multrigrain size model for Nautilus

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1 Introduction

Nautilus is now a multrigrain sizes code (Iqbal and Wakelam (2018)) which allows to give the abundances of species as a function of time with a full distribution of dust. From the perspective to use Nautilus in the context of circumstellar disk modelisations with a more realistic description of dust grains, we want to add dust settling and size distributions effects which both impact significantly the chemical evolution of the disk. In other words, this implies to obtain the dust density number $n_d(r, z, a)$ in Eq.1 at each coordinates (i.e. radius and altitude) for each grain species considered.

$$\frac{n_d(r, z, a)}{n_H(r, z)} \tag{1}$$

$n_H(r, z)$ is the Hydrogen density and a defines the grain species. In this documentation we first describe the disk model used to compute dust grain distribution then we comment the input files, scripts and how the output file is used by Nautilus. All scripts are written in Python 2.7.10.

2 disk model

In all the following description, g index always stands for gas and d always stands for dust. The index 0 stands for the reference radius. Unless specified, volumes are expressed in cm^3 and the mass in g. n always describes a number density while ρ always describe a mass density.

2.1 Gas description

The gas in the disk is considered to be in hydrostatic equilibrium. The gas vertical density is gaussian distributed and it is described by Eq.2 (Boehler et al (2013)). This density distribution is valid for H_2 and H_e. Unless specified, the gas profile, the gas surface density and the gas scale height will refer to the hydrogen nuclei (atomic or molecular) in the disk.

$$\rho_g(r, z) = \frac{\Sigma_g(r)}{H_g(r)\sqrt{2\pi}} \exp\left(\frac{-z^2}{2H_g(r)^2}\right) \tag{2}$$

Eq.2 can also be expressed as follows:

$$\rho_g(r, z) = \rho_{g,mid}(r) \exp\left(\frac{-z^2}{2H_g(r)^2}\right) \tag{3}$$

with $\rho_{g,mid}(r)$ the density of the gas in the midplane at radius $= r$ and $H_g(r)$ the gas scale height also given by Eq.4:

$$H_g(r) = H_{g,0}\left(\frac{r}{R_0}\right)^h \tag{4}$$

where $H_{g,0}$ is the scale height of the gas at the reference radius R_0 and $h = \frac{3}{2} - \frac{q}{2}$. q is the exponent in the power-law which defines the kinetic temperature T_k along the radius in the mid-plane

$$T_k(r, z=0) = T_k(R_0, z=0)\left(\frac{r}{R_0}\right)^{-q} \tag{5}$$

Assuming static vertical equilibrium, the scale height of the gas at reference radius is given by

$$H_{g,0} = \sqrt{\frac{k_b T_{mid} R_0^3}{\mu_m amu G M_\odot}} \tag{6}$$

The gas surface density $\Sigma_g(r)$ also follows a power law

$$\Sigma_g(r) = \Sigma_{g,0}\left(\frac{r}{R_0}\right)^{-p} \tag{7}$$

The gas is assumed to be in Keplerian rotation as an approximation (if the gas pressure is small and the disk mass limited).

$$v_g(r) = \sqrt{\frac{GM}{r}} \iff \Omega_g(r) = \sqrt{\frac{GM}{r^3}} \tag{8}$$

Then the disk scale height can be given by

$$H_g(r) = \frac{C_s(r)}{\Omega_g(r)} \tag{9}$$

where C_s is the sound speed in the disk which only depends on the radius since the equation of state is locally isothermal (Fromang and Nelson (2009)).
The total disk mass is

$$M_{disk} = M_{gas} + M_{dust} \tag{10}$$

Considering only the gas, the mass can be given as a function of the surface density by

$$M_{gas} = \int_{R_{in}}^{R_{out}} 2\pi r \Sigma_g(r) dr = \int_{R_{in}}^{R_{out}} 2\pi r \Sigma_{g,0}\left(\frac{r}{R_0}\right)^{-p} dr \tag{11}$$

where R_{out} is the outer radius of the gas disk and R_{in} is the inner radius. Eq.11 then becomes

$$M_{gas} = 2\pi\Sigma_{g,0} \int_{R_{in}}^{R_{out}} r\left(\frac{r}{R_0}\right)^{-p} dr \tag{12}$$

Integrating Eq.12 allows to obtain $\Sigma_{g,0}$

$$\Sigma_{g,0} = \frac{M_{gas} R_0^{-p}(2-p)}{2\pi(R_{out}^{2-p} - R_{in}^{2-p})} \tag{13}$$

For instance, for $R_{out} = 300$ au, $M_{gas} = 0.008$ M$_\odot$, $R_0 = 100$ au and $p = 1.5$, we get $\Sigma_{g,0} = 0.335$ g.cm^{-2}.

2.2 Dust description

2.2.1 Dust quantity

The material composition is distributed into two separate grain populations, one of silicate composition and the other of graphite composition, according to the MRN model (Mathis, Rumpl and Nordsieck (1977)). However, the code Nautilus uses a mean value, not two distinct populations of grains. We define the material density of the grains:

$$\rho_m = 2.5 g.cm^{-3}. \tag{14}$$

but the value can vary. Mathis, Rumpl and Nordsieck (1977), Draine and Lee (1984), Laor and Draine (1993), Weingartner and Draine (2001) also show that the number of species in the size interval [a, a + da] is given by

$$dn(a) = C n_H a^{-d} da \tag{15}$$

with C the normalised constant, n_H the number density of Hydrogen nuclei and dn(a) the number of grains in the size interval [a, a + da].

