

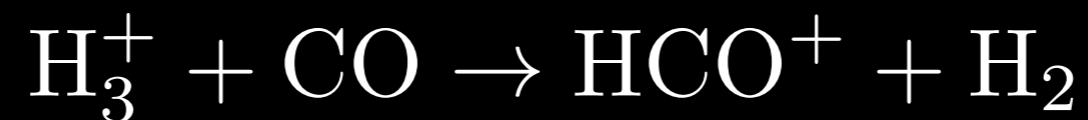
# Astrochem: a fast time- dependent code for astrochemistry

Sébastien Maret

Institut de Planétologie et d'Astrophysique de Grenoble

# Basics

- Let's start with an example:



- Let us call  $k_1$  and  $k_2$  the rates of these two reactions (in  $\text{cm}^3 \text{s}^{-1}$ ).

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

$$\frac{dn(\text{HCO}^+)}{dt} = k_1 n(\text{H}_3^+) n(\text{CO}) - k_2 n(\text{HCO}^+) n(e^-)$$

**Formation term**

**Destruction term**

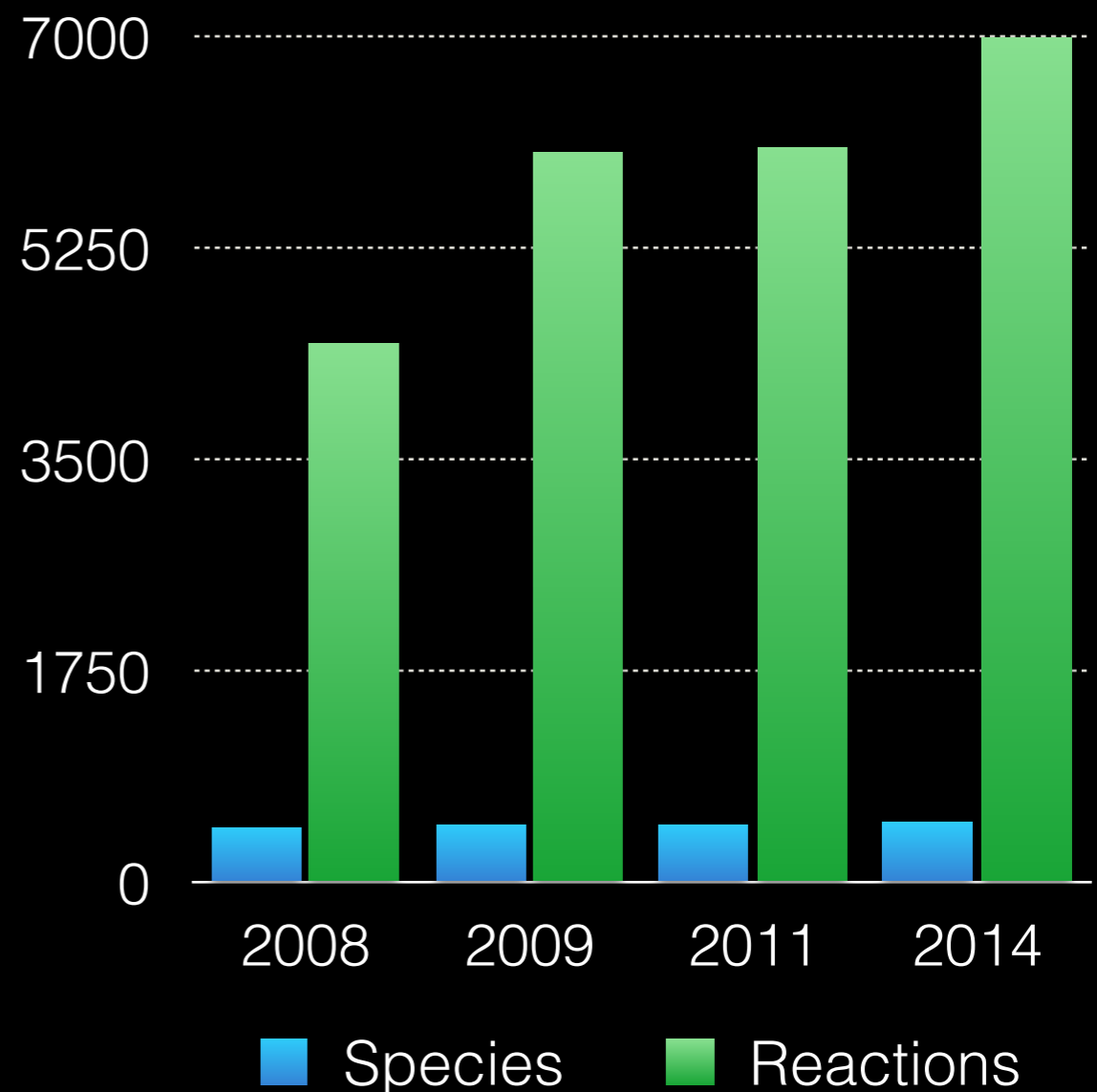
- Similar rate equations can be written for all species
- To compute the abundances of all species as a function of time, we need to solve a system of  $n_s$  ordinary differential equations (ODEs)

