KROME and RAMSES: when microphysics matters

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ISM chemistry/microphysics

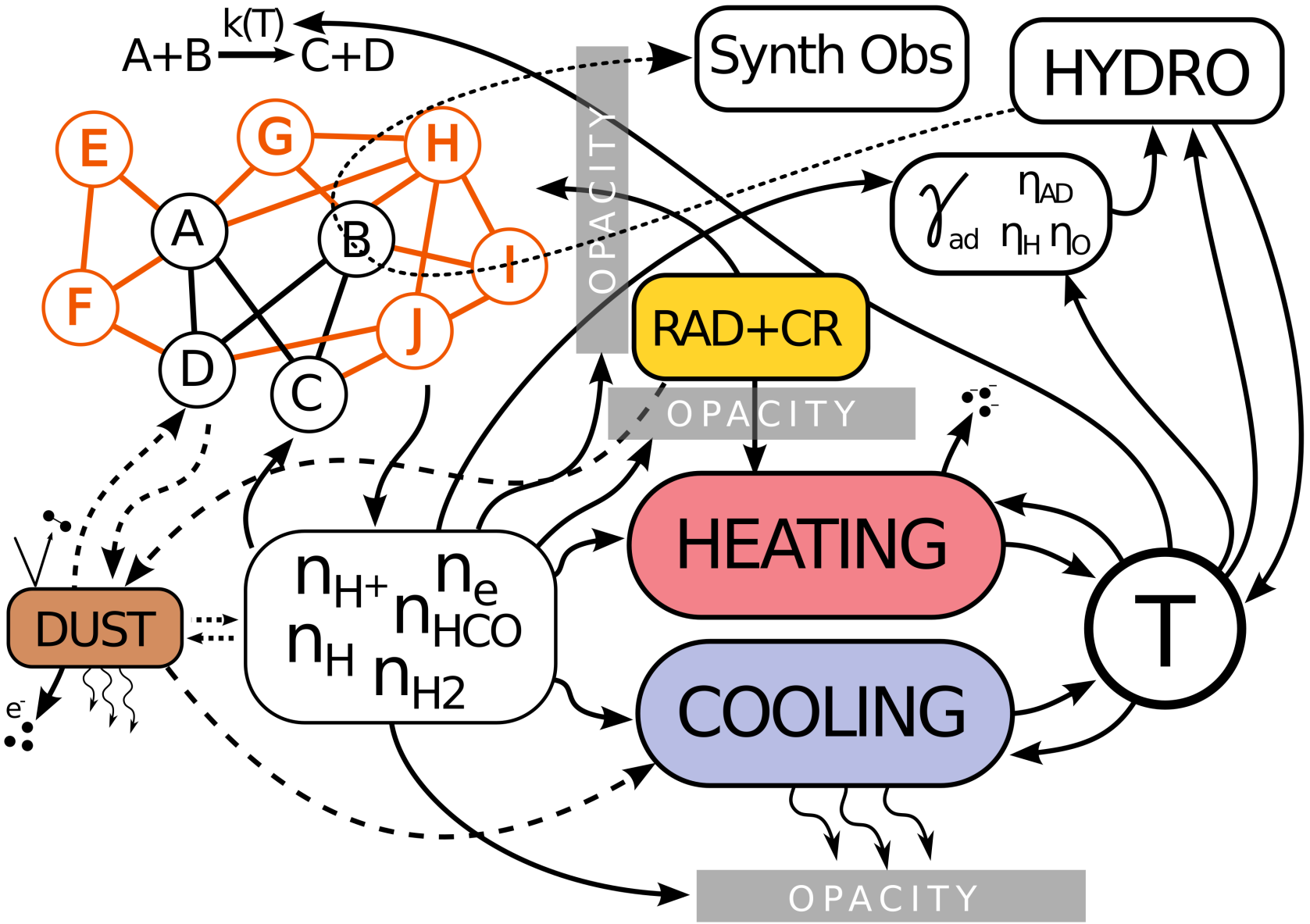
Why you need chemistry/microphysics (in numerical simulations)

- controls gas thermal evolution (cooling/heating)
- controls opacity (dust/gas)
- comparison with observations (abundances)
- adiabatic index, resistivity (non-ideal MHD), ...

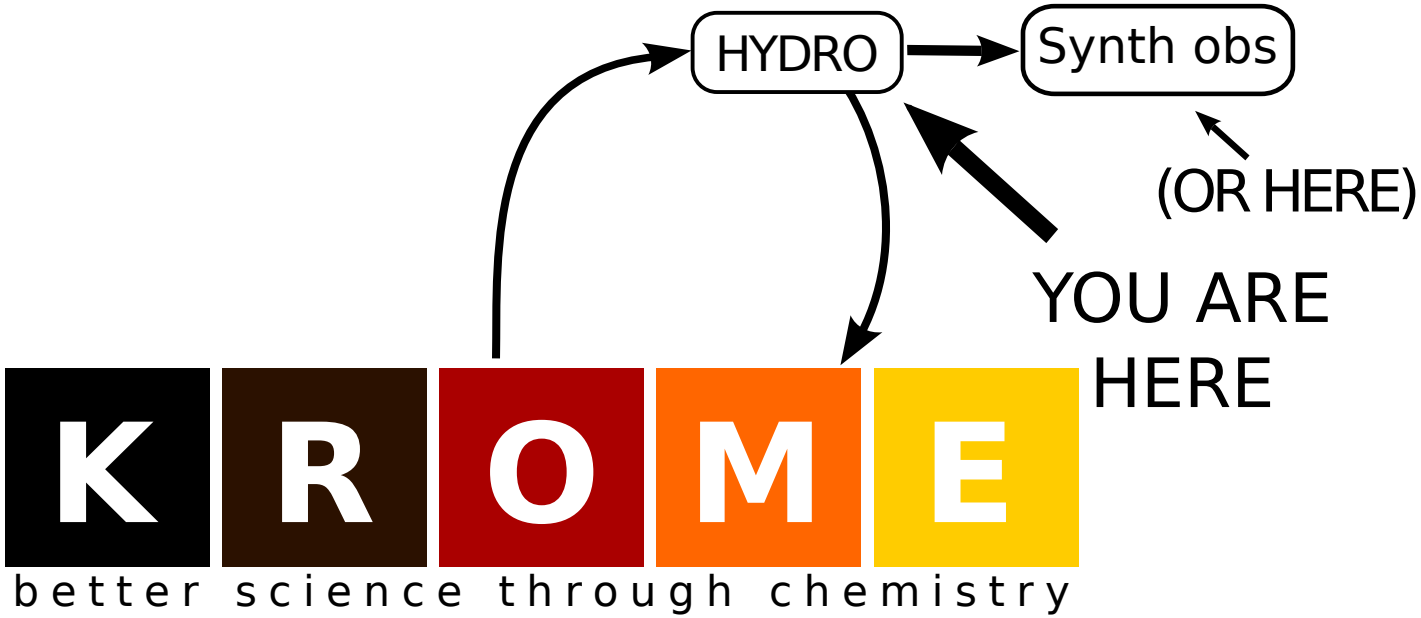
Why you don't like it (in numerical simulations)