We first consider a continuous grain size distribution. We can use Eq.15 to obtain the dust mass per unit of volume:

$$m_{dust} = \int_{a_-}^{a_+} m(a) dn(a) = \int_{a_-}^{a_+} \frac{4\pi}{3} \rho_m C n_H a^{3-d} da \tag{16}$$

where m(a) is the mass of grain species of size a per unit of volume and $\{a_-,a_+\}$ are the cutoff radii. The integration of Eq.16 gives

$$m_{dust} = \frac{4\pi}{3} \rho_m C n_H \frac{1}{4-d} (a_+^{4-d} - a_-^{4-d}) \tag{17}$$

The dust to gas ratio is

$$\zeta = \frac{m_{dust}}{m_{gas}} = \frac{m_{dust}}{n_H \mu_a m_H} \tag{18}$$

m_H is the mass of Hydrogen atom and μ_a is the mean molecular weight. The parameters are given in Table.2. Using Eq.17 and Eq.18 we isolate the normalization constant

$$C = \frac{3}{4\pi} \frac{\zeta \mu_a m_H}{\rho_m} (4-d) \frac{1}{(a_+^{4-d} - a_-^{4-d})} \tag{19}$$

We introduce the surface density of a species of size a following a radial power-law

$$\sigma_d(r,a) = \sigma_{d,0}(a) \left(\frac{r}{R_0} \right)^{-p} \tag{20}$$

where $\sigma_{d,0}(a)$ is the surface density of the dust species of size a at the reference radius R_0. We assume that the dust surface density follows the same law along the radius as the gas. We introduce the dust surface density integrated on all the grain sizes

$$\Sigma_d(r) = \int_a \sigma_d(r,a) da \tag{21}$$

2.2.2 Vertical distribution

$\sigma_d(r,a)$, the surface density at r for a grain size a (also given by Eq.20) can be expressed by integrating the dust mass density along the altitude:

$$\sigma_d(r,a) = \int_{-\infty}^{+\infty} \rho_d(r,z,a) dz \tag{22}$$

We assume that the mass density vertical profile also follows a Gaussian distribution for each grain species.

$$\rho_d(r,z,a) = \rho_{d,mid}(r,a) \exp\left(\frac{-z^2}{2H_d(r,a)^2} \right) \tag{23}$$

Using Eq.22 and Eq.23 we can write:

$$\rho_{d,mid}(r,a) = \frac{\sigma_d(r,a)}{\int_{-\infty}^{+\infty} \exp\left(\frac{-z^2}{2H_d(r,a)^2}\right) dz} \tag{24}$$

Solving the integral analytically gives

$$\rho_{d,mid}(r,a) = \frac{\sigma_d(r,a)}{\sqrt{2\pi} H_d(r,a)} \tag{25}$$

Unlike the gas, the dust is settled along the altitude. The dust scale height $H_d(r,a)$ is different from the gas scale height $H_g(r)$ and depends on the grain size a since the dust scale height depends on the settling.

2.2.3 Settling factor

The dust scale height and the gas scale height are differently characterized. We give a settling factor (Youdin et al (2007), Fromang and Nelson (2009), Boehler et al (2013), Dong et al (2015))

$$s(a,r) = \frac{H_d(a,r)}{H_g(r)} = \frac{1}{\sqrt{1 + T_{s,mid}\frac{S_c}{\alpha}}} \tag{26}$$

where S_c is the Schmidt number, α a viscosity coefficient and $T_{s,mid}$ the dimensionless stopping time of the dust in the midplane (Youdin et al (2007), Boehler et al (2013)). The Schmidt number is a dimensionless number defined by the ratio between the turbulent viscosity and the turbulent diffusion

$$S_c = \frac{\nu_t}{D_t} \tag{27}$$

which is a way to estimate the difference between the diffusion and viscosity turbulence (Shakura & Sunyaev (1973)). T_s, the dimensionless stopping time of the dust (also called Stokes number) at any altitude z is given by

$$T_s(r,z) = \tau_s \Omega(r,z) = \frac{a\rho_m}{\rho_g(r,z)C_s}\Omega(r) \tag{28}$$

in the Epstein regime. τ_s defines the stopping time of a dust particle which is the typical time for a dust particle initially at rest to reach the local gas velocity. The product of τ_s by $\Omega(r)$ is a way to compare the stopping time to the dynamical time in the disk. We note that the grain size depends linearly on T_s. Moreover, if we consider

$$\Omega(r) = \frac{C_s}{H_g(r)} \tag{29}$$

Eq.28 is also expressed by

$$T_s(r,z) = \frac{a\rho_m}{\rho_g(r,z)H_g} = \frac{\sqrt{2\pi}a\rho_m}{\Sigma_g(r)} \exp\left(\frac{-z^2}{2H_g(r)^2}\right) \tag{30}$$

At $z = 0$:

$$T_{s,mid}(r) = \frac{\sqrt{2\pi}a\rho_m}{\Sigma_g(r)} \tag{31}$$

We see that the ratio between H_d et H_g is directly dependant on the grain sizes a. We show that

$$\begin{aligned} \tau_s\Omega(r) \ll 1 &\implies \text{grains well coupled to the gas} \\ \tau_s\Omega(r) \gg 1 &\implies \text{grains settle toward midplane} \end{aligned} \tag{32}$$

which is well-characterised by Eq.26 as $H_g \to H_d$ when $\tau_s\Omega(r) \ll 1$. The settling ratio decreases as grains get bigger and settle toward the mid-plane. Big grains are mainly subject to gravitational interactions and turbulent diffusion which set their vertical distribution (Dong et al (2015)). Fig.1 shows the evolution of the settling factor as a function of the dimensionless stopping time at R_0 which is directly dependant on the grain sizes. We compare the model used in our study (Eq.26) from Dong et al (2015) to the models from Boehler et al (2013) and simulations from Fromang and Nelson (2009). This looks consistent with their results.

