Interstellar radiation, cosmic rays and their impact on the chemical evolution of star forming filaments

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Outline of the talk

- Heard a lot about:
  - theoretical background
  - how to setup KROME and basic usage
- Now: some application/experience from a (astrophysics) user
  - ~~problems~~ (of course there are none!), advantages (only!)
  - own modifications applied
  - details about usage + coupling to FLASH code (see also exercise)
- Code parts will be printed red
- physical + numerical results

FLASH code

- Astrophysical code to simulate 3D, magneto-hydrodynamical problems
- Uses Adaptive-Mesh-Refinement to resolve regions of interest with higher spatial resolution
- Block structure: Simulation domain divided in blocks/patches consisting of 8^3 cells
  - A block resides on one CPU in total (reducing communication)
  - Each block can be divided into 8 smaller blocks with half the linear size

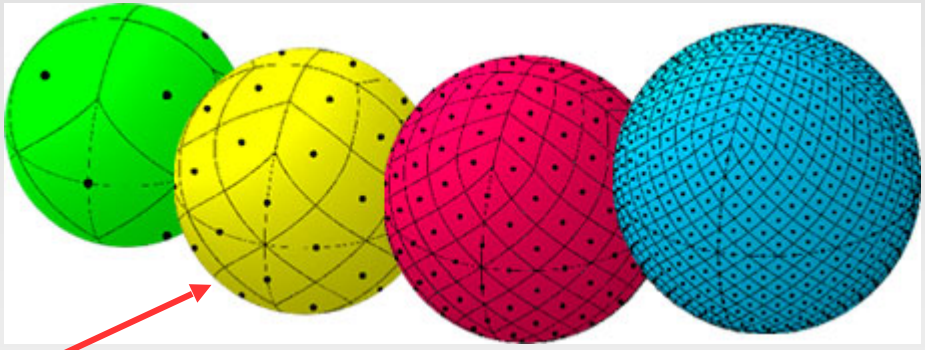
- FLASH is designed in a modular fashion:
  - Each module covers some physical process
  - Modules can be used individually or in combination
  - → Chemistry can easily be in-/excluded

FLASH modules

- Self-gravity:
  - Multigrid
  - Tree-code (usually faster by a factor of a few)
- Sink particles
  - Lagrangian particles accreting/ejecting mass
  - Interacting only gravitationally with gas
- Stellar feedback models (coupled to sinks)
  - Protostellar outflow, supernovae, stellar winds
- Radiative feedback of ionising and non-ionising radiation (optically thin gas)
- TreeCol: for (self-) shielding

TreeCol

- Tree-Col developed by P. Clark and R. Wünsch (Clark et al., 2012):
  - Calculates the mean optical depth / column density for each cell
- Makes use of the Healpix tool:
  - Divides sphere in regions of equal size
  - Calculates column density along each direction
  - Averages over all directions
  - Usually already 12 pixels are sufficient to receive accuracy of 10%

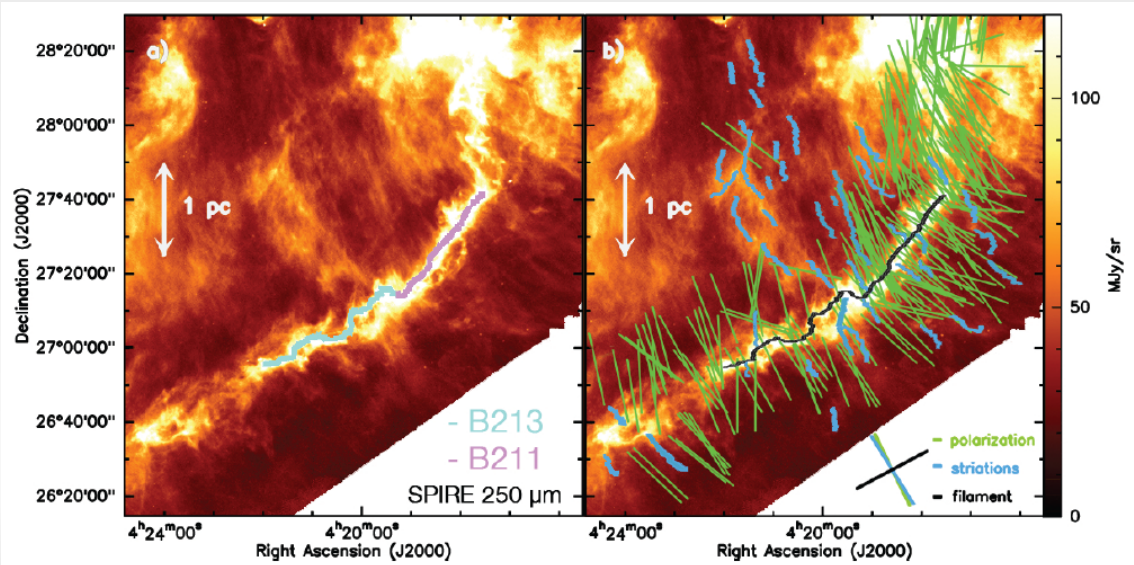


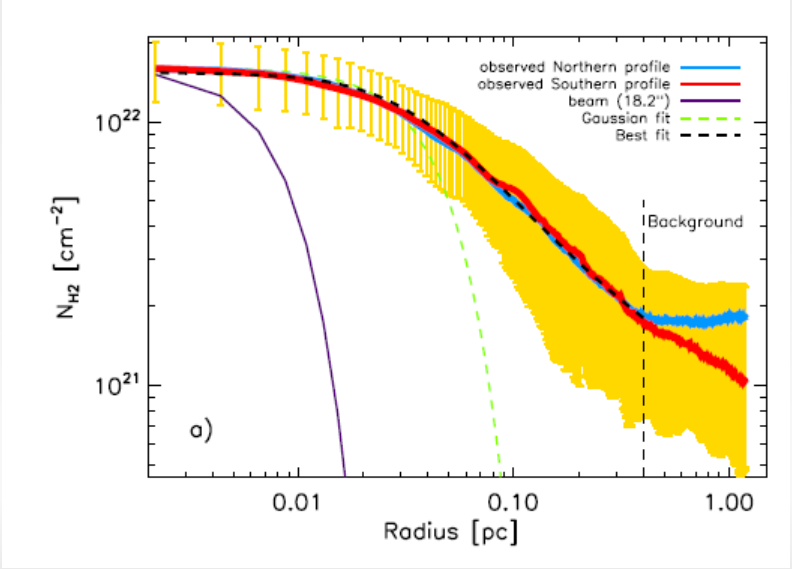
Picture taken from http://healpix.jpl.nasa.gov/

- Here 48 pixels are used
- We get: AV, H_2 self-shielding, CO column density N_{CO} …
  - Essential for chemistry to obtain proper ionisation + heating rates by incident radiation

Simulating interstellar filaments

- Filaments seem to be everywhere: „Filamentology“
- SF takes places in dense cores lining up along filaments
- Typical properties:
  - width of 0.1 pc
  - pervaded by magnetic fields
  - flat inner density part, at larger distances density falls off as r^{-2}

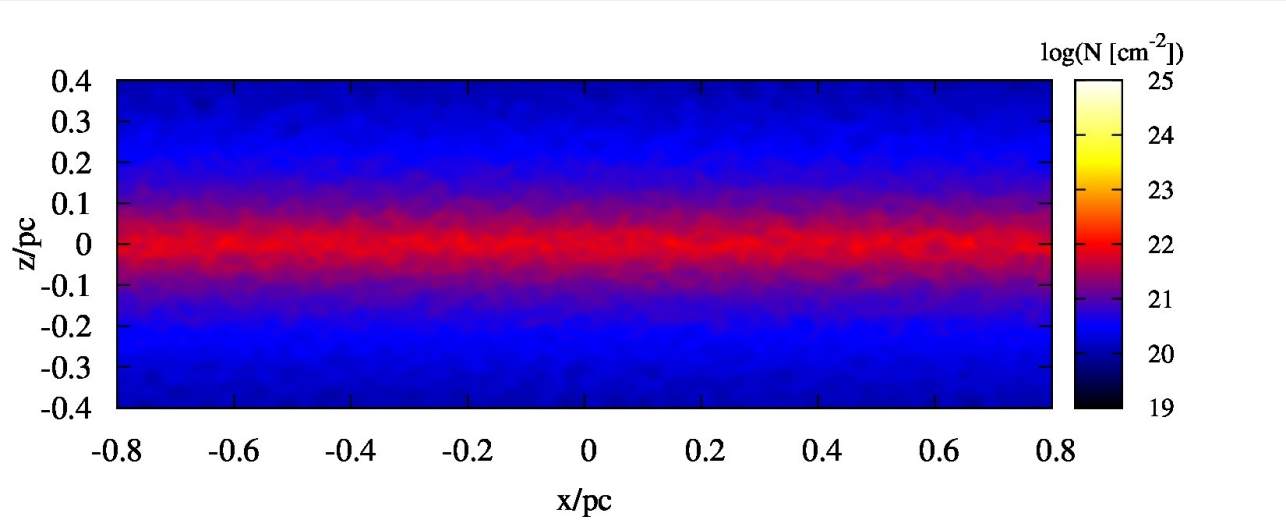




Palmeirim et al. 2013

Simulation setup

- Simulating filaments
  - Mass per length: 25 and 75 M_{sun}/pc
  - Central density of ~ 10^{-19} g/cm^{-3} , T = 15K
  - Without and with magnetic fields
    - Perpendicular and parallel to filaments, strength: 40 muG
  - Turbulent motions with M_{rms} ~ 1
  - Width ~ 0.1 pc, length 1.6 pc



