Modelling dust in KROME

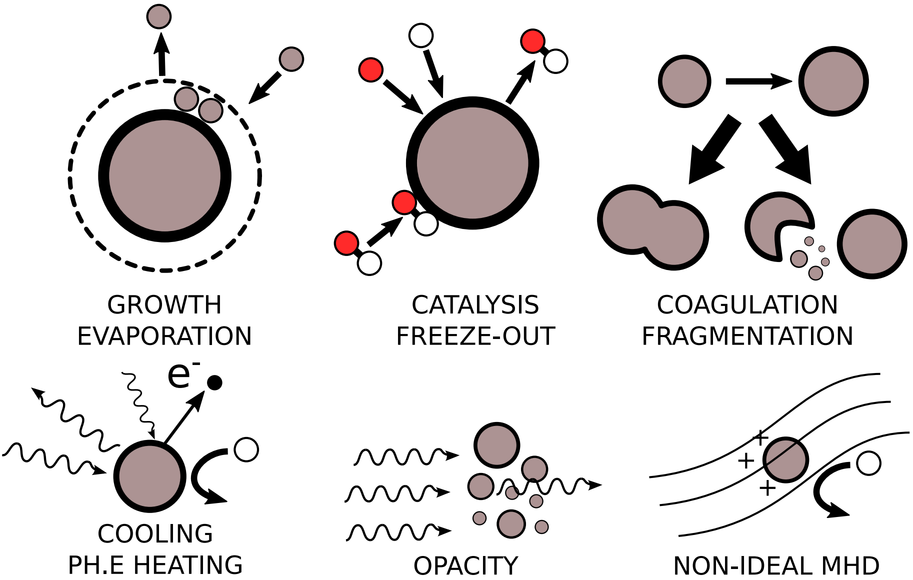
Tommaso Grassi
tgrassi@usm.lmu.de

USM/LMU, Munich

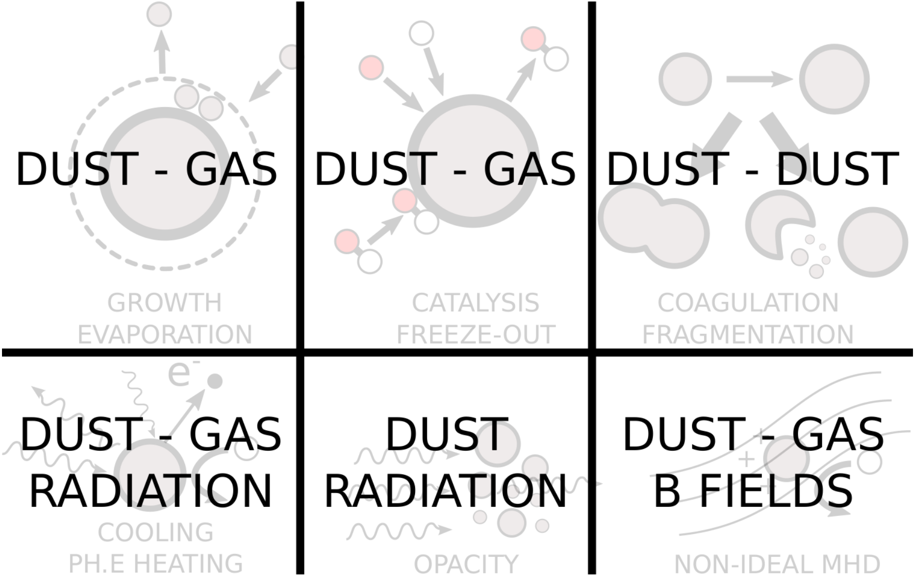
November 2018

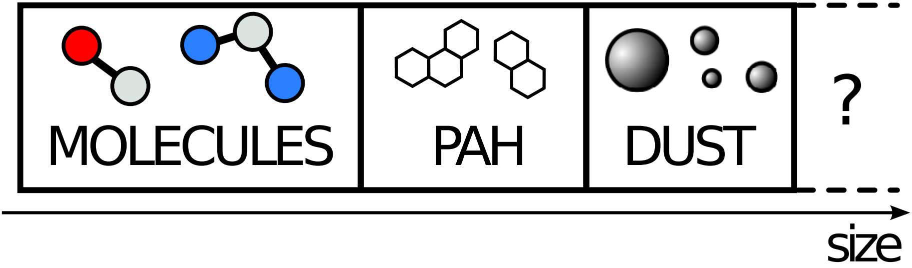
1. Recap of dust processes
2. Understand dust binning
3. how to model dust in KROME
4. H_2 formation on dust
5. Dust temperature and radiation balance