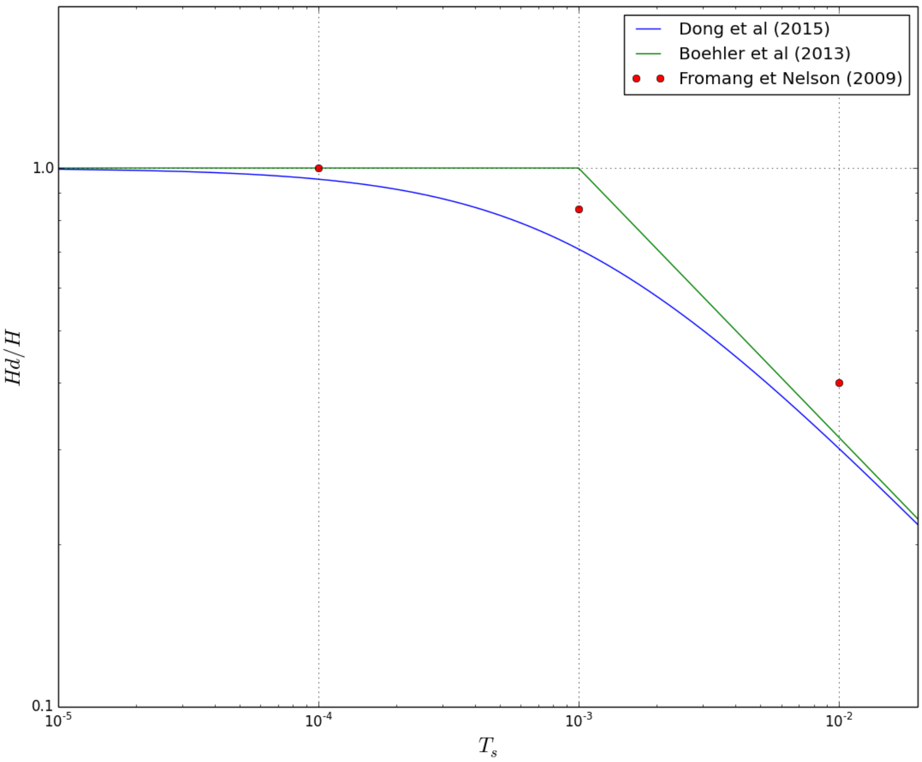

Figure 1: Settling factor as a function of the dimensionless stopping time at R_0, $\alpha = 0.001$ and $S_c = 1$. In green the model given by Boehler et al (2013), the red dots show the simulation values of Fromang and Nelson (2009) and the blue curve is the model we use (Dong et al (2015)).

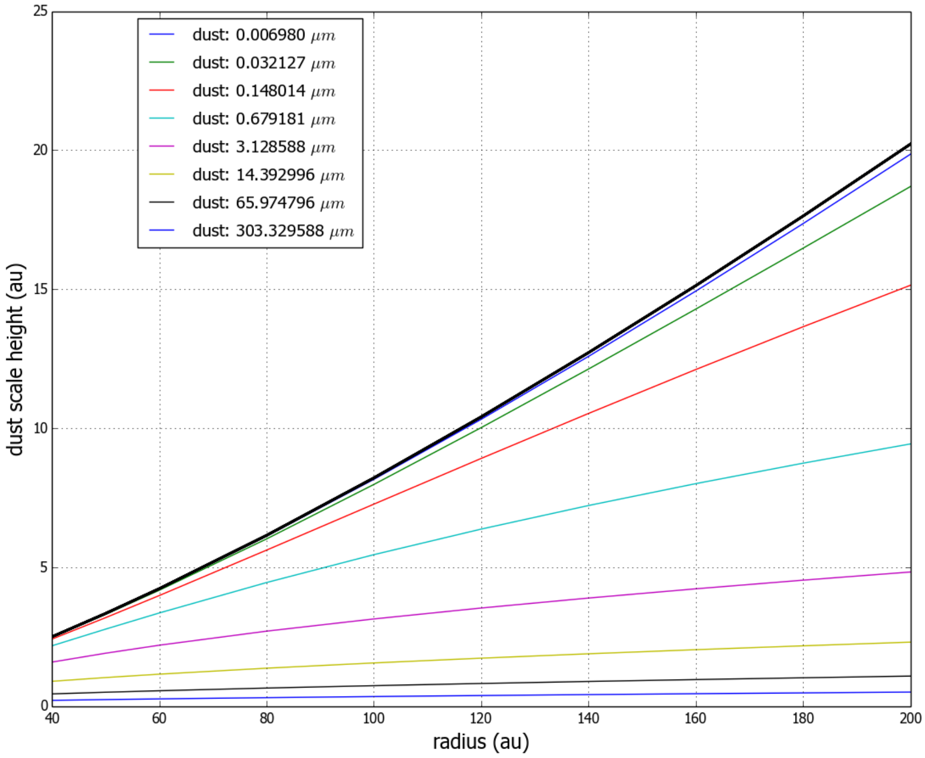

Figure 2: Scale heights of the dust as a function of the radius for different grain sizes. The black wide curve corresponds to the gas scale height.

Eq.33 is the dimensionless stopping time in the midplane $T_{s,t}$ at which the settling factor is x % smaller than the asymptotic value for small grains

$$T_{s,t} = \frac{\alpha}{S_c}\frac{(1 - s_{x\%}^2)}{s_{x\%}^2} \tag{33}$$

which is obtained from Eq.26. $T_{s,t}$ is the value at $z = 0$ but we don't use the index mid in order to simplify the notation. By definition $s_{x\%} = 0.01x$. For a viscosity coefficient $\alpha = 0.01$, a Stoke Number S_c set to 1 (which means that the turbulent viscosity and turbulent diffusion are equal) and $s_{90\%}$ we obtain $T_{s,t} = 2.35.10^{-3}$. This value is valid for all radius since $s_{90\%}$ is set to 0.9 regardless the radius. $T_{s,t}$ gives the transition between small and big grains for our model. Then we use Eq.31 and Eq.33 to set the grain size a_t that defines the transition size between small and big grains. we find:

$$a_t(r) = \frac{T_{s,t}\Sigma_g(r)}{\sqrt{2\pi}\rho_m} = \frac{T_{s,t}\Sigma_{g,0}}{\sqrt{2\pi}\rho_m}\left(\frac{r}{R_0}\right)^{-p} \tag{34}$$

$a_t(r)$ depends on the radius but also on $\Sigma_{g,0}$, which means that the transition size will vary as a function of the disk mass. Fig.3 illustrates the transition sizes (black fat curves) as a function of r for two disks of different mass, the Flying Saucer and DM tau. For a given disk, the grains above the black curve are considered big while the ones below are considered small in the model. We see that the transition size curve for DM tau is above the one of the Flying Saucer for any radius because DM tau is heavier.