- **very CPU demanding (solving stiff ODEs)**
- many different physical processes
- many atomic, molecular, thermochemical, ... data required

Microphysics, full story (25/25)



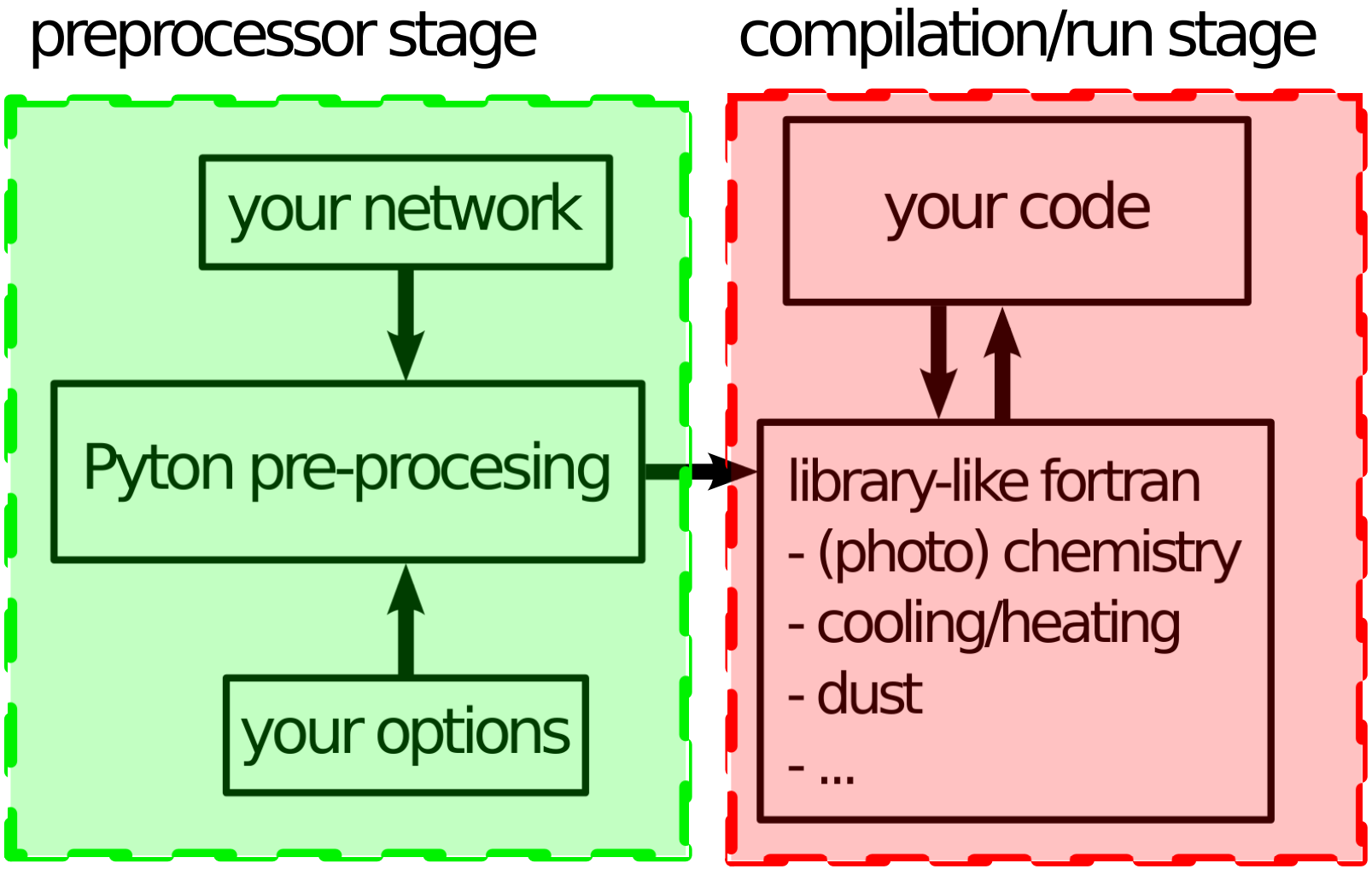
KROME



What is KROME?