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

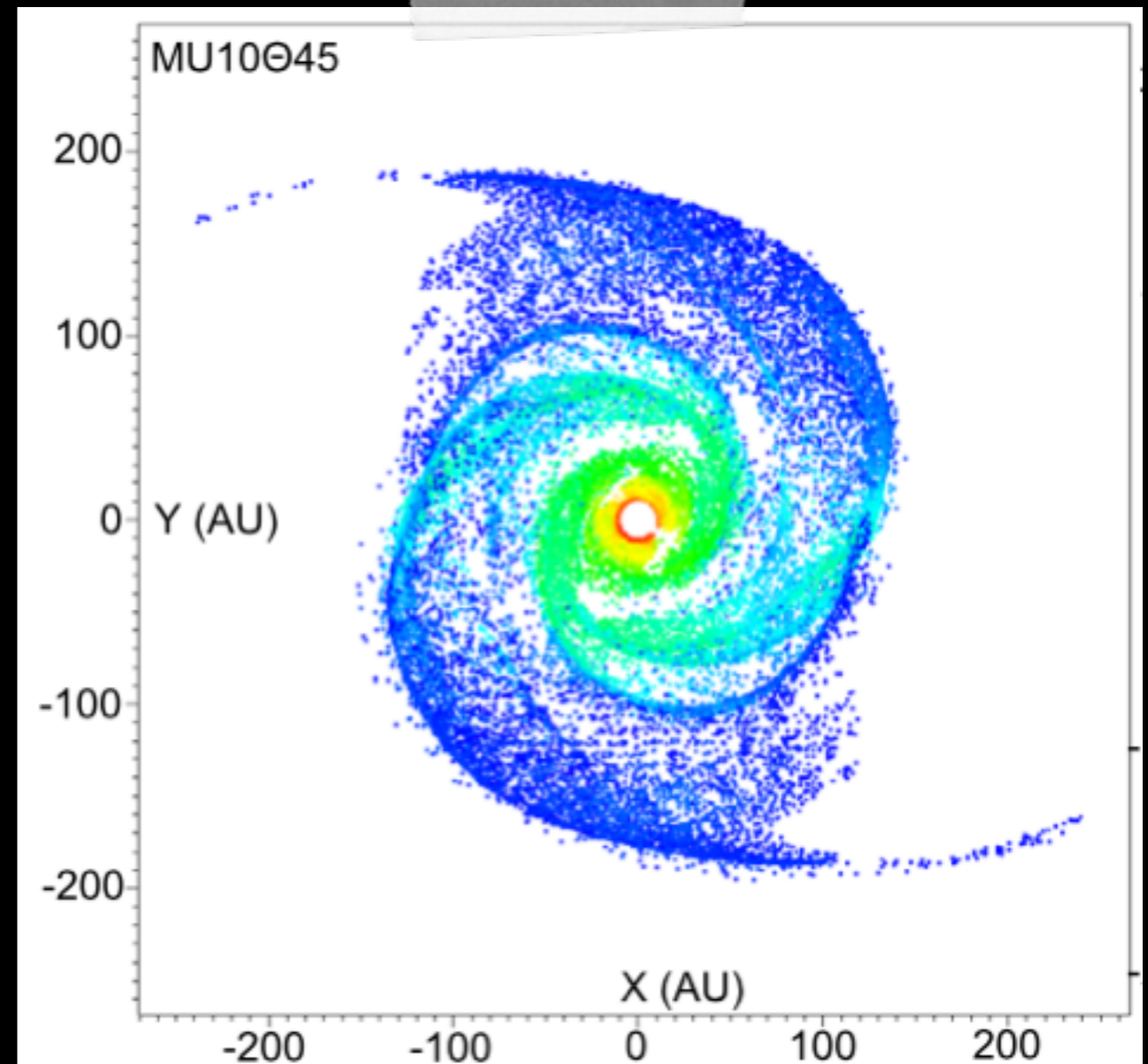
# The need for *fast* astrochemistry codes

