Recovering physical quantities from `DustEM` variables

Jacques Le Bourlot

21 April 2012

1 Dust mass distribution

The number dn_i of dust particle of kind i of size between a and $a + da$ is (in cm^{-3}):

$$dn_i = A_i \, n_{\mathrm{H}} \, f_i(a) \, da$$

In this expression, n_{H} is the hydrogen atom number density in cm^{-3}, a is the radius of the equivalent sphere in cm, $f_i(a)$ express the size variation of this distribution and A_i is a normalization factor. The aim of this note is to recover A_i from `DustEM` input.

From that expression, we deduce the mass of grain of type i in the same size range, with a mass density ρ_i:

$$dm_i = A_i \, n_{\mathrm{H}} \, \frac{4}{3} \pi \, a^3 \, \rho_i \, f_i(a) \, da$$

The total mass of dust of kind i is thus:

$$M_i = A_i \, n_{\mathrm{H}} \, \rho_i \, \frac{4}{3} \pi \int_{a_-}^{a_+} a^3 \, f_i(a) \, da$$

The mass of of gas[1] per unit volume is:

$$M_{\mathrm{H}} = m_{\mathrm{H}} \, n_{\mathrm{H}}$$

Then, the total dust to gas mass ratio is:

$$G = \frac{\sum_i M_i}{M_{\mathrm{H}}} = \frac{4\pi}{3 \, m_{\mathrm{H}}} \sum_i A_i \, \rho_i \int_{a_-}^{a_+} a^3 \, f_i(a) \, da$$

[1] Here "gas" means hydrogen only, whatever its chemical state. Helium and all other trace elements are explicitly excluded.

2 Link with DustEM variables

From DustEM documentation, we see that, for each component, the file GRAIN.DAT gives the dust-to-gas mass ratio and the grain mass density (in $\mathrm{g\,cm^{-3}}$). The dust-to-gas mass ratio is:

$$\frac{M_i}{M_\mathrm{H}} = \frac{4\pi}{3\,m_\mathrm{H}}\,A_i\,\rho_i \int_{a_-}^{a_+} a^3\,f_i(a)\,da = \frac{4\pi}{3\,m_\mathrm{H}}\,A_i\,\rho_i\,I_i$$

This quantity is known as `mprop(i)` in the code. The grain mass density is `rhom(i)`. The last equality defines the integral I_i.

2.1 Grid points

If there are n_i grid points between a_- and a_+, evenly spread in logarithmic scale, then:

$$da = \frac{\log(a_+) - \log(a_-)}{n_i - 1}$$

and the various size points are:

$$a_j = \exp\left(\log(a_-) + (j-1)\ da\right)$$

2.2 Power law distribution

This case corresponds to:

$$f_i(a) = a^\alpha$$

DustEM introduces a quantity "`ava(i,j)`" (written below $g_i(a)$) such that:

$$g_i(a) = \exp\left((4+\alpha)\ \log\left(a\right)\right) = a^{4+\alpha}$$

That is, we have:

$$g_i(a) = a^4\,f_i(a)$$

The integral in $\frac{M_i}{M_\mathrm{H}}$ is:

$$I_i = \int_{a_-}^{a_+} a^{3+\alpha}\,da = \left[\frac{a^{4+\alpha}}{4+\alpha}\right]_{a_-}^{a_+} = \frac{a_+^{4+\alpha} - a_-^{4+\alpha}}{4+\alpha} = \frac{g_i\left(a_+\right) - g_i\left(a_-\right)}{4+\alpha}$$

2.3 Log-Normal distribution

This case corresponds to:

$$f_i(a) = \frac{1}{a}\ \exp\left(-\frac{1}{2}\left(\frac{\log\left(a/a_0\right)}{\sigma}\right)^2\right)$$

where the centroid a_0 is in cm while the width is dimensionless.

The function $g_i(a)$ is:

$$g_i(a) = a^4\, f_i(a) = a^3\, \exp\left(-\frac{1}{2}\left(\frac{\log\left(a/a_0\right)}{\sigma}\right)^2\right)$$

$$g_i(a) = \exp\left[3\, \log\left(a\right) - \frac{1}{2}\left(\frac{\log\left(a\right) - \log\left(a_0\right)}{\sigma}\right)^2\right]$$

The integral in $\frac{M_i}{M_{\mathrm{H}}}$ is:

$$I_i = \int_{a_-}^{a_+} a^2\, \exp\left(-\frac{1}{2}\left(\frac{\log\left(a/a_0\right)}{\sigma}\right)^2\right)\, da = \int_{a_-}^{a_+} \frac{g_i(a)}{a}\, da$$

Let us write:

$$J(x) = \frac{1}{\sqrt{2\pi}} \int_0^x a^3\, \exp\left(-\frac{1}{2}\left(\frac{\log a - \log a_0}{\sigma}\right)^2\right)\, \frac{1}{\sigma}\, \frac{da}{a}$$

so that $J(\infty)$ is the third moment of the normalized log-normal distribution.