KROME Bootcamp 2018 - Dust process recap



KROME Bootcamp 2018 - Dust process recap





$$\rho_{gr} = 1 \text{ g/cm}^3 \quad (1)$$

$$a = 5 \times 10^{-7} \text{ cm} \quad (2)$$

$$M = \frac{4}{3}\pi a^3 \rho_{gr} \simeq 6 \times 10^{-19} \text{ g} \quad (3)$$

$$N = \frac{M}{m_C} \simeq 3 \times 10^4 \text{ atoms} \quad (4)$$

Reactions for grains

$$HC + H \rightarrow H_2 + C \quad (5)$$

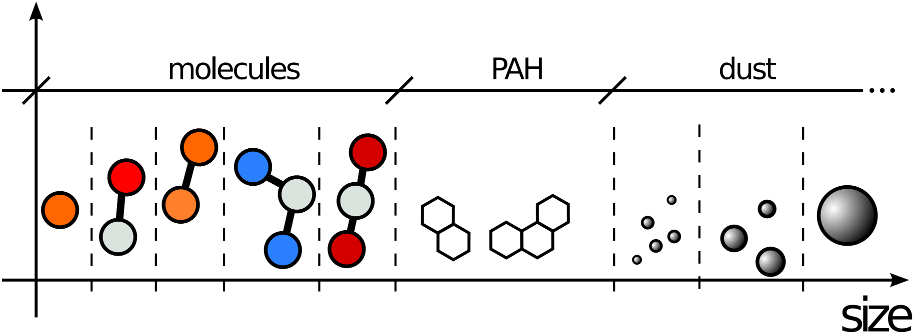
$$C_{24}H_{12} + e^- \rightarrow C_{24}H_{12}^- + \gamma \quad (6)$$

$$dust_{56222} \rightarrow dust_{16121} + dust_{40101} ???? \quad (7)$$

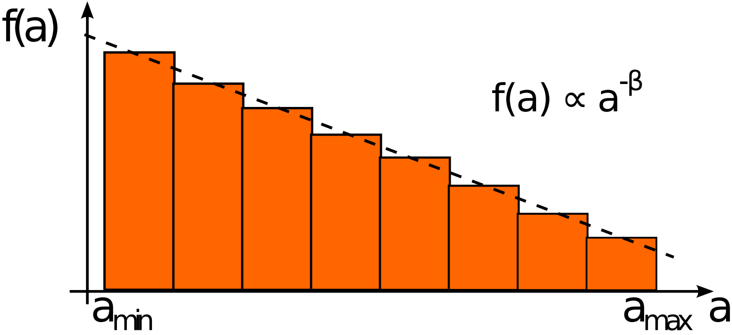
Expand chemical network

H, C, O
H_2, C_2, HC, ...
H_2O, CO_2, O_3, ...
CH_3, H_2O_2, H_2C_2, ...
HC_4, CH_4, H_2CO_2, C_5, C_2H_3, ...
...

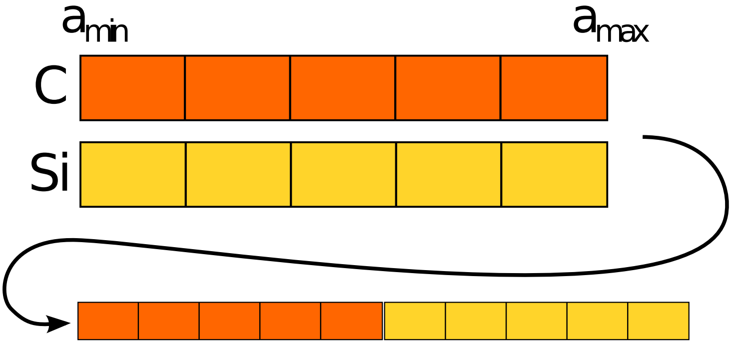
Yet antoher binning. . .



KROME Bootcamp 2018 - Bin distribution



$$\rho_d = \rho_g \mathcal{D} = C\frac{4\pi}{3}\rho_0 \int_{a_{min}}^{a_{max}} f(a) a^3 \mathrm{d}a$$




```
./krome mynetwork.ntw -dust=5,C,Si
```

krome_ndust $= 5 \times 2 = 10$

krome_ndustTypes $= 2$

Initialize the dust

```
call krome_init_dust_distribution(n(:), d2g, &
             a_low, a_up, beta)
call krome_init_dust_distribution(n(:), d2g)
```

