UV-driven chemistry in simulations of the ISM

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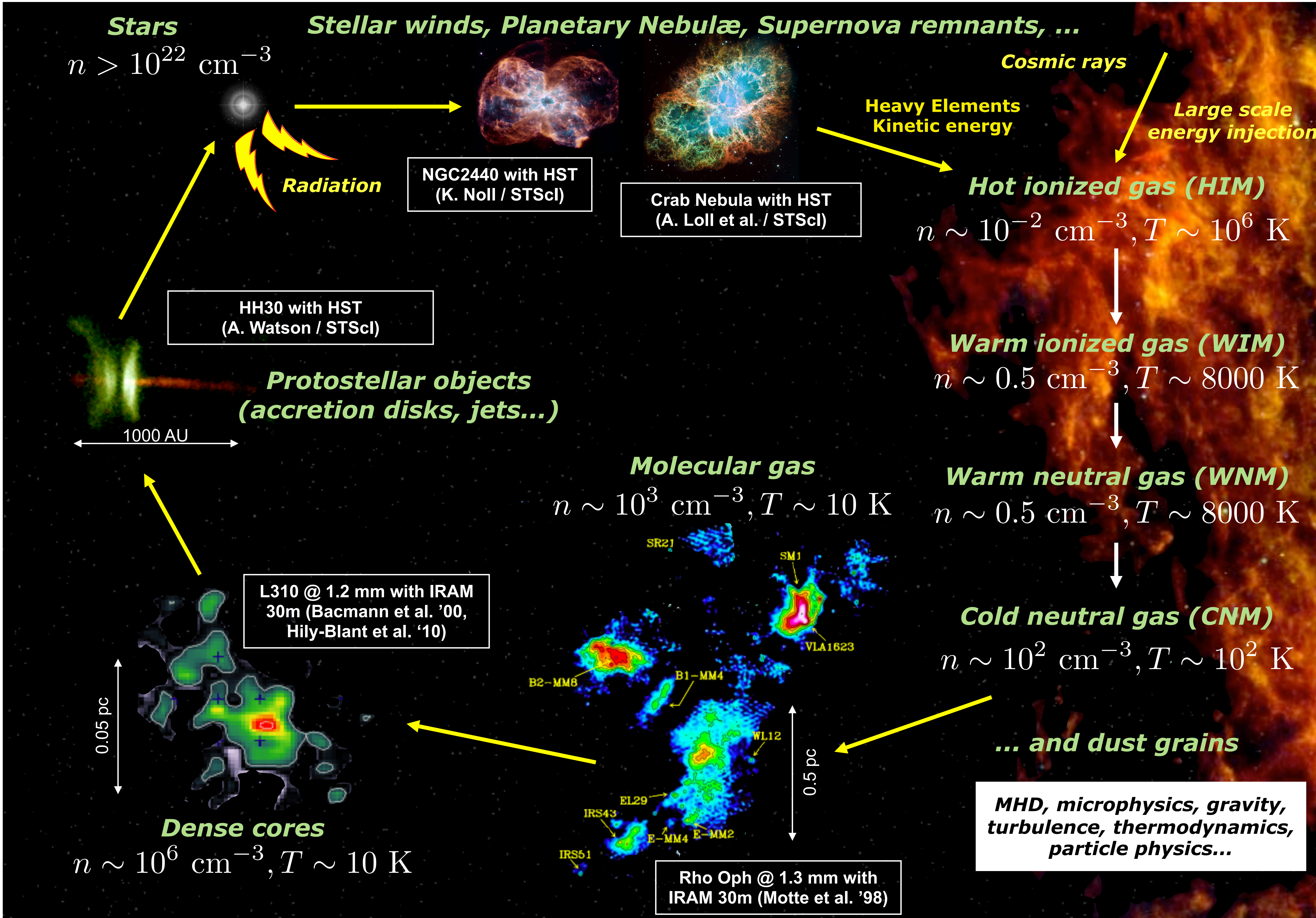
COSMIS kick-off meeting, Paris, 19-20 october 2011

Star formation and the cycle of interstellar matter



Motivations

Preparation of SPICA/SAFARI

SPICA : Joint JAXA/ESA infrared mission ~2020
SAFARI : wide field FTS 30-210 μm
Estimate the ability of SAFARI to map [CII] emission over large areas

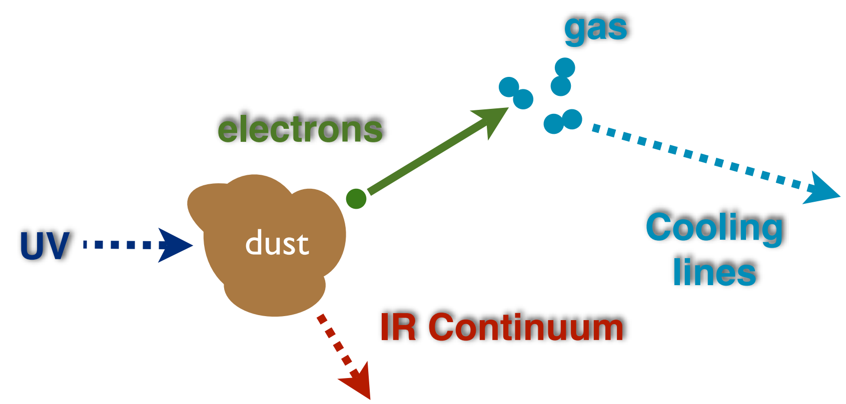
Dark neutral gas

Find out mass fraction of warm H_2 not traced by CO

Simulations of the ISM

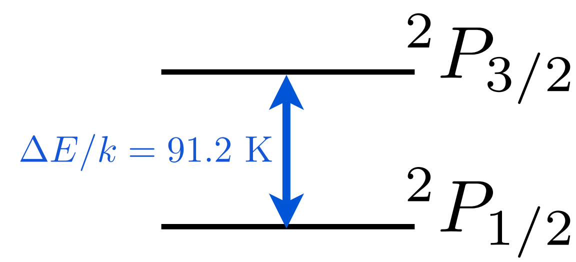
Include post-processed chemistry in MHD simulations of the ISM
MHD-PDR pipeline as part of the STARFORMAT project

