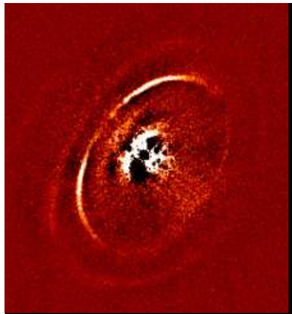
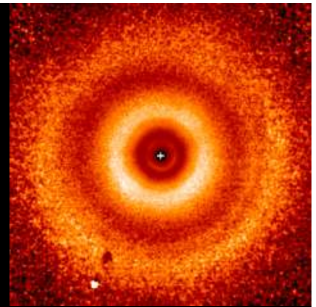
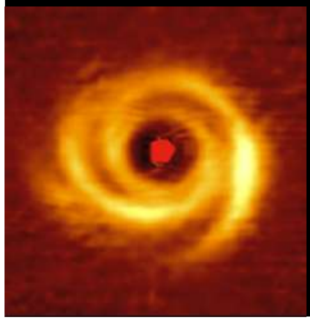
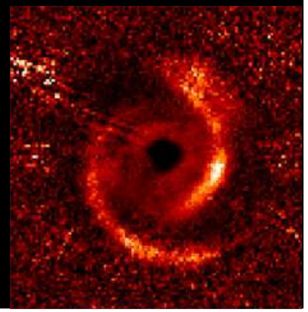


Dust and gas in SPH (part II): Simulating the dynamics of tightly-coupled dust grains with PHANTOM







Giovanni Dipierro

Main goal

Discretize and solve the equations for the conservation of mass and momentum and the internal energy equation in astrophysical continuous dust and gas mixture:

$$\frac{\partial \rho_{\mathrm{d}}}{\partial t} + \nabla \cdot (\rho_{\mathrm{d}} \mathbf{v}_{\mathrm{d}}) = 0$$

$$\frac{\partial \rho_{\mathrm{g}}}{\partial t} + \nabla \cdot (\rho_{\mathrm{g}} \mathbf{v}_{\mathrm{g}}) = 0$$

$$\rho_{\mathrm{g}} \left(\frac{\partial \mathbf{v}_{\mathrm{g}}}{\partial t} + \mathbf{v}_{\mathrm{g}} \cdot \nabla \mathbf{v}_{\mathrm{g}} \right) = K(\mathbf{v}_{\mathrm{d}} - \mathbf{v}_{\mathrm{g}}) + \rho_{\mathrm{g}} \mathbf{f}_{\mathrm{g}} + \rho_{\mathrm{g}} \mathbf{f}$$

$$\rho_{\mathrm{d}} \left(\frac{\partial \mathbf{v}_{\mathrm{d}}}{\partial t} + \mathbf{v}_{\mathrm{d}} \cdot \nabla \mathbf{v}_{\mathrm{d}} \right) = -K(\mathbf{v}_{\mathrm{d}} - \mathbf{v}_{\mathrm{g}}) + \rho_{\mathrm{d}} \mathbf{f}_{\mathrm{d}} + \rho_{\mathrm{d}} \mathbf{f}$$

$$\frac{\partial u}{\partial t} + (\mathbf{v}_{\mathrm{g}} \cdot \nabla) u = -\frac{P}{\rho_{\mathrm{g}}} (\nabla \cdot \mathbf{v}_{\mathrm{g}}) + K(\mathbf{v}_{\mathrm{g}} - \mathbf{v}_{\mathrm{d}})^2 + \Lambda_{\mathrm{visc}} + \Lambda_{\mathrm{heat}} - \Lambda_{\mathrm{cool}}$$

$$\mathbf{f}_{\mathrm{g}} = -\frac{\nabla P}{\rho_{\mathrm{g}}} + \mathbf{f}_{\mathrm{g,visc}}$$

$$\mathbf{f}_{\mathrm{d}} = 0$$

$$P = (\gamma - 1) \rho_{\mathrm{g}} u$$

$$K \equiv \frac{\rho_{\mathrm{d}} \rho_{\mathrm{g}}}{t_{\mathrm{s}} (\rho_{\mathrm{g}} + \rho_{\mathrm{d}})}$$

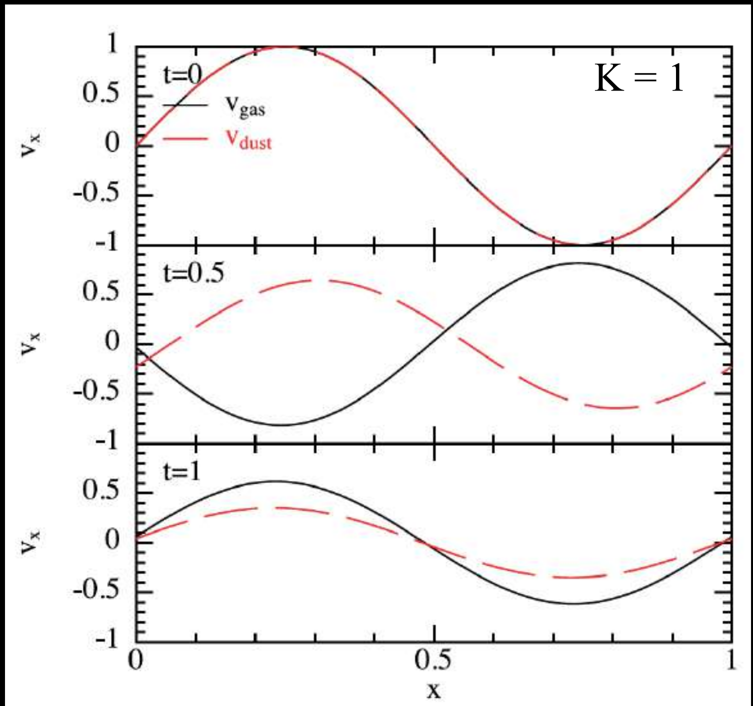
$$\mathrm{St} \equiv t_{\mathrm{s}} \Omega_{\mathrm{k}} = \frac{\rho_{\mathrm{grain}} s_{\mathrm{grain}} \Omega_{\mathrm{k}}}{(\rho_{\mathrm{g}} + \rho_{\mathrm{d}}) c_{\mathrm{s}}} \sqrt{\frac{\pi \gamma}{8}}$$