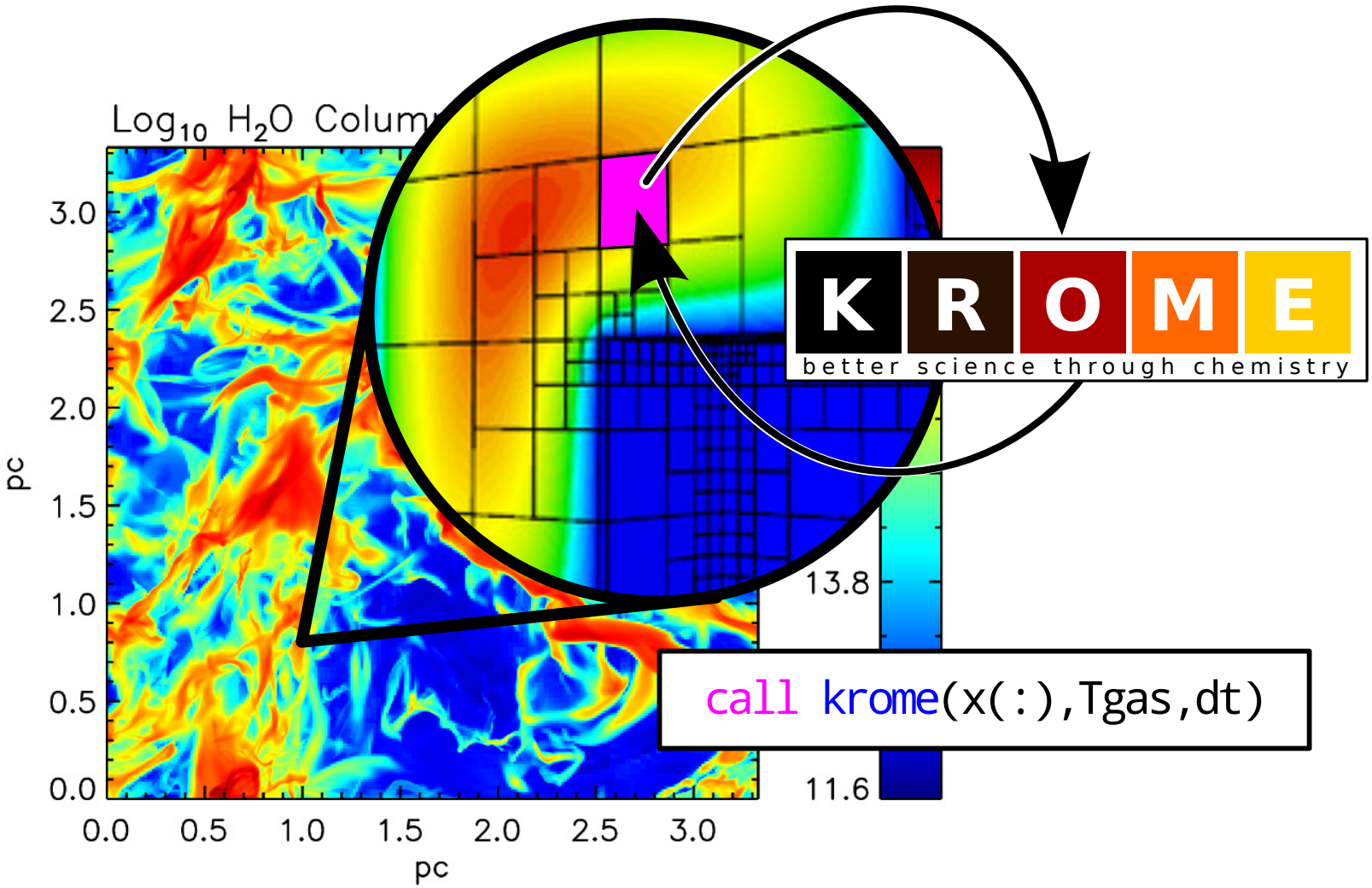
- Python pre-processor creates *ad hoc* optimized F90 modules
- Chemistry, dust-related physics, cooling, heating, photoionization, ...
- Open source, `kromepackage.org`, Grassi+2014 (MNRAS)
- Highly optimized code, based on "fast" solver (DLSODES)
- Can be coupled to hydrocodes, RAMSES, Enzo, FLASH, Gasoline, ...
- 26 papers (CEMP-stars, molecular clouds, BHs, AGBs, pp-disks, ...), 3 schools

Two-stages approach



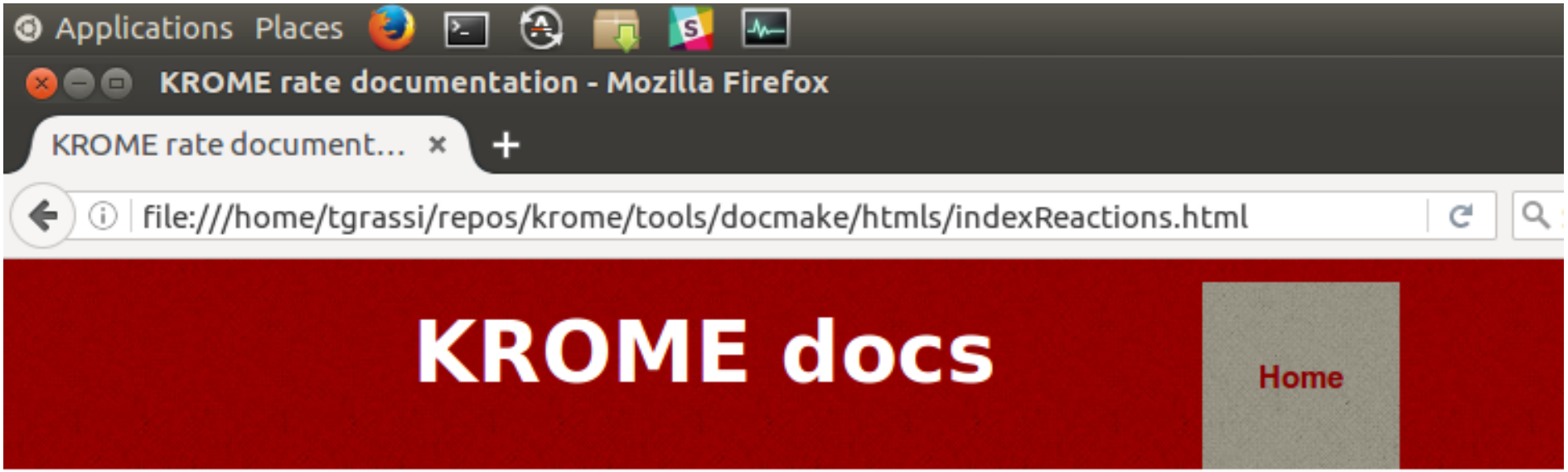

```
./krome -n myNetwork.dat -cooling=H2,CO -heating=CR
```

Cell-by-cell



- A set of one-zone models: one for each ijk-th cell
- i.e. the ijk-th cell doesn't see the neighbourhoods

