Stellar Physics at Paris Observatory Star formation with RANSES

Implementing new physics and performing challenging simulations



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 10^{-20}

10-17



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Accretion + Ejection

Protoplanetary disk

Matter ejected at the poles (winds and jets)



10 000 - 100 000 yrs



Protoplanetary disks

Quasi keplerian Gaz + dust

Planet formation by coagulation/fragmentation and accumulation of dust grains

Dispersal of the disk (Winds? Photo-evaporation?)

1 000 000 - 50 000 000 yrs



Introduction A key component: dust

Interstellar dust grains

Distribution

1% of the mass

Distribution in the diffuse ISM (MRN, Mathis et al., 1977)

$$\frac{\mathrm{d}n(s)}{\mathrm{d}s} \propto s^{-3.5}; s \in [5, 250] \text{ nm}$$

Larger grains in denser regions ?

1-10 microns in dense cores (Pagani et al., 2010)

- 10-100 microns around protostars (Kataoka et al., 2015; Sadavoy et al., 2018a, b, 2019; Galametz et al., 2019)
- 1-10 mm in protoplanetary disks

Crucial for

Observations : major tracer in star forming clouds Dynamics : Coupled with the gas and also the magnetic field. Thermodynamics : major cooling species and catalyser for molecule formation Planet formation : dust grains are the building blocks of planets

But .. Dust is challenging to take into account numerically !





Introduction Dust is a numerical challenge

different dynamical evolution

current method can handle all of them

exchange between sizes modelled by a non-linear integro-differential equation.

Difficulty 1 Dust grains are distributed in a spectrum of sizes -> Each dust size has a

Difficulty 2 Small grains are tightly coupled to the gas and large grains are completely decoupled (and very large grains are not in the fluid regime) -> 3 main regimes. No

- **Difficulty 3** Dust grain are coagulating and fragmenting during star formation -> Mass
- **Difficulty 4** Dust grains are typically charged and thus are coupled to the magnetic field





Methods Multifluid equations

(Saffman 1962)

 $\frac{\partial \rho_{g}}{\partial t} + \nabla \cdot \rho_{g} \overrightarrow{v}_{g} = 0$ $\frac{\partial \rho_{d}}{\partial t} + \nabla \cdot \rho_{d} \overrightarrow{v}_{d} = 0$

$$\frac{\partial \rho_{g} \overrightarrow{v}_{g}}{\partial t} + \nabla (\rho_{g} \overrightarrow{v}_{g} \otimes \overrightarrow{v}_{g} + P_{g} \mathbb{I}) = \rho_{g} \vec{f} + K \overrightarrow{\Delta v}$$
$$\frac{\partial \rho_{d} \overrightarrow{v}_{d}}{\partial t} + \nabla \rho_{d} \overrightarrow{v}_{d} \otimes \overrightarrow{v}_{d} = \rho_{d} \vec{f} - K \overrightarrow{\Delta v}$$
$$\frac{\partial E_{g}}{\partial t} + \nabla \cdot (E_{g} + P_{g}) \overrightarrow{v}_{g} = K \overrightarrow{\Delta v} \cdot \overrightarrow{\Delta v}$$

- Advantages:
- Simple
- Complete (in the fluid approximation)
 - Drawback:
 - 2 equations per dust species
 - Not convenient in Lagrangian codes
 - Intrusive for existing codes

 $\cdot \overline{\Delta v}$

Methods Dust and gas as one fluid

(Laibe & Price 2014a,b,c) See also Price & Laibe 2015; Lin & Youdin 2017; Hutchison et al., 2018 and Lebreuilly et al., 2019

Can we reformulate the multi-fluid equations using one fluid?

One density $\rho \equiv \rho_{\rm g} + \rho_{\rm d}$

One advection velocity $\vec{v} \equiv \frac{\rho_{\rm d} \vec{v}_{\rm d} + \rho_{\rm g} \vec{v}_{\rm g}}{\rho}$

Several phases (gas and each dust sizes) $\epsilon \equiv \rho_d / \rho$ and $\Delta \vec{v} \equiv \vec{v}_d - \vec{v}_g$

Note: Same as in magnetohydrodynamics (MHD) : ions, electrons and neutrals are all part of a monofluid.