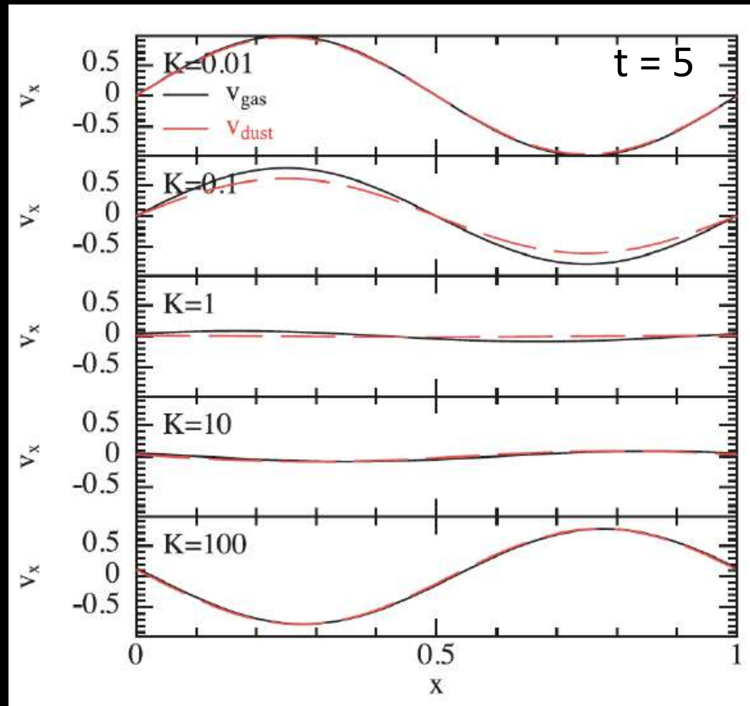
Epstein Regime (Epstein 1924)

What is the best way to benchmark an algorithm?

`DUSTYWAVE`: linear sound waves propagating in a uniform density two-fluid dust–gas (inviscid) medium with a linear dust/gas drag term (i.e K does not depend on Δv).

Full solution of the problem consists of a linear combination of three independent modes that take the form of exponentially decaying monochromatic waves (Laibe and Price 2011 -> see solutions in dustywaves.f90.. good luck!)



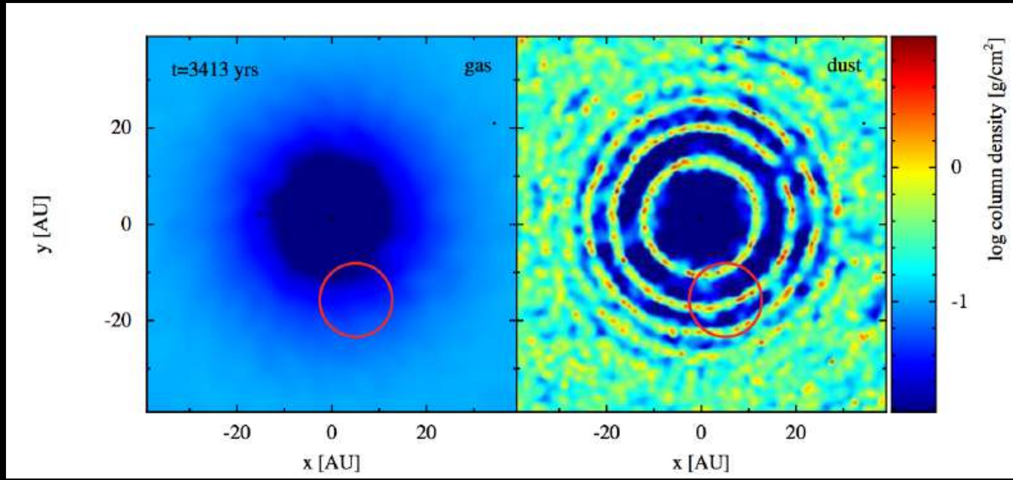


For perfectly coupled mixture ($t_s = 0$, $K=\infty$): 'acustic' waves propagating with a sound speed: $\tilde{c_s} = c_s \left(1 + \frac{\rho_d}{\rho_g}\right)^{-\frac{1}{2}}$

One-fluid method: the origins

Two-fluid methods: limitations

1. Artificial clumping of dust particles below the gas resolution



Artificial clumping when $h_{gas} > h_{dust}$

Requirements: $h_{gas} < h_{dust}$ and $h_{drag} = h_{gas}$

or $h_{drag} = \max(h_{gas}, h_{dust})$ along the simulations

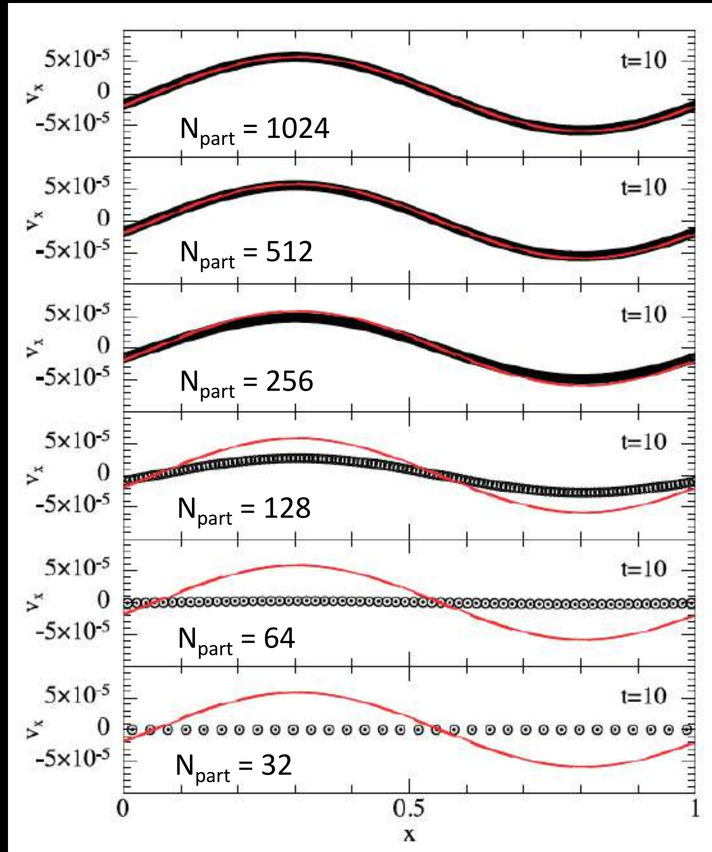
Laibe & Price (2012) - Price & Federrath (2010)

One-fluid method: the origins

Dustywave for strong drag (K = 100): $\tilde{c}_{\rm s} = c_{\rm s}\left(1+\frac{\rho_{\rm d}}{\rho_{\rm g}}\right)^{-\frac{1}{2}}$

Two-fluid methods: limitations

2. Infinite spatial resolution is required in the limit of infinite drag to resolve differential motion and prevent overdissipation of the kinetic energy



Laibe & Price (2012)

Spatial resolution $h < t_{\rm s} c_{\rm s} \xrightarrow[t_{\rm s}\to 0]{} 0$

One-fluid method: the origins

Two-fluid methods: limitations

3. Infinite temporal resolution is required in the limit of infinite drag to ensure numerical stability of explicit schemes

