2 \times 1.4 M_\odot$

1.3 & $1.4 M_\odot$



comparison Eulerian vs. Lagrangian



(Simulation Federrath)

1. Basics of Lagrangian fluid dynamics

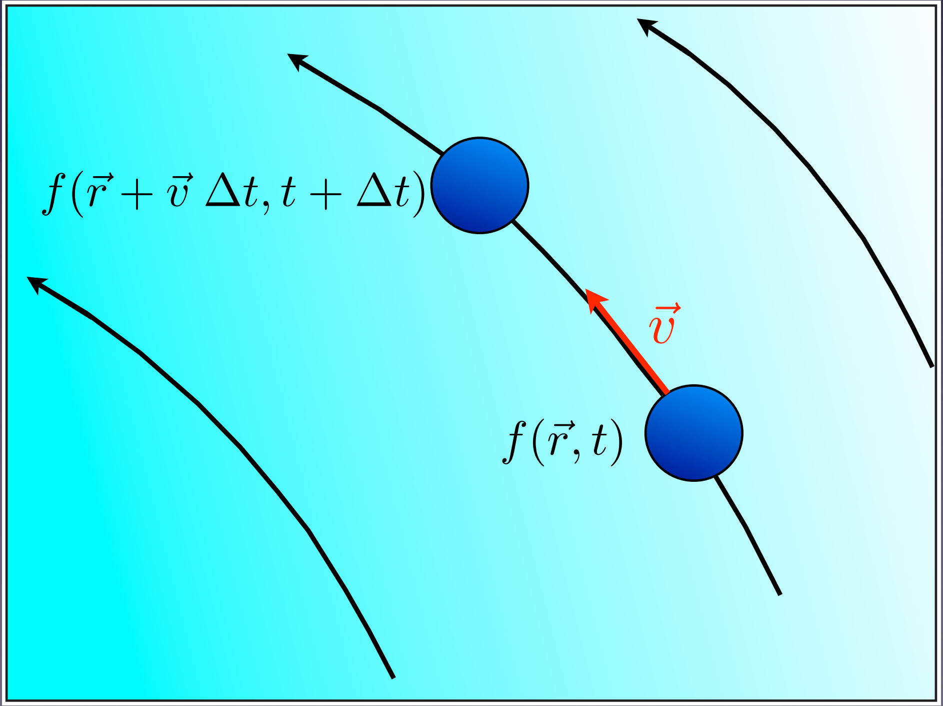
- in all of this lecture: restriction to ideal fluids (no viscosity, conductivity…)

- 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

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

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

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" → dU; ~~"change of entropy"~~ → ~~$T\,ds$~~; "work done via volume change" → $P\,dV$

- for our purposes: want quantities "per mass"

$$U \longrightarrow u \qquad \text{"energy per mass"}$$

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

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

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

- implications: a) evolution equation

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

b) for later use:

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

- 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

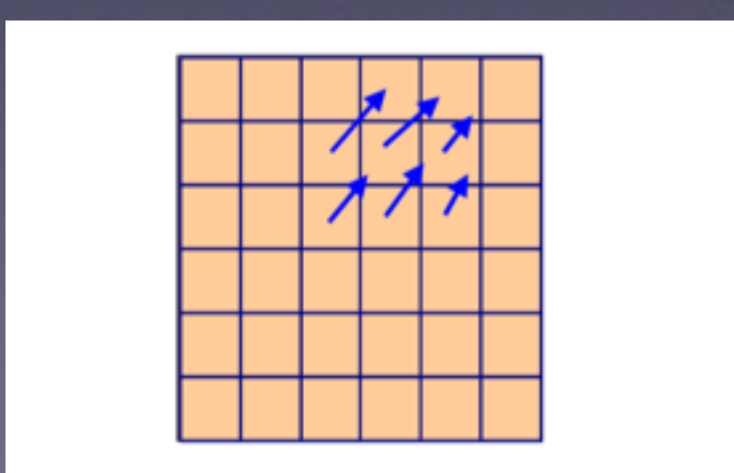
- long wish-list:

  - "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

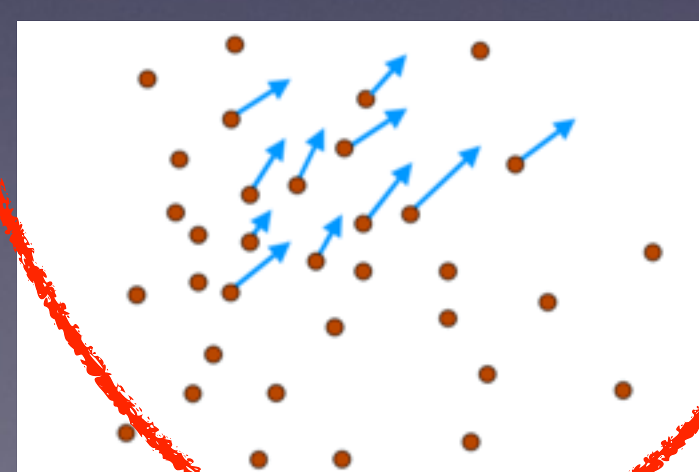
Eulerian

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



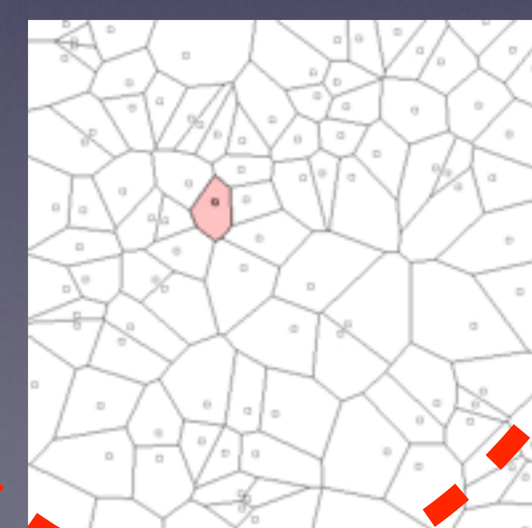
Lagrangian

- 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…



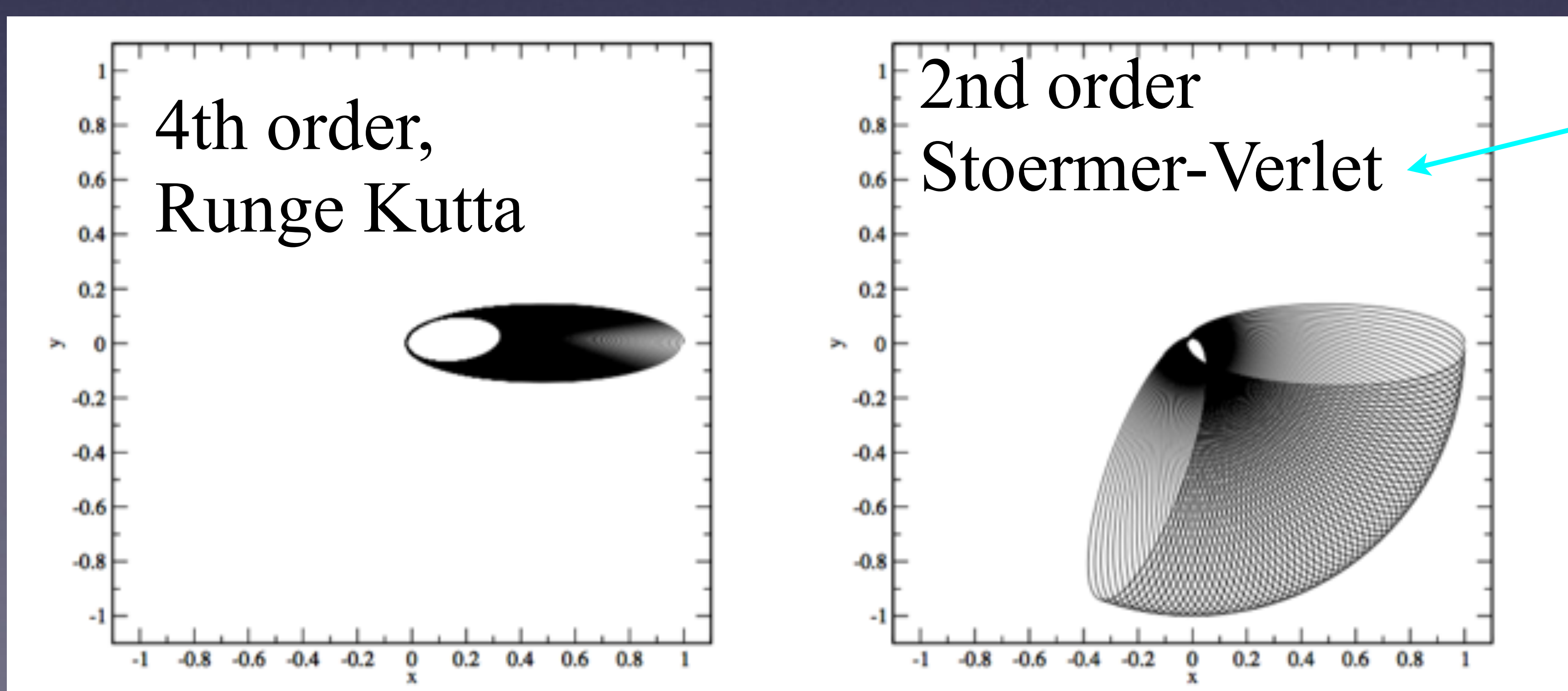
