Astrochem: a fast time-dependent code for astrochemistry

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Basics

- Let's start with an example:

$$\mathrm{H_3^+ + CO \rightarrow HCO^+ + H_2}$$

$$\mathrm{HCO^+ + e^- \rightarrow H + CO}$$

- Let us call $k1$ and $k2$ the rates of these two reactions (in $cm^3\ s^{-1}$).

- If we neglect other formation/destructions routes, the concentration of HCO^+ as a function of time is given by:

$$\frac{dn(\mathrm{HCO^+})}{dt} = k_1\, n(\mathrm{H_3^+})\, n(\mathrm{CO}) - k_2\, n(\mathrm{HCO^+})\, n(\mathrm{e^-})$$

Formation term Destruction term

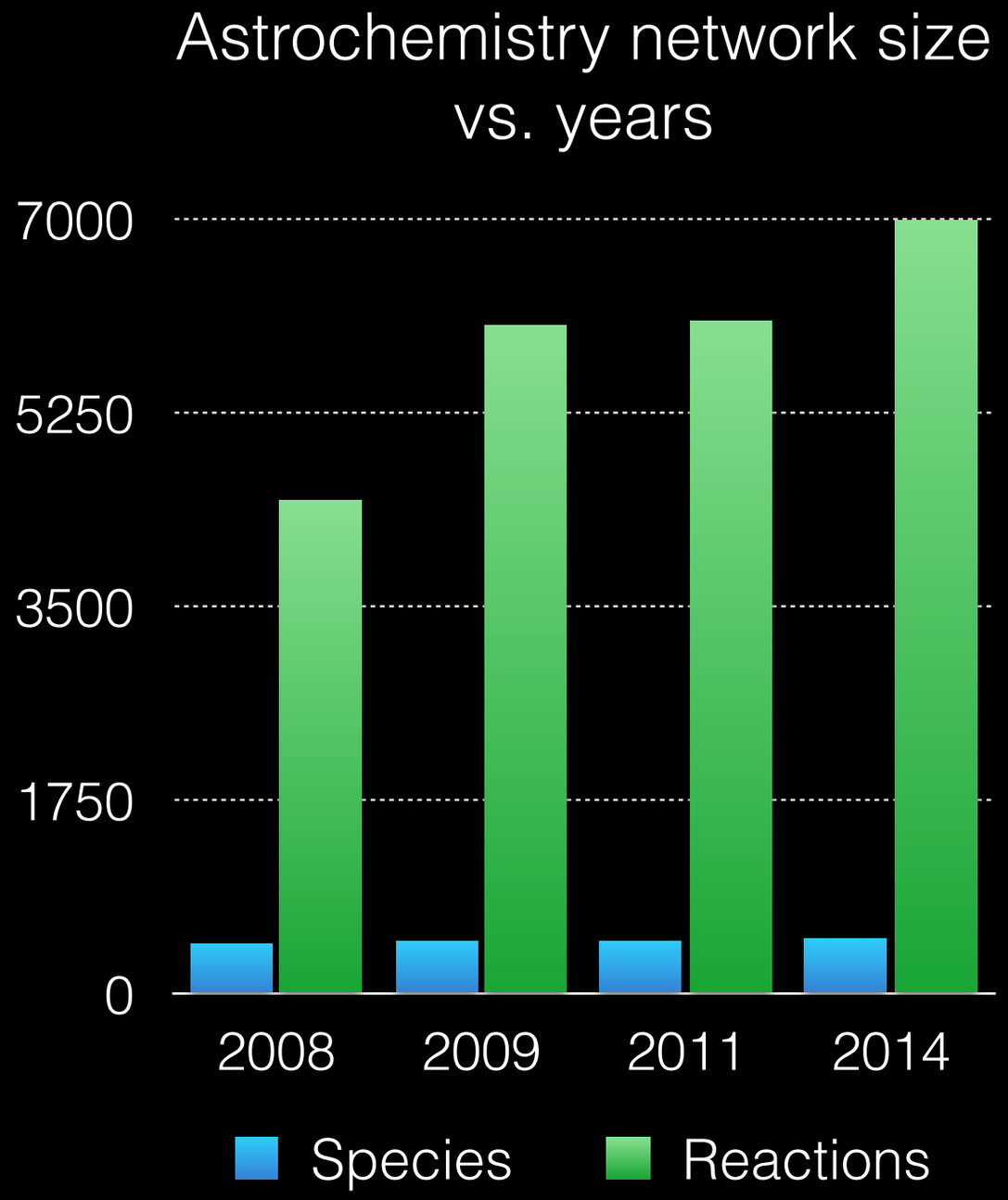
- Similar rate equations can be written for all species

- To compute the abundances of all species as a function of time, we need to solve a system of n_s ordinary differential equations (ODEs)