- 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

Astrochemistry network size vs. years



- 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
(...)
```

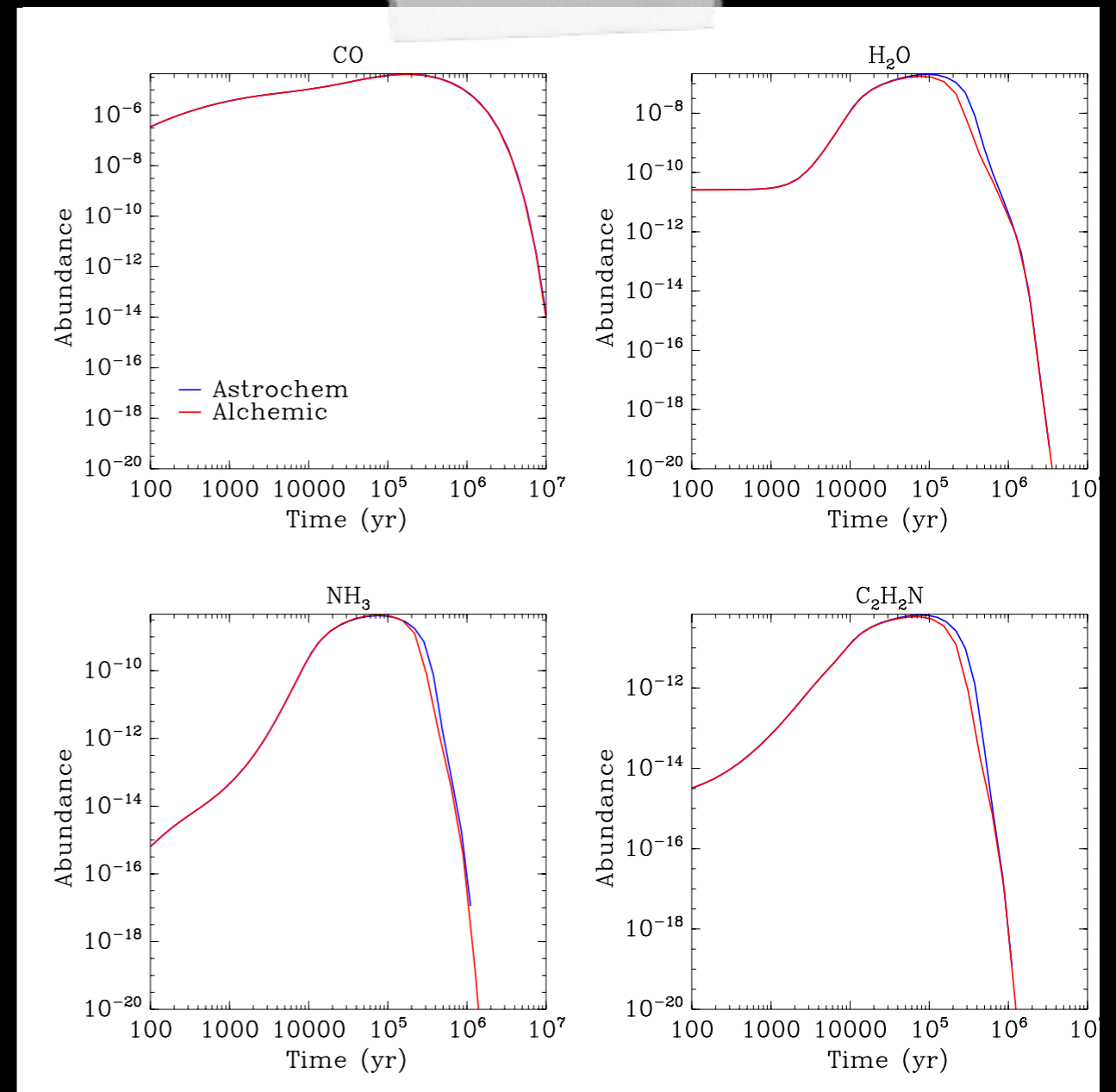
- Networks are simple text files (.chm format) that are easy to edit