Observations of the [CII] 158 μm line



UV to IR energy transfer via photoelectric effect

$E_{\text{ionization}} = 11.3 \text{ eV}$ ▶ Potentially exists where H is neutral, or even molecular



Fine structure of the ground state of C^+

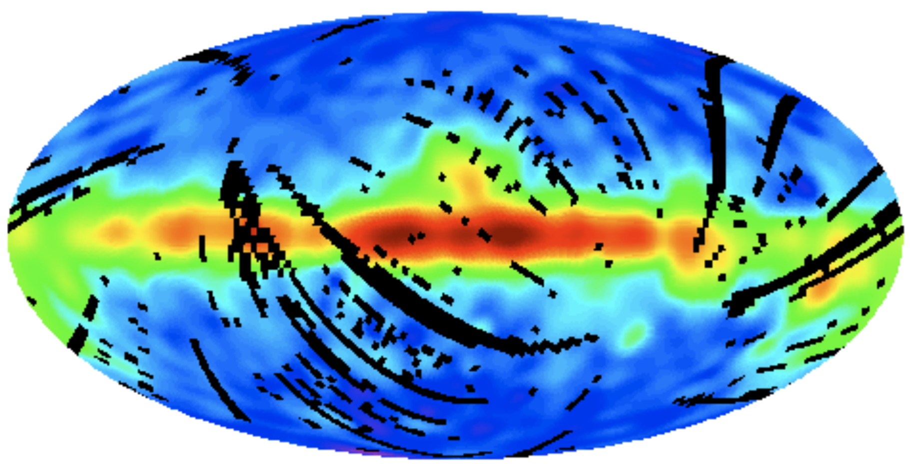
One of the dominant cooling lines of interstellar gas

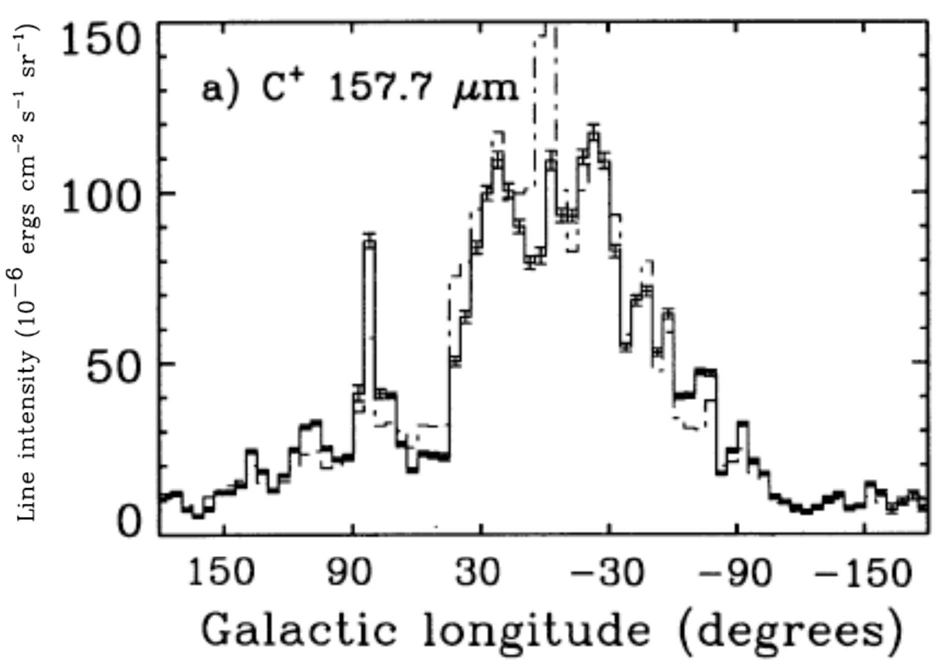
0.3% of the bolometric FIR emission of the Galaxy (*Wright et al. 91*)

Candidate tracer for "dark gas"

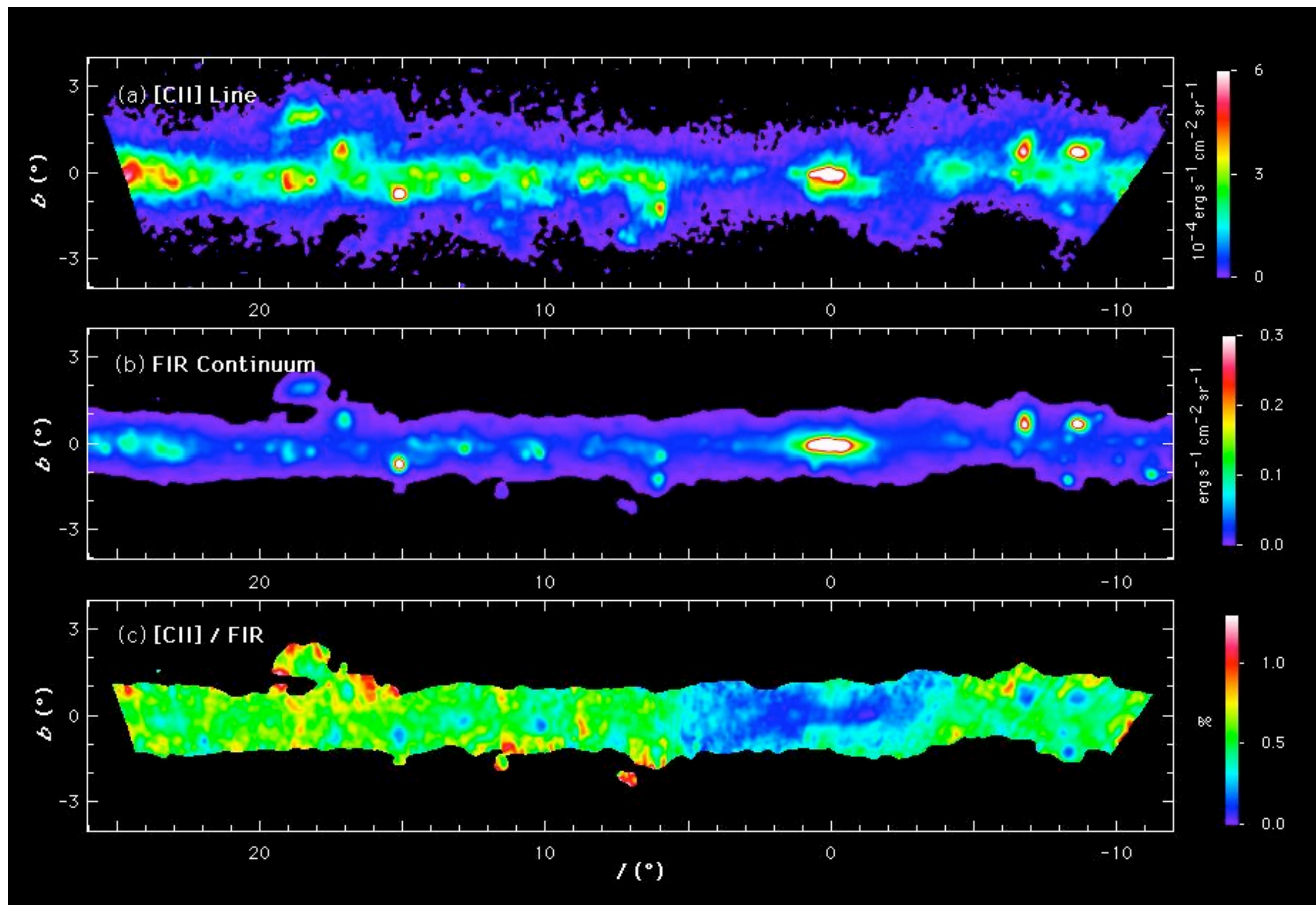
(*Joncas et al. 92, Grenier et al. 2005*)