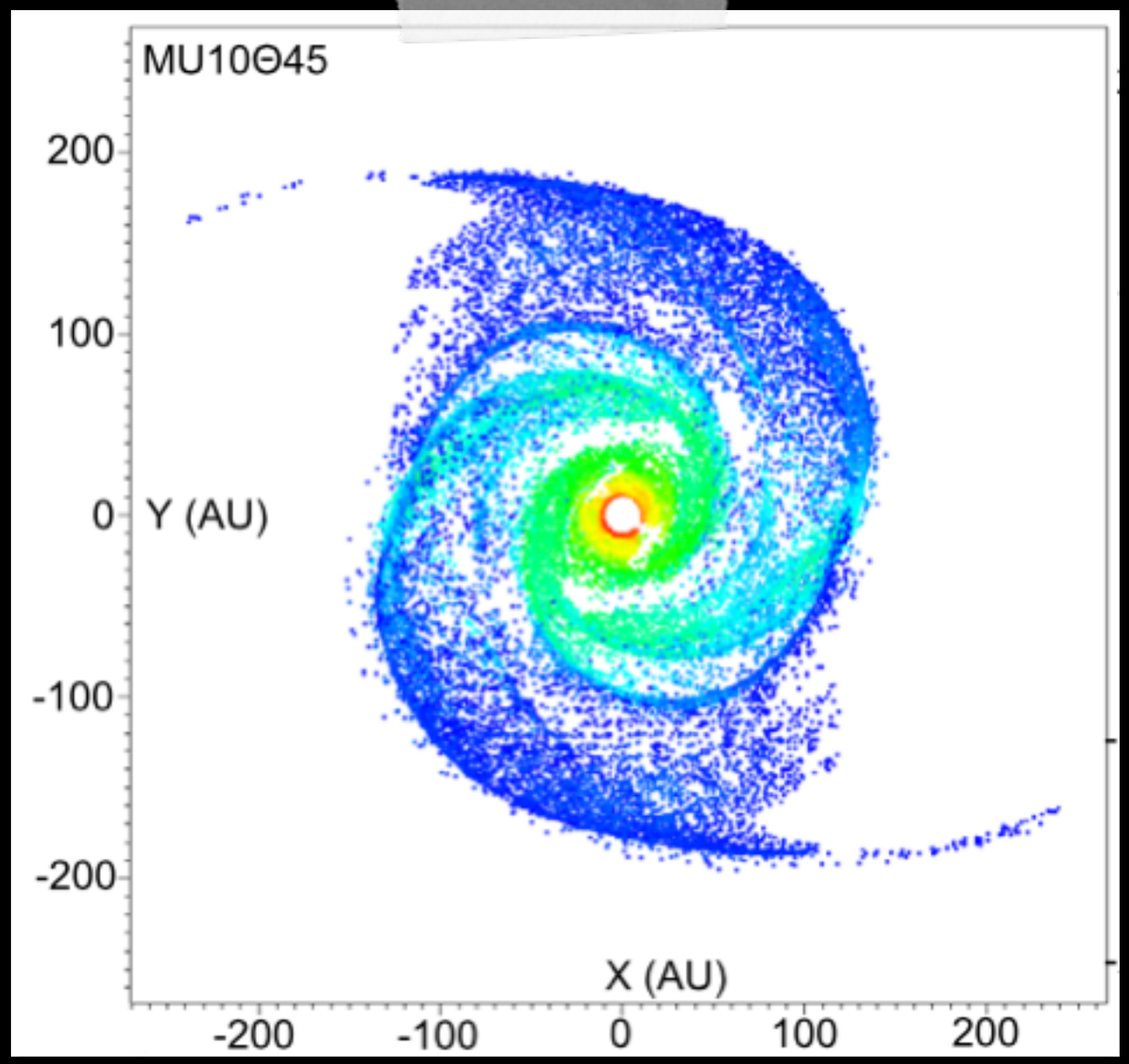
- This ODE system is *stiff* because the time constants are very different from one equation from the other
- Well studied numerical problem: librairies have been developed for many years: VODE, LSODE, CVODE (a.k.a. SUNDIALS)

The need for *fast* astrochemistry codes

- Astrochemistry networks becomes more a more complete over the years
  - more species (COMs, isotopologues, o/p) and reactions (surface reactions)
- Computational time for solving the ODE system goes as n_S^2, so we need efficient codes



- Astronomical sources (e.g. pre-stellar cores) have large density and temperature gradients
  - One need to sample the source in a large number of cells n_C
- Computational time goes as n_C (but this can be easily parallelized)



Hincelin et al. (2013)

What is Astrochem?