- A tool to convert from other formats (OSU and KIDA) to Astrochem format is provided



- 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<sub>2</sub> formation)

# Benchmark

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



TVMC model without freeze-out

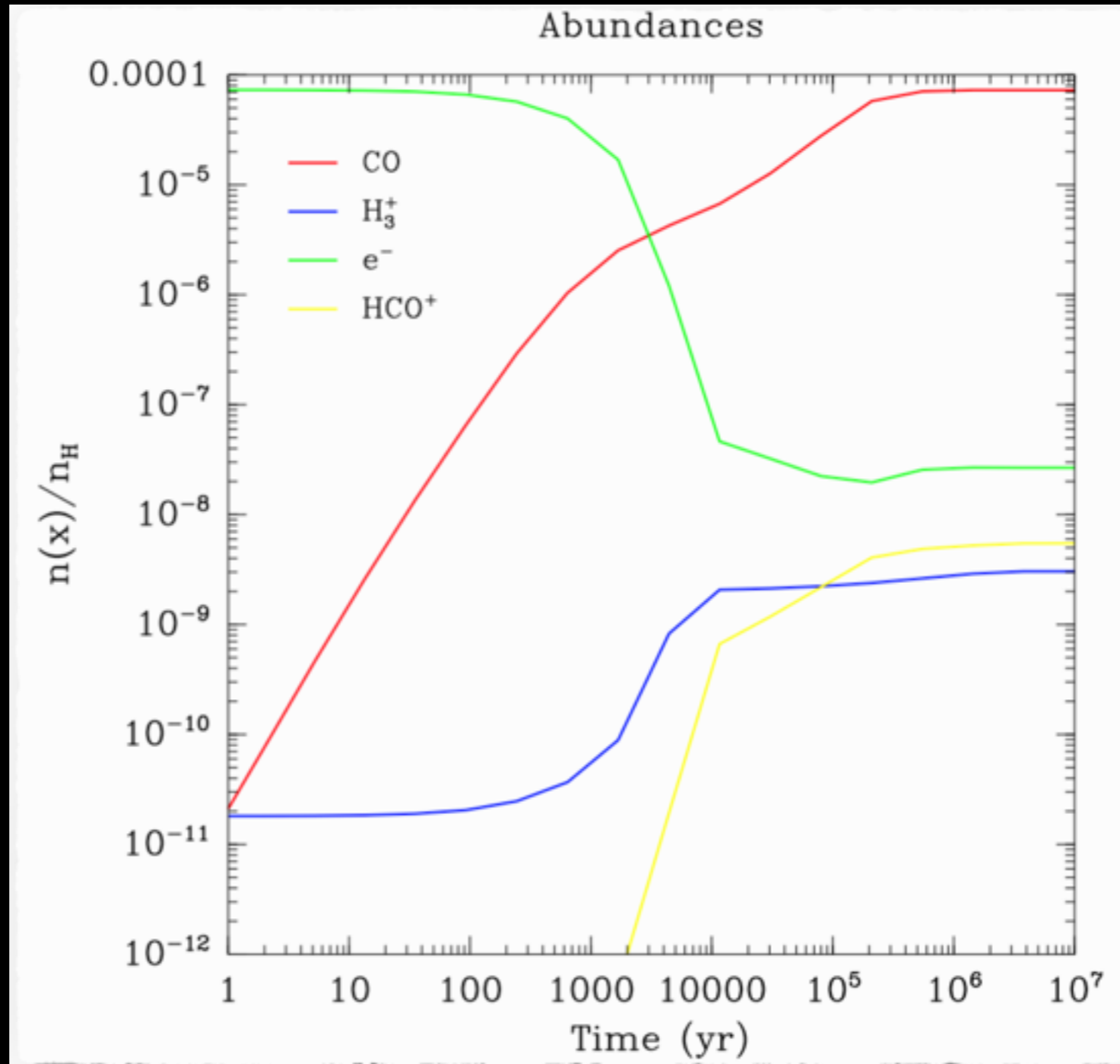
# Example of use