Useful dust functions

```
xdust(:) = krome_get_dust_distribution()
adust(:) = krome_get_dust_size()
call krome_set_Tdust_array(Tdust(:))
call krome_get_averaged_Tdust()
```

example

```
./krome -test=dust
```

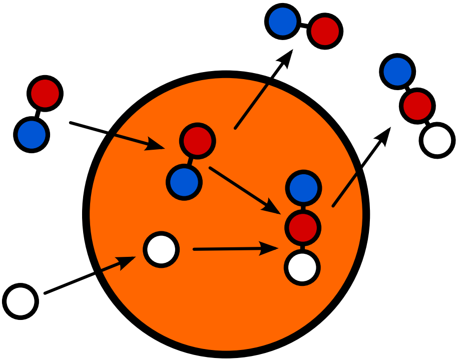
$$
\begin{aligned}
\dot{n}_i &= FORMATION - DESTRUCTION \pm DUST_{\mathrm{H}\rightarrow\mathrm{H}_2} \; [\times N_{gas}] \\
\dot{T} &= HEAT - COOL \pm DUST \qquad [\times 1] \\
\dot{n}_i &= COAGULATION - SPUTTERING \qquad [\times N_{dust} \times N_{type}] \\
\dot{a}_i &= GROWTH - EVAPORATION \qquad [\times N_{dust} \times N_{type}] \\
\dot{T}_{d,i} &= GAS + RADIATION \qquad [\times N_{dust} \times N_{type}]
\end{aligned}
$$

solve a system of stiff ordinary differential equations

H_2 on surface (Cazaux+2009)

$$\dot{n}_{\mathrm{H}_2} = \frac{\pi\, v_g\, n_{\mathrm{H}}}{2} \sum_{i \in bins} \epsilon_i\, n_{d,i}\, a_i^2\, S_{\mathrm{H}_2}(T_g, T_d)$$

```
./krome -n mynetwork.ntw -dust=10,C -dustOptions=H2
```



Gas-grain chemistry

- Adsorption (gas $\rightarrow$ dust)
- Desorption (dust $\rightarrow$ gas)
- Surface chemistry (dust $\rightarrow$ dust)

Adsorption (Hocuk+2015 and many others)

$\mathrm{X} \rightarrow \mathrm{X}_{dust}$

$$k_a = \pi a^2 v_g n_d S \quad (8)$$

$$S = \left(1 + 0.4\sqrt{T_g + T_d} + 0.2T_g + 0.08T_g^2\right)^{-1} \quad (9)$$

Desorption (Hocuk+2015 and many others)

$\mathrm{X}_{dust} \rightarrow \mathrm{X}$

$$k_e = \nu_0 \left[F_{bare} \exp\left(-\frac{E_{bare,i}}{T_d}\right) + F_{ice} \exp\left(-\frac{E_{ice,i}}{T_d}\right)\right] \quad (10)$$

(as it is: likely to be numerically unstable)

Adsorption

$X \rightarrow X_{dust}$

$$k_a = \frac{\pi v_g S \int a^2 \varphi(a)\, da}{4/3\pi\rho_0 \int a^3 \varphi(a)\, da}$$

```
1,CO,CO_dust,krate_stickSi(n, idx_CO, Tdust)
```

Desorption

$X_{dust} \rightarrow X$

$$k_e = \nu_0 \exp\left(-\frac{E_i}{T_d}\right)$$

```
2,CO_dust,CO,krate_evaporation(n, idx_CO, Tdust)
```

Non-thernal evaporation (Hollenback+2009 and many others)

$X_{dust} + \gamma/CR \rightarrow X$

$$k_{nt,CR} = f_{70}\nu_0 \exp(-E_b/k_B 70\,\mathrm{K})$$

$$f_{70} = 3 \times 10^{-16}\mathrm{s}^{-1}\frac{\zeta}{\zeta_0}$$

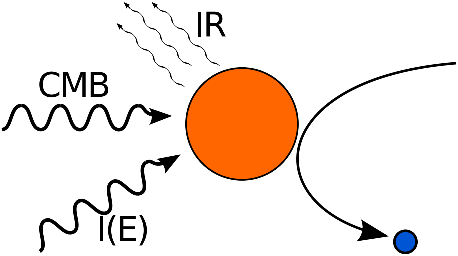
```
3,CO_dust,CO,krate_nonthermal_evaporation
                    (idx_CO, Gnot, Av, crflux, yield)
```

Surface chemistry (Hocuk+2015 and many others)

$\mathrm{X}_{dust} + \mathrm{Y}_{dust} \rightarrow \mathrm{XY}_{dust}$

$$k_{ij} = P_{ij}\,\nu_0 \left[\exp\left(-\delta \frac{E_i}{T_d}\right) + \exp\left(-\delta \frac{E_j}{T_d}\right)\right]$$

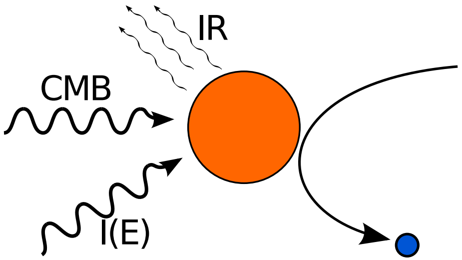
$$P_{ij} = \exp\left[-\frac{2b}{\hbar}\sqrt{2 m_{ij} k_B E_a}\right]$$