Physics applied

- Run with FLASH4, using
  - sink particles, possible without any further modifications
  - Spatial resolution of 40 AU
  - Self-gravity
  - TreeCol
- Following SF process over ~ 300 kyr
- We use either:
  - No chemistry, isothermal EOS
  - Chemistry for CO formation

Chemistry in present day SF

- Heard about chemistry in simulation of POPIII star formation
  - „Relatively“ simple: includes only light atoms, (almost) no metals
  - Computational costs are „moderate“

- For present day star formation (SF) metals + dust chemistry have to be included
- This makes chemistry unproportionally more expensive
  - Number of rate equations scales roughly as N^2 (N = number of species)

- Even for the most abundant (and simple) molecule CO
  - ~ 40 species
  - ~ 300 reaction

Chemistry network

- We use the react_COthin network
  - 37 species, 287 reactions, including CO, HCO+, H_2O
  - Abundances initialized with freeze-out taken into account (Flower et al. 2005)

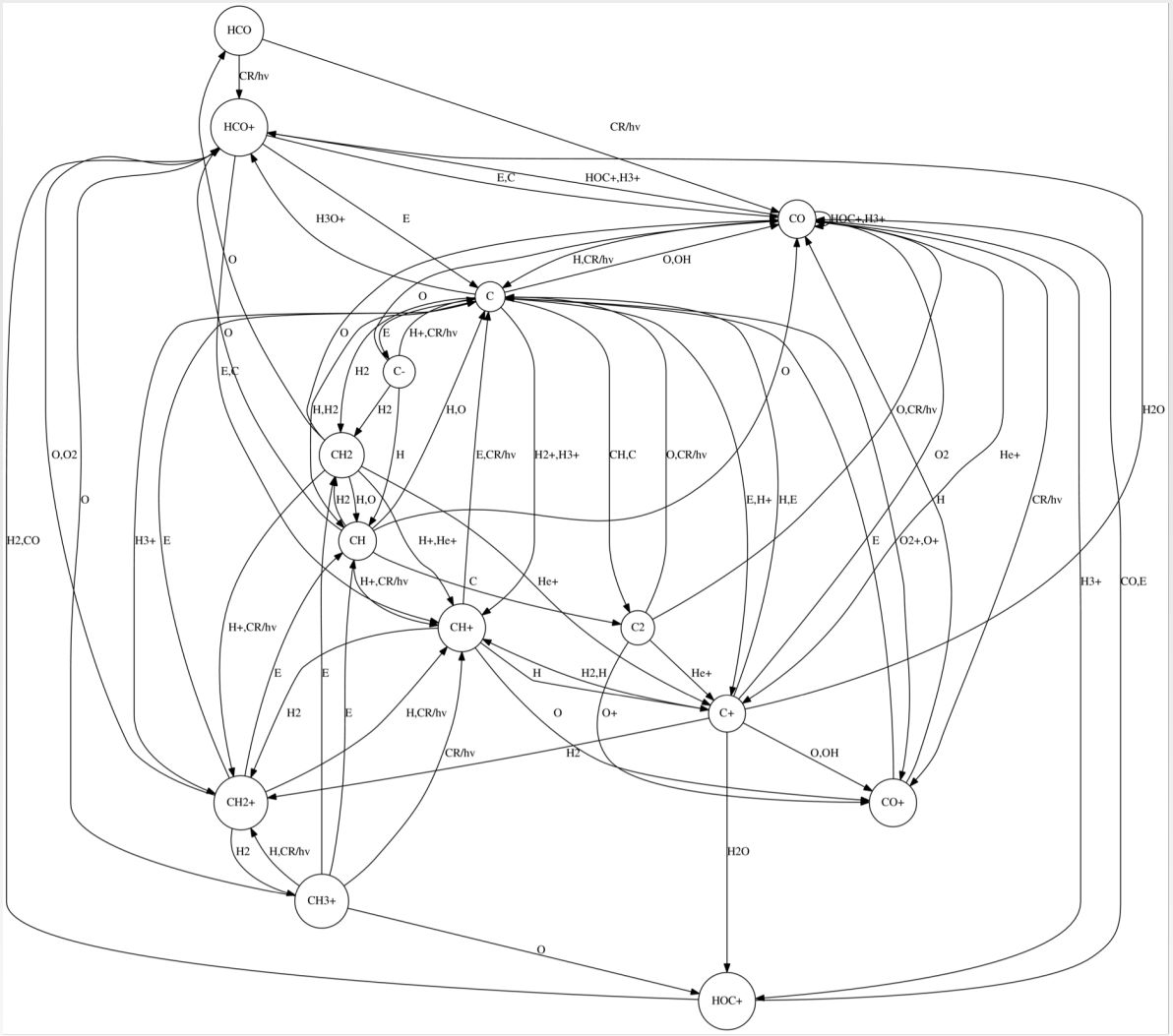
e^-	H	H^+	H^-	H_2	H_2^+	H_3^+	He	He^+	He^{2+}	C	C^+	C^-	C_2
CH	CH^+	CH_2	CH_2^+	CH_3^+	O	O^+	O^-	O_2	O_2^+	OH	OH^+	H_2O	H_2O^+
H_3O^+	HCO	HCO^+	HOC^+	CO	CO^+	Si	Si^+	Si^{2+}					

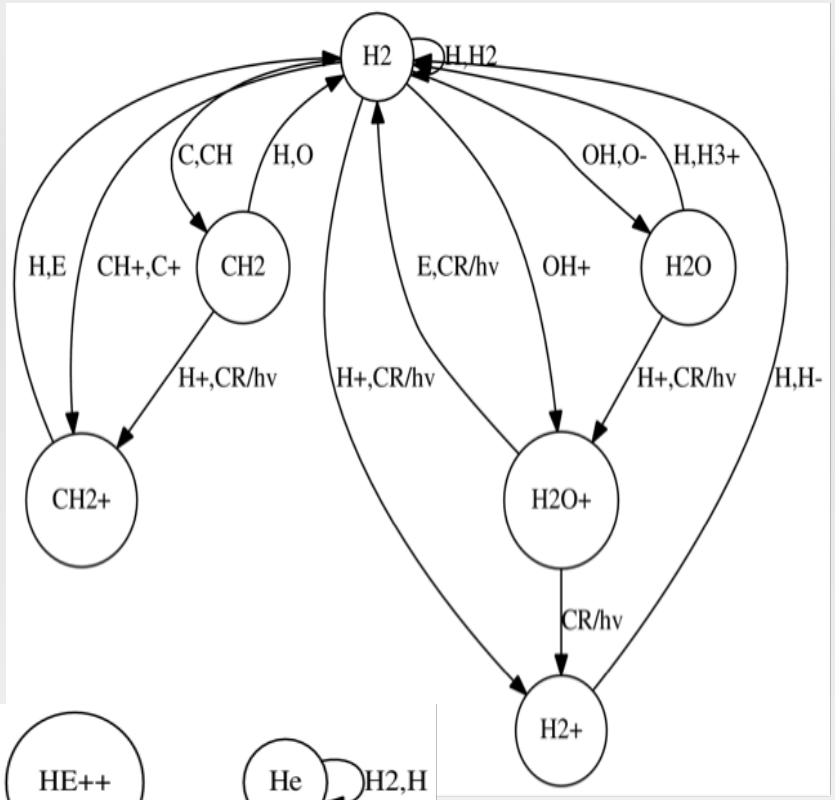
Element	mass fraction	fractional abundance
H	7.18(-1)	1
He	2.79(-1)	9.73(-2)
C^+	7.13(-4)	8.27(-5)
O	1.42(-3)	1.24(-4)
Si	6.78(-5)	3.37(-6)

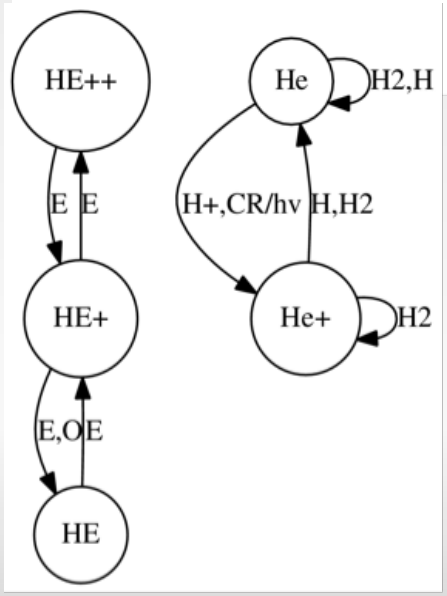
Chemistry network

- There is a nice tool in KROME to graphically represent (parts of) the network:
  - in the tools/ folder: pathway.py script
  - ./pathway any_network figure.eps <species>
    - <species>: gives a subselection of the network showing reactions including <species> as a reactant/product
  - graphviz package must be installed
    - sudo aptitude install graphviz
  - e.g. ./pathway.py react_COthin C-figure.eps C gives …..