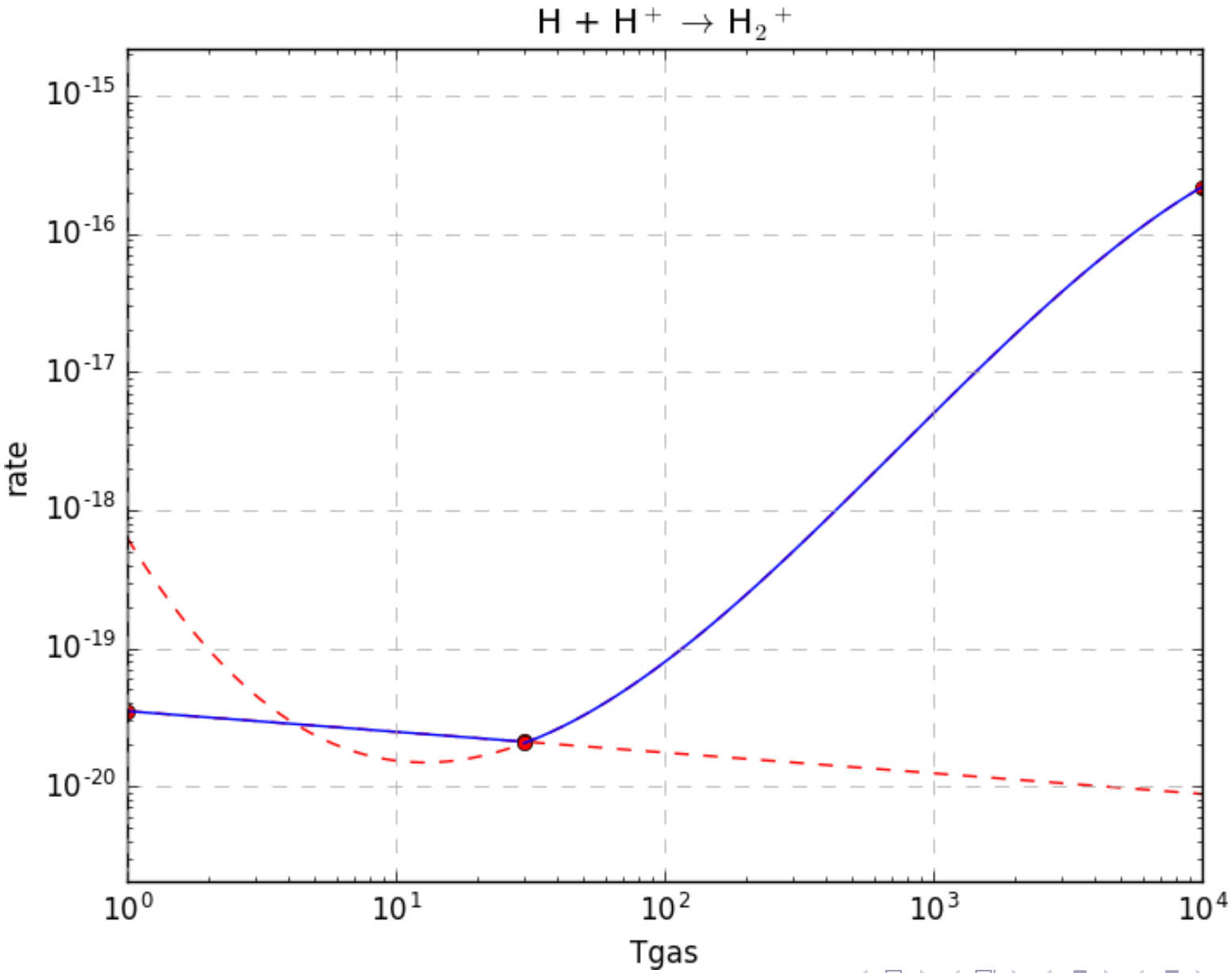
Documentation/1



Reactions

H^-	+	H	→	H	+	H	+ e^-	details
H_2	+	e^-	→	H	+	H	+ e^-	details
H^-	+	H	→	H_2	+	e^-		details
H^-	+	e^-	→	H	+	e^-	+ e^-	details
H_2	+	e^-	→	H	+	H^-		details
H^-	+	H^+	→	H	+	H		details
He^+	+	e^-	→	He^{++}	+	e^-	+ e^-	details