```
[files]
source = source.mdl
chem = osu2009.chm
# Physical parameters
[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
```

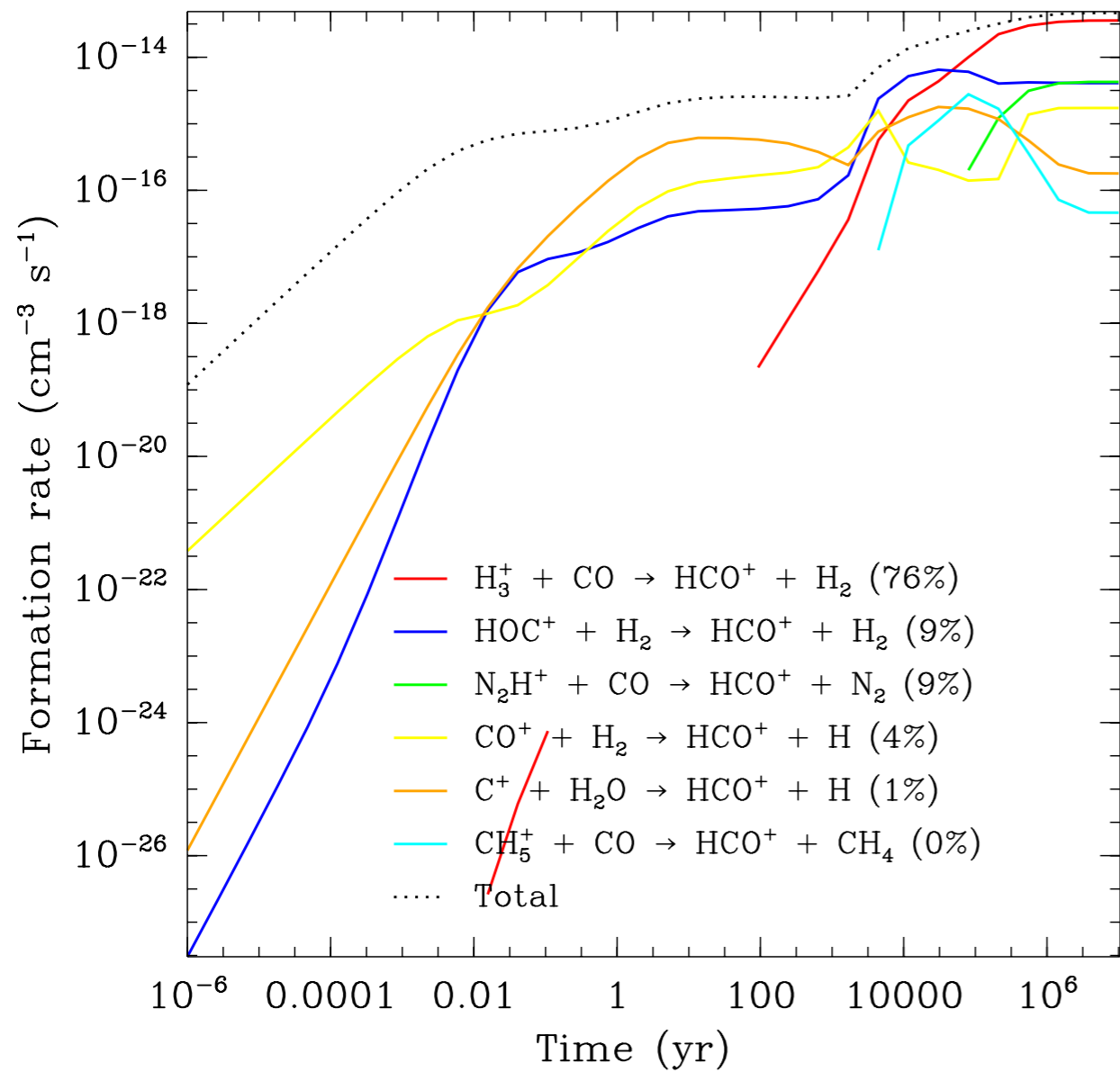
```
% astrochem input.ini
Reading input from input.ini.
Reading source model from source.mdl.
Reading reactions network from osu2009.chm... done.
Found 6046 reactions involving 468 species.
Computing abundances in cell 0...
Done with cell 0.
Writing abundances in output files... done.
Writing formation/destruction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