Chemistry network

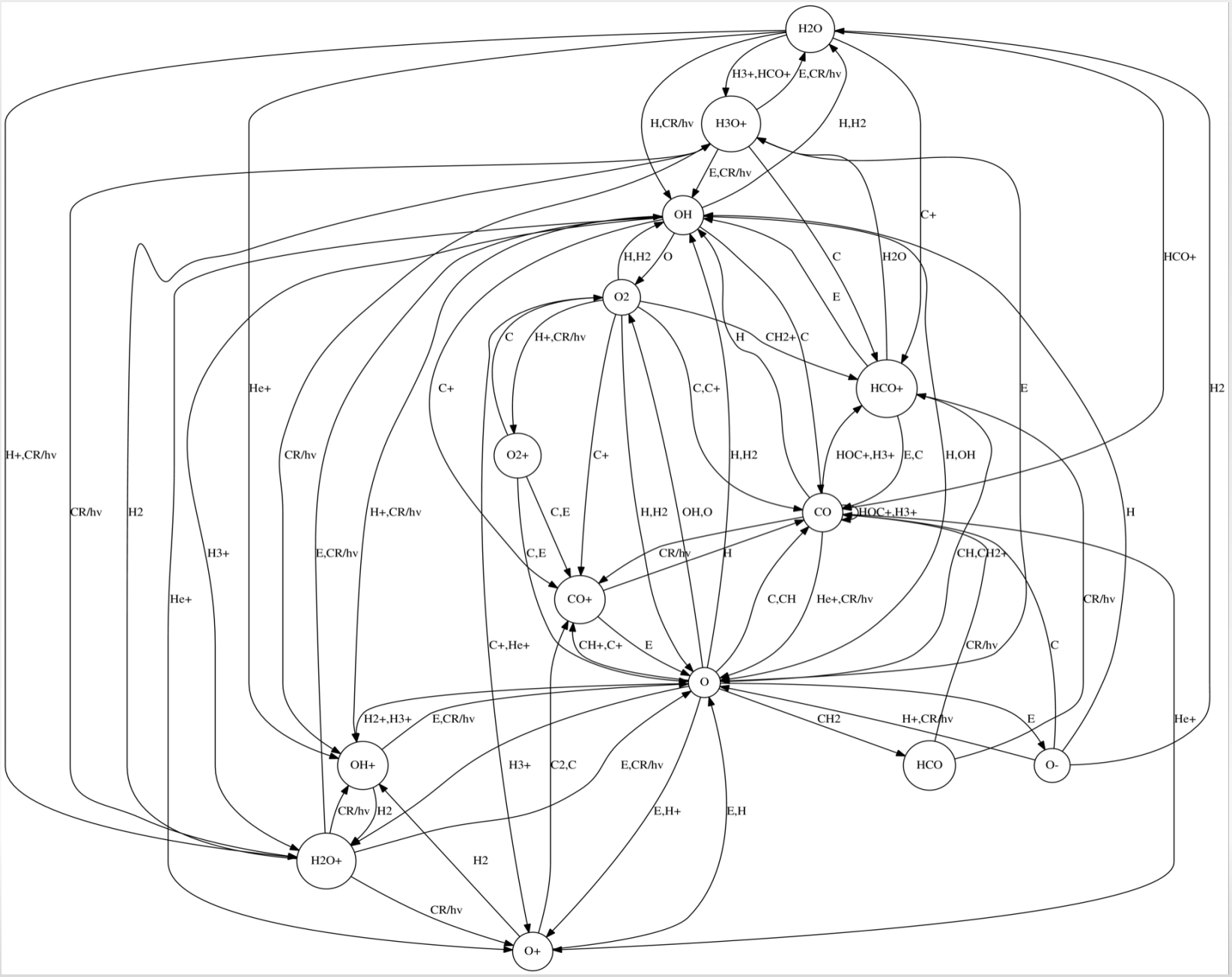


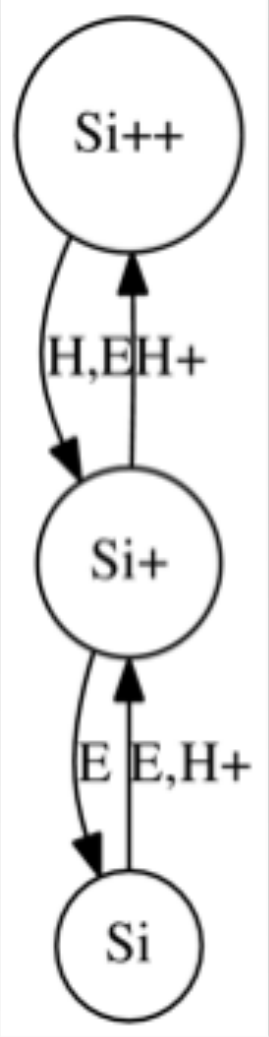




- ./pathway react_COthin C-figure.eps C

Chemistry network





Cosmic rays and ISRF

- We want to investigate impact of interstellar radiation field (ISRF) and cosmic rays (CR)
- Ionisation by incident CR:
  - In Krome: variable crate set to $1.3 \cdot 10^{-17}$ s^{-1} and $1 \cdot 10^{-16}$ s^{-1} (to account for uncertainties)
  - In KromeChemistry_init: call krome_set_user_crate(crate)
- Strength of ISRF:
  - In network react_COthin: create new variable Ghab
  - Correct all reactions depending on Ghab by Ghab/1.7
  - Ghab set to 1.7 and 8.5,
  - In KromeChemistry_init: call krome_set_user_Ghab(Ghab)
- Strength of ISRF evaluated in each cell by attenuation (TreeCol)

Chemistry network

- H_2 formation on dust in parametrised form, dust temperature self-consistently from simulation
  - Before EACH krome call: call krome_set_user_Tdust(t_dust)
- Optical depth AV, H_2 self-shielding, and CO column density self-consistently from TreeCol
  - Before EACH krome call: call krome_set_user_Av(AV)
  - Before EACH krome call: call krome_set_user_H2self(H2self)
  - Before EACH krome call: call krome_set_user_NCO(NCO)
- -useN: KROME by default uses number densities
  - Flash uses mass fractions
  - Make sure that conversion is done properly!
    - Use same masses of species as stored in KROME

Chemistry network

- three further options:
- -compact:
  - summarizes all Krome functions in krome_all.f90
- -gamma full:
  - use individual gammas for different species
  - check that your code does the same
- -flash:
  - make interface for Flash
  - just copy folders/code to Flash source code

Take a breath…

- Hydrodynamics taken care of by Flash
- „Chemistry“ by using network react_COthin
- Radiation by TreeCol (+ KROME)
- **Missing description of thermal evolution**

Cooling processes

- KROME cooling mechanisms:
  - -cooling H2, CHEM, CIE, CI, CII, OI, OII, SiI, SiII,CO
  - For CO: N_{CO} required → from TreeCol (new variable user_NCO)
    - In code set v3 = user_NCO
  - CO cooling from ^{13}CO and $C^{18}O$ included
    - Necessary if gas gets optically thick for ^{12}CO
    - Scale user_NCO and resulting cooling rate by 1/69 and 1/557
  - -coolingQuench 10: terminates cooling below 10 K

Cooling processes

- KROME cooling mechanisms:
  - For dust: own defined cooling routine
    - Does not require the usage of dust within KROME (memory saving)
    - Integrated over dust particles sizes

$$\Lambda_{\rm coll}(T_{\rm dust,eq}) + \Gamma_{\rm ISRF}(T_{\rm dust,eq}) \stackrel{!}{=} \Lambda_{\rm BB}(T_{\rm dust,eq})$$

→ Calculated once before Krome call to calculate Tdust
→ set user_Tdust

$$\Gamma_{\rm ISRF} = 5.8 \times 10^{-24}\, \chi\, n_{\rm H,tot}\, G_0\, {\rm erg\, s^{-1}\, cm^{-3}}\,.$$

$$\Lambda_{\rm BB}(T_{\rm dust}) = 4.68 \times 10^{-31}\, T_{\rm dust}^6\, n_{\rm H,tot}\, {\rm erg\, s^{-1}\, cm^{-3}}\,.$$

$$\Lambda_{\rm coll}(T_{\rm dust}) = 2\times 10^{-33}\, n_{\rm H_2}^2 \sqrt{\frac{T_{\rm gas}}{10.0}}\, (T_{\rm gas} - T_{\rm dust})\, {\rm erg\, s^{-1}\, cm^{-3}}$$

