Modelling the dust in KROME

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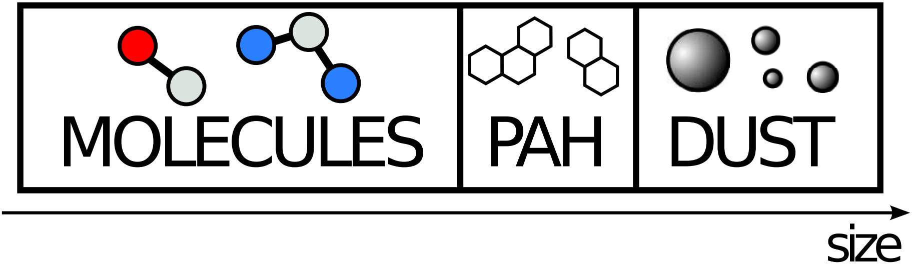
STARPLAN CENTRE FOR STAR AND PLANET FORMATION

KROME better science through chemistry

Aims of this talk

1. Understand that ~~photochemsitry~~ dust is a mess
2. Realize that KROME saves your day

- another one bites the dust
(Queen)



$$\rho_{gr} = 1.22 \text{ g/cm}^3 \quad (1)$$

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

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

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

Reactions for grains

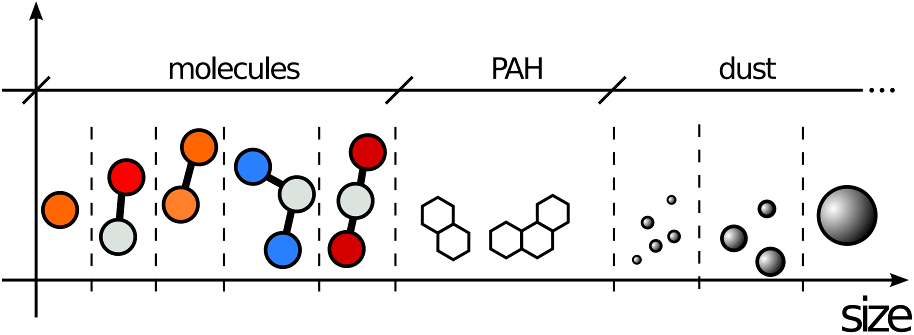
$$\mathrm{HC} + \mathrm{H} \rightarrow \mathrm{H_2} + \mathrm{C} \quad (5)$$

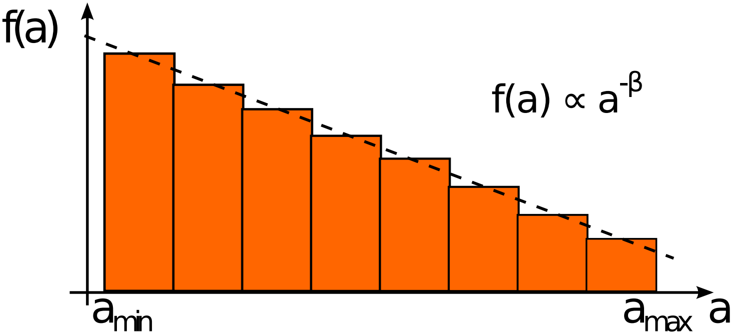
$$\mathrm{C_{24}H_{12}} + e^- \rightarrow \mathrm{C_{24}H_{12}^-} + \gamma \quad (6)$$

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

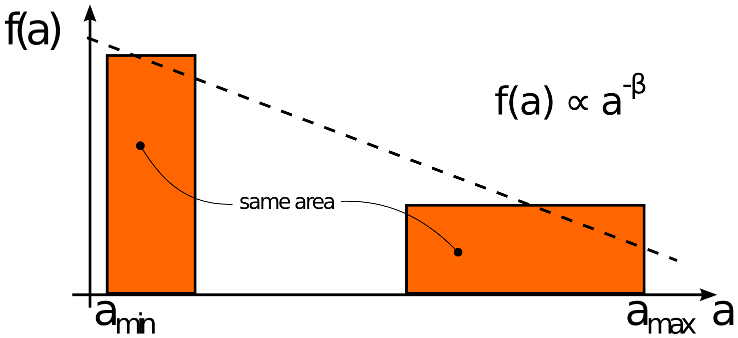
Expand chemical network

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, . . .