- Astrochem is code to compute the chemical abundances as a function of time in a variety of astronomical sources (molecular clouds, prestellar cores, protostars disks)
- Uses the CVODE solver from the SUNDIALS library, with explicit computation of the Jacobian of the ODE system
  - Fast (< 1 second for a typical model)
  - Parallel (OpenMP)
- Can be used with several chemistry networks (including KIDA)

Networks and reactions

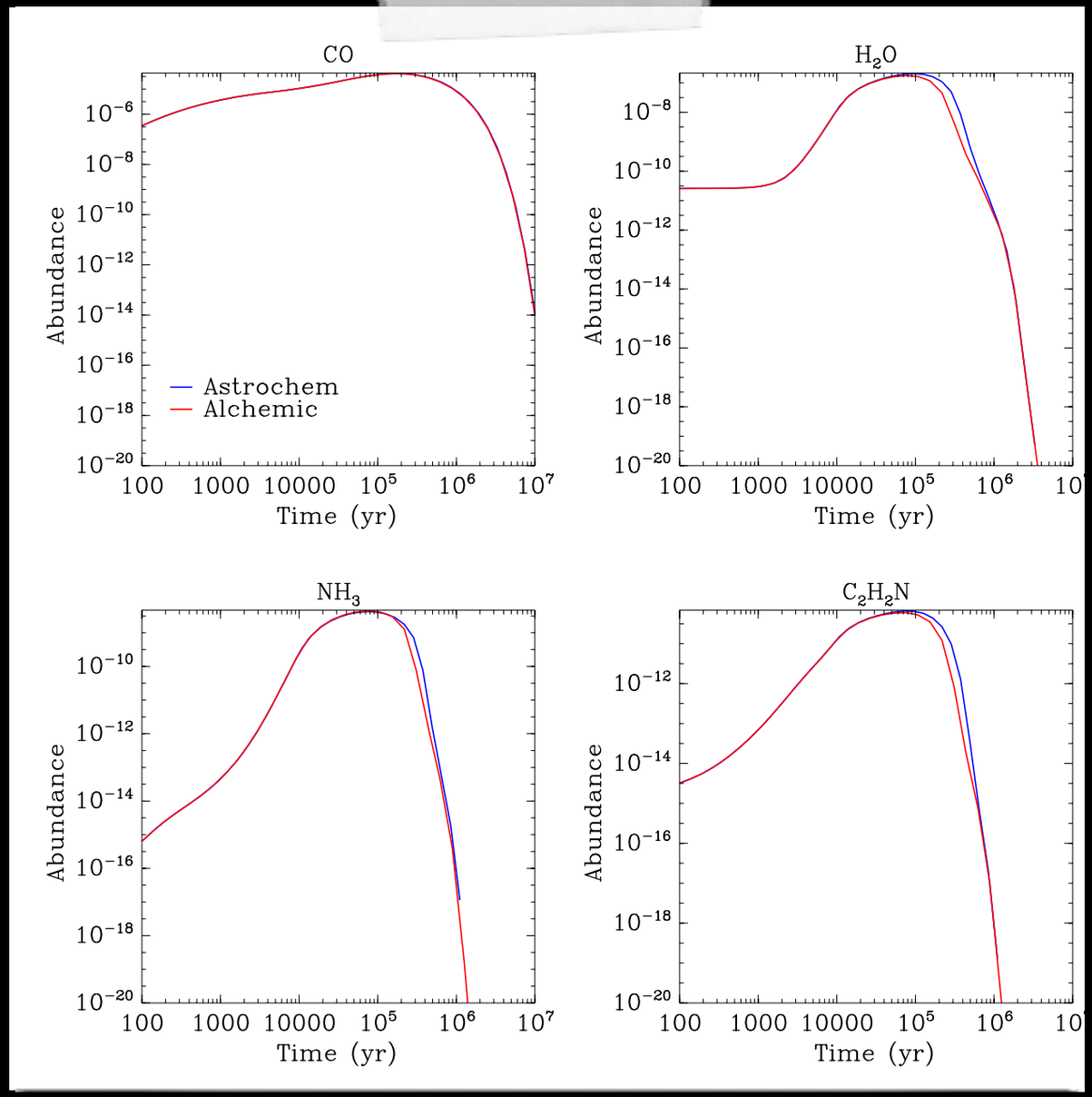
```
# A few reactions extracted from osu2008.chm
H      + H           -> H2                4.95e-17  5.00e-01  0.00e+00  0    1
H2     + cosmic-ray  -> H2(+)  + e(-)     9.30e-01  0.00e+00  0.00e+00  1   39
H3(+)  + CO          -> HCO(+) + H2       1.61e-09  0.00e+00  0.00e+00  2 1756
H3(+)  + e(-)        -> H      + H    + H  4.36e-08 -5.20e-01  0.00e+00  9 3746
CO     + uv-photon   -> C      + O        3.10e-11  0.00e+00  2.54e+00 13 4297
(...)
```

- Networks are simple text files (.chm format) that are easy to edit
- A tool to convert from other formats (OSU and KIDA) to Astrochem format is provided

- Several type of reactions are included:
  - Gas-phase reactions
  - Gas-grain interactions
    - Depletion
    - Desorption (thermal desorption, photo-desorption and cosmic-ray induced photo-desorption)
- No grain surface chemistry yet (except fo H_2 formation)

Benchmark

- Model results have been compared to the Alchemic and Nautilus codes (Semenov et al. 2010)
- Excellent agreement between the three codes