→ Last term affects gas + dust: Also used during Krome evaluation as additional gas cooling process

Heating processes

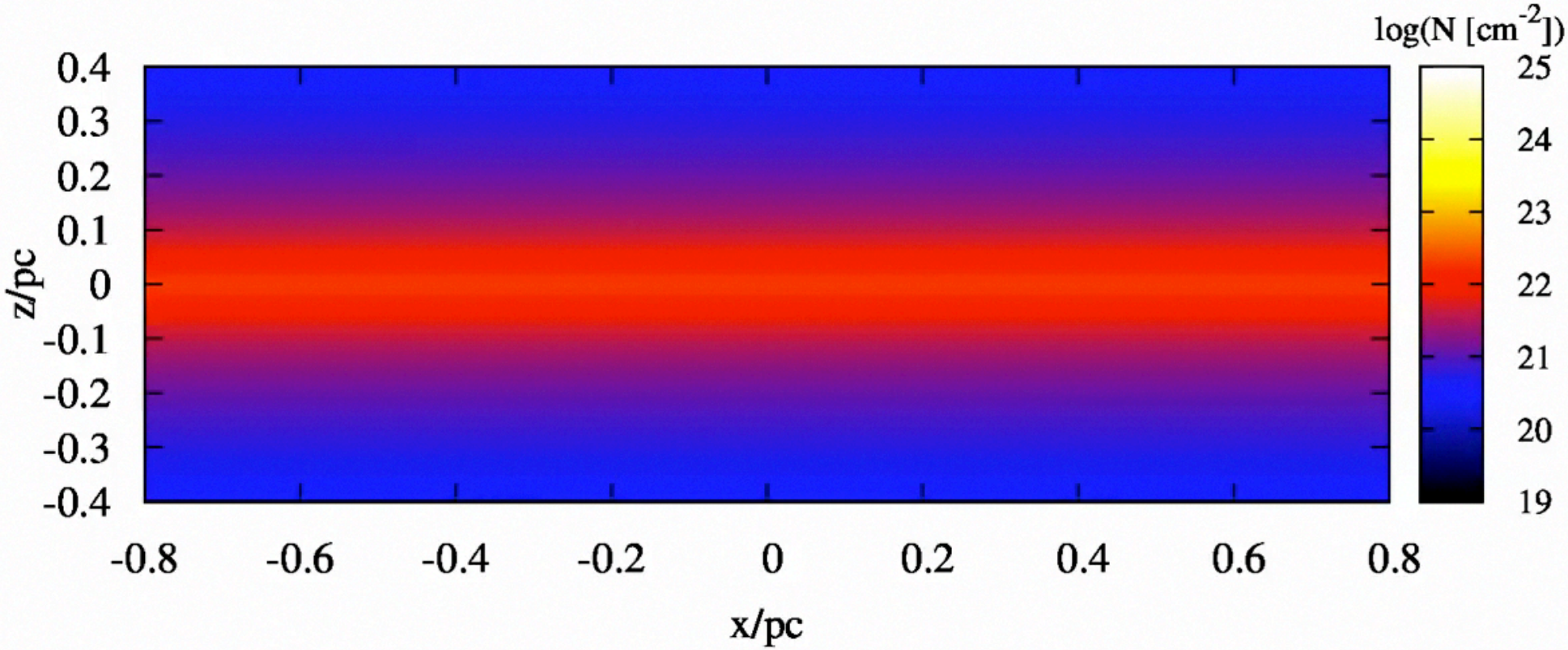
- KROME heating mechanisms:
  - -heating CHEM, CR, PHOTODUST
  - For PHOTODUST set Ghab = user_Ghab * exp(-2.5 user_AV)

- To summarize: KROME set up with:

```
./krome -n react_COthin -heating CHEM,CR,PHOTODUST
-cooling H2,CHEM,CIE,CI,CII,OI,OII,SiI,SiII,CO
-coolingQuench 10 -gamma FULL -useN -compact
-flash
```

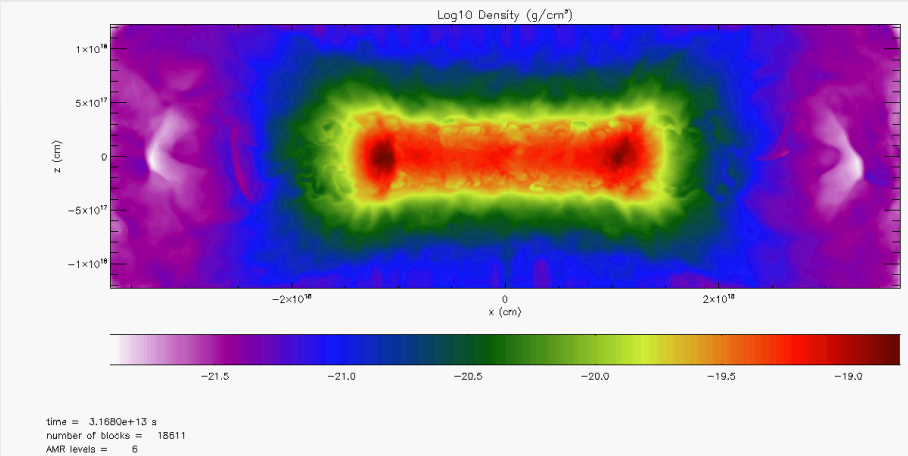
FINALLY:

Time for some MOVIES

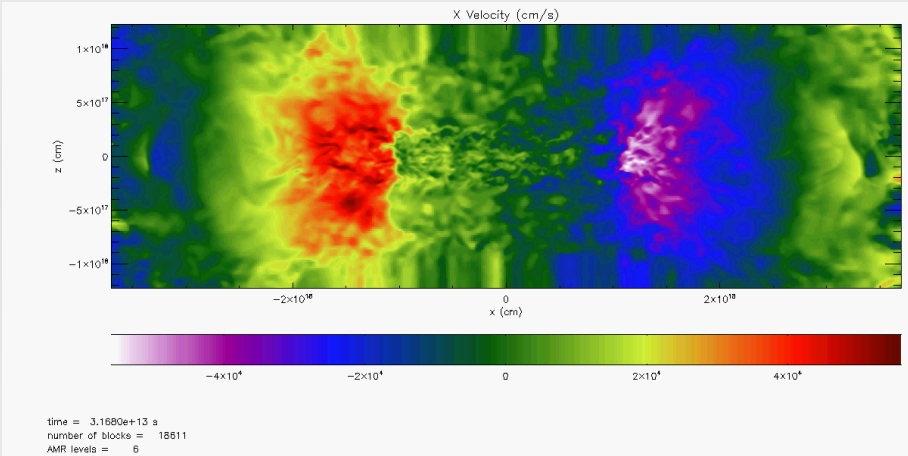

log(N [cm^{-2}])
25
24
23
22
21
20
19
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
z/pc
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
x/pc

Time evolution

Density



Velocity



- Edge-on collapse, condensations form first at outer edges, gravitational focussing (Pon et al. 11)
- Fragmentation properties depend on magnetic field configuration and mass of the filaments
- Filaments get rather narrow (< 0.1 pc) ↔ observations

Results

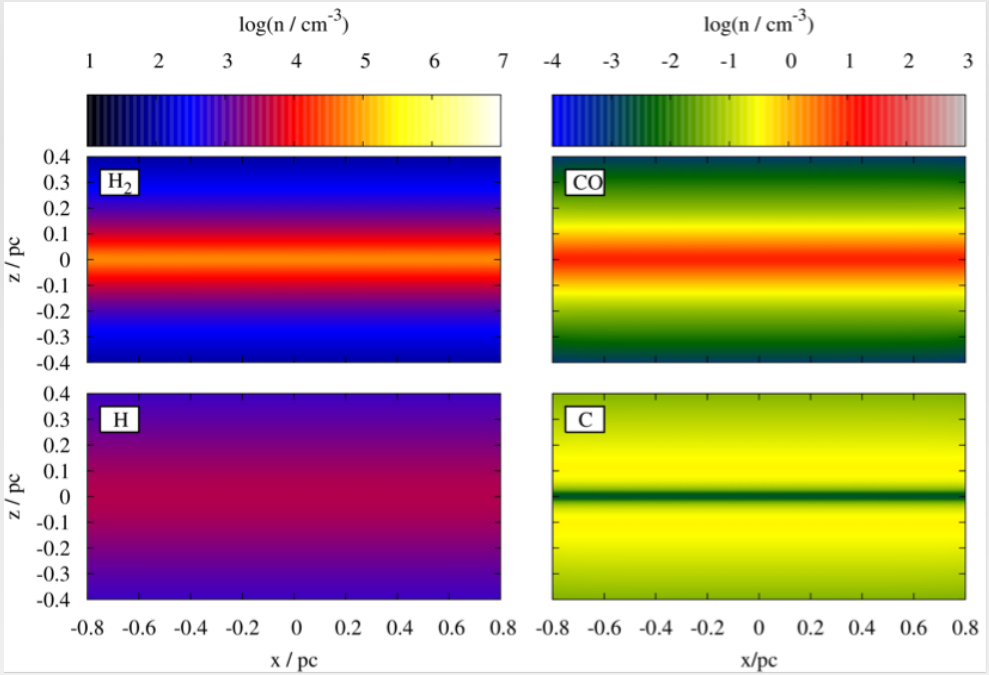
- So far we have considered runs without chemistry