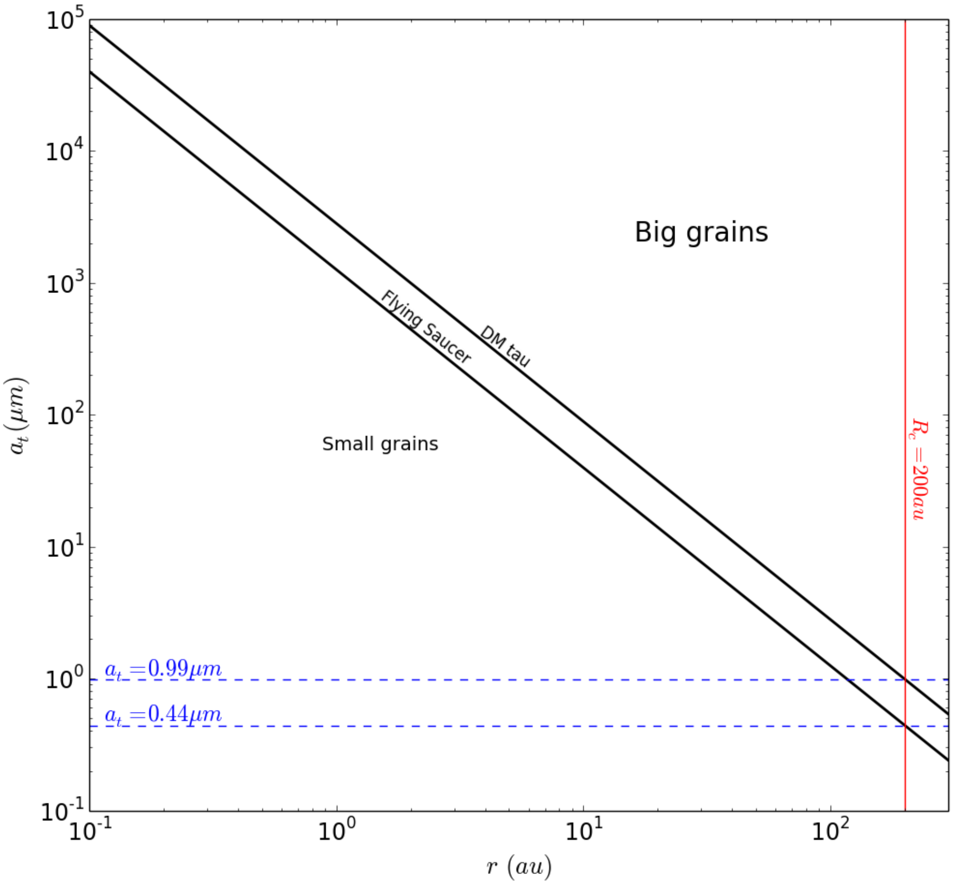

Figure 3: the transition grain size a_t in μm as a function of the radius of two disks, the Flying Saucer (M = 0.008 $M_\odot$) and DM tau (M = 0.03 $M_\odot$). All the grains above the black curve of a disk are considered big while all the grains below are considered small. For instance, with $s_{90\%}$, $\alpha = 0.01$ and at $R_c = 200$ au we find $a_t = 3.26$ μm for DM tau while a_t= 0.44 μm for the Flying Saucer.

The model herein will divide the disk into an inner part and an outer part from where only small grains survive. This division is given by the radius R_c. Then the size that separates small and big grains at R_c is defined by a_t as given by Eq.34. To sum up, the model determines that from the radius R_c every grains of size $a < a_t$ stop existing (Fig.4).

	Flying Saucer[a]	DM tau[b]
Disk mass (solar mass)	0.008	0.03
surface density at reference (g.cm^{-2})	0.335	0.75
R_c(au)	200	200
a_t with $s_{90\%}$ (μm)	0.44	0.99
a_t with $s_{50\%}$ (μm)	5.67	12.7

Table 1: List of parameters for two example disks. The values of mass and surface density are from references. a: Dutrey et al. (2017). b: Guilloteau et al. (2011); Pietu et al. (2007). The values of a_t are given by the model introduced herein.

2.2.4 Dust to gas ratio

Fig.2 and Fig.4 show the evolution of the settling seen edge-on for different grain sizes. We assume that only small dust grains remain beyond R_c as previously said. Therefore we have to define two dust to gas ratios

$$
\begin{aligned}
\zeta_{in} &= \langle \frac{\Sigma_d(r,a)}{\Sigma_g(r)} \rangle = \frac{1}{100} \text{ for r} < R_c \\
\zeta_{out} &= \langle \frac{\Sigma_d(r,a)}{\Sigma_g(r)} \rangle = \frac{1}{1000} \text{ for r} \geq R_c
\end{aligned}
\tag{35}
$$

Or in other words the integrated dust surface densities is a factor of the gas surface density as

$$
\begin{aligned}
\int \sigma_d(r,a)da &= \zeta_{in}.\Sigma_g(r) \text{ for r} < R_c \\
\int \sigma_d(r,a)da &= \zeta_{out}.\Sigma_g(r) \text{ for r} \geq R_c
\end{aligned}
\tag{36}
$$