Methods Monofluid, mass conservation

(Laibe & Price 2014a,b,c) See also Price & Laibe 2015; Lin & Youdin 2017; Hutchison et al., 2018 and Lebreuilly et al., 2019



$$\frac{\partial \rho_{\rm d}}{\partial t} + \nabla \cdot \rho_{\rm d} \overrightarrow{v}_{\rm d} = 0 \quad \longrightarrow \quad \frac{\partial \rho_{\rm d}}{\partial t}$$

$$+ \frac{\partial \rho_{d}}{\partial t} + \nabla \cdot \rho_{g} \overrightarrow{v}_{g} + \nabla \cdot \rho_{d} \overrightarrow{v}_{d} = 0$$

$$\downarrow$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \overrightarrow{v} = 0 \quad \text{Remember}: \overrightarrow{v} \equiv \frac{\rho_{d} \overrightarrow{v}_{d} + \rho_{g} \overrightarrow{v}_{g}}{\rho}$$

$$\varepsilon = \nabla \left[\exp(\overrightarrow{v}_{d} + (1 - v) \overrightarrow{A_{v}}) \right] = 0$$

 $+ v \cdot |\rho \epsilon (v + (1 - \epsilon) \Delta v)| = 0$

Methods Full monofluid equations

(in a Lagrangian formulation)

$$\begin{aligned} \frac{\mathrm{d}\rho}{\mathrm{d}t} &= -\rho(\overrightarrow{\nabla}\cdot\overrightarrow{v}),\\ \frac{\mathrm{d}\overrightarrow{v}}{\mathrm{d}t} &= -\frac{\nabla P_{\mathrm{g}}}{\rho} + \overrightarrow{f} - \frac{1}{\rho}\nabla\cdot\left(\epsilon(1-\epsilon)\rho\overrightarrow{\Delta v}\otimes\overrightarrow{\Delta v}\right),\\ \frac{\mathrm{d}\epsilon}{\mathrm{d}t} &= -\frac{1}{\rho}\overrightarrow{\nabla}\cdot\left(\epsilon(1-\epsilon)\rho\overrightarrow{\Delta v}\right)\\ \frac{\mathrm{d}\overrightarrow{\Delta v}}{\mathrm{d}t} &= \frac{\nabla P_{\mathrm{g}}}{(1-\epsilon)\rho} - \frac{\overrightarrow{\Delta v}}{t_{\mathrm{s}}} - (\overrightarrow{\Delta v}\cdot\overrightarrow{\nabla})\overrightarrow{v} + \frac{1}{2}\nabla\left((2\epsilon-1)\overrightarrow{\Delta v}\cdot\overrightarrow{\Delta v}\right)\\ &+ (1-\epsilon)\overrightarrow{\Delta v}\times(\nabla\times(1-\epsilon)\overrightarrow{\Delta v}) - \epsilon\overrightarrow{\Delta v}\times(\nabla\times\epsilon\overrightarrow{\Delta v}),\\ \frac{\mathrm{d}e_{\mathrm{g}}}{\mathrm{d}t} &= -\frac{P_{\mathrm{g}}}{\rho(1-\epsilon)}\nabla\cdot\left(\overrightarrow{v} - \epsilon\overrightarrow{\Delta v}\right) + (\epsilon\overrightarrow{\Delta v}\cdot\nabla)e_{\mathrm{g}} + \epsilon\frac{\overrightarrow{\Delta v}\cdot\overrightarrow{\Delta v}}{t_{\mathrm{s}}}\\ &t_{\mathrm{s}} \equiv \rho_{\mathrm{d}}\rho_{\mathrm{g}}/(\rho K)\end{aligned}$$



See also Price & Laibe 2015; Lin & Youdin 2017; Hutchison et al., 2018 and Lebreuilly et al., 2019



Methods Monofluid, strong coupling regime

(Laibe & Price 2014a,b,c) See also Price & Laibe 2015; Lin & Youdin 2017; Hutchison et al., 2018 and Lebreuilly et al., 2019

Stopping time $t_{\rm s} \equiv \rho_{\rm d} \rho_{\rm g} / (\rho K) \approx \frac{\rho_{\rm grain} s_{\rm grain}}{\rho c_{\rm s}}$.