Documentation/2



Documentation/3

KROME docs Home

H^-

back

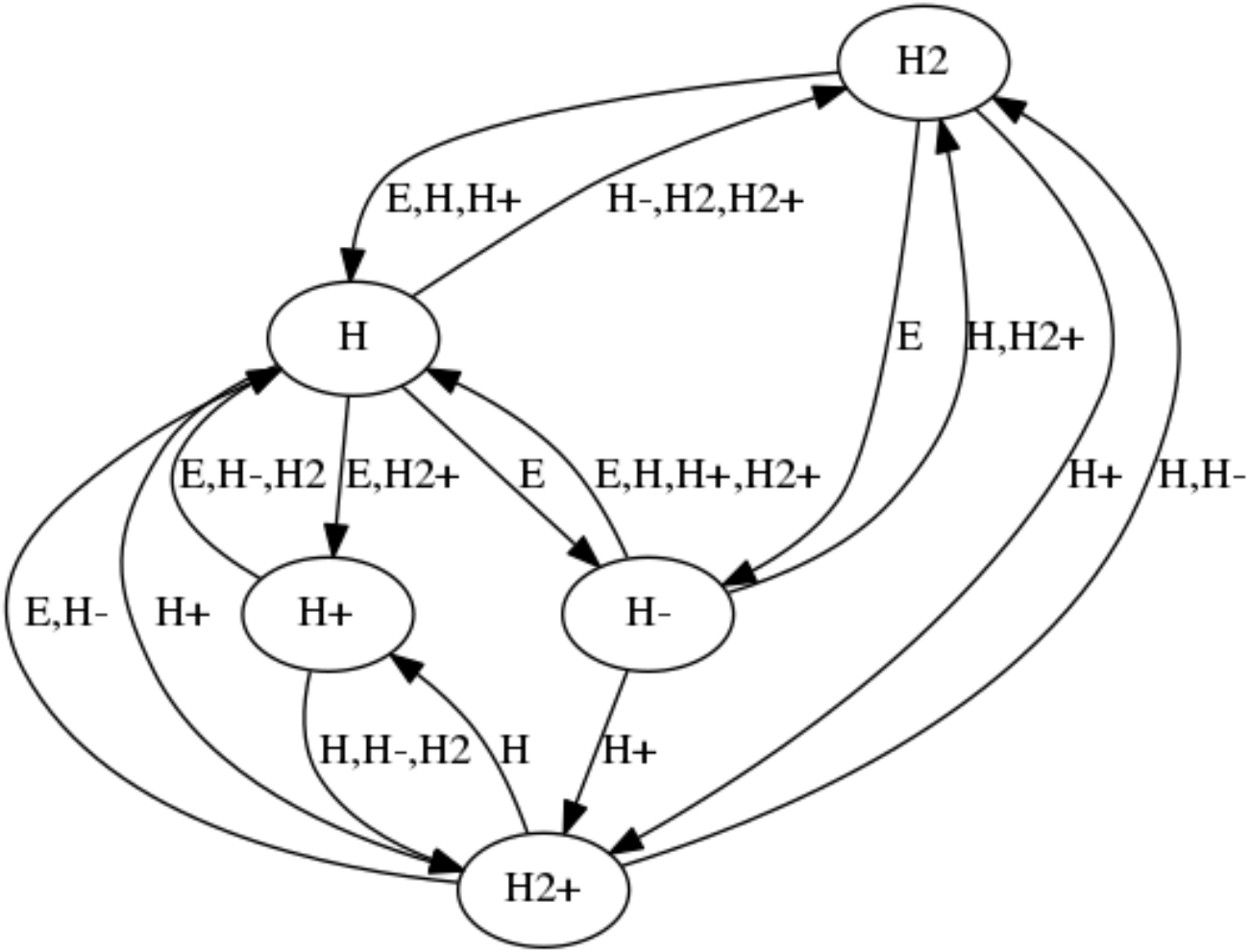
Formation channels

H_2	+	e^-	→	H	+	H^-		details
H	+	e^-	→	H^-				details

Destruction channels

H^-	+	H	→	H	+	H	+ e^-	details
H^-	+	H	→	H_2	+	e^-		details
H^-	+	e^-	→	H	+	e^-	+ e^-	details
H^-	+	H^+	→	H	+	H		details
H_2^+	+	H^-	→	H	+	H_2		details

Documentation/4



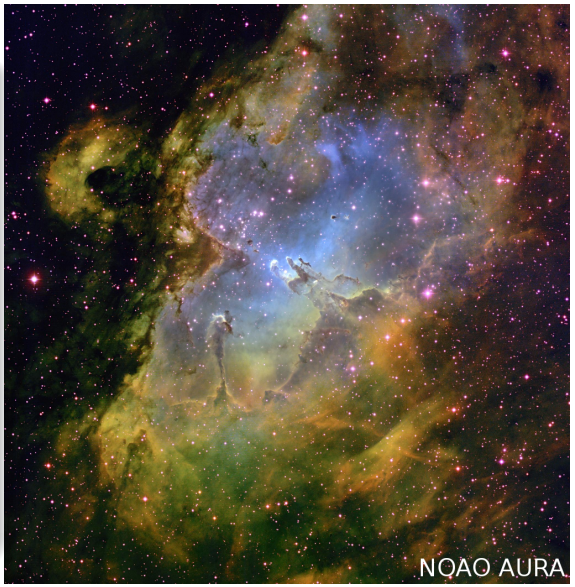
HTML documentation ready to be uploaded on your own server

Application: Molecular Clouds (3D MHD)

Molecular Clouds

Aim: IMF + understand the role of microphysics in star-forming regions + chemical abundances (w/ T.Haugbølle)

- Complex structures at all scales
- Molecular richness (mainly H-C-O-N, but also F-S)
- Large CO variability
- CO-to-H_2 conversion factor still under investigation
- Mass tracers (N_2H^+, HF, OH, CH_3OH, . . .)
- Chemical clocks, ortho/para, and isotopologues



Caveats and bottlenecks (computational)

- Multi-scale interaction
- Chemistry/microphysics at different scales (“hierarchical chemical legacy”)
- Non-trivial coupling between “pure” chemistry, microphysics, and dynamics
- Radiative-transfer and other (not negligible) amenities

Molecular Clouds/2

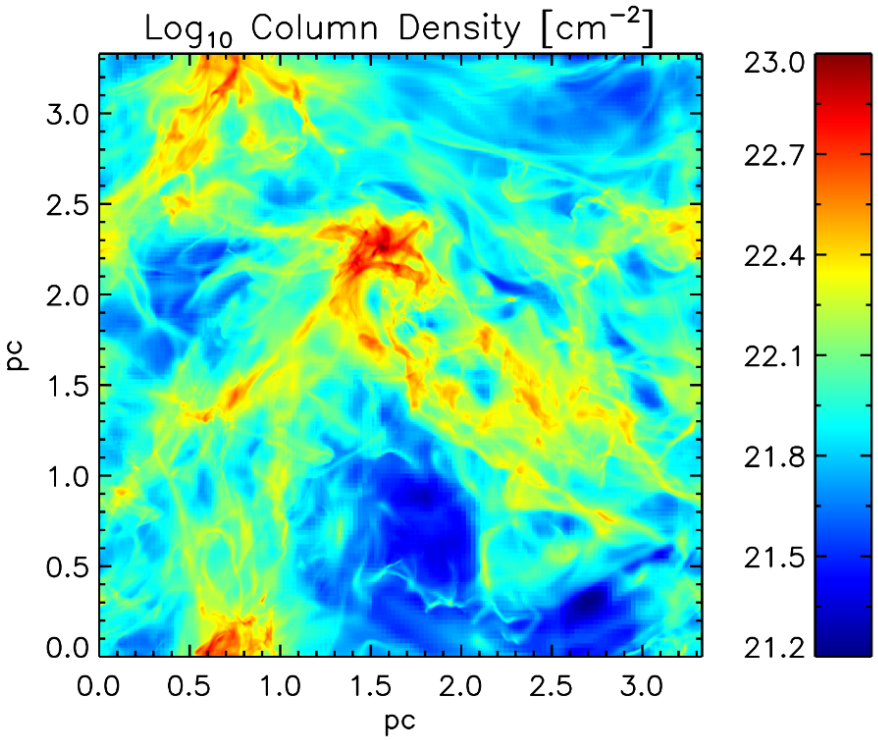
RAMSES-CPH (+KROME)