Then:

$$I_i = \sigma\, \sqrt{2\pi}\, \left(J\left(a_+\right) - J\left(a_-\right)\right)$$

Now, using $\frac{\log a - \log a_0}{\sigma} = u$, $a = a_0\, \exp\left(\sigma\, u\right)$ and $\frac{1}{\sigma}\, \frac{da}{x} = du$, we have:

$$J(x) = \frac{1}{\sqrt{2\pi}}\, a_0^3 \int_{-\infty}^{\frac{\log x - \log a_0}{\sigma}} \exp\left(3\sigma\, u - \frac{1}{2}\, u^2\right)\, du$$

Then $v = \frac{1}{\sqrt{2}}\, (u - 3\sigma)$, so $u = \sqrt{2}\, v + 3\sigma$ and $\sqrt{2}\, dv = du$:

$$J(x) = \frac{1}{\sqrt{\pi}}\, a_0^3\, \exp\left(\frac{1}{2}\, 3^2\sigma^2\right) \int_{-\infty}^{v_x} \exp\left(-v^2\right)\, dv$$

with $v_x = \frac{1}{\sigma\sqrt{2}}\, (\log x - \log a_0 - 3\sigma^2)$. And we can use the definition of the erf function to write:

$$J(x) = \frac{1}{2}\, a_0^3\, \exp\left(\frac{9}{2}\, \sigma^2\right)\, \mathrm{erf}\left(\frac{\log x - \log a_0 - 3\sigma^2}{\sigma\, \sqrt{2}}\right)$$

And finally:

$$I_i = \sigma\, \sqrt{\frac{\pi}{2}}\, a_0^3\, \exp\left(\frac{9}{2}\, \sigma^2\right)\, \left[\mathrm{erf}\left(\frac{\log a_+ - \log a_0 - 3\sigma^2}{\sigma\, \sqrt{2}}\right) - \mathrm{erf}\left(\frac{\log a_- - \log a_0 - 3\sigma^2}{\sigma\, \sqrt{2}}\right)\right]$$

If various modifications (curvature or exponential decay) are applied to the distribution function, then a numerical integration is required:

$$I_i = \frac{1}{2} \sum_{j=1}^{n_i - 1} \left(a_{j+1} - a_j\right)\, \left(\frac{g_i(a_j)}{a_j} + \frac{g_i(a_{j+1})}{a_{j+1}}\right)$$

2.4 Normalization factor

Once that integral is computed, the normalization factor can be recovered:

$$A_i = \frac{3\,m_{\rm H}}{4\pi}\,\frac{M_i}{M_{\rm H}}\,\frac{1}{\rho_i\,I_i}$$

This allows to compute mean quantities over the various dust components for a given size, weighted by the mass of each component in the specific bin. E.g., for the mean temperature, we have:

$$\bar{T}(a) = \frac{\sum_i \bar{T}_i(a)\,dm_i}{\sum_i dm_i} = \frac{\sum_i \bar{T}_i(a)\,A_i\,\rho_i\,f_i(a)}{\sum_i A_i\,\rho_i\,f_i(a)}$$

2.5 `DustEM` output

One specific output file is "`SDIST.RES`", which gives for each grain component the quantity
`ava(i,j) * mprop(i) * xmp / masstot(i)`
Let us see how this relates to the previous calculation.

The quantity "`masstot`" is (from `DM_inout.f90`, line 747):

$$\mathrm{masstot(i)} = \int_{a_-}^{a_+} a^3\,f_i(a)\,\rho_i(a)\,\frac{4\pi}{3}\,da = \frac{M_i}{A_i\,n_{\rm H}}$$

So, the quantity computed is (if we take $m_p \simeq m_{\rm H}$):

$$a^4\,f_i(a)\,\frac{M_i}{m_{\rm H}\,n_{\rm H}}\,m_p\,\frac{A_i\,n_{\rm H}}{M_i} = A_i\,a^4\,f_i(a) = \frac{1}{n_{\rm H}}\,a^3\,\frac{dn_i}{d\log a}$$