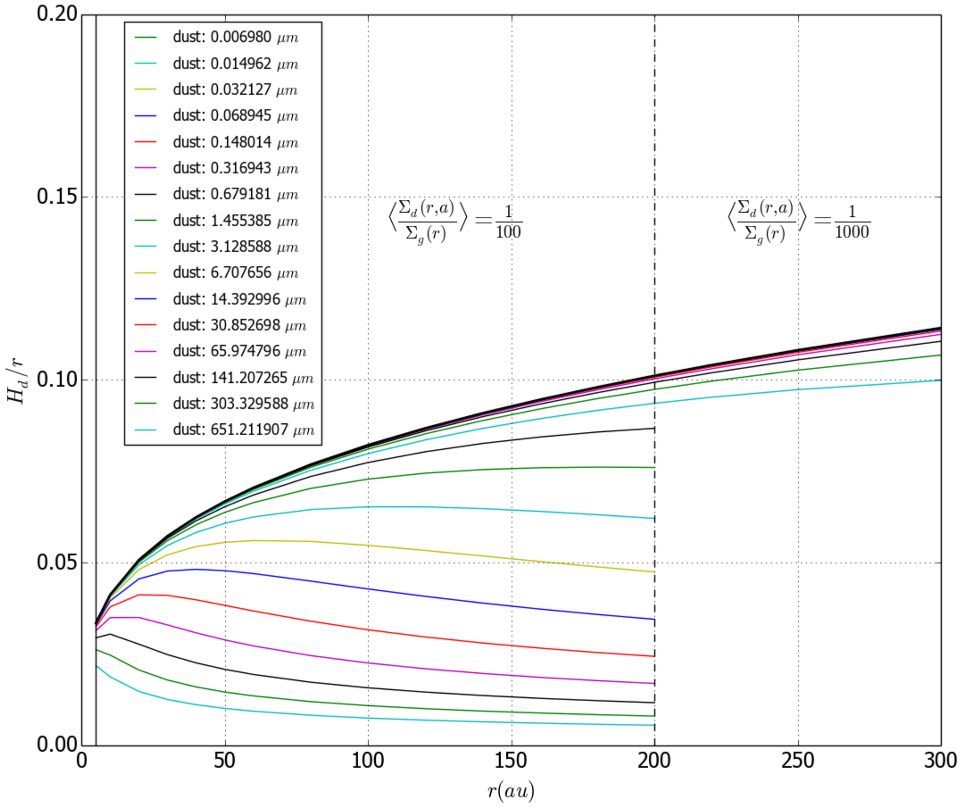

Figure 4: Illustration of the dust settling along the radius of the disk. It gives H_d/r as a function of the radius r. The cut radius R_c at which the dust to gas ratio changes from 1/100 to 1/1000 is given by the vertical dotted line and is set to 200 au in this example. Beyond this line, only the small grains are considered. $\alpha = 10^{-3}$ and $a_t = 4.43$ μm.

Therefore we define two dust surface densities, one for small grains the other for big grains as follows

$$\Sigma_s = \int_{a_-}^{a_c} \sigma_d(r,a)da$$
$$\Sigma_b = \int_{a_c}^{a_+} \sigma_d(r,a)da \quad (37)$$

And as a result

$$\Sigma_d(r) = \Sigma_s(r) + \Sigma_b(r) \quad (38)$$

3 Model implementation in Nautilus multi-grain code

3.1 Illustration of the implementation in Nautilus

This section is purely illustrative. We show herein how to implement the dust distribution model in Nautilus code for chemistry simulations. We discretize the grains size from now on. We give an example with a set of 4 different arbitrary grain sizes given in terms of stopping time $\Omega\tau_1 = 1e^{-2}$, $\Omega\tau_2 = 1e^{-3}$, $\Omega\tau_3 = 1e^{-4}$ and $\Omega\tau_4 = 1e^{-5}$. Fig.5 shows the density (in arbitrary units) as a function of the altitude z at the reference radius R_0 (see Table.3) and for $H_0 = 8.2105au$ (values from the Flying Saucer). The distribution is Gaussian distributed for the gas and the dust.

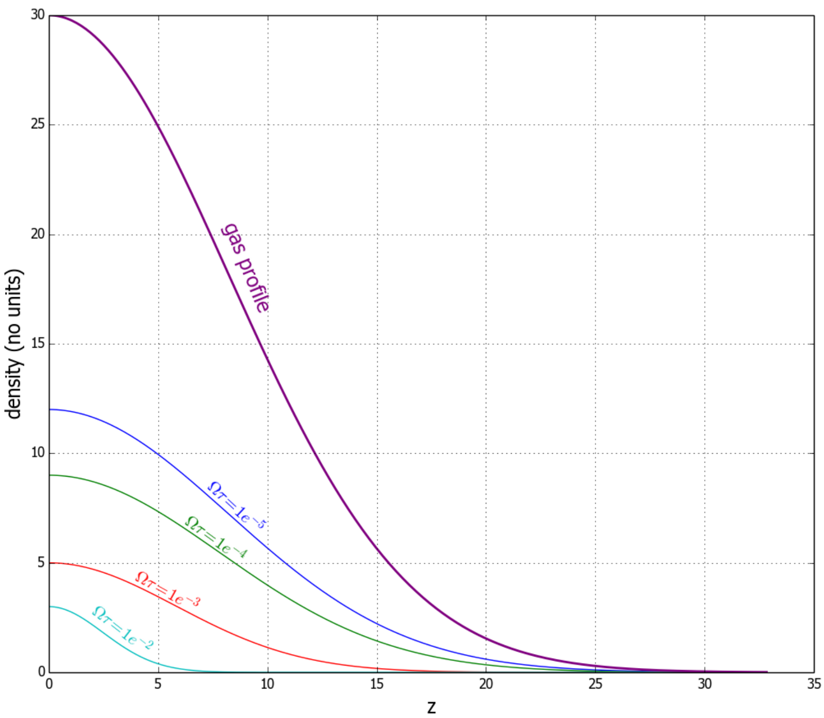

Figure 5: Density vertical profile of the dust and the gas in au at reference radius $R_0 = 100$ au. The density units are arbitrary. We show the disk only above the midplane.

Nautilus considers the abundance distribution according to the total number of Hydrogen (atomic and molecular) in gas phase, so the gas profile (in purple) will be that of the Hydrogen. The total size of the box is $z/H = 4$. So we convert the altitude z(au) to z/H in a 4 box to fit in Nautilus with H being the scale height of the Hydrogen.

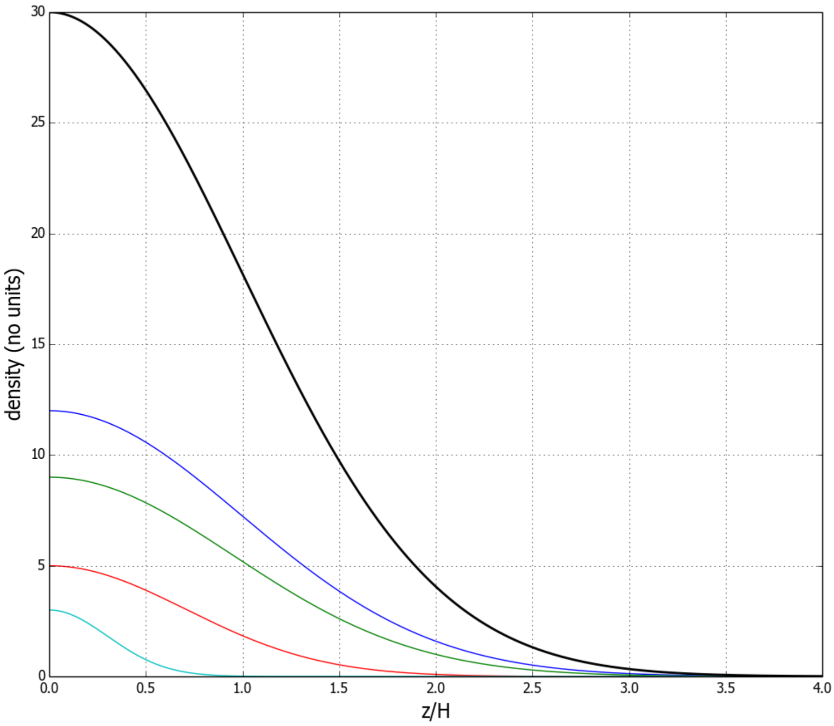

Figure 6: Density vertical profile as a function of z/H in the 4 box at reference radius $R_0 = 100$ au. The gas profile (black curve) would be that of the Hydrogen. We show the disk only above the midplane.