TMC1 model without freeze-out

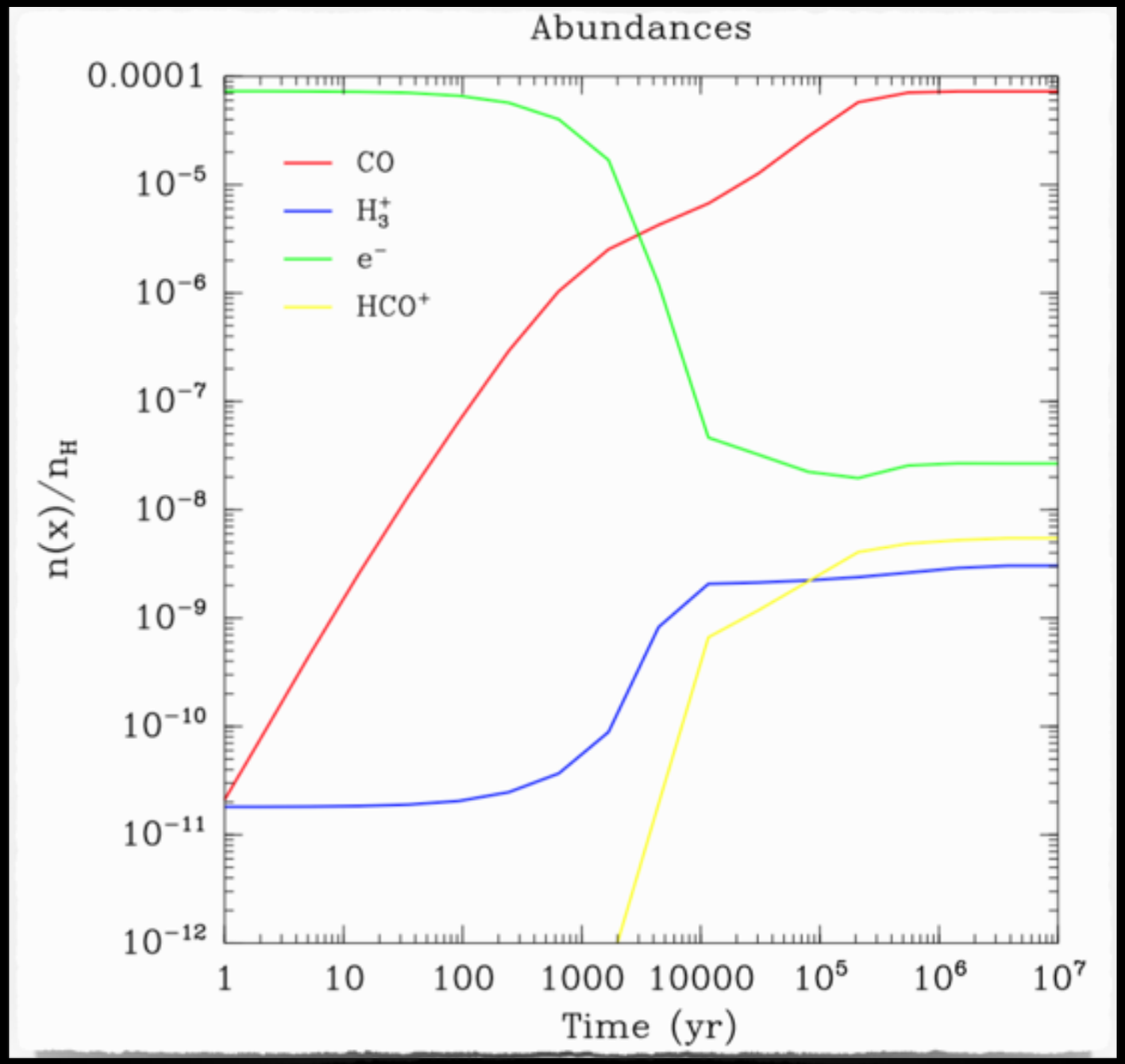
Example of use

```
[files]
source = source.mdl
chem = osu2009.chm
# Physical paramaters
[phys]
chi = 1.0
cosmic = 1.3e-17
# Solver parameters
[solver]
ti = 1e-6
tf = 1e7
# Initial abundances
[abundances]
H2      = 0.5
He      = 0.14
N       = 2.14e-5
O       = 1.76e-4
C(+)    = 7.30e-5
S(+)    = 8.00e-8
Si(+)   = 8.00e-9
Fe(+)   = 3.00e-9
Na(+)   = 2.00e-9
Mg(+)   = 7.00e-9
P(+)    = 2.00e-10
Cl(+)   = 1.00e-9
F       = 6.68e-9
e(-)    = 7.31012e-5
# Output
[output]
abundances = H3(+),e(-),CO,HCO(+)
trace_routes = 1
```