Bennett et al. 94 (COBE / FIRAS)





Nakagawa et al. 98 (BICE)



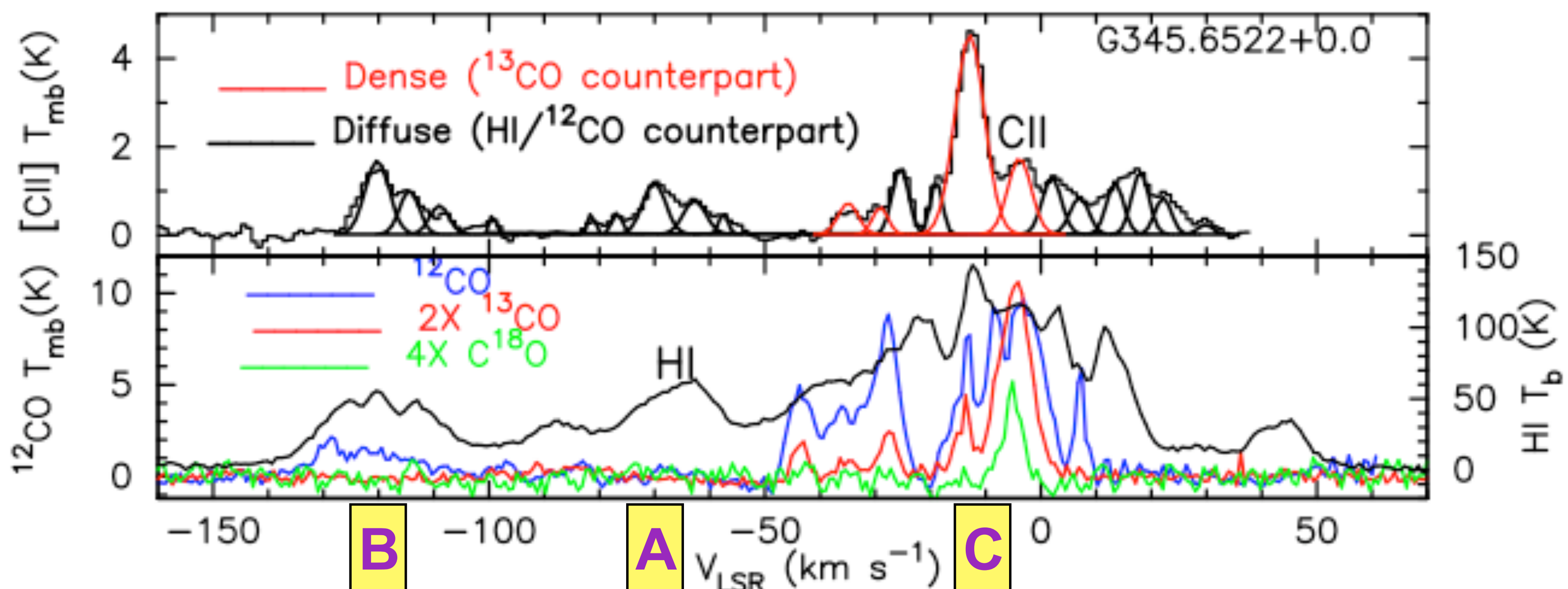
Herschel Galatic [CII] observations

GOTC+ OT key program

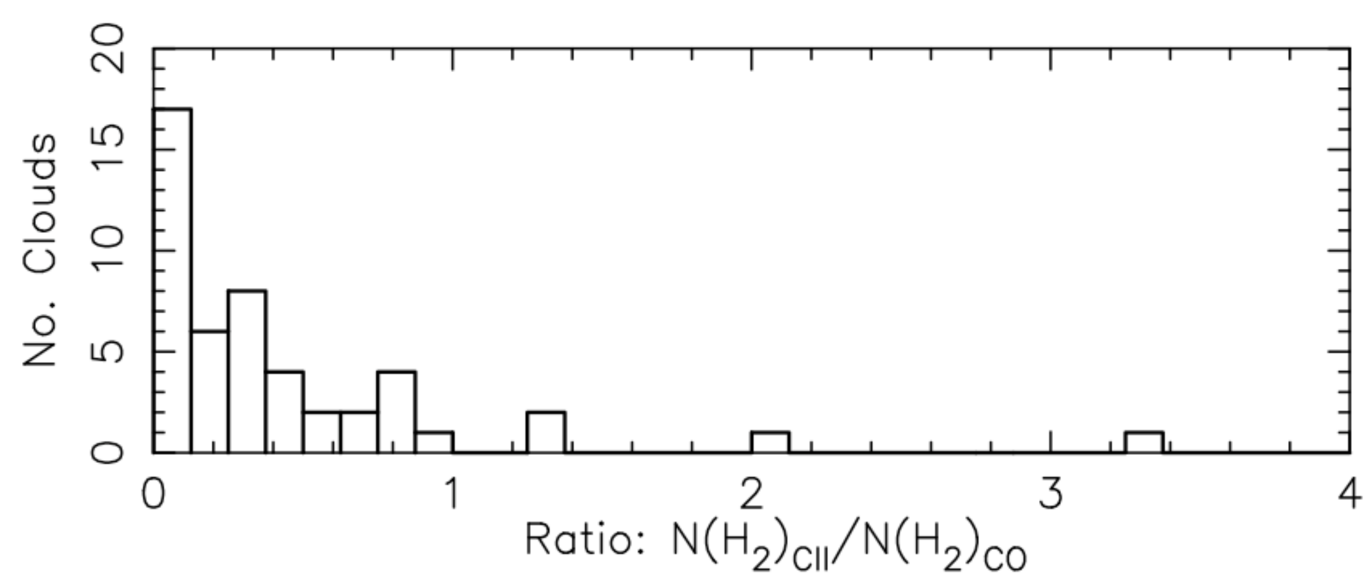
Langer, Velusamy, Pineda, Goldsmith, Li, Yorke