Importance of conservation

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

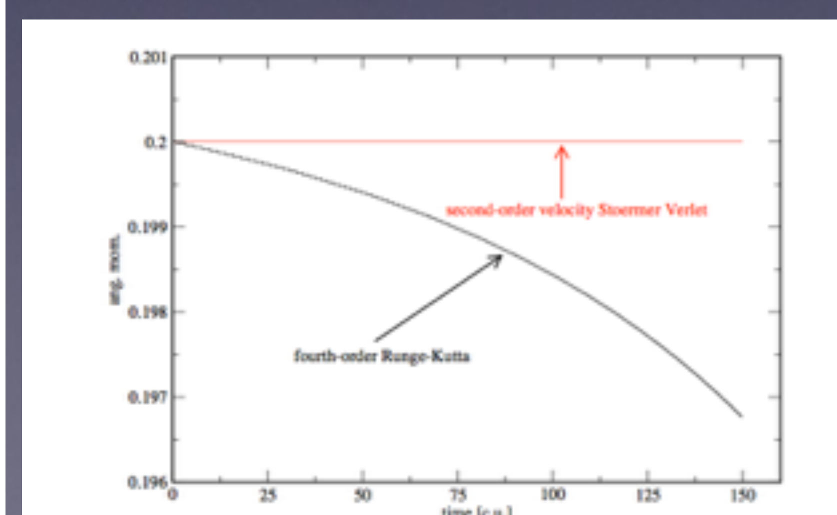
$\Rightarrow$ if conservation is “hardwired” (independent of resolution), we can hope to stay close to the real, physical solution

- Example 1: “Order vs. Conservation”