Requirement for numerical stability of the explicit two-fluid scheme (Laibe & Price 2012)

$$\Delta t < t_{\mathrm{s}} = \frac{\rho_{\mathrm{g}}\rho_{\mathrm{d}}}{K\left(\rho_{\mathrm{g}} + \rho_{\mathrm{d}}\right)} \xrightarrow[K \to \infty]{} 0$$

$$K \sim \frac{4\pi}{3}\rho_{\mathrm{g}}\rho_{\mathrm{d}}\frac{s_{\mathrm{grain}}^{2}}{m_{\mathrm{grain}}}\sqrt{\frac{8}{\pi\gamma}}c_{\mathrm{s}} \propto s_{\mathrm{grain}}^{-1}$$

Epstein Regime (Epstein 1924)

This problem can be handled using implicit timestepping methods (Laibe & Price 2012b) or alternative 2-fluid + semi-analytical methods but limitation (2) holds

One-fluid method: the origins

Two-fluid methods: limitations

1. Artificial clumping of dust particles below the gas resolution $$h_{\mathrm{gas}} < h_{\mathrm{dust}}$$

2. Infinite spatial resolution is required in the limit of infinite drag to resolve differential motion and prevent overdissipation of the kinetic energy $$h < t_{\mathrm{s}} c_{\mathrm{s}}$$

3. Infinite temporal resolution is required in the limit of infinite drag to ensure numerical stability of explicit schemes $$\Delta t < t_{\mathrm{s}}$$

One fluid to rule them all

Main idea: gas and dust are described as a single fluid made of two different phases, referred to as the mixture, moving with the barycentric velocity $\mathbf{v}$. The differential velocity $\Delta\mathbf{v}$ between the two phases and the dust fraction ϵ are internal properties of the mixture.

$$\mathbf{v} = \frac{\rho_{\mathrm{g}}\mathbf{v}_{\mathrm{g}} + \rho_{\mathrm{d}}\mathbf{v}_{\mathrm{d}}}{\rho_{\mathrm{g}} + \rho_{\mathrm{d}}} \qquad \Delta\mathbf{v} = \mathbf{v}_{\mathrm{d}} - \mathbf{v}_{\mathrm{g}}$$

$$\rho = \rho_{\mathrm{g}} + \rho_{\mathrm{d}} \qquad \epsilon = \frac{\rho_{\mathrm{d}}}{\rho}$$

Lagrangian frame comoving with the fluid barycentric velocity

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v} \qquad \frac{\mathrm{d}}{\mathrm{d}t} \equiv \frac{\partial}{\partial t} + (\mathbf{v}\cdot\nabla)$$

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\left(\nabla\cdot\mathbf{v}\right)$$

$$\frac{\mathrm{d}\epsilon}{\mathrm{d}t} = -\frac{1}{\rho}\nabla\cdot\left[\epsilon(1-\epsilon)\rho\Delta\mathbf{v}\right]$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{\nabla P}{\rho} - \frac{1}{\rho}\nabla\cdot\left[\epsilon(1-\epsilon)\rho\Delta\mathbf{v}\Delta\mathbf{v}\right] + (1-\epsilon)\mathbf{f}_{\mathrm{g,visc}} + \mathbf{f}$$

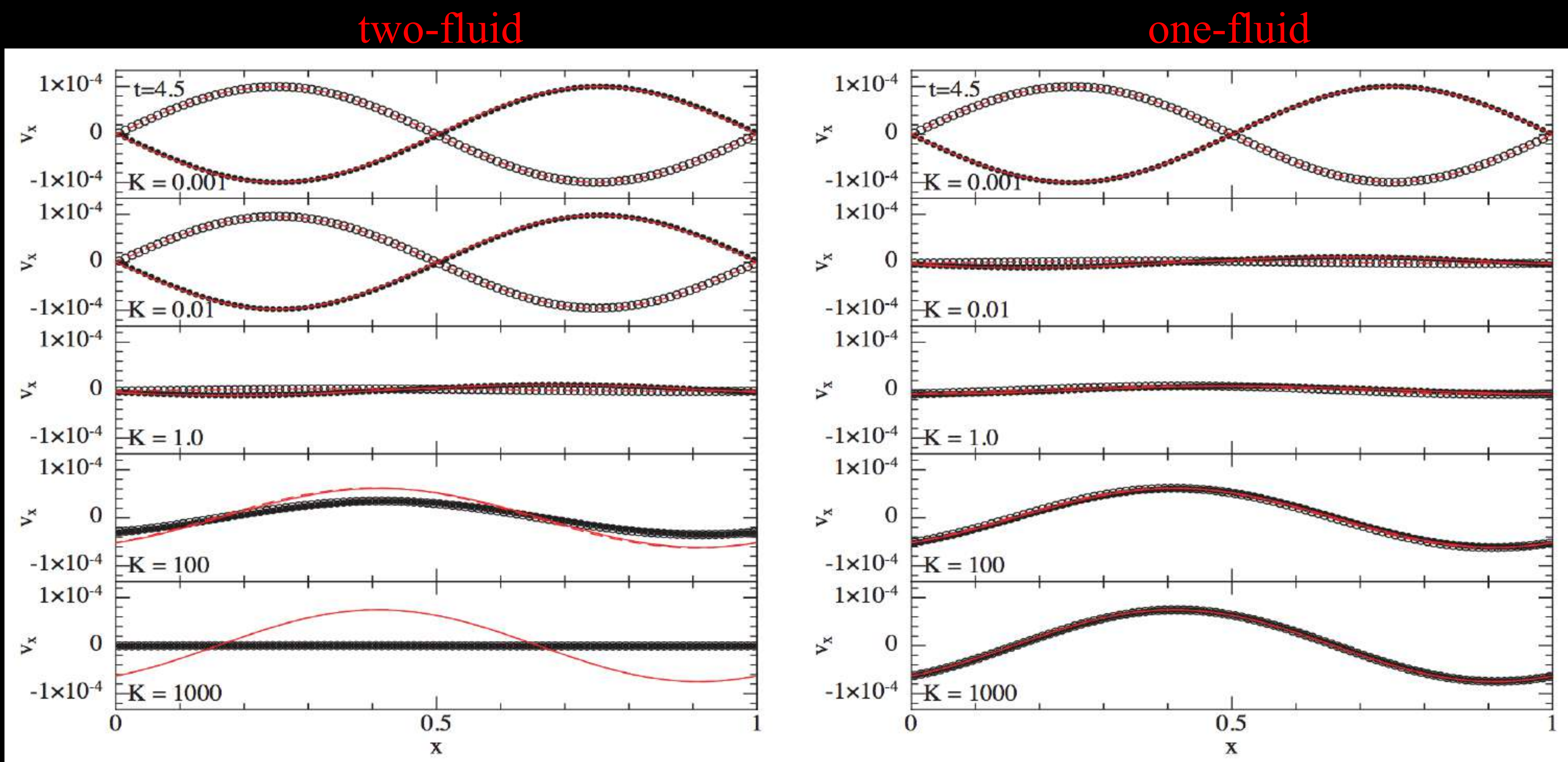
$$\frac{\mathrm{d}\Delta\mathbf{v}}{\mathrm{d}t} = -\frac{\Delta\mathbf{v}}{t_{\mathrm{s}}} + \frac{\nabla P}{(1-\epsilon)\rho} - \mathbf{f}_{\mathrm{g,visc}} - (\Delta\mathbf{v}\cdot\nabla)\mathbf{v} + \frac{1}{2}\nabla\left[(2\epsilon-1)\Delta\mathbf{v}\Delta\mathbf{v}\right]$$