Nautilus divides the edge-on disk into a finite number of radius and altitudes

$$
\begin{aligned}
r &: (r_1, r_2, ..., r_k, ..., r_R) \\
z &: (z_1, z_2, ..., z_j, ..., z_S)
\end{aligned}
\tag{39}
$$

with R being the number of implemented radii and S the number of altitudes implemented that are called spatial points. Therefore, the disk is divided into cells with each cell having defined coordinates (r_k, z_j). As in Fig.7, the dus density profiles are discretized according to the spatial points.

Each cell at (r_k, z_j) in the grid receives the densities from all the grain species at the considered coordinates. The local $\zeta_{d/g}$ varies with z and r because of differential dust settling, but the vertically averaged $\zeta_{d/g}$ is given by the input model as a function of r.

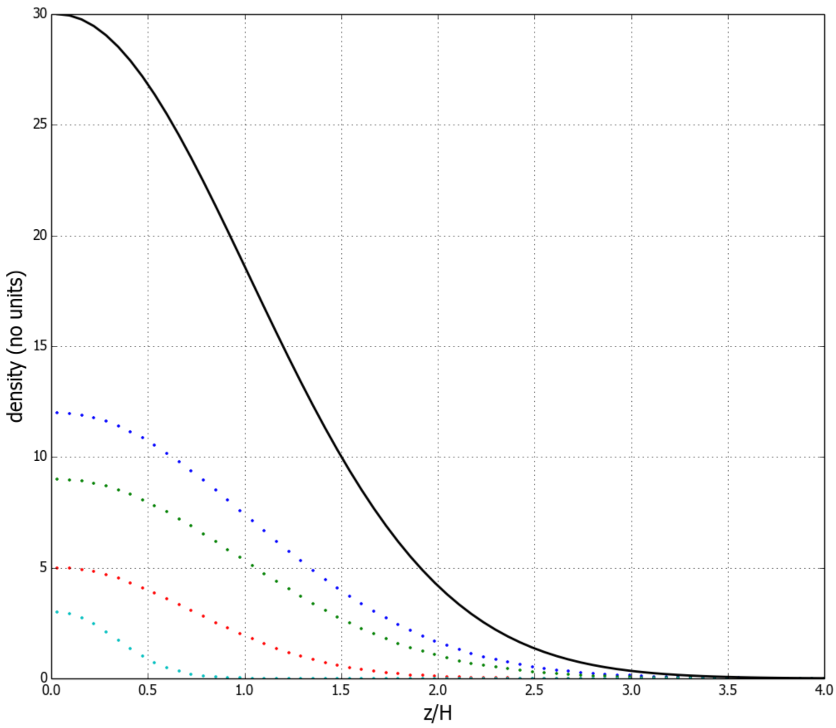

Figure 7: Vertical density profile above the midplane as a function of z/H in the 4 box with the profile being discretized as spatial points.

3.2 Computation of the surface density at reference radius of each species

We discretize the size intervals and write a_i the size of the ith species. The dust to gas ratio can be expressed as

$$\Sigma_d(r) = \zeta \Sigma_g(r) \tag{40}$$

Moreover, we assume that the dust surface densities follow the law as written in Eq.20. So this equation can be given as

$$\Sigma_{d,0} = \zeta \Sigma_{g,0} \tag{41}$$

Considering the grain species Eq.41 is also

$$\sum_i \sigma_{d,0}(a_i) = \zeta \Sigma_{g,0} \tag{42}$$

In other words, $\sigma_{d,0}(a_i)$ is a fraction x_{a_i} of the gas surface density:

$$\sigma_{d,0}(a_i) = x_{a_i} \zeta \Sigma_{g,0} \tag{43}$$

Using Eq.17 we can express the fraction as

$$x_{a_i} = \frac{m_{a_i}}{\sum_i m_{a_i}} \tag{44}$$

Then the fraction x_{a_i} allows to express the surface density at the reference radius of the ith grain species $\sigma_{d,0}(a_i)$.

3.3 Computation of the dust density

The surface densities of the dust at reference radius give the dust densities at all coordinates:

$$\rho_d(r,z,a_i) = \frac{\sigma_d(r,a_i)}{\sqrt{2\pi}H_g(r)}\sqrt{1+\frac{T_sS_c}{\alpha}}\exp\left(\frac{-z^2(1+\frac{T_sS_c}{\alpha})}{2H_g(r)^2}\right) \tag{45}$$

Which is used to express the dust to mass ratio at each coordinates:

$$\zeta(r,z,a_i) = \frac{\rho_d(r,z,a_i)}{n_H(r,z)\mu_a m_H} = \frac{\rho_d(r,z,a_i)}{2\rho_g(r,z)} \tag{46}$$

The factor of 2 is to take into account the fact that Nautilus computes the total H column density from H_2 densities.