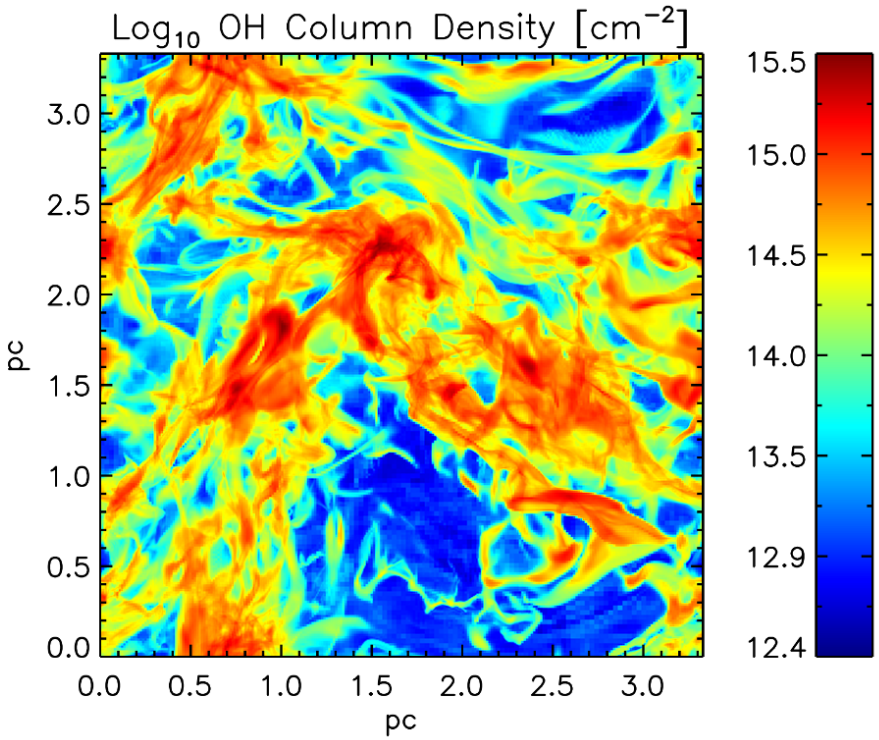
- Non-equilibrium H-C-O chemistry (+CRs, +photo, ∼Glover+2009)
- Fully coupled thermochemistry (on-the-fly fine-structure +tables, ∼Maio+2007)
- Consistent adiabatic index (partition functions, Boyle+2007)
- Dust chemistry (H_2,Cazaux+2009), dust cooling/photoheating (Grassi+2016)
- RT workaround: local density-based photochemisty, i.e. $A_v = f(n_{\rm tot})$
- Testing: tracer particles and RT (w/ T. Frostholm)
- with access to photochemistry-based opacity (RT-ready)

Molecular cloud model details

- MHD
- $\simeq (3.5\ \mathrm{pc})^3$, $\Delta x = 800$ AU
- Turbulence: Mach 11 @ 10 K
- $\langle B \rangle \simeq 7\ \mu$G
- > 18 Mcells
- 4.7 Myr $\simeq 3.5\,\tau_d \simeq 4.5\,\tau_{ff}$
- ~ 300 rates, ~ 40 species
- Grassi+2016

RAMSES+KROME results

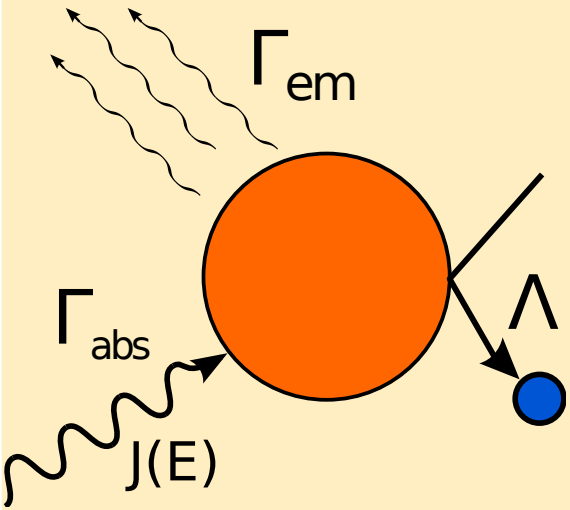




(More in Grassi+2016)

Dust: cooling / heating

Radiation-dust-gas interaction: Kirchoff's law



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

$$\int_{a_{min}}^{a_{max}} a^2 \varphi(a) \int_0^{\infty} \frac{Q_{abs}(a,E) B\left[E, T_d(a)\right]}{h} \mathrm{d}E \, \mathrm{d}a$$

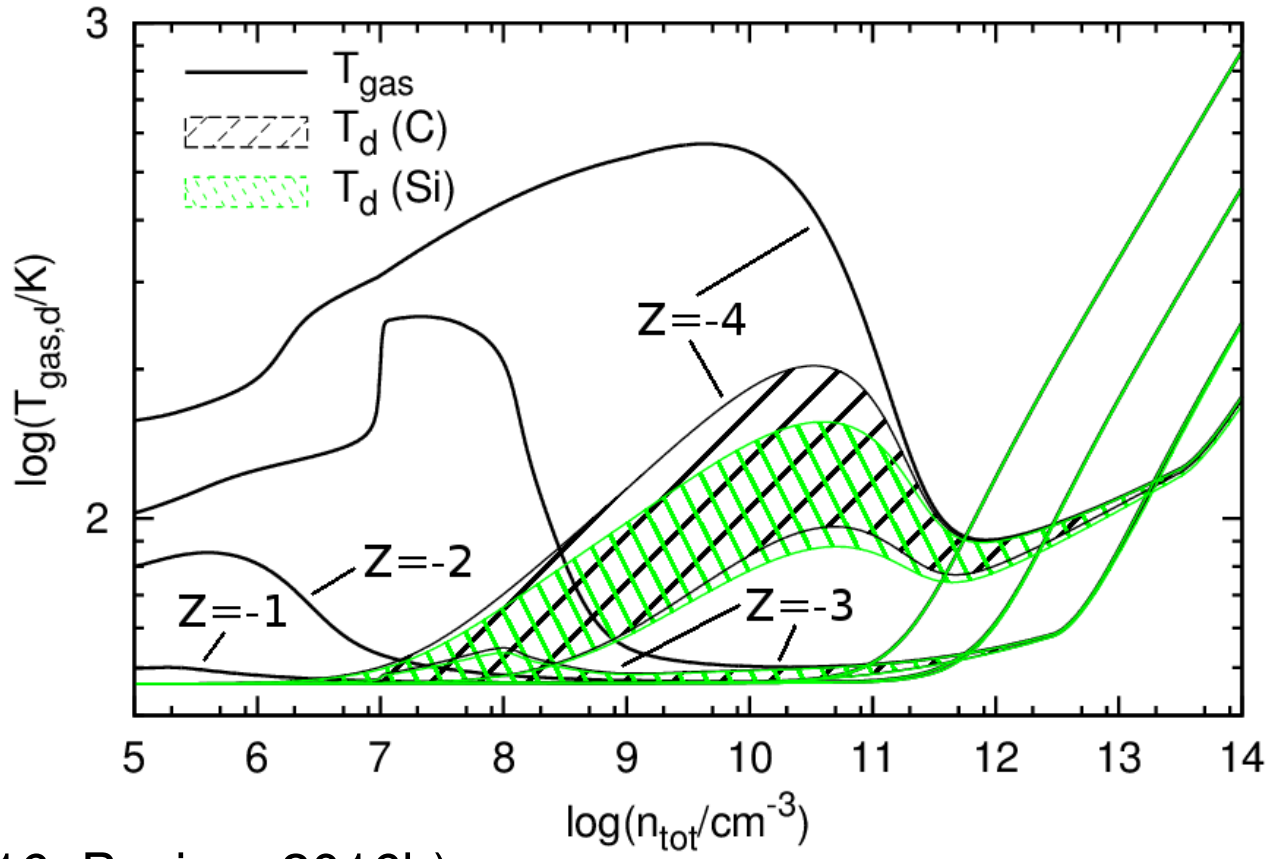
$$= \int_{a_{min}}^{a_{max}} a^2 \varphi(a) \int_0^{\infty} \frac{Q_{abs}(a,E) [J(E)]}{h} \mathrm{d}E \, \mathrm{d}a$$