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{P}{(1-\epsilon)\,\rho}\nabla\cdot(\mathbf{v}-\epsilon\Delta\mathbf{v}) + \epsilon\left(\Delta\mathbf{v}\cdot\nabla\right)u + \epsilon\frac{\Delta\mathbf{v}^2}{t_{\mathrm{s}}} + \Lambda_{\mathrm{heat}} - \Lambda_{\mathrm{cool}}$$

$$\mathbf{f}_{\mathrm{g}} = -\frac{\nabla P}{(1-\epsilon)\rho} + \mathbf{f}_{\mathrm{g,visc}}$$

$$\mathbf{f}_{\mathrm{d}} = 0$$

Improvements



Propagation of waves in a dust-gas mixture, showing dust and gas velocities for the two-fluid (left) compared to a one-fluid (right) numerical solution (black solid and open circles for gas and dust, respectively). The two fluid approach (left) leads to overdamping in the limit of strong coupling (lower panels in left Figure), since the resolution criterion $h < c_s t_s$ is not satisfied.

One-fluid method

advantages

1) The equations can be solved on a single fluid that moves with the barycentric velocity v, rather than requiring two fluids. This avoids the particle trapping under the gas resolution
2) Drag does not have to be explicitly evaluated, reducing it to a simple exponential decay
3) The spatial resolution criterion $h < c_s t_s$ is no longer required (there is no physical separation between the two phases)

limitations

1) If explicit timestepping is used, the usual criterion $\Delta t < t_s$ is required. However, it's simpler to implement an implicit method but it is nevertheless an extra complication to the algorithm…

…but for very strong drag (short t_s) an alternative, a much simpler and faster method can be derived…

Simplifying equations for strong drag/small grains

We assume that drag forces adjust quasi-statically to pressure and viscous forces. In other words, the differential velocity between the gas and dust is instantaneously dissipated by the drag (Youdin and Goodman 2005)

$$\frac{\mathrm{d}\Delta\mathbf{v}}{\mathrm{d}t} = -\frac{\Delta\mathbf{v}}{t_\mathrm{s}} + \frac{\nabla P}{(1-\epsilon)\rho} + \mathbf{f}_{\mathrm{g,visc}} - (\Delta\mathbf{v}\cdot\nabla)\mathbf{v} + \frac{1}{2}\nabla\cdot\left[(2\epsilon-1)\Delta\mathbf{v}\Delta\mathbf{v}\right] \longrightarrow \Delta\mathbf{v} = t_\mathrm{s}\left[\frac{\nabla P}{(1-\epsilon)\,\rho} - \mathbf{f}_{\mathrm{g,visc}}\right]$$

To first order in t_s/T, where T is the timescale for a sound wave to propagate over a typical distance L (h in SPH simulations), the equations describing the evolution of a dust-gas mixture (with $\mathbf{f}_{g,visc} = 0$) can be written in the form

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\left(\nabla\cdot\mathbf{v}\right)$$

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

$$\frac{\mathrm{d}\epsilon}{\mathrm{d}t} = -\frac{1}{\rho}\nabla\cdot\left(\epsilon t_\mathrm{s}\nabla P\right)$$

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{P}{(1-\epsilon)\,\rho}(\nabla\cdot\mathbf{v}) - \frac{\epsilon t_\mathrm{s}}{(1-\epsilon)\,\rho}\left(\Delta P\cdot\nabla u\right) + \Lambda_\mathrm{heat} - \Lambda_\mathrm{cool}$$

The only differences to the usual equations of hydrodynamics are:

1. extra equation that describes the evolution of the dust fraction
2. Extra term in the evolution of the internal energy
3. the gas pressure gradient is divided by the total density of the fluid

Extra equation that describes the evolution of the dust fraction or dust-to-gas ratio:

$$\frac{\mathrm{d}\epsilon}{\mathrm{d}t} = -\frac{1}{\rho}\nabla \cdot (\epsilon t_{\mathrm{s}} \nabla P) \qquad \text{or, equivalently} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\rho_{\mathrm{d}}}{\rho_{\mathrm{g}}}\right) = -\frac{\rho}{\rho_{\mathrm{g}}^2}\nabla \cdot \left(\frac{\rho_{\mathrm{g}}\rho_{\mathrm{d}}}{\rho}\left[\frac{\nabla P}{\rho_{\mathrm{g}}} t_{\mathrm{s}}\right]\right)$$

The source term ($\propto \nabla P$, neglecting viscous forces, magnetic, etc) produces a relative drift tends to accumulate dust in the pressure maxima and, by conservation of momentum, pushes the gas outside.

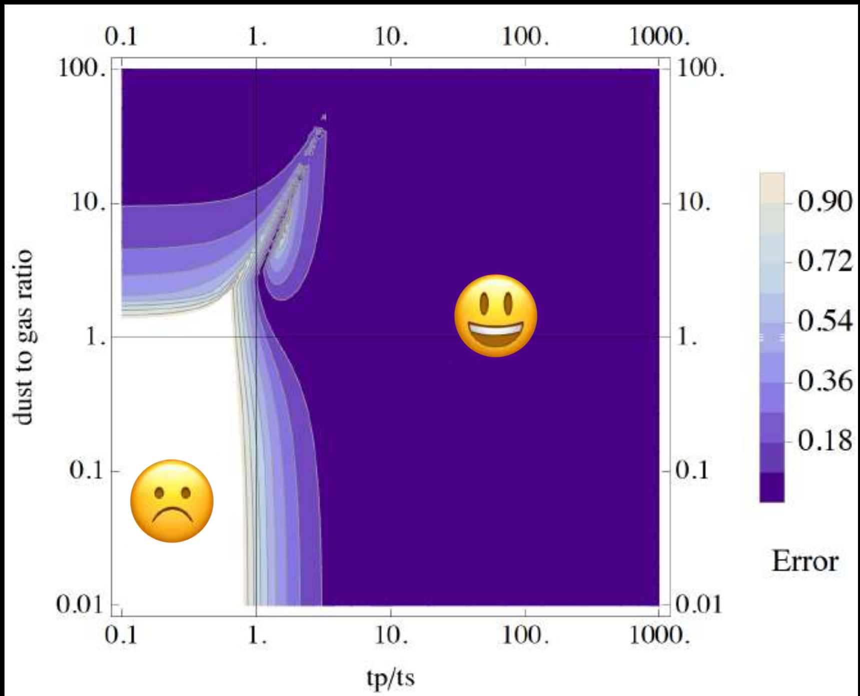
This term acts to diffuse the dust-fraction on timescales $\propto \frac{1}{c_{\mathrm{s}}^2 t_{\mathrm{s}}}$

the addition of the dust fraction equation adds a further constraint on the timestep (assuming $\nabla\epsilon = 0$): $\Delta t < C_0 \frac{h}{\sqrt{\tilde{c_{\mathrm{s}}} + \epsilon^2 t_{\mathrm{s}}^2 c_{\mathrm{s}}^4 / h^2}}$ with $\tilde{c}_{\mathrm{s}} = c_{\mathrm{s}}\left(1 + \frac{\rho_{\mathrm{d}}}{\rho_{\mathrm{g}}}\right)^{-\frac{1}{2}}$

In what drag regime the terminal velocity approximation can be safely used?