molecules
PAH
dust
...
size



$$C \int_{a_{min}}^{a_{max}} f(a) \mathrm{d}a = C \sum_{i=0}^{N_{dust}} f_i^{dust} \Delta a_i = 1$$



$$x_i^{dust} = f_i^{dust} \Delta a_i = \frac{1}{N_{dust}} \qquad \forall i$$

How KROME computes the bin size

$$\zeta = \int_{a_{min}}^{a_{max}} a^{-\beta} \mathrm{d}a \tag{8}$$

$$\zeta = \frac{a_{max}^{1-\beta} - a_{min}^{1-\beta}}{1-\beta} \tag{9}$$

$$\frac{\zeta}{N} = \int_{a_0}^{a_1} a^{-\beta} \mathrm{d}a \tag{10}$$

$$a_1 = \left[\frac{\zeta}{N}(1-\beta) + a_0^{1-\beta}\right]^{1/(1-\beta)} = g(a_0) \tag{11}$$

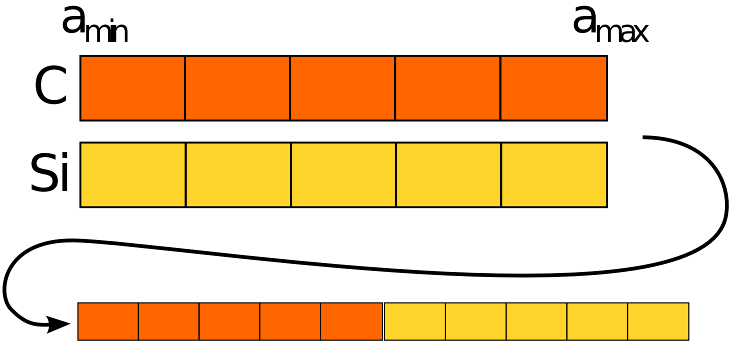
$$a_{i+1} = g(a_i) \tag{12}$$

Internal variables

```
xdust(ndust)
krome_dust_asize(ndust)
krome_dust_asize2(ndust)
krome_dust_asize3(ndust)
krome_dust_aspan(ndust)
krome_dust_partner_ratio(ndust)
krome_dust_partner_ratio_inv(ndust)
krome_dust_partner_idx(ndustTypes)
krome_dust_T(ndust)
```

$$a_{span} = \Delta a \quad (13)$$

$$r_{par} = \frac{a^3 \rho_{gr}}{m_{par}} \quad (14)$$




```
./krome my_favourite_network -dust=5,C,Si
```

ndust $= 5 \times 2 = 10$

ndustTypes $= 2$

Initialize the dust

```
call krome_set_dust_distribution(alow=5d-7, &
             aup=2.5d-5, beta=-3.5d0)
call krome_set_dust_distribution()
call krome_scale_dust_gas_ratio(ratio, x(:))
call krome(x(:), Tgas, dt)
```

Old way (not supported any more)

```
call krome_set_dust_distribution(adust(:),xdust(:),&
          ratio,alow=5d-7, aup=2.5d-5, beta=-3.5d0)
call krome(x(:), Tgas, dt, adust(:), xdust(:))
```

```
xd(:) = krome_get_dust_distribution()
ad(:) = krome_get_dust_size()
```

```
./krome -n awsome_network -dust=10,C -dustOptions=GROWTH
```

Growth equations (Dwek+1998)

$$R_+ = c_d \, \pi \, a^2 \, (n_d + \varepsilon) \, n_p \, S\left(T_d, T_g\right) \, v_g \quad (15)$$

$$v_g = \sqrt{\frac{8 k_b}{\pi m_p} T_g} \quad (16)$$

$$c_d = 10^{-4} \quad (17)$$

$$\varepsilon = 10^{-12} \quad (18)$$

$$S(T_g, T_d) = c_0 T_g \, (c_1 \, T_d + c_2) \, e^{-c_3 \, T_g} \quad (19)$$

```
./krome -n lovely_network -dust=10,C -dustOptions=SPUTTER
```

Thermal sputtering equations (Nozawa+2006)

$$R_{-} = \pi\, a^2\, n_d\, v_g \sum_{i \in ions} n_i\; Y_i(T_g) \tag{20}$$

$$v_g = \sqrt{\frac{8k_b}{\pi m_p} T_g} \tag{21}$$

$$Y_i = \frac{e^{-c_0 \log T_g}}{c_1 + c_2 \log T_g} + c_3 \tag{22}$$

KROME Bootcamp 2014 - Flags: H_2 catalysis

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

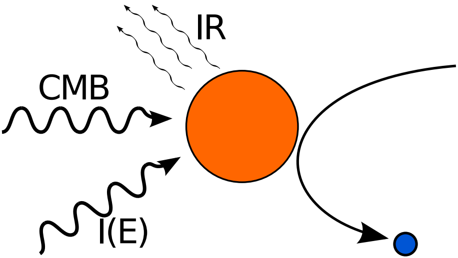
H_2 on surface, equations (Cazaux+2009)