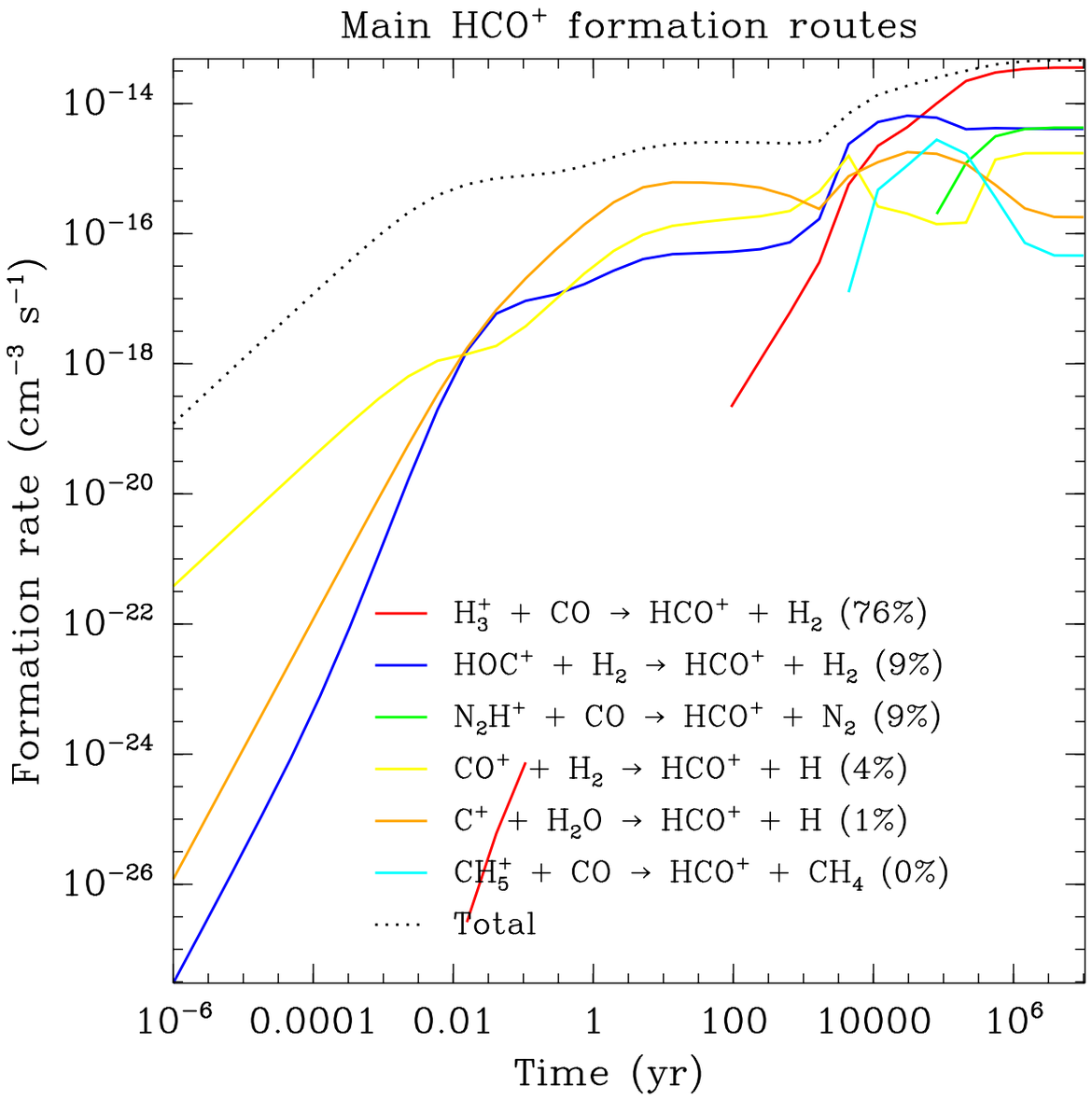
```
# Source model file example
# cell number, Av [mag], nH [cm^-3], Tgas [K], Tdust [K]
#
0   20.0    1e+04   10.0    10.0
```