Dusty wave for strong drag

Terminal velocity approximation: the drag-induced decay of the differential velocity or, equivalently, the dissipation of the relative kinetic energy ($\propto \Delta v^2$) occurs very fast and Δv reaches the terminal value..



Contour plot of the relative error in the dissipation timescale when using the terminal velocity approximation compared to the full dustywave problem

When the ratio between the pressure timescale

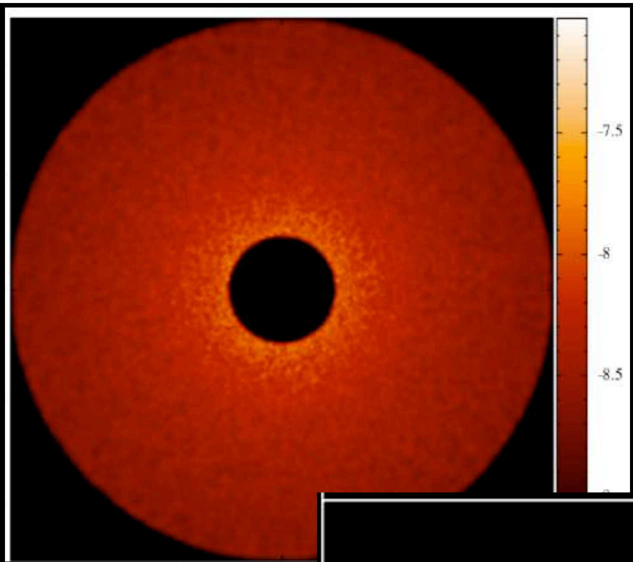
$$t_{\rm p} \approx \frac{\lambda}{2\pi c_{\rm s}}$$

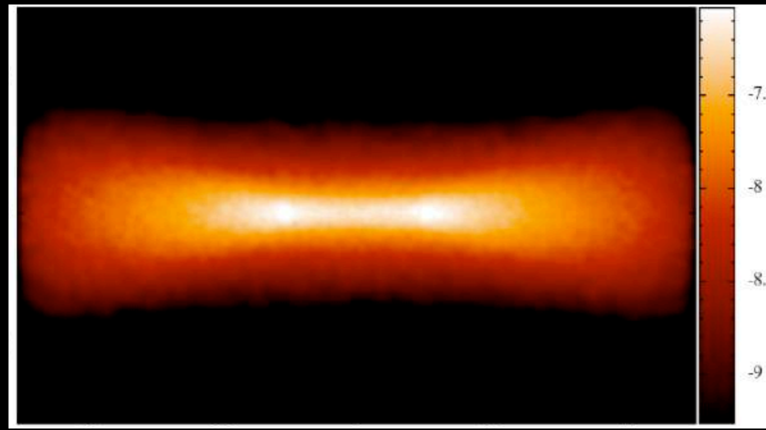
(i.e. typical time for a sound wave to propagate across one wavelength) and the stopping time t_s is > 1-10, the terminal velocity can be used.

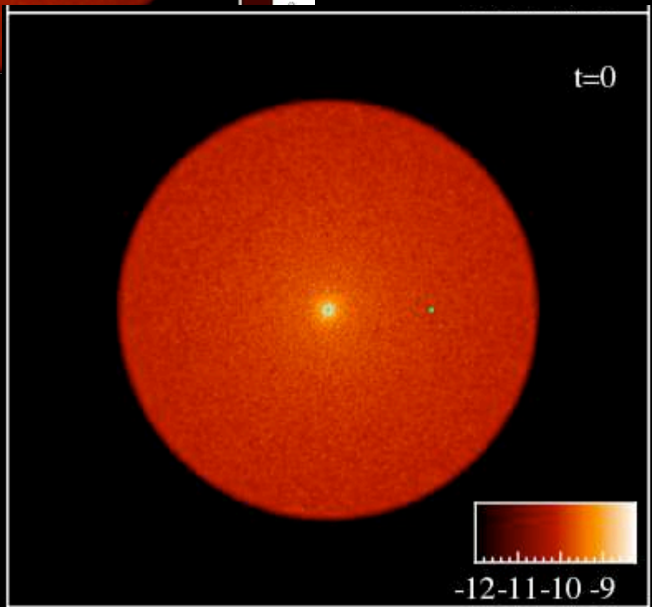
Conditions for the validity of the diffusion approximation in numerical simulations:

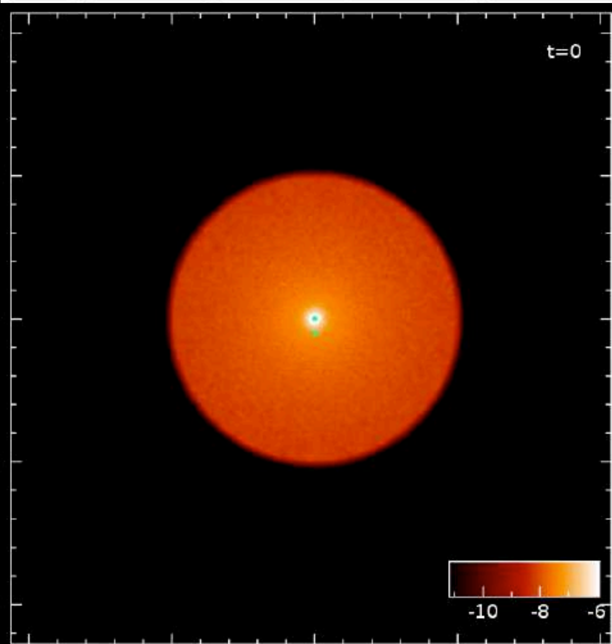
$$t_{\rm s} \lesssim \frac{\Delta t}{2\pi} \sim \frac{1}{2\pi}\frac{\Delta x}{c_{\rm s}} \xrightarrow{\rm SPH} t_{\rm s} \lesssim \frac{h}{c_{\rm s}} \rightarrow t_{\rm s}\Omega \lesssim \frac{h}{H}$$

Bugs!!