- 900 Galactic lines of sight planned (2% completed)
- 146 clouds detected in [CII]

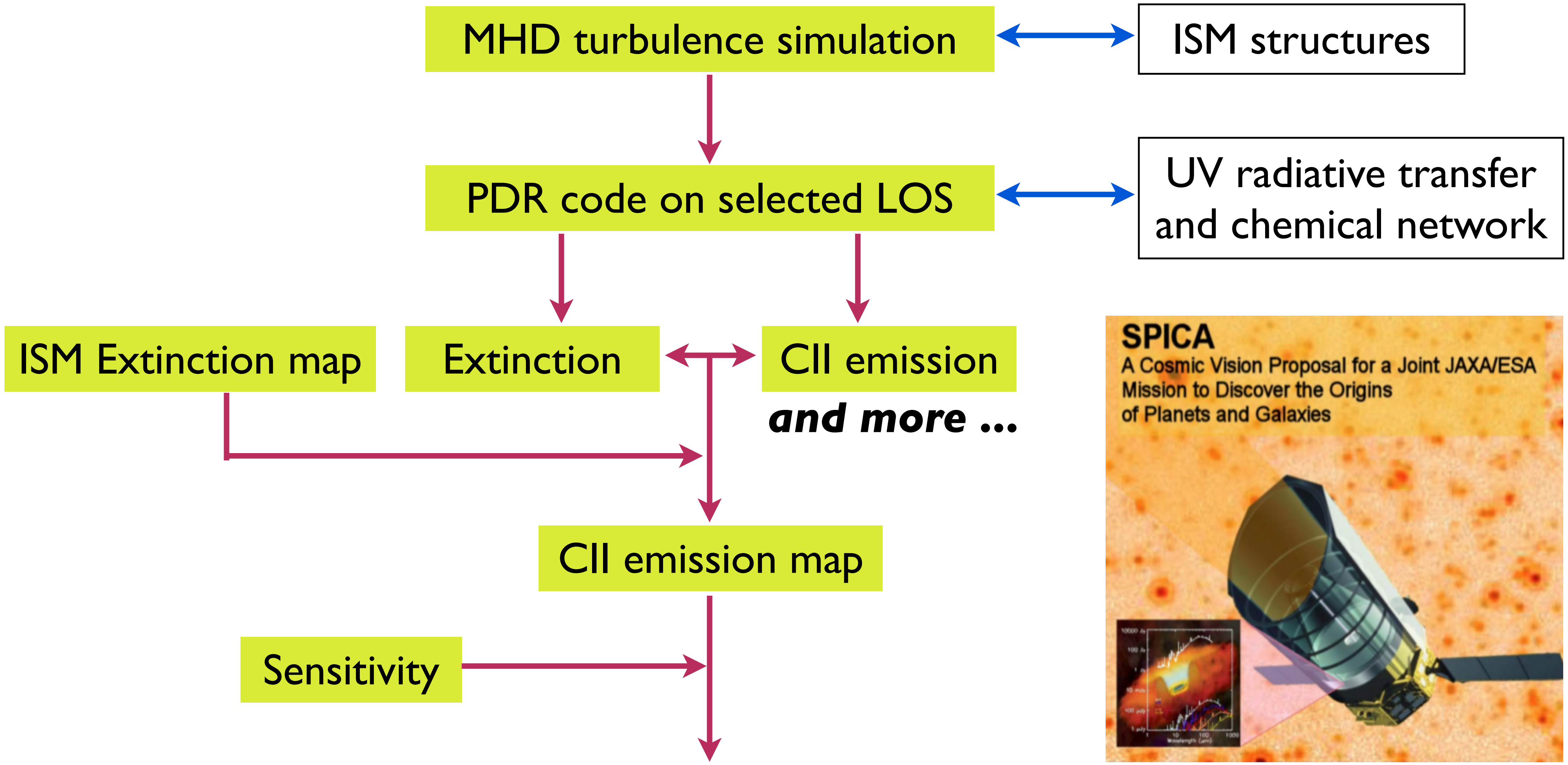
  - 35 **A** • Diffuse atomic clouds detected in HI, [CII] but not CO
  - 53 **B** • Transition clouds and PDRs detected in HI, [CII], ^{12}CO but not ^{13}CO
  - 58 **C** • Dense molecular clouds detected in HI, [CII], ^{12}CO, ^{13}CO and sometimes $C^{18}O$



B ~24% of the total H_2 column density is in the H_2/C^+ layer not traced by ^{12}CO