3.4 Computation of the averaged grain sizes

To discretize the grain sizes, we divide the range into logarithmically distributed intervals. The cutoff of each interval i is defined by a maximum value $a_{max,i}$ and a minimum value $a_{min,i}$. We want to express the averaged grain size value of each interval. By using Eq.15 we can derive the averaged grain size of the ith interval $a_{av,i}$ as follows:

$$\frac{4\pi}{3}Cn_H\int_{a_{min,i}}^{a_{max,i}} a^3a^{-d}da = \frac{4\pi}{3}Cn_Ha_{av,i}^3\int_{a_{min,i}}^{a_{max,i}} a^{-d}da \tag{47}$$

$$\Longleftrightarrow \int_{a_{min,i}}^{a_{max,i}} a^{3-d}da = a_{av,i}^3\int_{a_{min,i}}^{a_{max,i}} a^{-d}da \tag{48}$$

Then by integrating we can isolate the averaged grain size:

$$\Longleftrightarrow a_{av,i} = \left(\frac{1-d}{4-d}\cdot\frac{a_{max,i}^{4-d}-a_{min,i}^{4-d}}{a_{max,i}^{1-d}-a_{min,i}^{1-d}}\right)^{\frac{1}{3}} \tag{49}$$

3.5 input

The input parameters for the procedure are as follows:
The full package contains four input files:
grainsizes.in
radius.in
spatial_resolution.in
source_parameters.in

They are all used by the routine "*dust_distribution.py*" written in Python 2.7.10.

grainsizes.in gives all the logarithmically distributed intervals of grain sizes in μm.
radius.in gives a list of radius at each Nautilus will compute physical and chemical parameters.
source_parameters.in gives a list of input parameters characterising the disk. The parameters are listed in table 1.

symbol	definition	unit
σ	stiffness of the temperature profile	-
q	exponent for the radial variation of temperature	-
T_{mid}	midplane temperature at the reference radius	K
R_{ref}	reference radius for parametric laws	au
R_c	tapered edge radius	au
R_{in}	inner radius	au
R_{out}	outer radius	au
M_{star}	mass of the central object	$M_\odot$
M_{gas}	total mass of the gas in unit of star mass	$M_\odot$
ρ_m	material density of the grains	g.cm^{-3}
ζ_{in}	dust to gas ratio below the tapered edge radius	-
ζ_{out}	dust to gas ratio beyond the tapered edge radius	-
d	size distribution exponent	-
p	surface density exponent	-
$\Sigma_g, 0$	Surface density at the reference radius	g.cm^{-2}
S_c	Schmidt number	-
α	viscosity coefficient	-

Table 2: Input parameters

3.6 output

The output parameters computed by the procedure are as follows:

symbol	definition	unit
$H_{g,0}$	gas scale height at reference radius	cm
$H_g(r)$	gas scale height	cm
$\Sigma_g(r)$	gas surface density	g.cm^{-2}
C	normalisation constant in the MRN equation	cm$^{2.5}$
$\sigma_{d,0}$	dust surface density at reference radius	g.cm^{-2}
$\sigma_d(r)$	dust surface density	g.cm^{-2}
$\rho_d(r, z, a)$	dust mass density	g.cm^{-3}
a_{av}	averaged size grain	cm
T_s	dimensionless stopping time	-
$H_d(r)$	dust scale height	cm

Table 3: Output parameters

The main output files created by the procedure simply give the grain size and its corresponding abundance at each spatial point as given by Eq.1. These output files are meant to be read by the Nautilus multigrain code for chemical simulation in disks next. There is one file per radius. For instance, "1D_grain_sizes_040.in" for $r = 40au$.

3.7 EXAMPLE

Here is a example with input parameters as follows:

symbol	definition	value
σ	stiffness of the temperature profile	2
q	exponent for the radial variation of temperature	0.4
T_{mid}	midplane temperature at the reference radius	10 K
R_{ref}	reference radius for parametric laws	100 au
R_{in}	inner radius	1.5 au
R_{out}	outer radius	300 au
M_{gas}	mass of the gas	0.008 $M_{\odot}$
ρ_m	material density of the grains	2.5 g.cm^{-3}
ζ_{in}	dust to gas ratio below the tapered edge radius	0.01
ζ_{out}	dust to gas ratio beyond the tapered edge radius	0.001
d	size distribution exponent	3.5
p	surface density exponent	1.5
$\Sigma_g, 0$	Surface density at the reference radius	0.335 g.cm^{-2}
S_c	Schmidt number	1
α	viscosity coefficient	0.001

Table 4: Input example

and with 16 logarithmically distributed intervals of grain sizes:

averaged grain size (μm)	% of total dust mass	cumulative %
0.00698	0.10	0.10
0.0149	0.15	0.25
0.0321	0.22	0.47
0.0689	0.33	0.80
0.148	0.48	1.28
0.317	0.70	1.98
0.679	1.03	3.01
1.45	1.51	4.52
3.13	2.20	6.72
6.71	3.23	9.95
14.4	4.73	14.7
30.9	6.90	21.6
65.9	10.1	31.7
141	14.8	46.5
303	21.7	68.2
651	31.8	100

Table 5: Average grain sizes and their corresponding percentage of total dust mass.

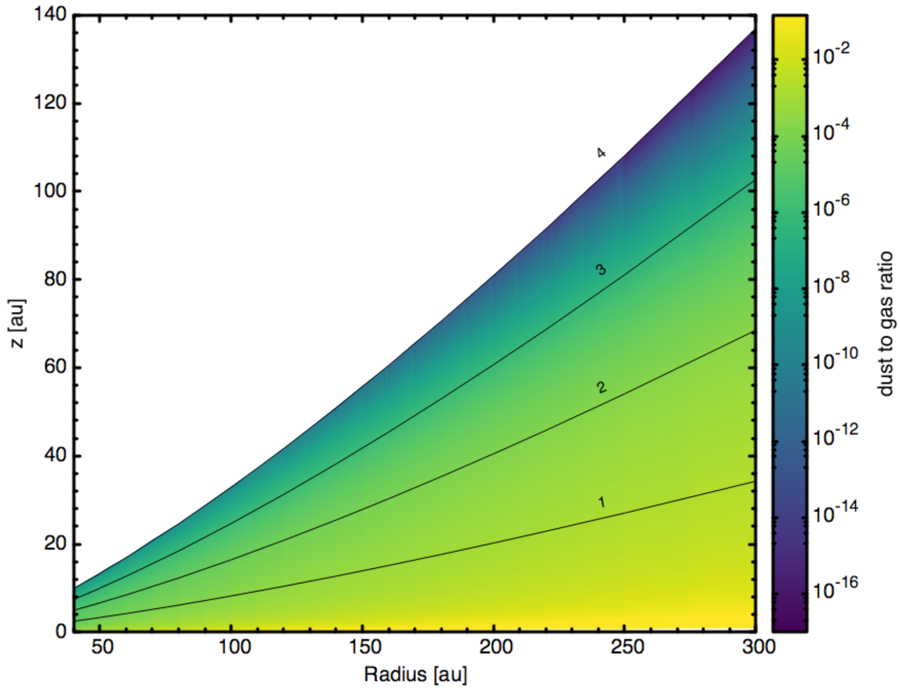

Figure 8: Altitude as a function of the radius. The color scale gives the map of the dust to gas mass ratio.