  $\Rightarrow$ Kepler problem with too large a time step

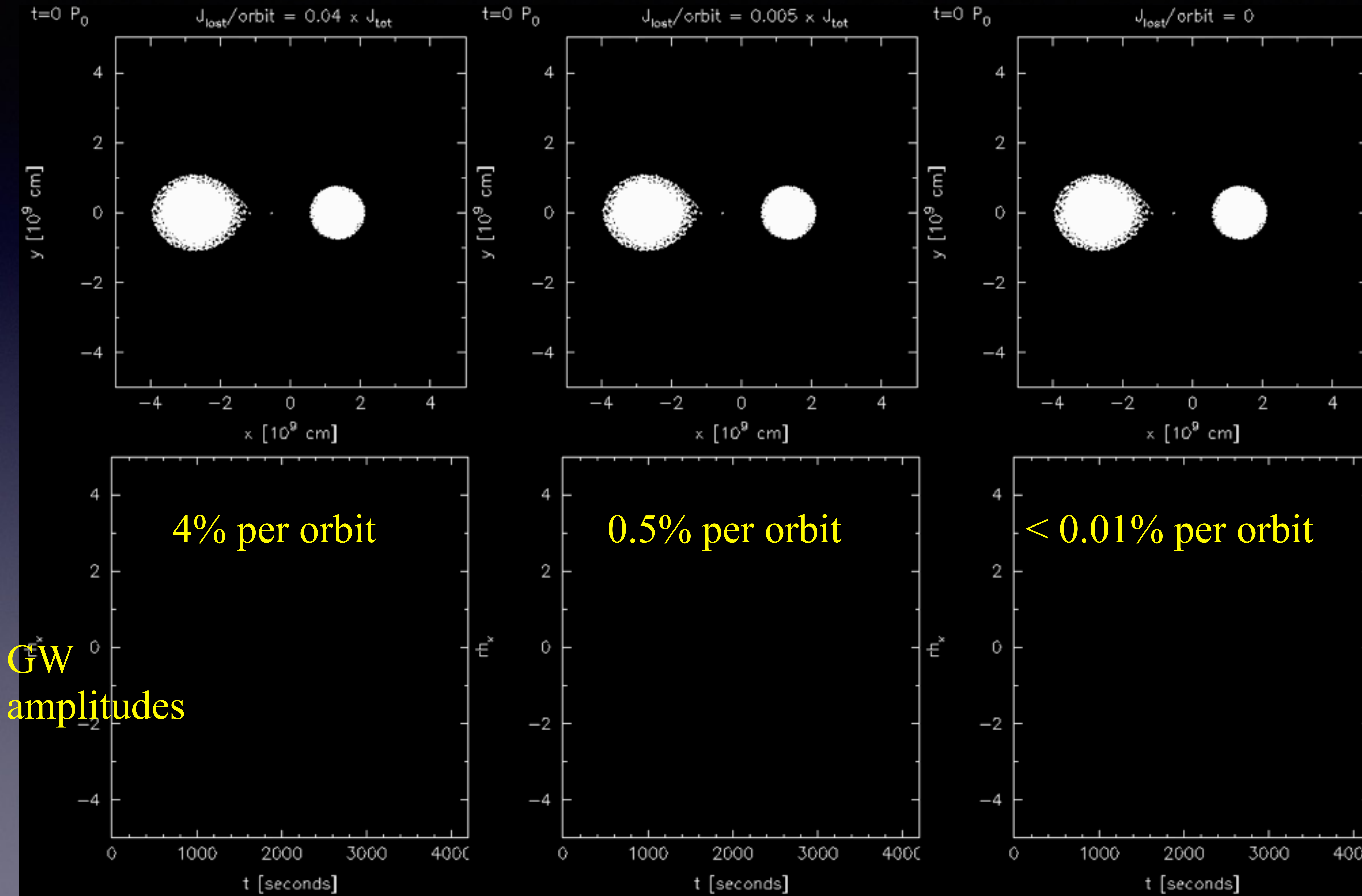


angular momentum conservation built-in!