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

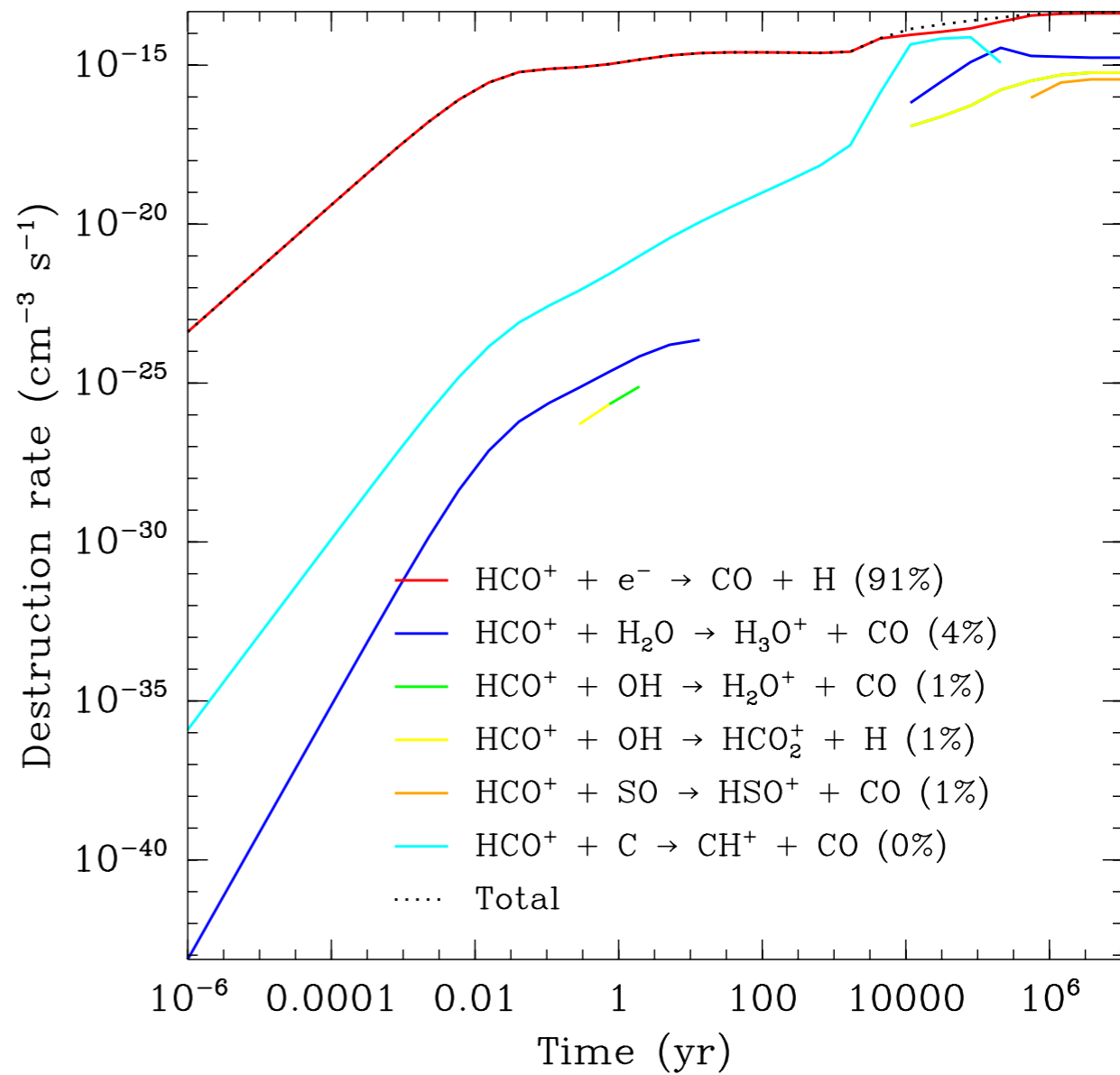


% plroute astrochem\_output.h5 HCO(+)