$$+ \quad 2 f v_g n_{tot} \int_{a_{min}}^{a_{max}} a^2 \varphi(a) k_B \left[T_g - T_d(a)\right] \mathrm{d}a \,,$$

Dust: tables

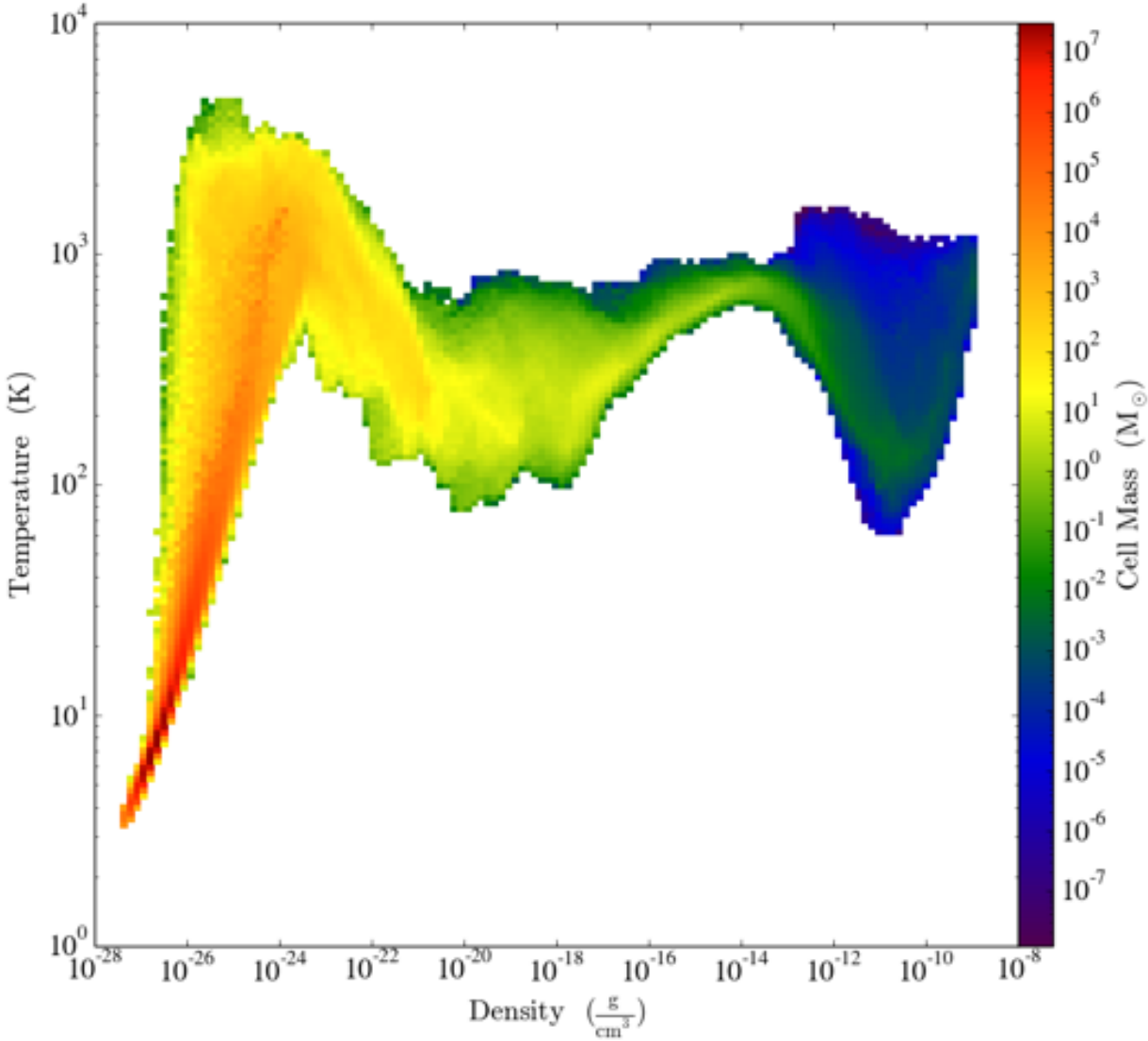
Parameters and table

$$\Lambda = f_\Lambda(n_g, T_g)\,\mu_g$$
$$\dot{n}_{H_2} = f_{H_2}(n_g, T_g)\,\mu_g\,n_H$$