Stokes number $St = t_s/t_{dyn}$, where t_{dyn} is the dynamical timescale of the gas. In the ISM grains are 'small', we typically have St<1, we are in a strong coupling regime between the gas and the dust.

Methods Monofluid, strong coupling regime

(Laibe & Price 2014a,b,c) See also Price & Laibe 2015; Lin & Youdin 2017; Hutchison et al., 2018 and Lebreuilly et al., 2019

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho(\overrightarrow{\nabla}\cdot)$$

$$\frac{\mathrm{d}\overrightarrow{v}}{\mathrm{d}t} = -\frac{\nabla P_{\mathrm{g}}}{\rho} + \overrightarrow{f} - \frac{1}{\rho}\nabla\cdot\left(\epsilon(1-\epsilon)\rho\overrightarrow{\Delta v}\otimes\overrightarrow{\Delta v}\right)$$

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

$$\frac{\mathrm{d}\overrightarrow{\Delta v}}{\mathrm{d}t} = \frac{\nabla P_{\mathrm{g}}}{(1-\epsilon)\rho} - \frac{\overrightarrow{\Delta v}}{t_{\mathrm{s}}} - (\overrightarrow{\Delta v}\cdot\overrightarrow{\nabla})\overrightarrow{v} + \frac{1}{2}\nabla\left((2\epsilon-1)\overrightarrow{\Delta v}\cdot\overrightarrow{v}\right)$$

$$+(1-\epsilon)\overrightarrow{\Delta v}\times(\nabla\times(1-\epsilon)\overrightarrow{\Delta v}) - \epsilon\overrightarrow{\Delta v}\times(\nabla\times\epsilon\overrightarrow{v})$$

$$\frac{\mathrm{d}\epsilon_{\mathrm{g}}}{\mathrm{d}t} = -\frac{P_{\mathrm{g}}}{\rho(1-\epsilon)}\nabla\cdot\left(\overrightarrow{v}-\epsilon\overrightarrow{\Delta v}\right) + (\epsilon\overrightarrow{\Delta v}\cdot\nabla)e_{\mathrm{g}} + \epsilon\frac{\overrightarrow{\Delta v}}{t_{\mathrm{s}}}$$



Second order in Stokes First order in Stokes/Decaying in a stopping time



Methods Monofluid, strong coupling regime

(Laibe & Price 2014a,b,c) See also Price & Laibe 2015; Lin & Youdin 2017; Hutchison et al., 2018 and Lebreuilly et al., 2019



Advantages:

Still one fluid.

Less intrusive for a code

Fewer equations (drift velocity directly computed from the force balance)

Easier to implement

Drawback:

Incomplete (St<1).

Methods Monofluid in strong coupling regime

(With multiple species)



With
$$\mathscr{C} \equiv \sum_{l=1}^{\mathcal{N}} \epsilon_l, T_{s,k} \equiv \frac{t_{s,k}}{1 - \epsilon_k} - \sum_{l=1}^{\mathcal{N}} \frac{\epsilon_l}{1 - \epsilon_l} t_{s,l} \text{ and } \mathcal{T}_s \equiv \frac{1}{\mathscr{C}} \sum_{l=1}^{\mathcal{N}} \epsilon_l T_{s,l}$$

-), <u>Advantages:</u>
 - Still one fluid.
 - Less intrusive for a code
 - Fewer equations (drift velocity directly computed from the force balance)
 - Easier to implement
 - Drawback:
 - Incomplete (St<1).