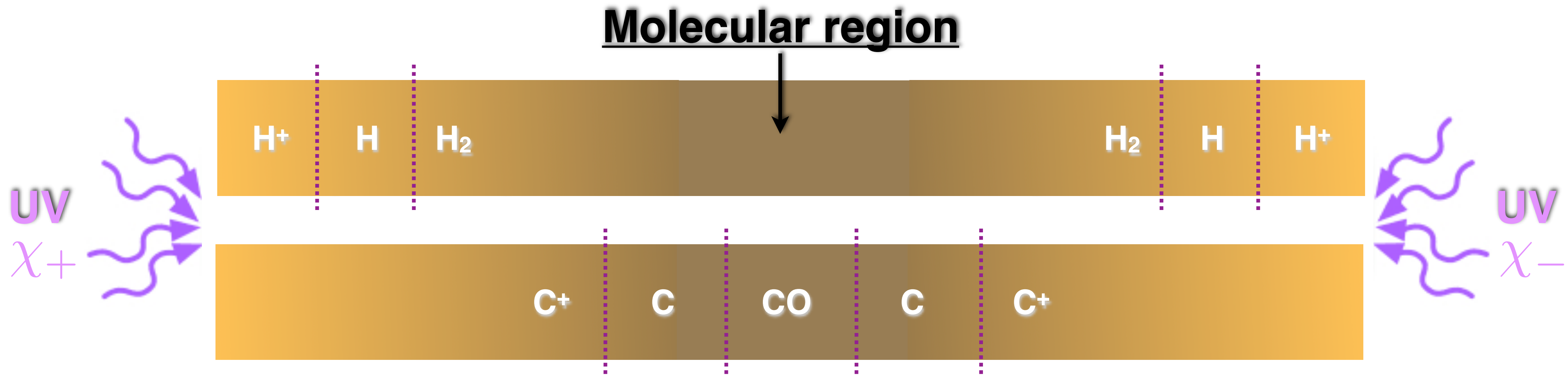
UV-driven chemistry of a simulated ISM



SPICA / SAFARI (Joint JAXA / ESA)

- Sample lines of sight in the MHD simulation cube
- Extract "clouds" by applying a simple density threshold
- Use these as input density profiles in the PDR code
- Derive 158 μm [CII] line intensity versus visual extinction
- Use that relationship to estimate mapping speed for the diffuse ISM

The Meudon PDR code



Stationary 1D model, including :

- UV radiative transfer:
  - Absorption in molecular lines
  - Absorption in the continuum (dust)
  - 10000's of lines
- Chemistry :
  - Several hundred chemical species
  - Network of sevral thousand chemical reactions
  - Photoionization
- Statistical equilibrium of level populations
  - Radiative and collisional excitations and de-excitations
  - Photodissociation
- Thermal balance:
  - Photoelectric effect
  - Chemistry
  - Cosmic rays
  - Atomic and molecular cooling

Outputs :

- Local quantities :
  - Abundance and excitation of species
  - Temperature of gas and duts
  - Detailed heating and cooling rates
  - Energy density
  - Gas and grain temperatures
  - Chemical reaction rates
- Integrated quantities on the line of sight :
  - Species column densities
  - Line intensities
  - Absorption of the radiation field
  - Spectra

Le Bourlot et al. 1999
Le Petit et al. 2006
Goicoechea & Le Bourlot 2007
Gonzalez-Garcia et al. 2008

http://pdr.obspm.fr/

STARFORMAT

The StarFormat DataBase

The StarFormat database contains results of heavy numerical simulations computed in order to study the problem of star formation, essentially molecular cloud formation, evolution and collapse.

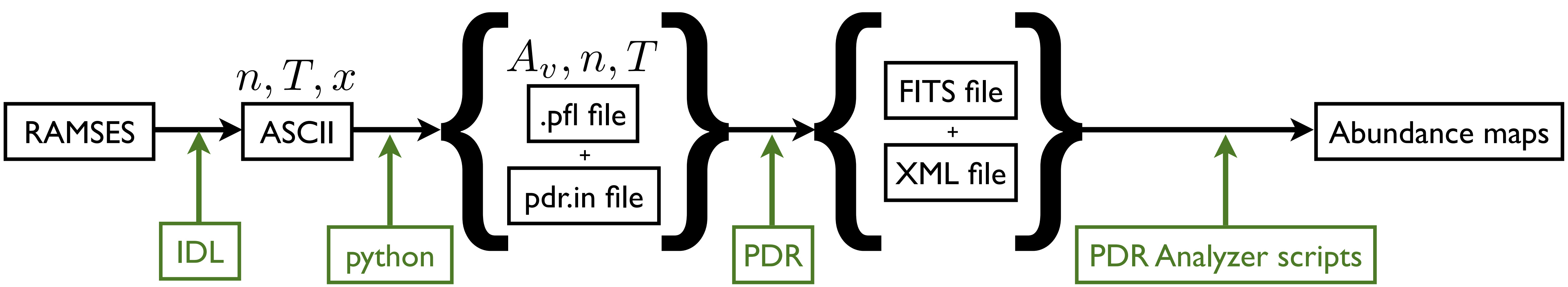
Understanding the dynamical evolution of the interstellar medium (ISM) and its relation to stellar birth is a key challenge in astronomy and astrophysics. The **STAR FORMAT** project aims at providing observers and theorists studying formation and evolution of molecular clouds, their morphological and kinematical characteristics, and the formation of stars in their interior with a set of theoretical tools and a database of models to aid in the analysis and interpretation of current and future observations.

The goal of this database is to give access to observers, or more generally to any scientist working on a related field, to the results of these numerical simulations, which could be useful to help prepare or analyze observations.

Available projects:

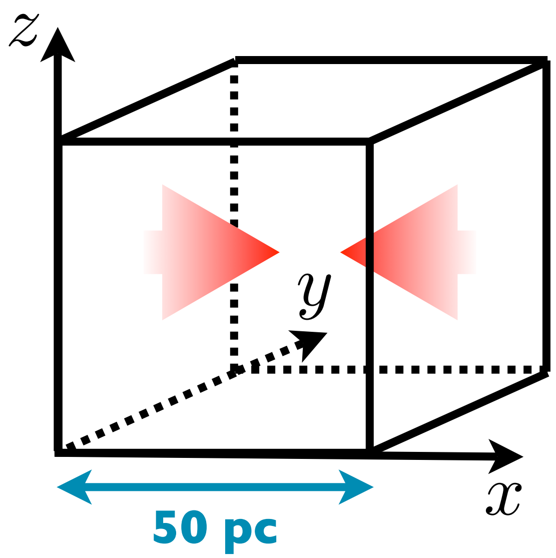
PROJECT	DESCRIPTION
Molecular cloud evolution with decaying turbulence	This project aims at describing the evolution of a turbulent molecular cloud in which the turbulence is decaying.
Barotropic dense core simulations	This project aims at describing the gravitational collapse of magnetized molecular dense cores.
Colliding flow simulations	This project aims at describing self-consistently the formation of molecular clouds starting from the very diffuse atomic interstellar medium.
Solenoidal vs. Compressive Turbulence Forcing	This project investigates the influence of different forcing (i.e., kinetic energy injection) on turbulent flows in the interstellar medium.