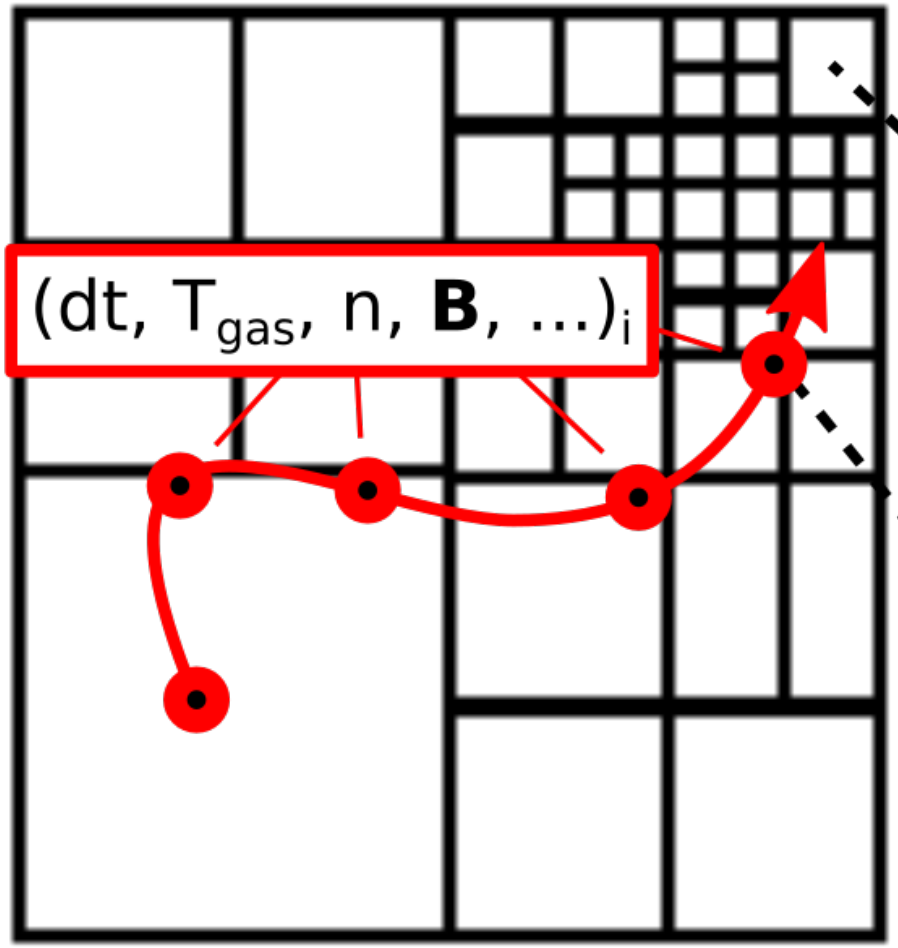
(Grassi+2016, Bovino+2016b)

Dust 3D in ENZO (w/S.Bovino+D.Schleicher)



(Grassi+2016, Bovino+2016b)

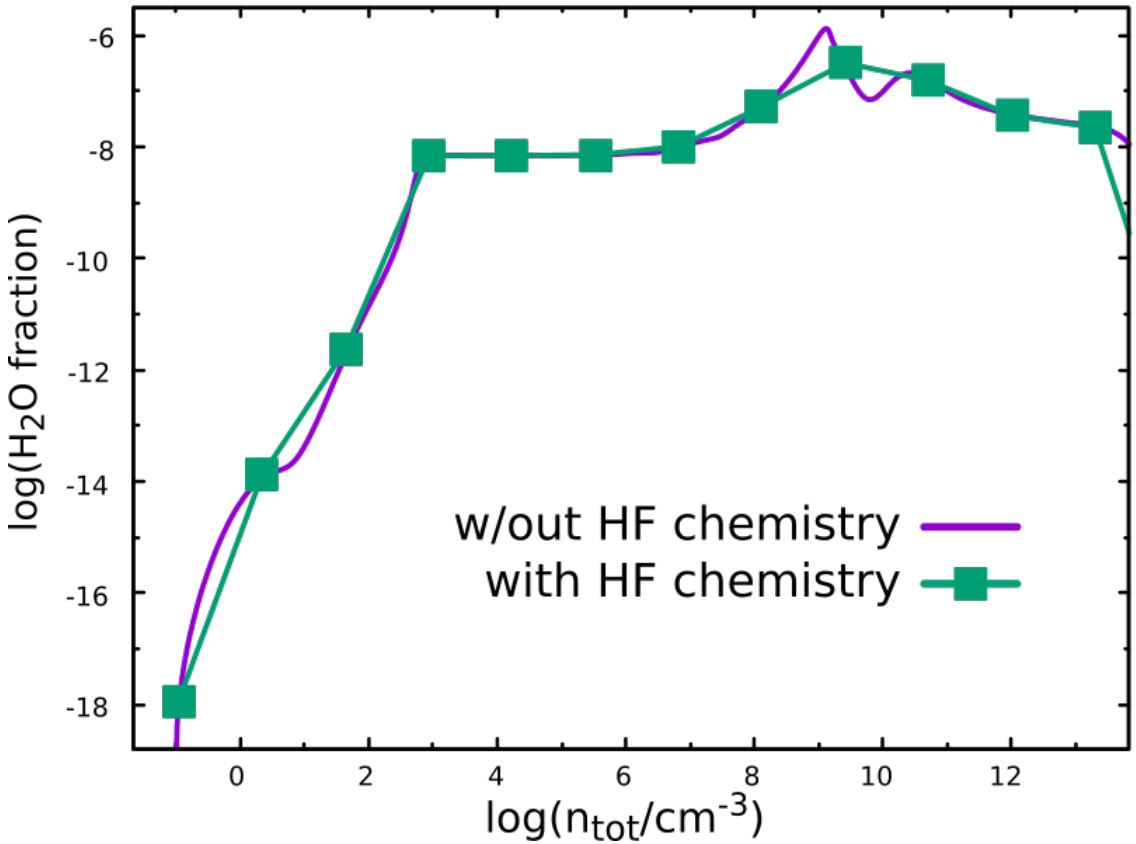
Tracer particles post-processing/1



1
Run "thermally interesting" chemistry on the AMR grid at run-time (e.g. H_2, CO, H_2O, ...)

2
Run full chemistry on tracer particles as post processing (e.g. HF)

Tracer particles post-processing/2



- Add more complicated chemistry at post-processing (observations!)
- Check the validity of “reduced” networks
- Play with parameters and add additional physics
- Optimize microphysics machinery using “cooked” data

Summary/Outlook

KROME

- KROME is a state-of-the-art code for microphysics, open-source
- self-consistent non-equilibrium microphysics/chemistry
- flexible (change ingredients with ease)
- successfully coupled with 3D simulations (but not only)
- HTML documentation and source help benchmarking and reproducibility

Take-home message

YOU NEED MICROPHYSICS!

Perspective

- Tracer particles in MCs (w/T.Haugbølle)
- MCs+RT (w/T. Frostholm, P Padoan) and synth observations (w/S. Frimann)
- Non-ideal MHD (global disk sims. w/O. Gressel, C. McNally, jets w/J. Ramsey)
- Chemistry in planetary atms. (PATMO code w/E. Simoncini, A. Chiavassa)