Non–conservation of dust mass: fatal numerical errors in the evolution of the dust fraction ϵ, especially in the upper/outer disc regions

Problems in the computation of the evolution of ϵ

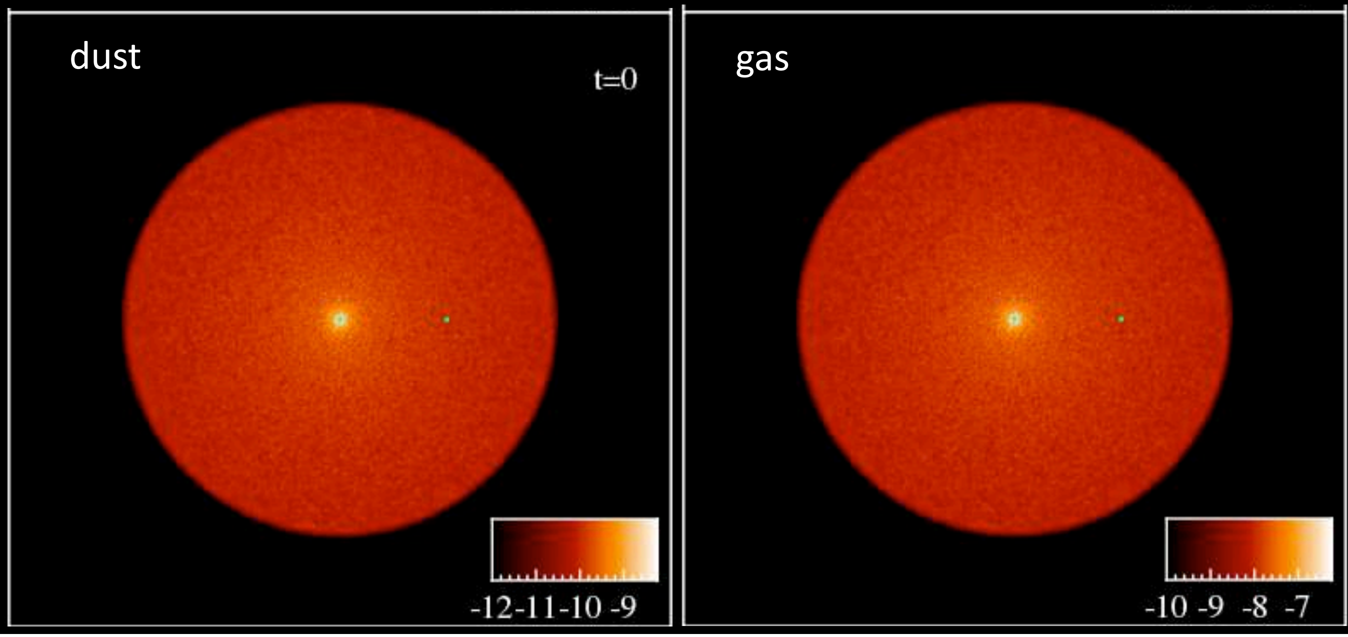
$$\frac{\mathrm{d}\epsilon}{\mathrm{d}t} = -\frac{1}{\rho}\nabla\cdot(\epsilon t_{\mathrm{s}}\nabla P)$$

ϵ is simply evolved via a differential equation, without the constraint $0 < \epsilon < 1$

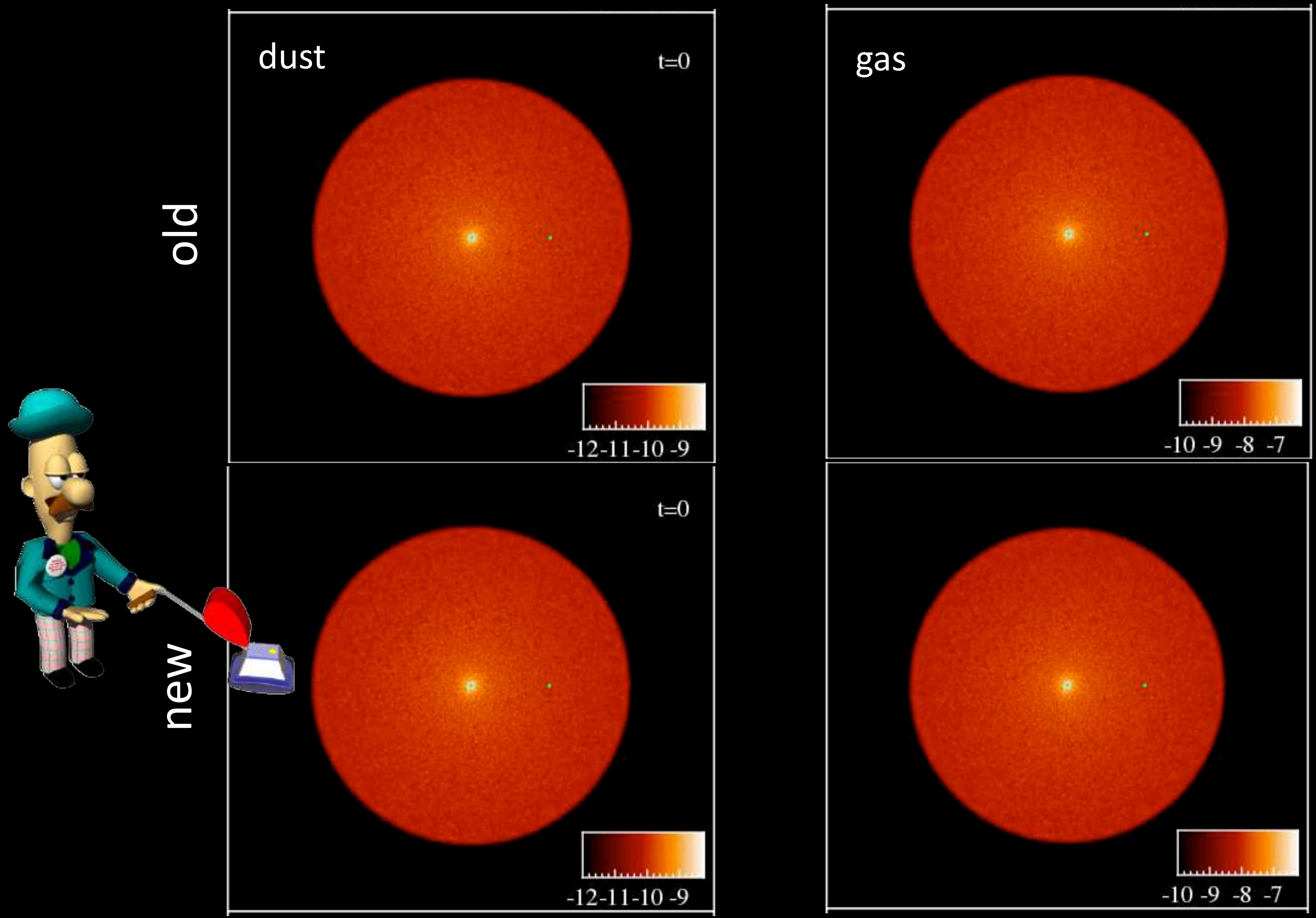
The dust diffusion, i.e. $\propto t_s \nabla P$, in outer/upper disc regions might be strong due to the steep gradients in the pressure and the presence of particles with large stopping time

$$t_{\mathrm{s}} \approx \frac{\pi}{2}\frac{\rho_{\mathrm{grain}} s_i}{\Sigma_{\mathrm{g}}\Omega_{\mathrm{k}}}\exp\left[\frac{z^2}{2H_{\mathrm{g}}^2}\right]$$

as the dust front diffuse in the outer disc regions, ϵ can become negative or larger than 1, leading to an incorrect computation of the dust and gas dynamics