Fig.9, Fig.10 and Fig.11 show the vertical density profile of single grain species compared to that of the Hydrogen nuclei vertical density profile at $r = 50$ au. Fig.10 and Fig.11 show big sized grain, which explains why the vertical distribution of dust doesn't extend to the total 4 box. This illustrates well the settling of big grains.

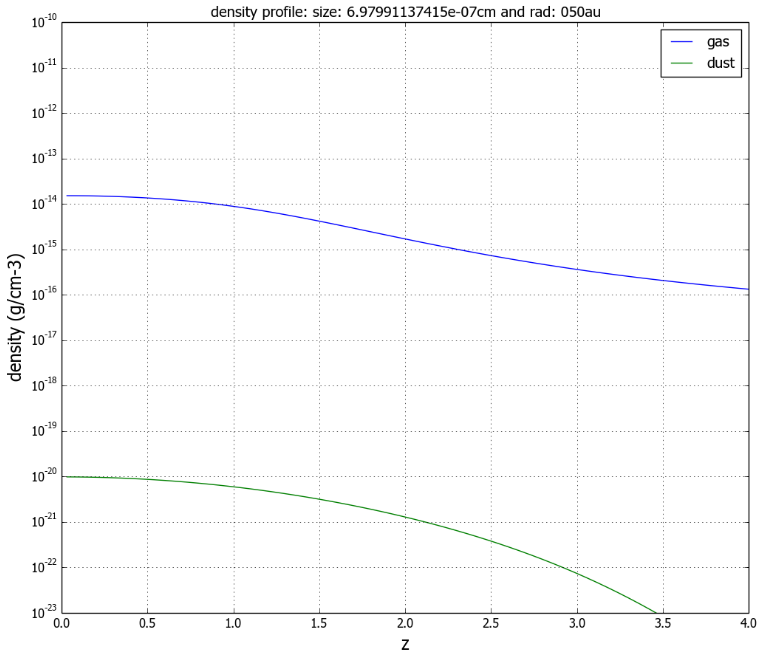

Figure 9: Dust vertical density profile (green) and Hydrogen nuclei vertical density profile (blue) at $r = 50$ au. The grain size is 6.97 nm. The y-axis is the mass density (g.cm^{-3}) given as a function of the altitude z in unit of gas scale height.

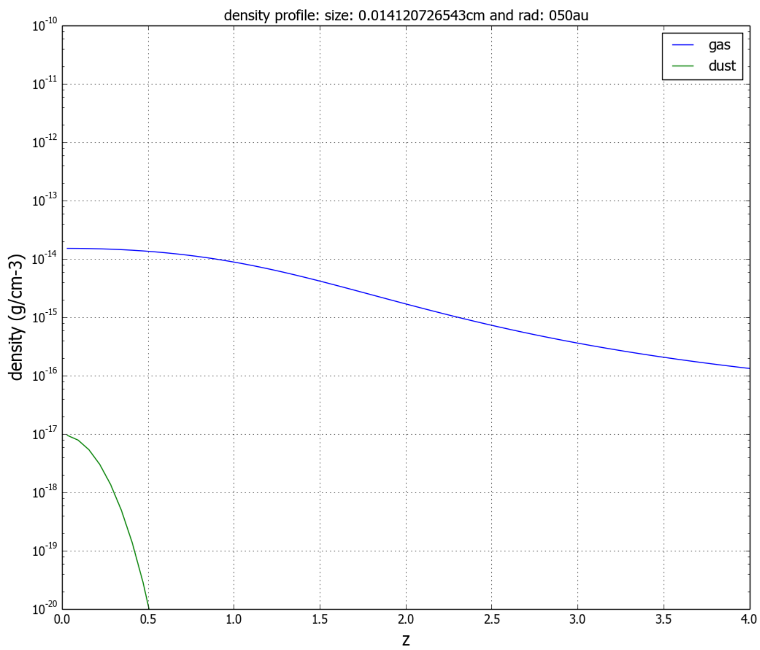

Figure 10: Dust vertical density profile (green) and Hydrogen nuclei vertical density profile (blue) at $r = 50$ au. The grain size is 141 μm. The y-axis is the mass density (g.cm^{-3}) given as a function of the altitude z in unit of gas scale height.

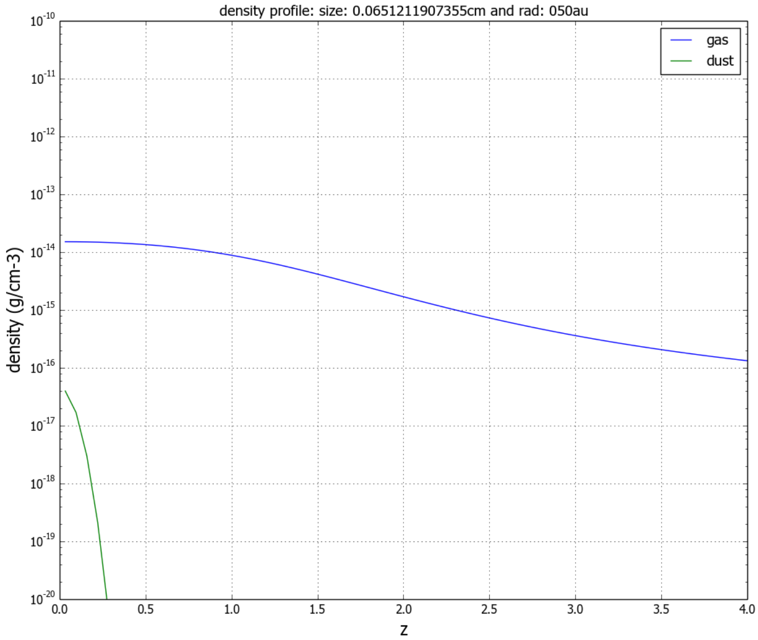

Figure 11: Dust vertical density profile (green) and Hydrogen nuclei vertical density profile (blue) at $r = 50$ au. The grain size is 651 μm. The y-axis is the mass density (g.cm^{-3}) given as a function of the altitude z in unit of gas scale height.