- Problems with IC
  - Unavoidable for every kind of simulation
  - Even more severe for simulations including chemistry:
    - With which chemical configuration do we start
    - Chemical equilibrium? → probably better choice than „random“ ICs

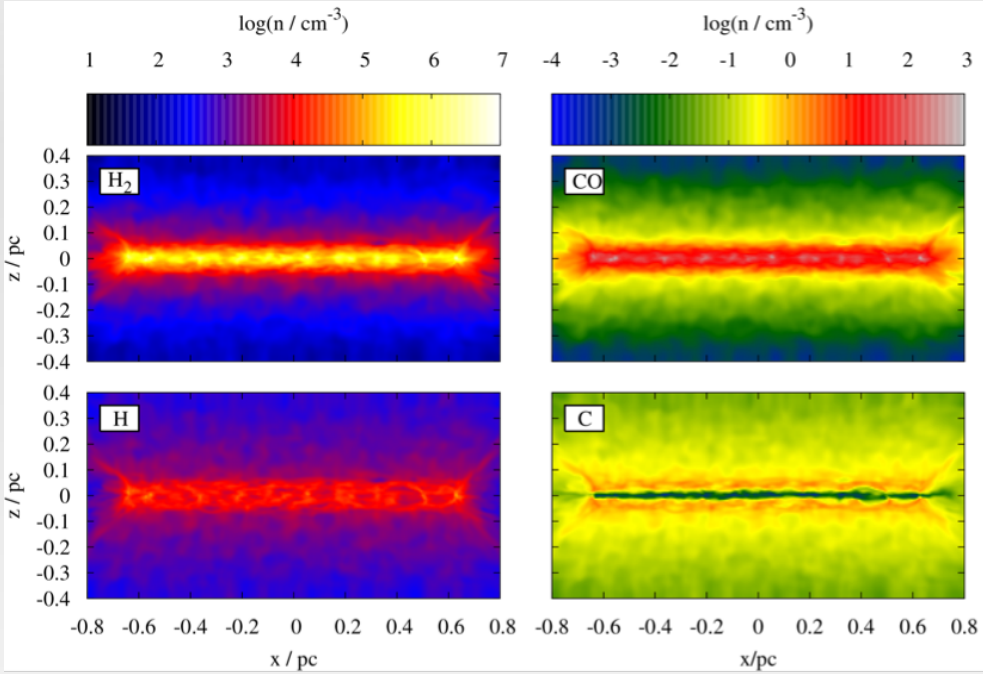
- Start with purely atomic species (carbon in C^+ instead of C)
- Relax for 500 kyr
  - Hydrodynamics not evolved
  - Sufficient to reach rough chemical equilibrium
  - 500 kyr ~ H_2 formation time at $n = 10^5$ cm^{-3}

Results

T = 0 (after relaxation)



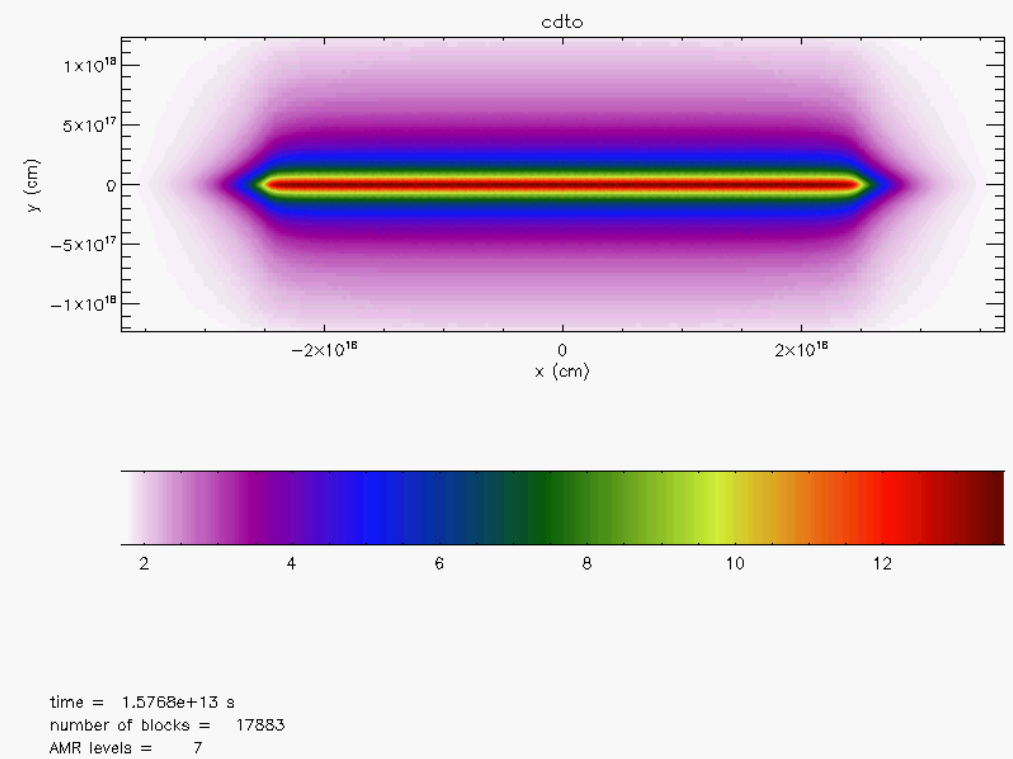
T = 300 kyr



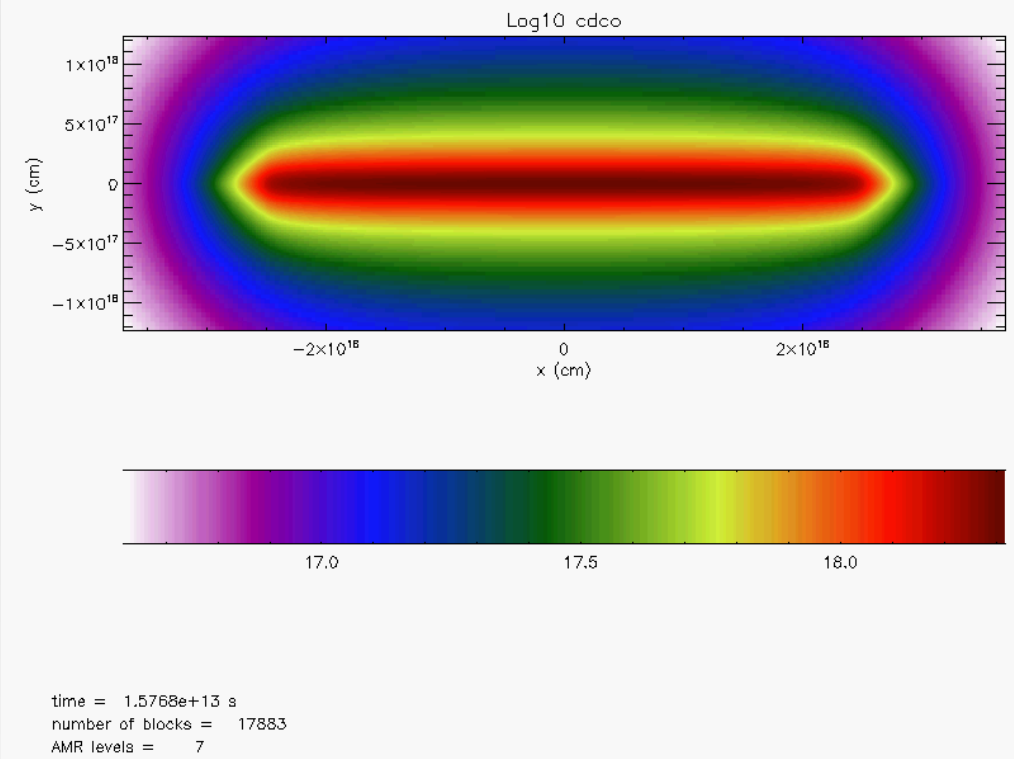
- In center of the filament
  - hydrogen mainly in form of H_2
  - Carbon almost completely in CO
- Impact of turbulent motions recognisable