http://starformat.obspm.fr/

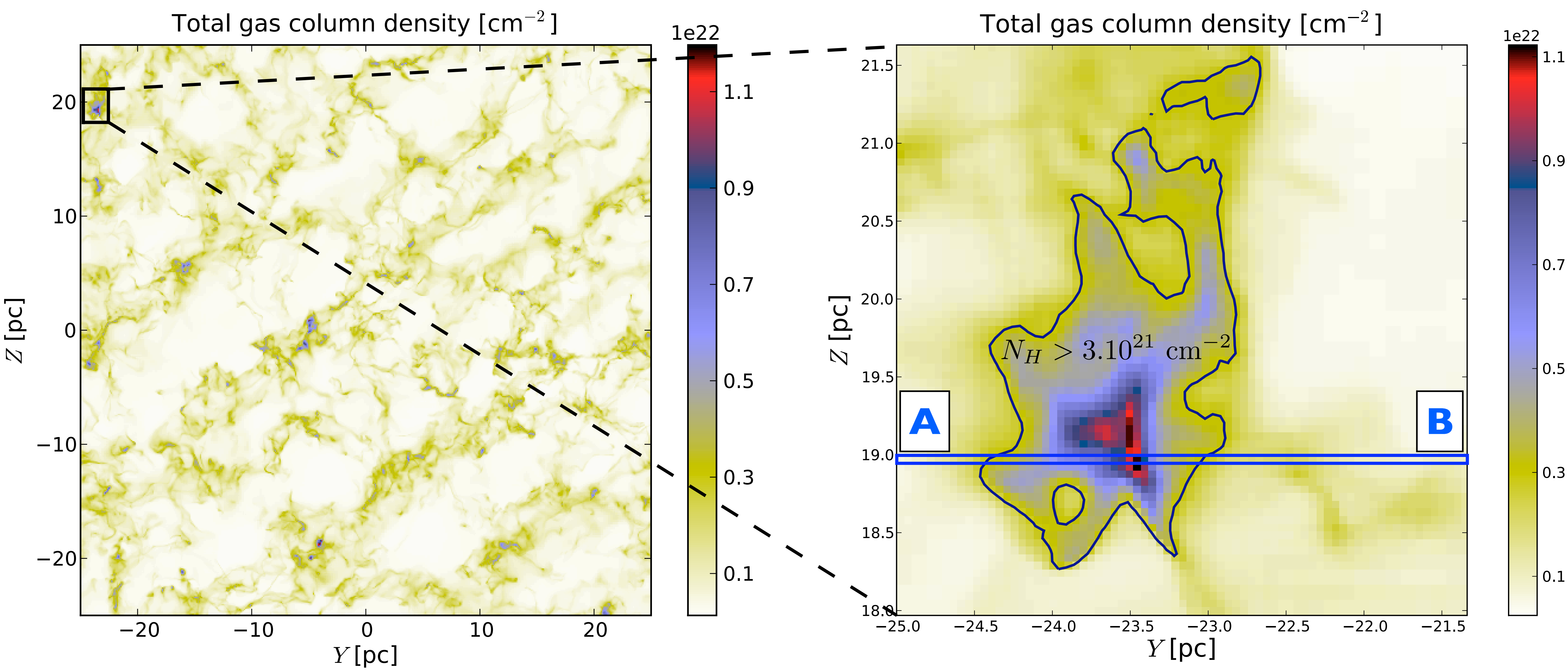


Compressible MHD turbulence simulation

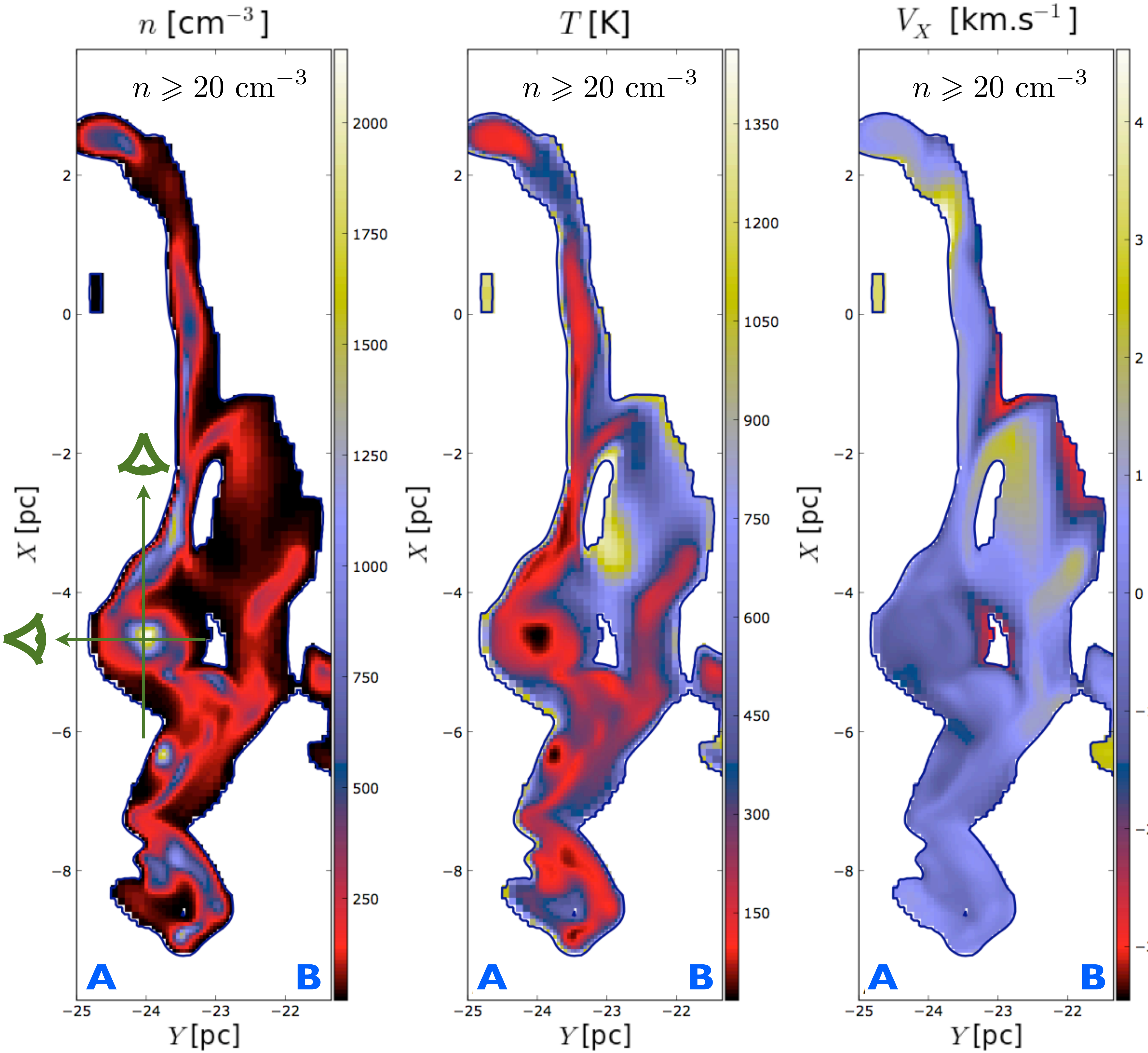
Hennebelle et al. 2008



- RAMSES code (Teysier 2002, Fromang et al. 2006)
- Adaptive Mesh Refinement with up to 14 levels
- Converging flows of warm (10,000 K) atomic gas
- Periodic boundary conditions on remaining 4 sides
- Includes magnetic field, atomic cooling and self-gravity consistently
- Covers scales 0.05 pc - 50 pc
- Heavy computation : ~30,000 CPU hours ; 10 to 100 GB