Reminder for a pure gas

Conservative form

$$\begin{split} & \frac{\partial \mathbb{U}}{\partial t} + \nabla \cdot \mathbb{F}(\mathbb{U}) = 0 \\ & \mathbb{U} \equiv \left(\rho_{\rm g}, \rho_{\rm g} \mathbf{v}_{\rm g}, E_{\rm g} \right); \ \mathbb{F}(\mathbb{U}) \equiv \left(\rho_{\rm g} \mathbf{v}_{\rm g}, \rho_{\rm g} \mathbf{v}_{\rm g} \otimes \mathbf{v}_{\rm g} + P_{\rm g} \mathbb{I}, \mathbf{v}_{\rm g}(E_{\rm g} + P_{\rm g}) \right) \end{split}$$

Integral over a control volume

$$\int_{x_{\text{left}}}^{x_{\text{right}}} \left(\mathbb{U}\left(T\right) - \mathbb{U}\left(0\right) \right) dx + \int_{0}^{T} \left(\mathbb{F}(x_{\text{right}}) - \mathbb{F}(x_{\text{left}}) \right) dt = 0$$

Godunov Scheme (Godunov 1959) & Riemann problem $\mathbb{U}_{i}^{n+1} = \mathbb{U}_{i}^{n} - \left(\mathbb{F}_{i+1/2}^{n+1/2} - \mathbb{F}_{i-1/2}^{n+1/2}\right) \frac{\Delta t}{\Delta x}; \mathbb{F}_{i\pm 1/2}^{n+1/2} = \mathbb{F}^{\star}\left(\mathbb{U}_{i}^{n}, \mathbb{U}_{i-1}^{n}\right)$

Stability constrain (Courant et al., 1928)

$$\Delta t \equiv C_{\rm CFL} \frac{\Delta x}{c_{\rm fastest}}$$

Now with the dust (see Lebreuilly et al., 2019)

Conservative form $\frac{\partial \mathbb{U}}{\partial t} + \nabla \cdot \mathbb{F}_{H}(\mathbb{U}) + \nabla \cdot \mathbb{F}_{\Delta}(\mathbb{U}) = 0$

 $\mathbb{U} \equiv \left(\rho, \rho \mathbf{v}, E, \rho_{\mathrm{d},k}, \dots\right); \mathbb{F}_{\mathrm{H}}(\mathbb{U}) \equiv \left(\rho \mathbf{v}, \rho \mathbf{v} \otimes \mathbf{v} + P_{\mathrm{g}}\mathbb{I}, \mathbf{v}(E + P_{\mathrm{g}}), \mathbb{V}_{\mathrm{H}}(\mathbb{U})\right)$

We perform the integration in two distinct steps (operator sp

1. We treat the 'barycentre' terms (almost already done in RAMSES) 2. We treat the differential advection of the dust terms represented by the flux : \mathbb{F}_{Λ}

The dust 'source' term $\nabla \cdot \mathbb{F}_{\Lambda}(\mathbb{U})$ is computed in two steps 1. Predictor step : variables computed at cell interfaces and half timesteps (using slope limiters and finite differences) 2. Flux computed by solving a Riemann problem a cell discontinuities and added in a conservative way using the Godunov scheme

Note that this is exactly what was already done for the gas fluxes !

$$,\rho_{\mathrm{d},k}\mathbf{v},\dots);\mathbb{F}_{\Delta}(\mathbb{U})\equiv\left(0,0,\frac{P_{\mathrm{g}}}{\gamma-1}\frac{\mathscr{CT}_{\mathrm{s}}}{1-\mathscr{C}}\frac{\nabla P_{\mathrm{g}}}{\rho},\rho_{\mathrm{d},k}\frac{T_{\mathrm{s},k}\nabla P_{\mathrm{g}}}{\rho},\dots\right)$$

plitting)

Validation tests (see Lebreuilly et al., 2019)

Diffusion (DUSTYDIFFUSE)





Shock (DUSTYSHOCK)

Damping of sound waves (DUSTYWAVE)



Validation tests (see Lebreuilly et al., 2019)

Settling in protoplanetary disks

1 microns



Validation tests (see Lebreuilly et al., 2019)

Settling in protoplanetary disks



Application The protostellar collapse (see Lebreuilly et al., 2020)

Gas (left) and dust (right) densities

 $\log(\rho)$ [g cm⁻³]