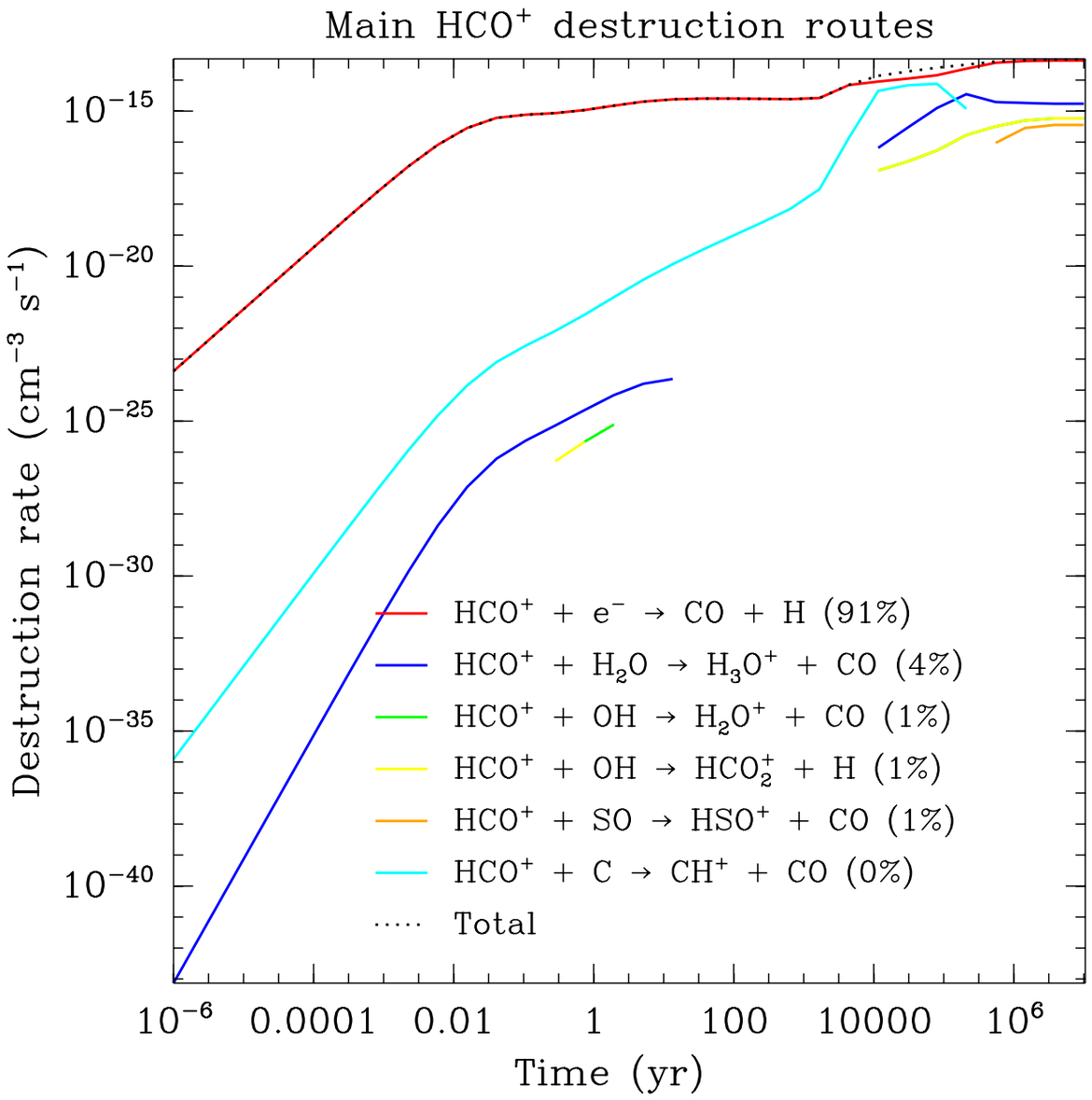
```
% astrochem input.ini
Reading input from input.ini.
Reading source model from source.mdl.
Reading reactions network from osu2009.chm... done.
Found 6046 reactions involving 468 species.
Computing abundances in cell 0...
Done with cell 0.
Writing abundances in output files... done.
Writing formation/destruction in output files... done.
%
```

```
% plabun --xrange=1,1e7 --yrange=1e-12,1e-4 astrochem_output.h5 CO H3(+) e(-) HCO
```



```
% plroute astrochem_output.h5 HCO(+)
```