Main HCO<sup>+</sup> formation routes



Main HCO<sup>+</sup> destruction routes



# 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 development

This repository Search Explore Gist Blog Help smaret +- ⚙️

smaret / astrochem Unwatch 2 Unstar 1 Fork 1

A code to compute the abundances of chemical species in the interstellar medium  
<http://smaret.github.com/astrochem> — Edit

273 commits 6 branches 5 releases 2 contributors

branch: master astrochem / +

Document the grain properties

smaret authored on Feb 10 latest commit db9ed3a64f

doc	Document the grain properties	2 months ago
m4	Add m4 macro for hdf5 library	3 months ago
networks	Remove PYTHONPATH from network/Makefile.am	3 months ago
python	Add species mass/charge in the network structure	3 months ago
src	Fix merge errors in Python scripts	3 months ago
tests	Fix benchmark	3 months ago
.gitignore	Update .gitignore file	3 months ago
.travis.yml	Don't install texlive on Travis CI	3 months ago
AUTHORS.md	Better formatting of markdown files	8 months ago
CONTRIBUTING.md	Add instructions for contributors	8 months ago
COPYING.md	Convert COPYING to markdown format	8 months ago
INSTALL.md	Add missing dependencies in INSTALL.md	2 months ago
Makefile.am	Include all Python code in same module	3 months ago
README.md	Fix ReadTheDocs badge in README.md	2 months ago
bootstrap	Use autoreconf in the bootstrap script	8 months ago
configure.ac	Convert the user manual to rst	3 months ago

Code

- Issues 7
- Pull requests 2
- Wiki
- Pulse
- Graphs
- Settings

SSH clone URL  
git@github.com:smz

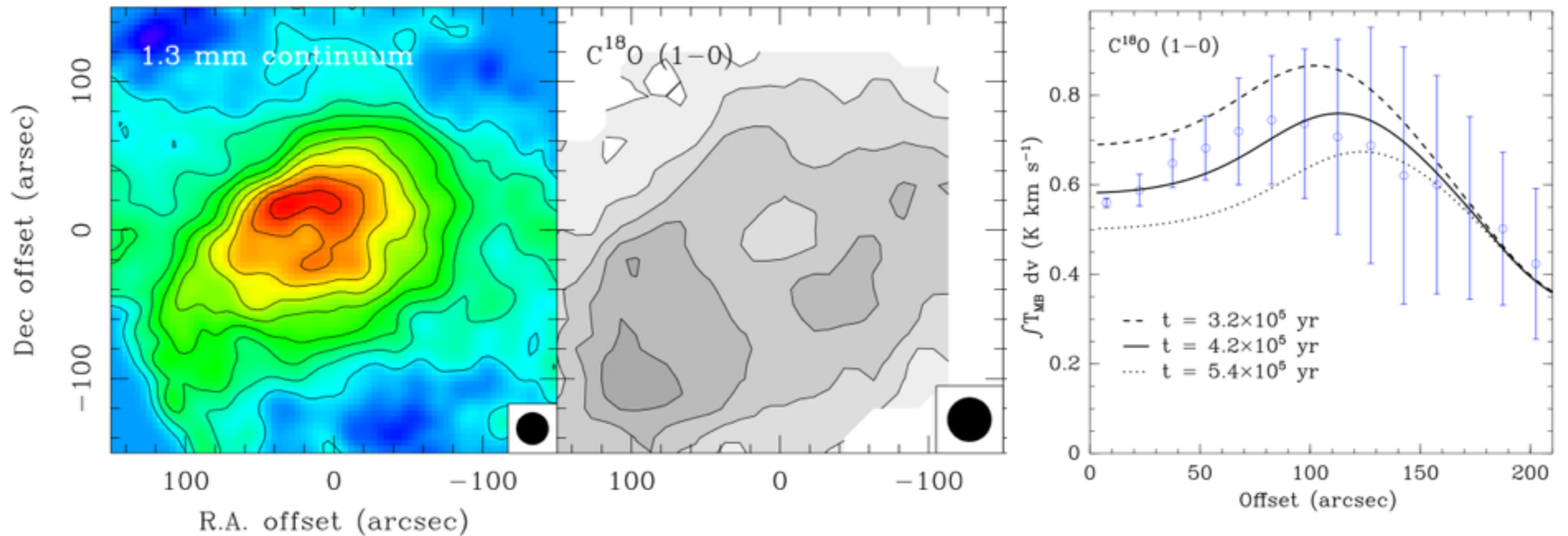
You can clone with HTTPS, SSH, or Subversion.