Dust enrichment in the different objects





Application Current sheets in protoplanetary disks (Lebreuilly et al., sub)

Current sheets



Dust concentration variations in the current sheets







Application Turbulent molecular clouds (Commerçon et al, in prep)







Next stage Dust growth

There are two possibilities to take into dust growth. 1. Solve the full coagulation equation (Smoluchowski) that considers mass exchange between bins. 2. Only follow the evolution of the peak of the distribution: "monodisperse growth" We consider one species: but of varying size $s_d(\vec{r}, t)$

$$\frac{\partial \rho_d \, s_d}{\partial t} + \nabla \cdot \rho_d \, s_d \overrightarrow{v}_d = A_{\text{gain,loss}} \frac{\rho_d \, s_d}{t_{\text{growth}}}, \text{ we also}$$

What we can get from that:

- 1. Typical grain size (in terms of mass)
- 2. Dust mass content of disks
- 3. Spatial repartition of large dust grains
- 4. Better synthetic observations

While I am used to both methods. The first one is still tricky in 3D so I'll present only the second one.

o advect dust grain as passive scalars at $\overrightarrow{v}_d \neq \overrightarrow{v}_g$

Next stage Dust growth

Gas density



Dust-to-gas ratio



Goals

- 1. To generate synthetic self-consistent populations of disks and constrain (statistically) the initial conditions of planet formation
- 2. To predict the internal structure (gas, temperature, magnetic field) of protoplanetary disks
- 3. To predict the dust content (in mass and size) of protoplanetary disks
- 4. To provide a physical interpretation of young disk observations

Methods

Several clump collapse calculations with different initial conditions (magnetic field, Mach number, size, mass) and physical processes (non-ideal MHD, radiative feedback, dust)

Rezooms on some specific disks to get the internal structure ! Synthetic observations with radiative transfer code

Ressources

32.7 million CPU hours (so far ~70% used) on the JUWELS cluster -1 Run is about 3-4 million CPU hours on ~1000 CPUs.

See Lebreuilly et al., (2021) for a similar previous work

















PRACE Disk extraction



$$v_{\phi} > 2v_{r}$$
$$v_{\phi} > 2v_{z}$$
$$\frac{1}{2}\rho v_{\phi}^{2} > 2P_{th}$$
$$n > n_{thre} = 10^{9} \text{ cm}^{-3}$$

Joos et al., 2012

PRACE Disks variety









26.730







PRACE Disk populations





PRACE Synthetic observations



ALL CREDITS for the synthetic obs go to Tung Ngo Duy

PRACE Rezooms



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PRACE Impact of the magnetic field



WEAK FIELD = FIDUCIAL / 5

How to get PRACE time?

https://prace-ri.eu/hpc-access/calls-for-proposals/ Call for proposals every 6 months (spring and autumn) Proposal (template available at the previous link): mine was about 17 pages.

- 1. Key scientific contribution (for example disk populations in my case)
- 2. Detailed plan, justification for the ressources, scientific overview of the project
- 3. Code presentation, performances, ressources needed & data management
- 4. Detailed presentation of the HPC performances of the code (strong, weak scaling on the setup proposed)
- 5. Work plan : Gantt chart, publication plan, communication plan

Why/When asking a PRACE?

If a lot of ressources are needed -> You can do a lot with PRACE time. It's about 10 times what the CPU time I was used to get.

If you can propose something useful for the community (in my case catalogues of disks and clumps to compare with observations)

My experience

Ask help from people who got a PRACE in the past !

Time consuming: needs preparation and requires a perfect work plan.







DUSTY RAMSES

We have implemented dust (dynamics and growth) in RAMSES. We have extensively tested the implementation We have been using this module in the context of: Protostellar collapse Protoplanetary disks Turbulent molecular clouds

PRACE "Synthetic populations of protoplanetary disks"

We can now predict the initial properties of protoplanetary disks self-consistently in massive protostellar clumps (as a function of B, Mach, the cloud size, ...) For the community: future open access of the simulations <u>http://www.galactica-simulations.eu/db/</u> (previous ones published in Lebreuilly et al., 2021 are already there)