Results of TreeCol

AV

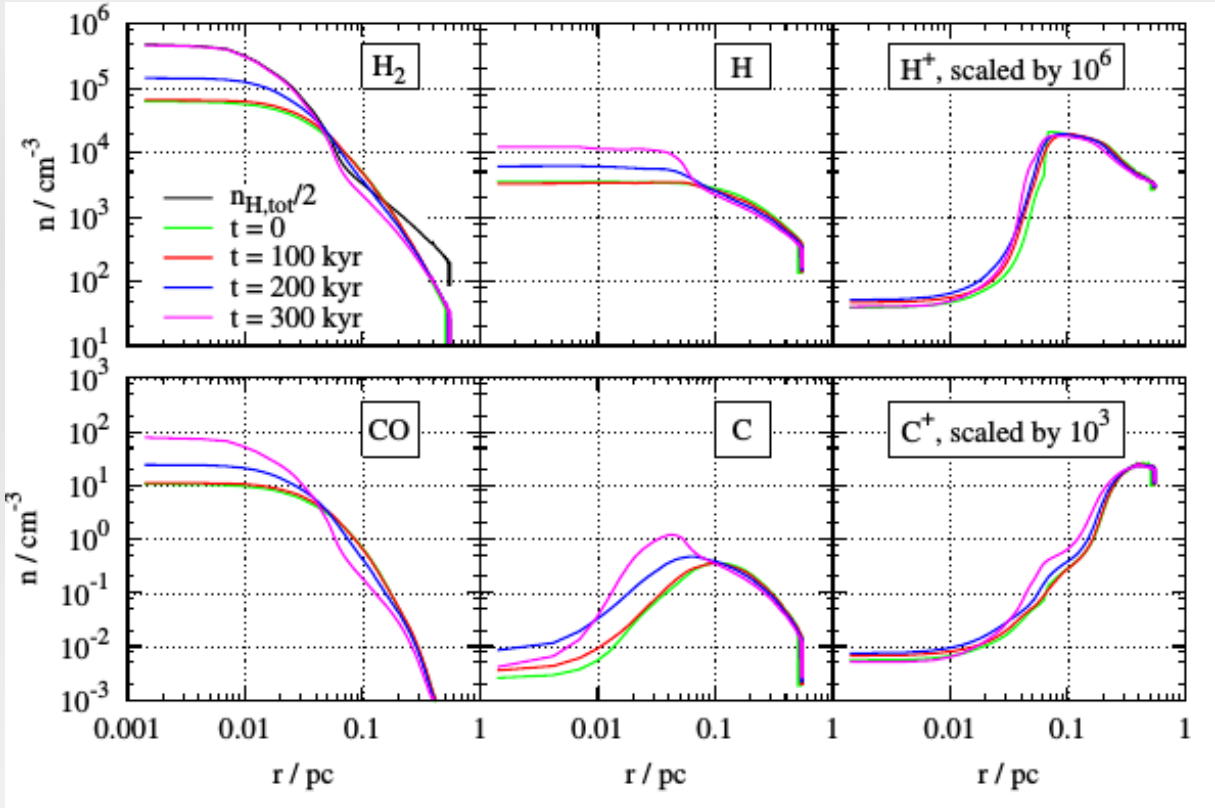


CO column density



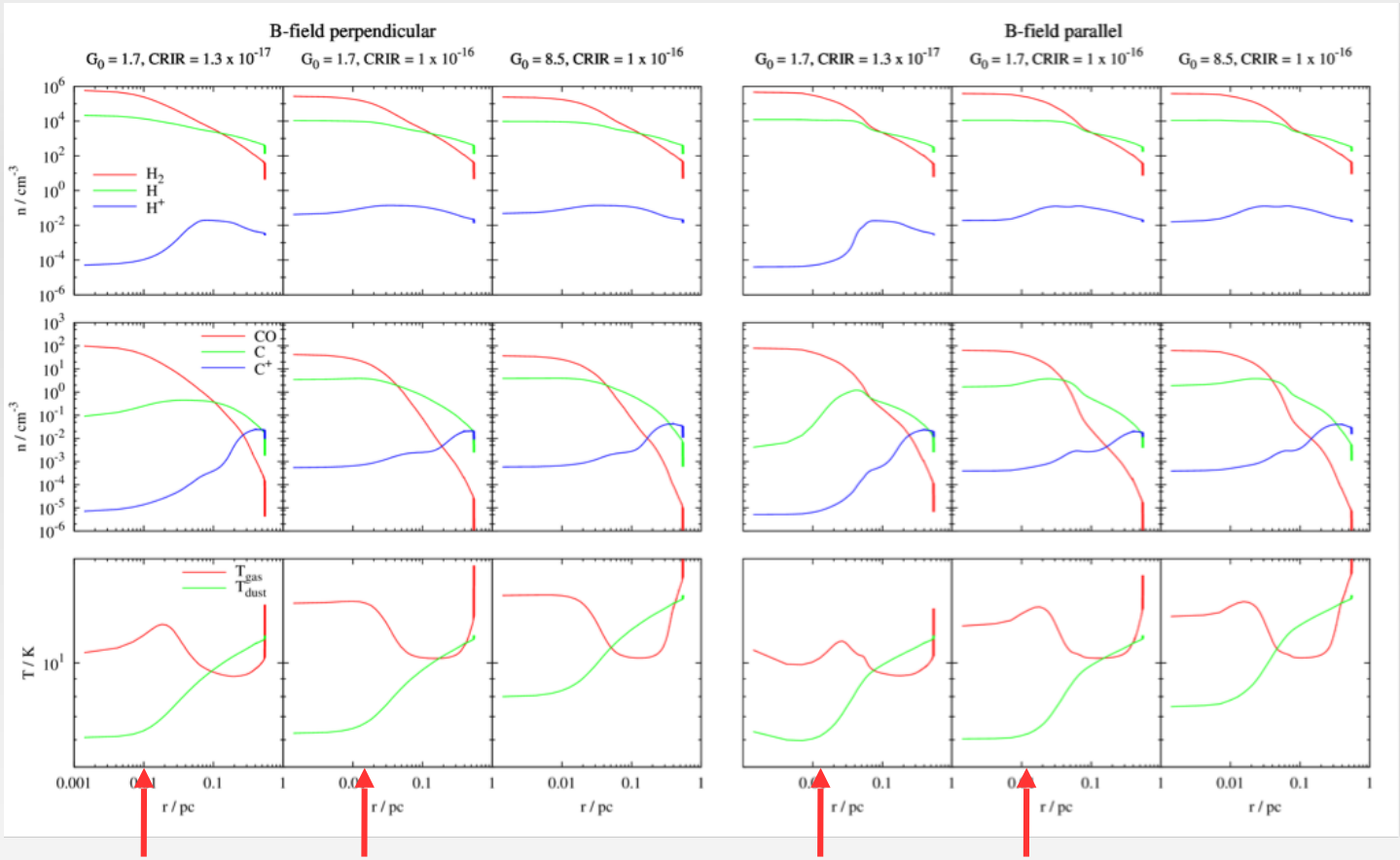
- Optical depth increasing strongly towards center
- CO column density between 10^{16} and 10^{19} cm^{-2}