Clone in Desktop

Download ZIP

README.md

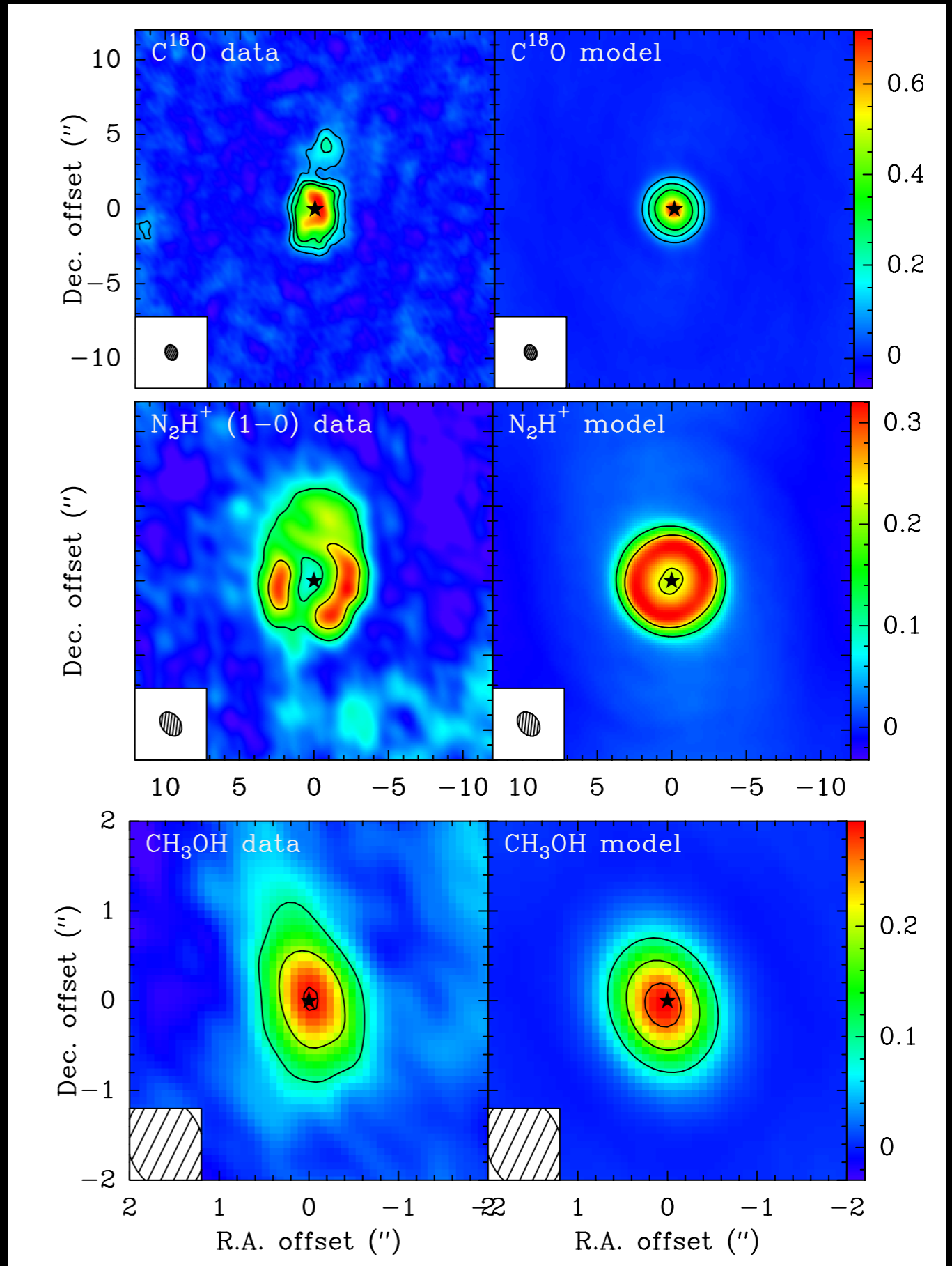
# A few recent results



- C<sup>18</sup>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  $CH_3OH$  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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