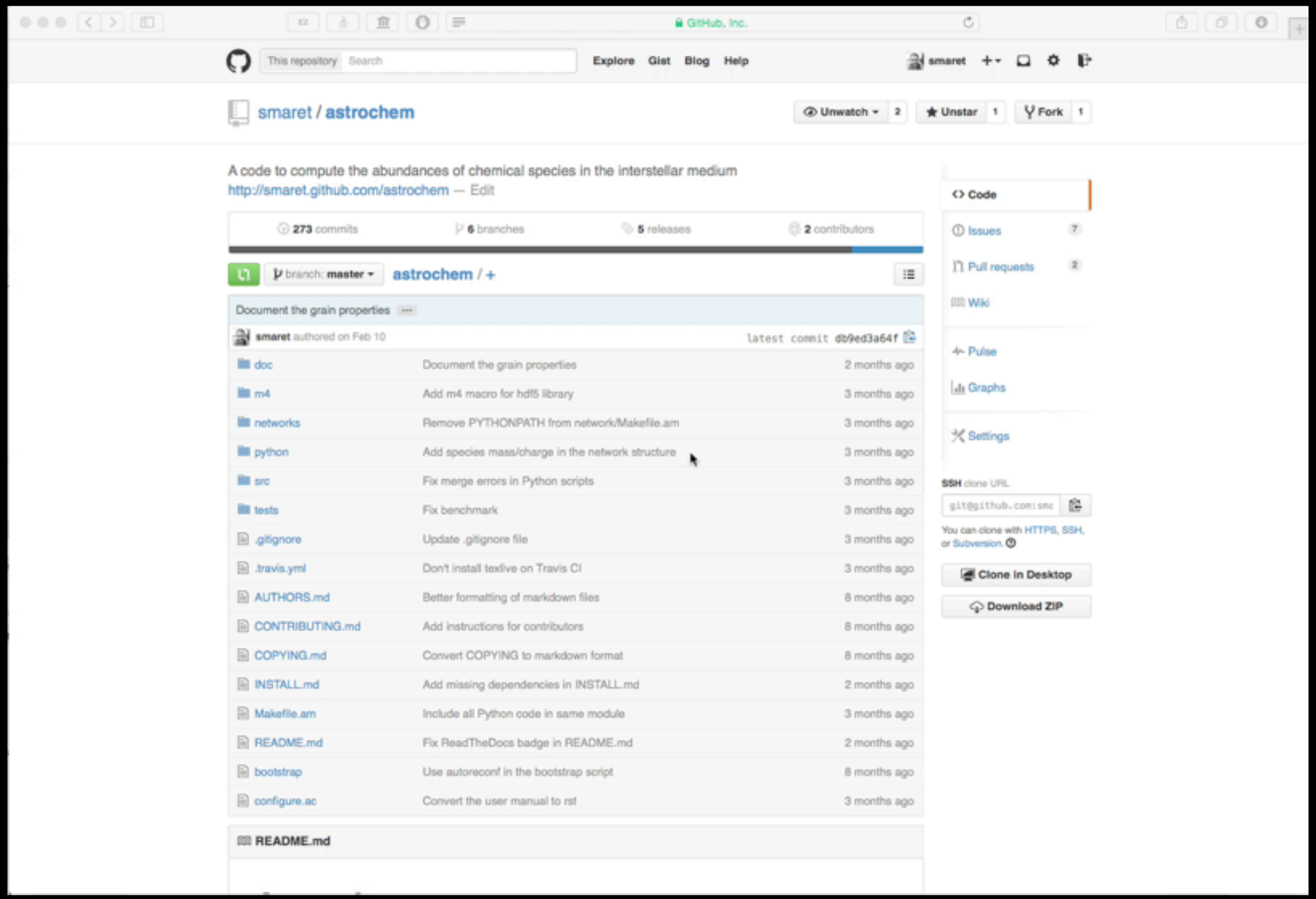




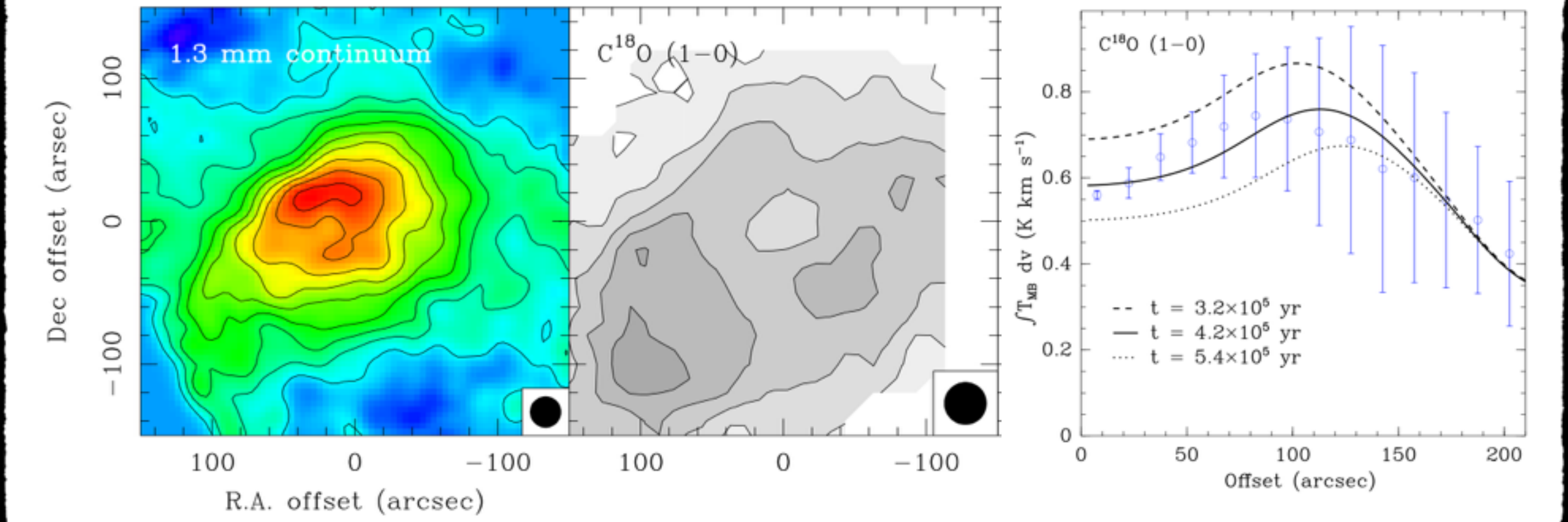
Advanced features

- Astrochem can be used to study sources which time-varying physical conditions e.g.:
    - Gravitational collapse of a protostar
    - Post-processing of MHD simulations
- Can also be embedded directly in HD/MHD simulations
    - Interface in both Python and C languages