Kirchoff's law

$$\Gamma_{em} = \Gamma_{abs} \quad (11)$$

$$\int_E Q_{abs} B_{T_d} = \sum_i \int_E Q_{abs} J_i \quad (12)$$



Gas coupling

$$\Gamma_{em} = \Gamma_{abs} + \Lambda_{dust} \quad (13)$$

$$\Lambda_{dust} = 2\pi\, a^2\, n_g\, n_d\, v_g\, k_b\, (T_g - T_d) \qquad \mathrm{erg\,cm^{-3}\,s^{-1}} \quad (14)$$

Bisection

```
./krome -n mynetwork.ntw -dust=10,C -dustOptions=T
        -cooling=DUST
```

solve $\Gamma_{em}(T_d) = \Gamma_{abs} + \Gamma_{CMB} + \Lambda(T_d, T_g)$ for T_d

Actual ODE

```
./krome -n mynetwork.ntw -dust=10,C -dustOptions=dT
        -cooling=DUST
```

$$\frac{\mathrm{d}T_{d,i}}{\mathrm{d}t} = A\frac{\mathrm{d}T_g}{\mathrm{d}t}\left[A + \int_0^\infty \frac{\mathrm{d}B(E, T_{d,i})}{\mathrm{d}T_{d,i}} Q_i(E)\mathrm{d}E\right]^{-1}$$

$$A = 2\, f\, n_g\, v_g\, k_B$$

$$T_{d,i}(t_0 + \Delta t) = T_{d,i}(t_0) + \mathrm{d}T_{d,i}/\mathrm{d}t$$

(Grassi+2017)

Collapsing cloud - fully consistent

$$\left[\Gamma_{\rm em}(T_{d,i}) - \Gamma_{\rm abs}\right] \beta_{esc}(T_{d,i}) = \Lambda(T_{d,i}, T_g) \quad (15)$$

$$\beta_{esc,i} = \tau_{d,i}^{-2} \quad (16)$$

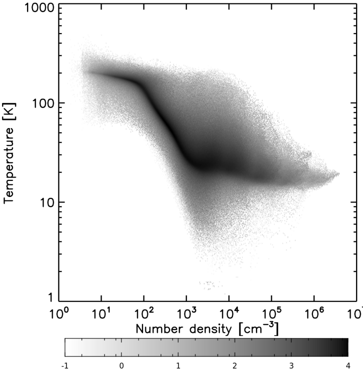
$$\tau_{d,i} = \lambda_J \pi \sum_{j\in bins} n_{d,j}\, a_j^2 \frac{\int_0^\infty Q(E, a_j) B(E, T_{d,j}) \mathrm{d}E}{\int_0^\infty B(E, T_{d,j}) \mathrm{d}E} \quad (17)$$

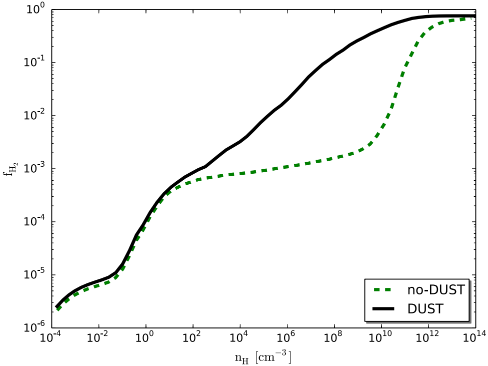
Parameters and table

- dust to gas ratio (metallicity)
- dust distribution (exponent, size range)

$$\Lambda_{collapse} = f(n_g, T_g)$$
$$\Lambda_{cloud} = f(n_g, T_g, A_v)$$

(Grassi+2016)


1000
100
10
1
Temperature [K]
10^0 10^1 10^2 10^3 10^4 10^5 10^6 10^7
Number density [cm^{-3}]
-1 0 1 2 3 4


10^0 10^{-1} 10^{-2} 10^{-3} 10^{-4} 10^{-5} 10^{-6}
f_{H_2}
10^{-4} 10^{-2} 10^0 10^2 10^4 10^6 10^8 10^{10} 10^{12} 10^{14}
n_H [cm^{-3}]
no-DUST
DUST

What KROME does

- Fully-consistent temperature and cooling/heating (rad-dust-gas)
- Fully-consistent growth and evaporation (dust-gas)
- Fully-consistent H_2 formation (dust-gas)
- Optimized table cooling

What KROME “does”

- Reaction-based surface chemistry (gas-dust)

Whislist

- Fragmentation (dust-dust)
- Coagulation (dust-dust)
- ...

All models are wrong, some are useful

(George E. P. Box)