Time evolution of radially averaged quantities



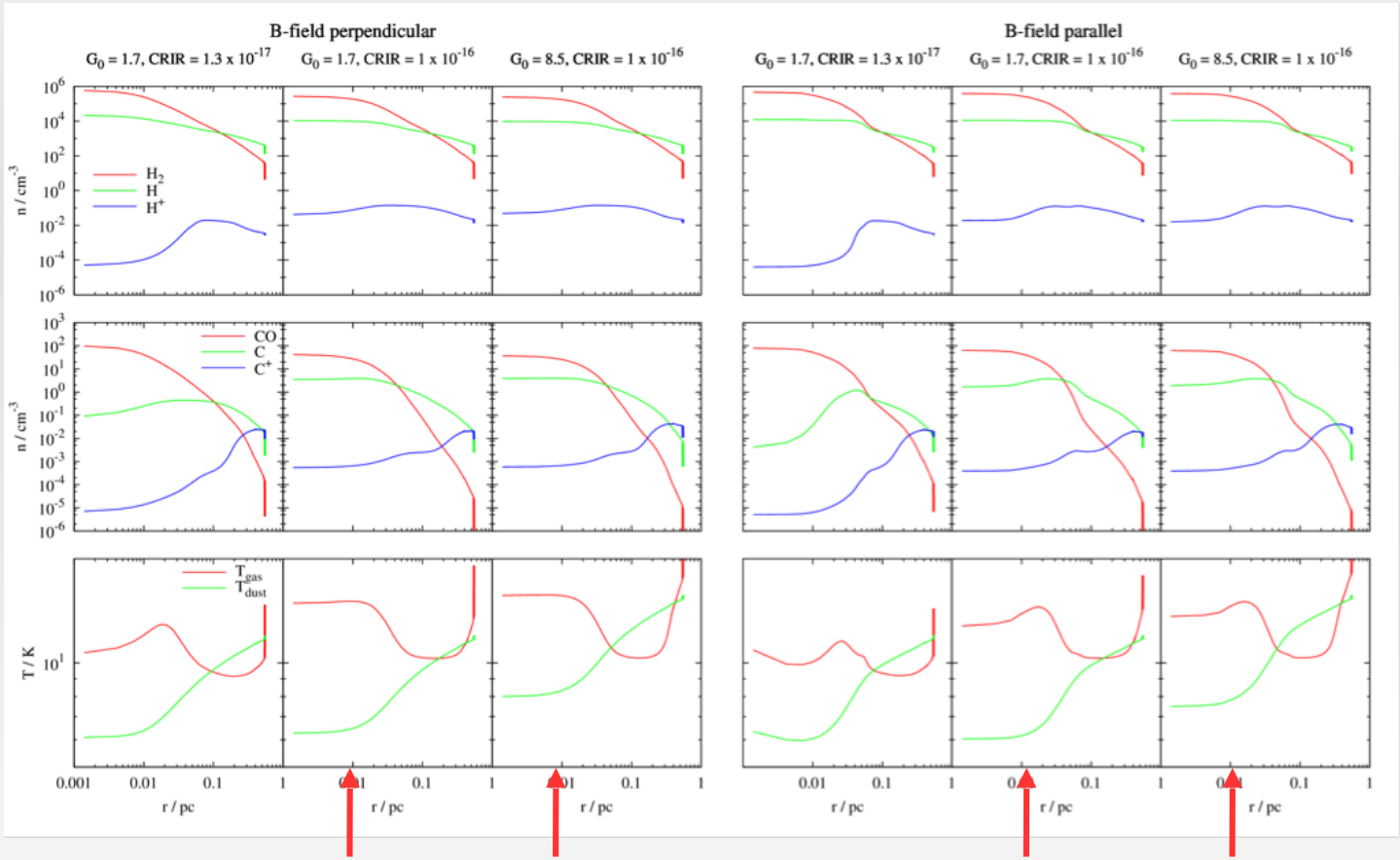
- Increase of H_2, H, and CO over time
- H^+, C, and C^+ remain rather unchanged
  - Quick conversion into other species
- Wit decreasing radius: Gradual conversion of $H^+ \rightarrow H \rightarrow H_2$ and $C^+ \rightarrow C \rightarrow CO$

Impact of ISRF and CR



- Increasing CR ionisation rate:
  - Higher abundances of H^+ and C^+ (1 – 2 order of mag.)
  - Slightly increased gas temperature due to energy released by dissociation reactions

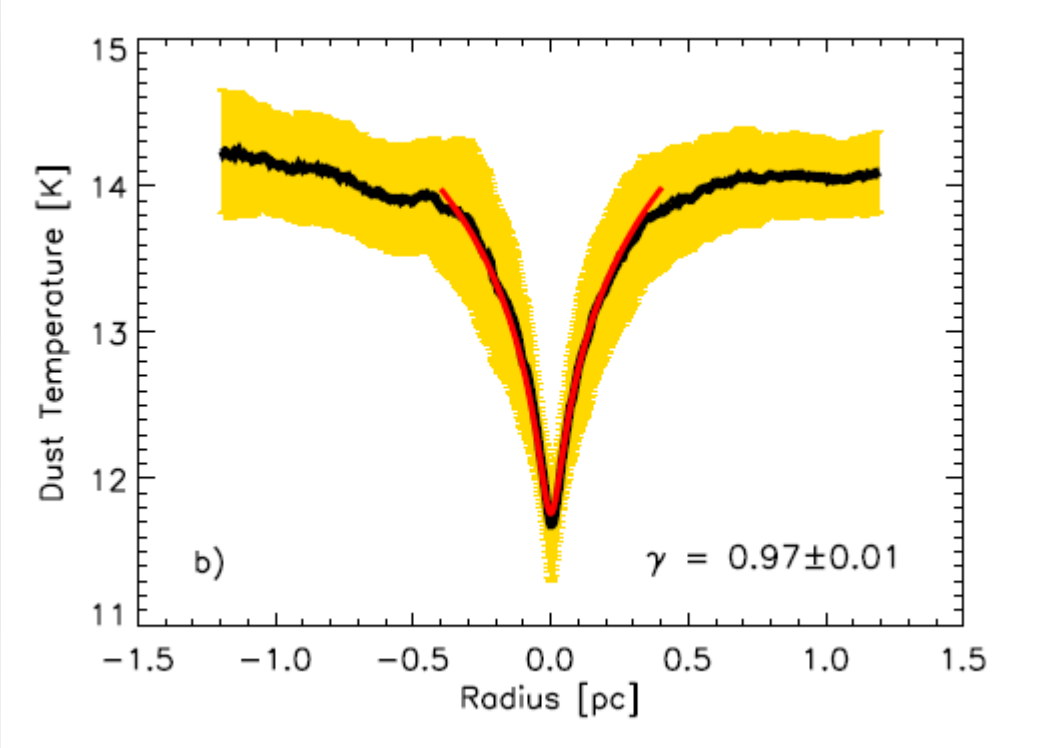
Impact of ISRF and CR



- Increasing ISRF:
  - Chemical composition only marginal affected
  - Gas + dust temperature increase by a few K due to enhance PE heating
- Note: Gas and dust temperature are markedly different

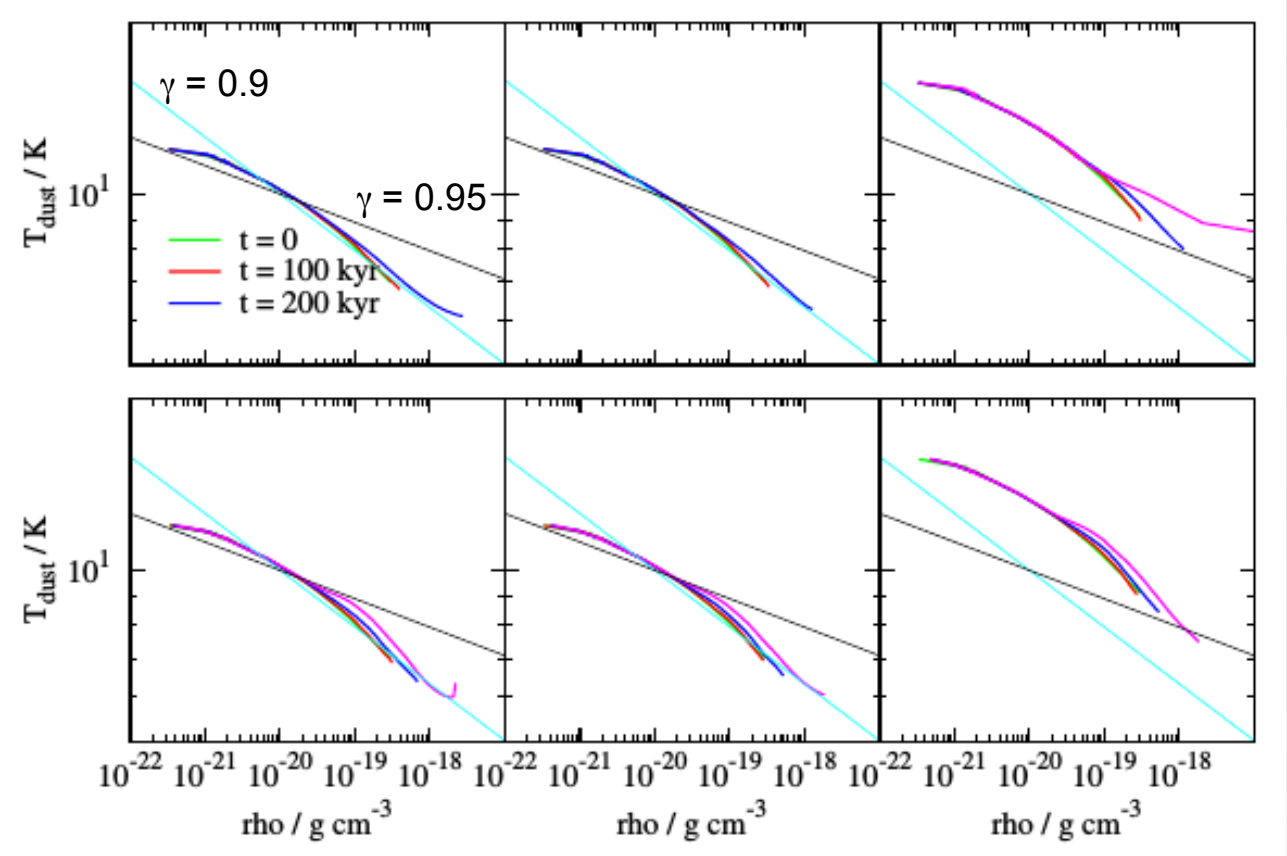
EOS

- KROME allows to accurately describe thermal evolution of gas and dust
- Palmeirim et al. 2013 found decrease of T_{dust} towards center
  - Similar do we
- Fit of polytropic EOS: $T \sim \rho^{\gamma - 1}$
- $\rightarrow \gamma = 0.97$
- How does this compare to our results?