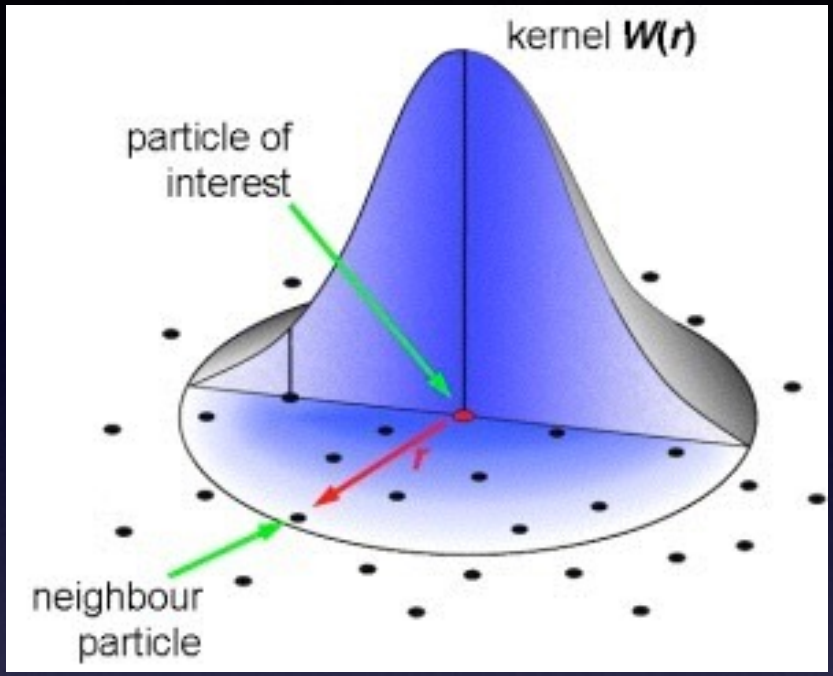


- Example 2: "How much non-conservation can we tolerate?"

  ⇒ 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

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

$$\Downarrow$$

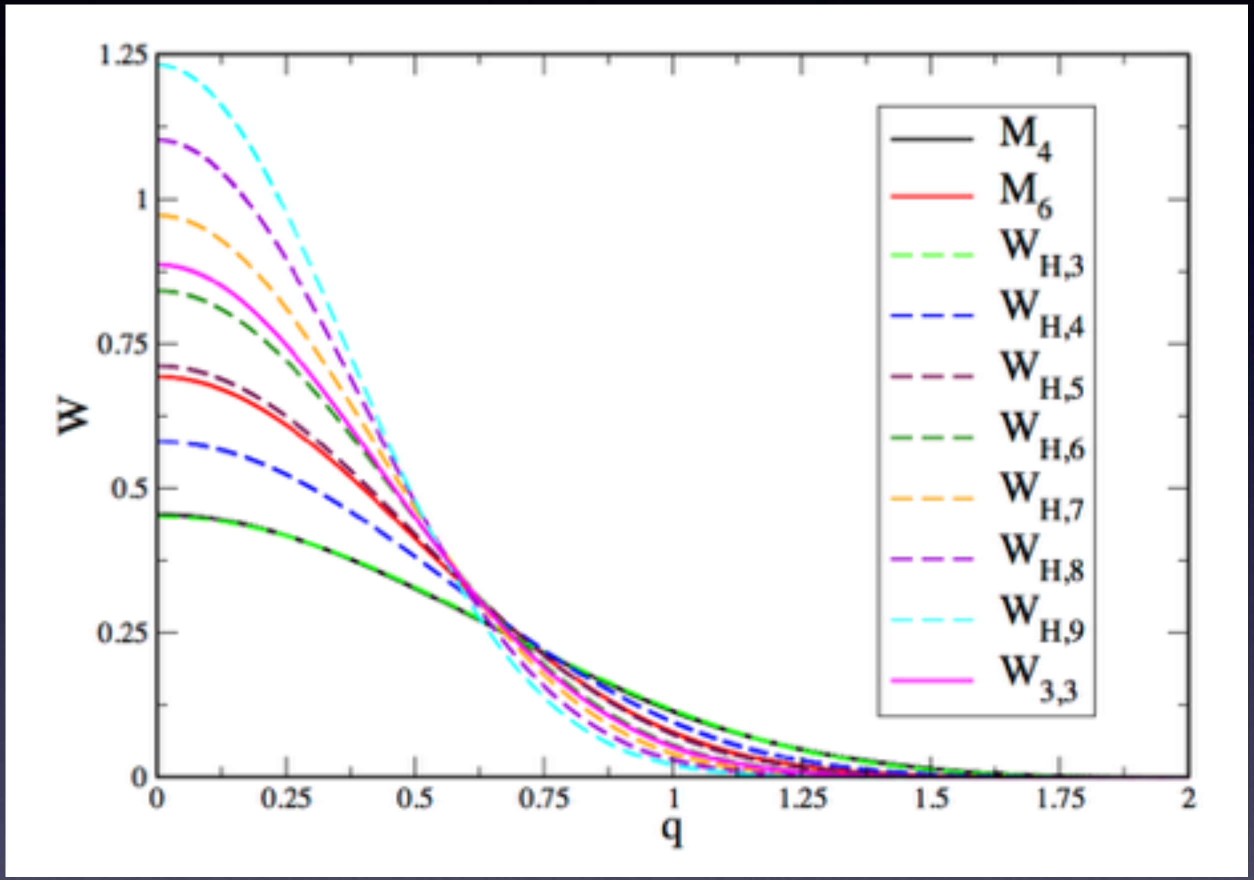
$$\nabla A(\vec{r}) = \sum_a \frac{m_a}{\rho_a} A_a \nabla W(|\vec{r} - \vec{r}_a|, h)$$