Astrochem developement



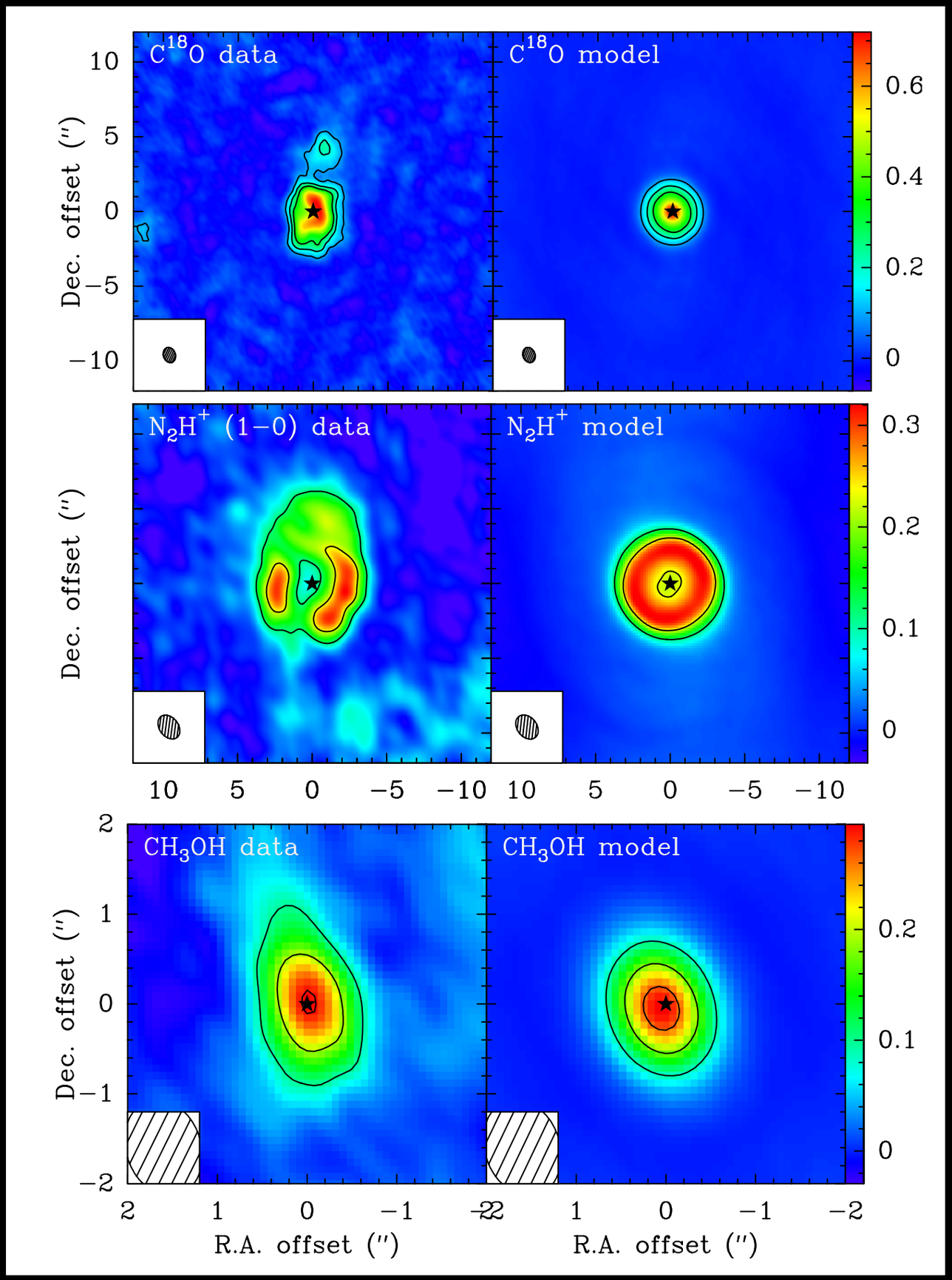
A few recent results



- $C^{18}O$ depletion in the L1498 prestellar core (Maret, Bergin & Tafalla 2013)
- Model with Astrochem using the OSU 2009 network coupled with RATRAN for the line excitation and transfer

- $C^{18}O$, N_2H^+ and CH3OH distributions in NGC1333-IRAS4B (Anderl, Maret et al. in prep.)

- Model with Astrochem using the OSU 2009 network coupled with RATRAN for the line excitation and transfer and GILDAS to simulate observations



Conclusions

- Fast and versatile gas-phase chemistry code that can be used with a variety of chemical networks (e.g. KIDA)
- Can be used make simple computations (e.g. check the influence of a rate) or more realistic astrophysical models (dense cores, protostars)
- Can also be used for post-processing of HD/MHD simulations, or even be directly embedded in such simulations

http://smaret.github.com/astrochem

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