Palmeirim et al 2013

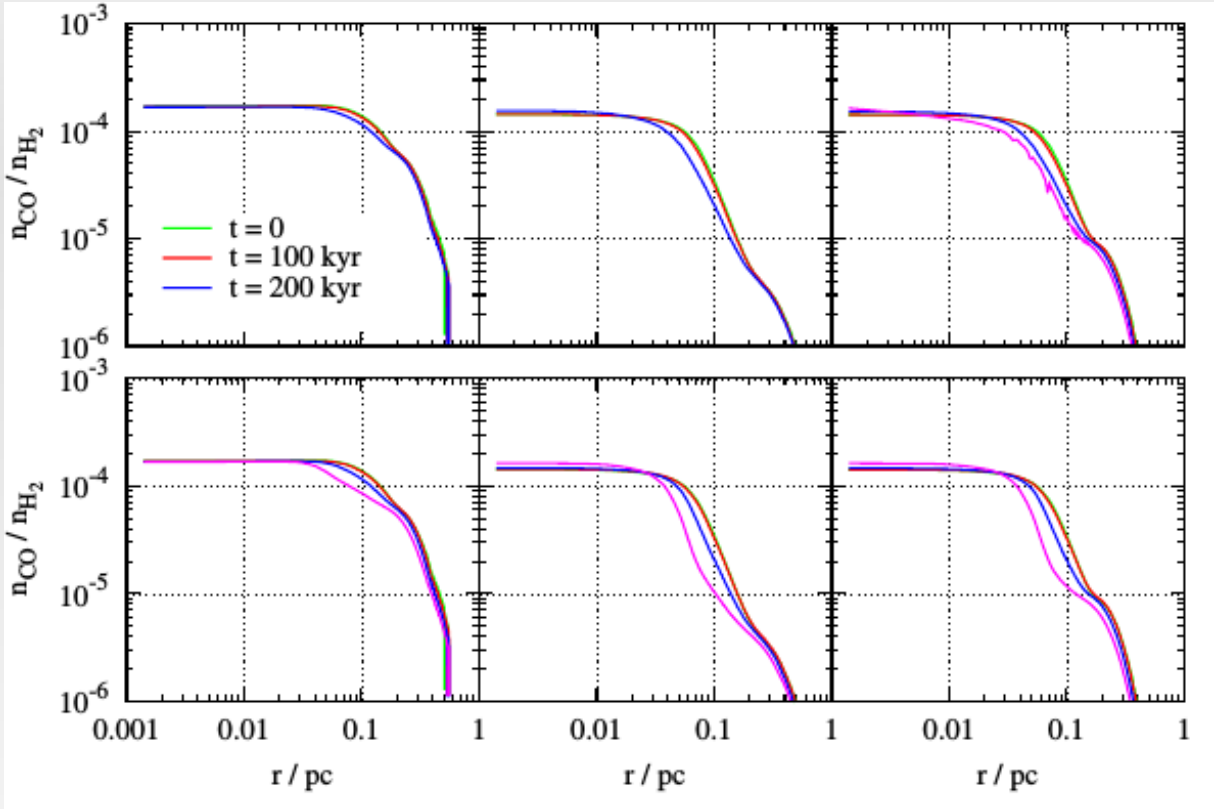
EOS



- γ = 0.90 – 0.95
  - Independent of CR and ISRF
  - In reasonable agreement with observations

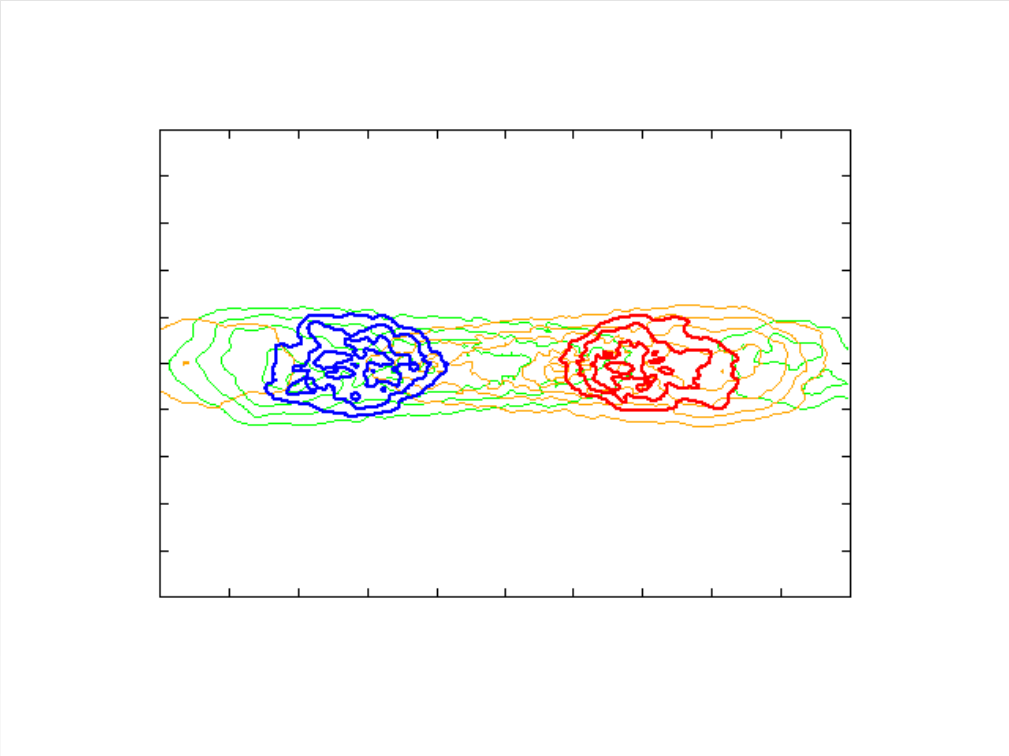
CO-H_2 conversion factor

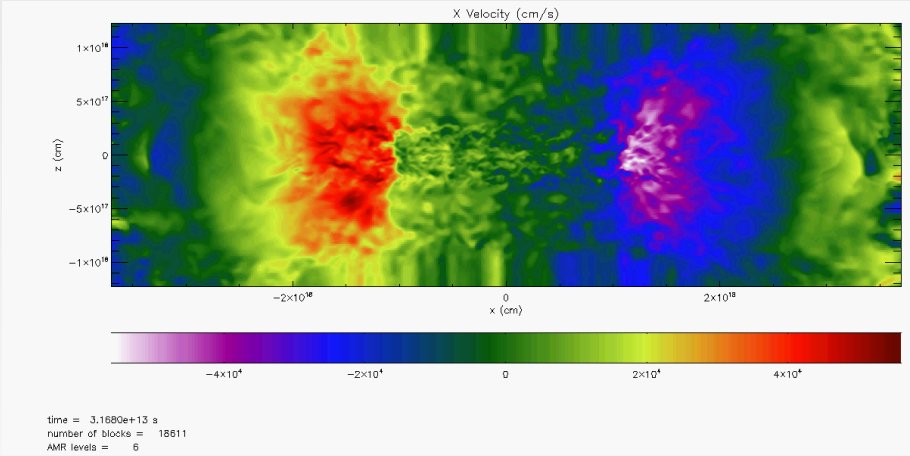
- Often a fixed conversion between CO and H2 is assumed
  - Around 10^{-4}
- Good agreement in central region
- Drop by 2 orders of mag. in outer regions
- Affect of ISRF and CR mainly in outer regions
- Variation affects X-factor
  - Caution when converting CO line intensities to gas masses



Synthetic observations – Preliminary results

- Usage of data for line transfer calculations:
  - CO-channel maps (RADMC-3D) reflect velocity structure





Numerical performance

- Some technical details
  - Simulation runs on SuperMUC at LRZ/Garching, + JUROPA in Juelich
  - Use of 500 blocks/CPU, standard cpus (~ 1.5 GB – 3 GB memory / CPU)

- Numerical costs:
  - Measured against a simulation without any chemistry
  - naturally some small (unavoidable) differences
  - Computational cost increased by a **factor of 7**

Conclusions

- KROME can by used „on-the-fly“ even with a complex network
  - 37 species, ~ 300 reactions
  - Runs on typical machines with 2 GB memory / CPU
  - Slow down by a factor of 7
- Applied to a collapsing filament
  - Promising physical results

- Potential for future applications
  - Synthetic observations
  - Compare „observed“ filament width with „real“ (3D) width
  - Constrains on the X-factor
  - Inclusion of nitrogen chemistry (necessary for important tracers)