- 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"
⇒ zero outside of given radius
⇒ determined by "smoothing length" h
⇒ sum over local neighbours
(avoid N^2-behaviour)



(b) "bell-shaped"

(c) "radial":

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

⇒ 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

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

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

$\nabla_a W_{ab} = -\nabla_b W_{ab}$

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.

$$\frac{d\vec{v}_a}{dt} = -\frac{\nabla P}{\rho} = -\frac{P}{\rho^2}\nabla\rho - \nabla\left(\frac{P}{\rho}\right)$$

$$= -\frac{P_a}{\rho_a^2}\sum_b m_b \nabla_a W_{ab} - \sum_b \frac{m_b}{\rho_b}\frac{P_b}{\rho_b}\nabla_a W_{ab}$$

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

- 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:

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

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

- 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…

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

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

  for the velocity divergence:

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

- 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:

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

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

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

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

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

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

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

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

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

$$\frac{dE}{dt} = \sum_a m_a \left[\frac{P_a}{\rho_a^2}\sum_b m_b \vec{v}_{ab} \cdot \nabla_a W_{ab} - \vec{v}_a \cdot \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right) \nabla_a W_{ab}\right]$$

$$= \sum_{a,b} m_a m_b \frac{P_a}{\rho_a^2} \vec{v}_a \cdot \nabla_a W_{ab} - \sum_{a,b} m_a m_b \frac{P_a}{\rho_a^2} \vec{v}_b \cdot \nabla_a W_{ab}$$

$$- \sum_{a,b} m_a m_b \frac{P_a}{\rho_a^2} \vec{v}_a \cdot \nabla_a W_{ab} - \sum_{a,b} m_a m_b \frac{P_b}{\rho_b^2} \vec{v}_a \cdot \nabla_a W_{ab}$$

$$= - \sum_{a,b} m_a m_b \left(\frac{P_a \vec{v}_b}{\rho_a^2} + \frac{P_b \vec{v}_a}{\rho_b^2}\right) \nabla_a W_{ab} = 0$$

symmetric / antisymmetric
w.r. a ⟺ b

→ same "tricks" as before,
energy conserved by construction