$$\dot{n}_{\mathrm{H}_2} = \frac{\pi\, v_g\, n_{\mathrm{H}}}{2} \sum_{i\in bins} \sum_{j\in types} \epsilon_j \left[T_g, T_d(i)\right] n_d(i)\, a_i^2\, S_{\mathrm{H}_2}(T_g, T_d)$$

$$v_g = \sqrt{\frac{8k_b}{\pi m_p} T_g} \qquad (23)$$

$$S_{\mathrm{H}_2} = \left[1 + 0.4\sqrt{T_{g*} + T_{d*}} + 0.2T_{g*} + 0.08T_{g*}^2\right]^{-1} \qquad (24)$$

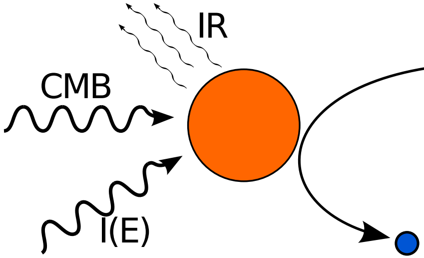
$$\epsilon_j \left[T_g, T_d(i)\right] = a\, nice\, LaTeX\, exercise + typo \qquad (25)$$



Kirchoff's law:
"and in the end / the radiation you take / is equal to the one / you make"

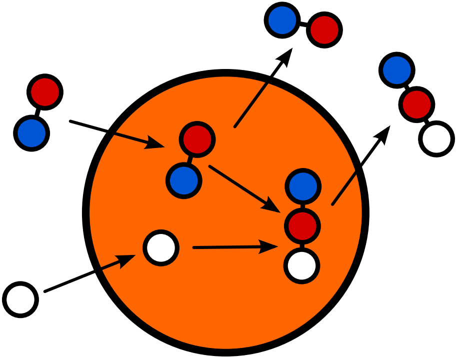
$$\Gamma_{em} = \Gamma_{abs} + \Gamma_{CMB} \quad (26)$$

$$\int Q(a,E)\, B\left[E, T_d(a)\right] \mathrm{d}E = \int Q(a,E)\, I(E) \mathrm{d}E + \int Q(a,E)\, B\left[E, T_{CMB}\right] \mathrm{d}E \quad (27)$$



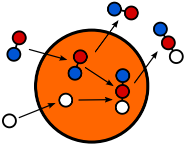
Gas coupling

$$\Lambda_{dust} = 2\pi a^2 n_g n_d v_g k_b (T_g - T_d) \quad \mathrm{erg\,cm^{-3}\,s^{-1}} \tag{28}$$



Gas-grain chemistry

- Adsorption (gas → dust)
- Desorption (dust → gas)
- Surface chemistry (dust → dust)



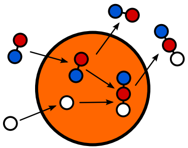
$$\mathrm{O} \rightarrow \mathrm{O}_{dust}$$

Adsorption

$$k_a = \pi\, a^2\, v_g\, n_d(a)\, S_a[T_g, T_d(a)] \quad (29)$$

$$S_a(T_g, T_d) = \left[1 + 0.4\sqrt{T_{g*} + T_{d*}} + 0.2 T_{g*} + 0.08 T_{g*}^2\right]^{-1} \quad (30)$$

$$v_g = \sqrt{\frac{8k_b}{\pi m_j} T_g} \quad (31)$$



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

Desorption

$$k_e = \nu_0 \left[F_{bare} \exp\left(-\frac{E_{bare,i}}{T_d}\right) + F_{ice} \exp\left(-\frac{E_{ice,i}}{T_d}\right) \right] \quad (32)$$

$$F_{ice} = \min \left| \left[\frac{n_{\mathrm{H_2O}}}{n_d n_s}, 1 \right] \right| \qquad F_{bare} = 1 - F_{ice} \quad (33)$$

$$n_d n_s = \phi = n_d \sigma_d \frac{4}{a_{pp}^2} \quad (34)$$

- solver
- GPU porting
- improve CR heating
- please, more plot tools (gnuplot is nice, but...)
- improve partition functions
- upgrade some interfaces
- new tools
- new user functions
- ...

Feedback form

password: ****************

Thank you for your attention!

"Given enough eyeballs, all bugs are shallow."
(Eric S. Raymond)

http://kromepackage.org/
http://kromepackage.org/bootcamp