Possible solution: evolve the new quantity $s = \sqrt{\dfrac{\epsilon}{1-\epsilon}}$ such that $\epsilon = \dfrac{s^2}{1+s^2}$, thus enforcing $0 < \epsilon < 1$

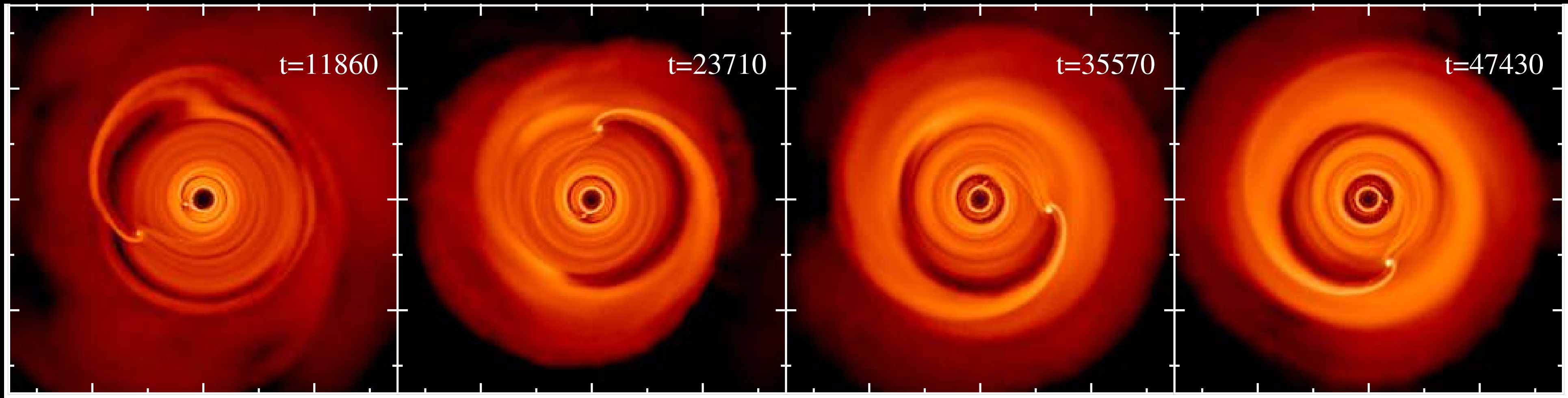


Ballabio et al. 2018

Note that Mark is working on a new parameterisation to achieve a better numerical stability $s = \sin^{-1}(\sqrt{\epsilon})$
(currently implemented in PHANTOM)

Still problems!!

despite the conservation ensured by the spatial discretisation of the fluid equations and regularization of ϵ in [0,1] (Ballabio et al 2018), non-conservation may still arise due to timestepping errors



In the presence of strong gradient of ϵ (typically in the outer disc) we need to reduce the timestep to account for $\nabla\epsilon$

$$\Delta t < C_0 \frac{h}{\sqrt{\tilde{c}_\mathrm{s} + \epsilon^2 t_\mathrm{s}^2 c_\mathrm{s}^4 / h^2}} \; \frac{2a}{a^2 + b^2} \quad \text{with} \quad a = 1 - h^2 \frac{\nabla^2 \epsilon}{\epsilon}, \quad b = 2h \frac{|\nabla \epsilon|}{\epsilon}$$

But…

we see numerical inaccuracies when such strong gradients are present in the disc for particles with large stopping time…

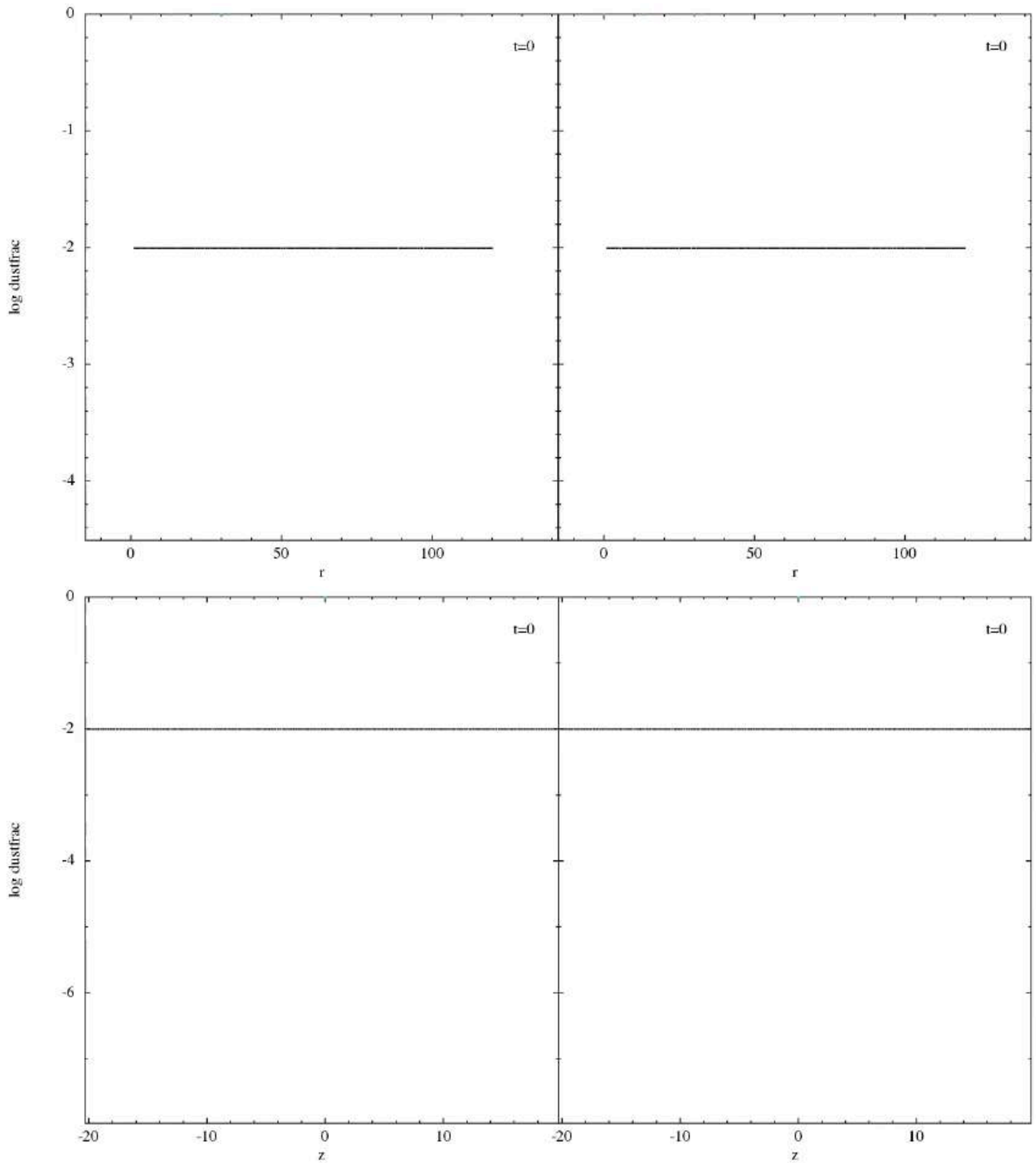
Tests: stop the evolution of particles with $t_{\rm s} > \dfrac{h}{c_{\rm s}}$

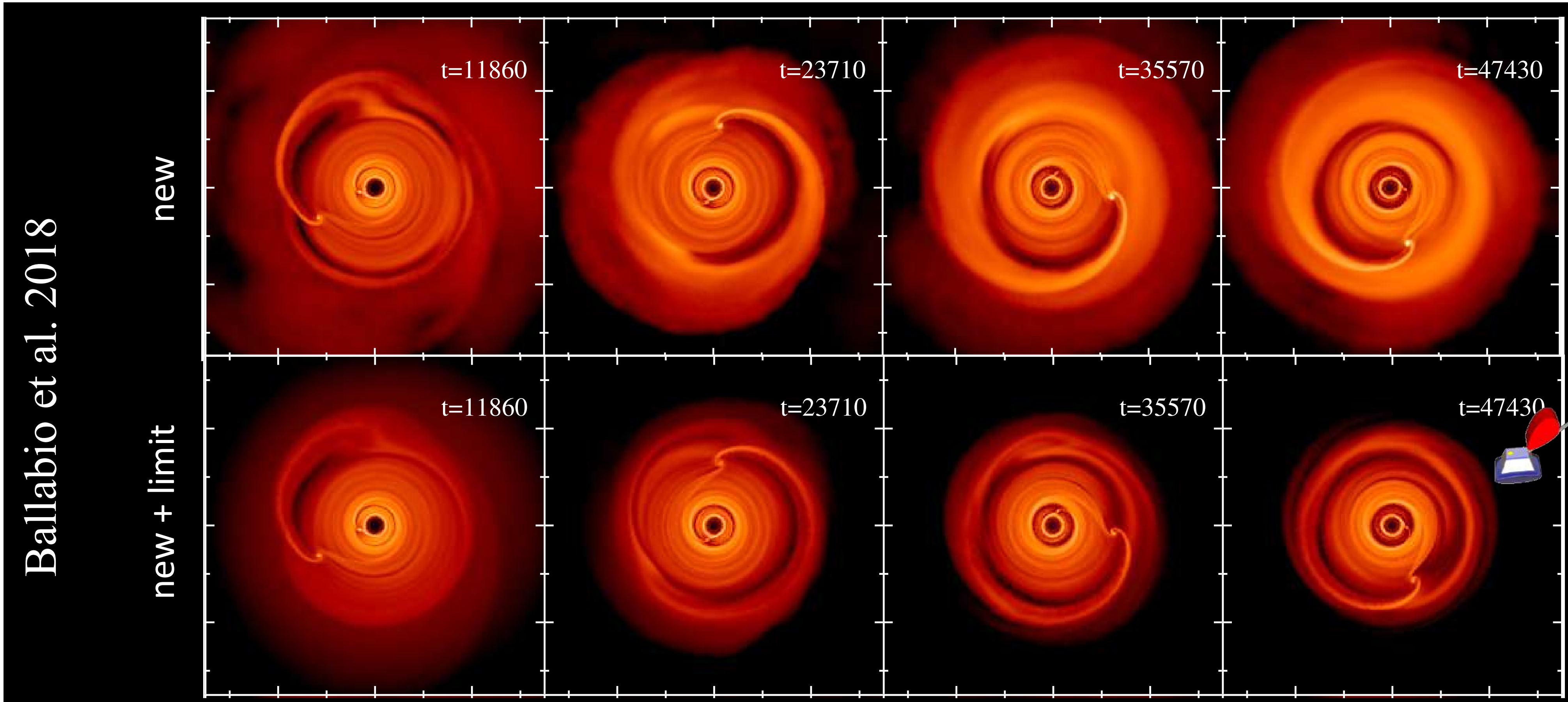
(limit of validity of the terminal velocity approximation)

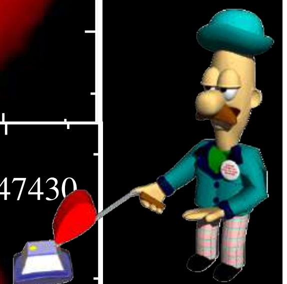
How to ‘fix’ the problem?: enforcing the following limit on the stopping time or Stokes Number:

$$\tilde{t_{\rm s}} = \min\left(t_{\rm s}, \frac{h}{c_{\rm s}}\right) \Longleftrightarrow \tilde{\rm St} = \min\left({\rm St}, \frac{h}{H}\right)$$

ilimitdustflux = T in the input file







Warning: limiting the stopping time leads to an underestimate of the radial flux of large grains with $t_{\rm s} > \dfrac{h}{c_{\rm s}}$

Even using a better timestepping/numerical scheme, the dynamics of grains with $t_{\rm s} > \dfrac{h}{c_{\rm s}}$ is not correct with the one fluid + terminal velocity approximation

Use with care!!

Take home messages

two-fluid method (dust_method = 2 in setup_disc.F90)

Best use: simulate the dynamics of large grains in weak drag regime (i.e. large Stokes numbers).

Warning: It can be used to simulate tightly coupled dust grains but the timestep will be constrained by t_s and you need to make sure that the resolution $h < c_s t_s$. If you want to use it, do a detailed resolution study and prepare to wait!

one-fluid + diffusion method (dust_method = 1 in setup_disc.F90)

Best use: simulate the dynamics of small grains in strong drag regime (i.e. small Stokes numbers).

Warning: make sure the Stokes number of the dust grains in your simulation is $St < h/H$!!
Even if the scheme appears numerically stable, the dynamics might be incorrect.

For system with a large dynamical range in, e.g., gas density, a single grain size can be strongly-coupled in one region of the disc and weakly-coupled in another. Thus, you need to make sure your algorithm is best suited to simulate dust dynamics

Possible solution: a hybrid scheme that marries the two approaches

Thanks for your attention!