Structures along the LOS

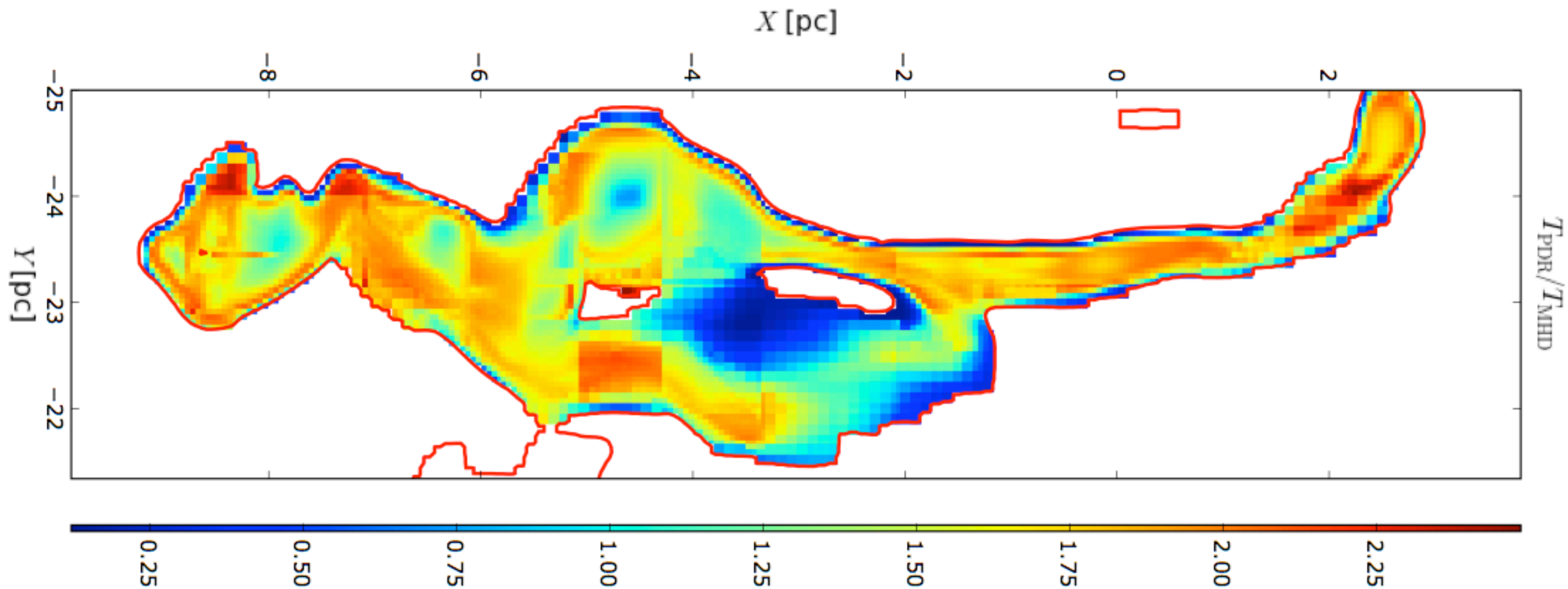


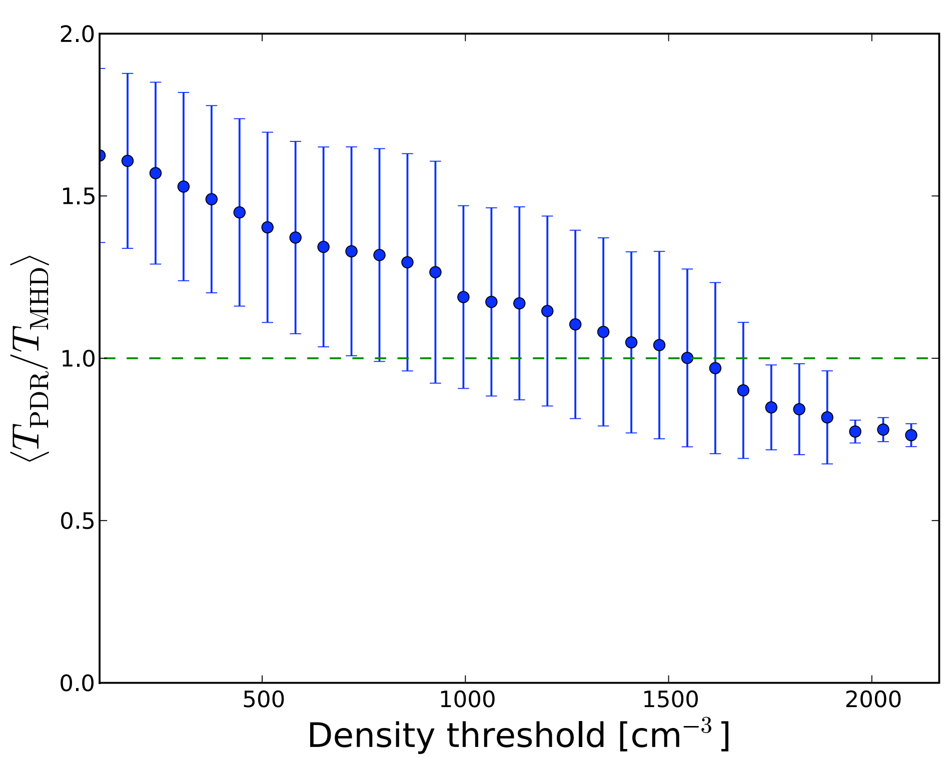
PDR code run on 1D density profiles above 20 cm^{-3} extracted along lines of sight either parallel to X or Y.

Outputs (temperature, chemical abundances) combined in 2D arrays.

Temperature comparison

Ratio of the temperature computed by the PDR code and the temperature from the MHD simulation





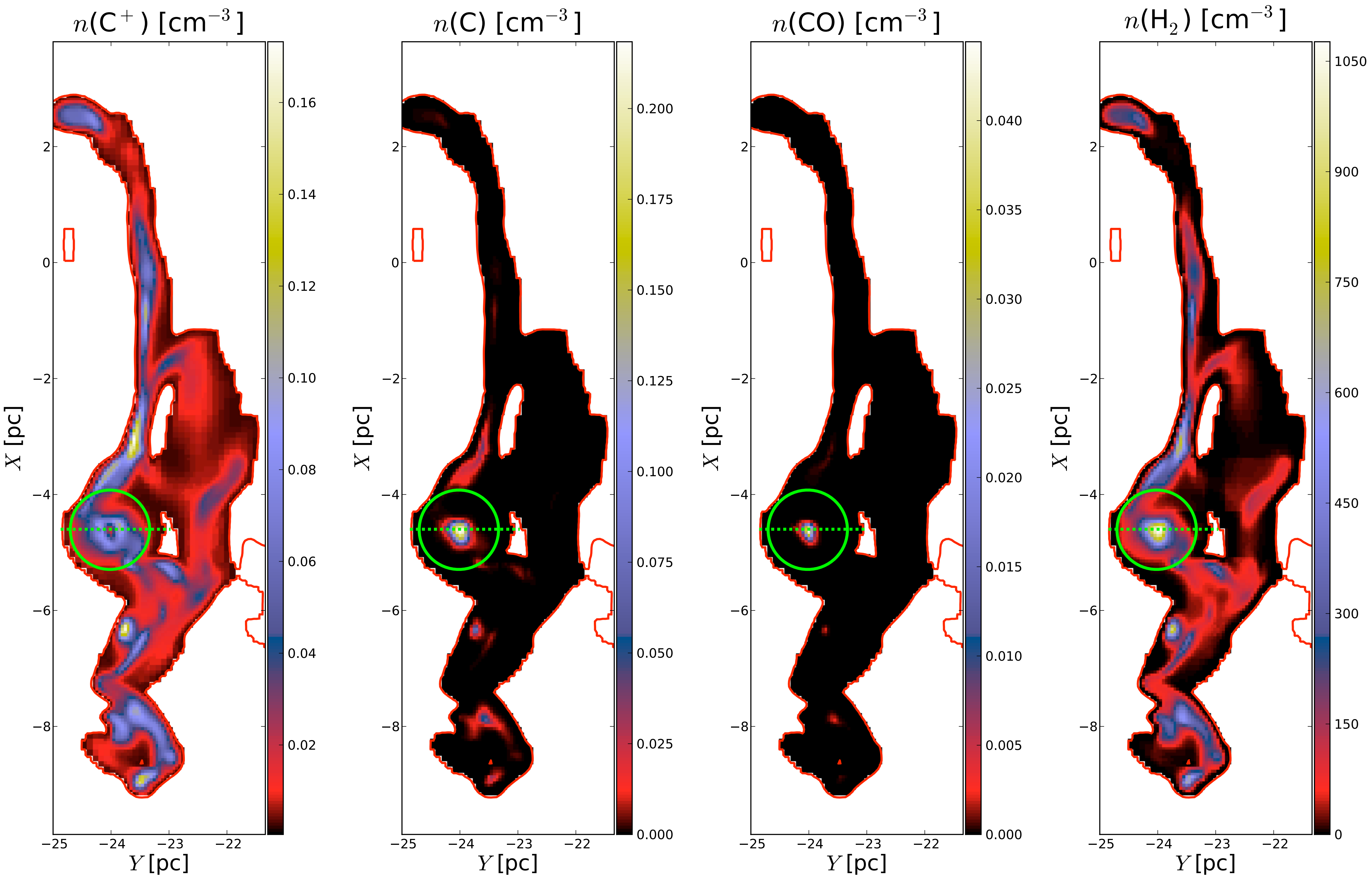
- **Different cooling functions**
- **Steady-state versus dynamical**
- **1D versus 3D**

and yet...

$$0.3 \lesssim \frac{T_{\rm PDR}}{T_{\rm MHD}} \lesssim 2$$

“Dark neutral gas”

Levrier et al. (in prep)



- C^+ closely follows the total gas density, except in the densest regions.
- Significant fraction of the molecular gas not traced by CO, but rather by C and C^+.

"Dark neutral gas" fraction through the cloudlet

Fractions in volume densities

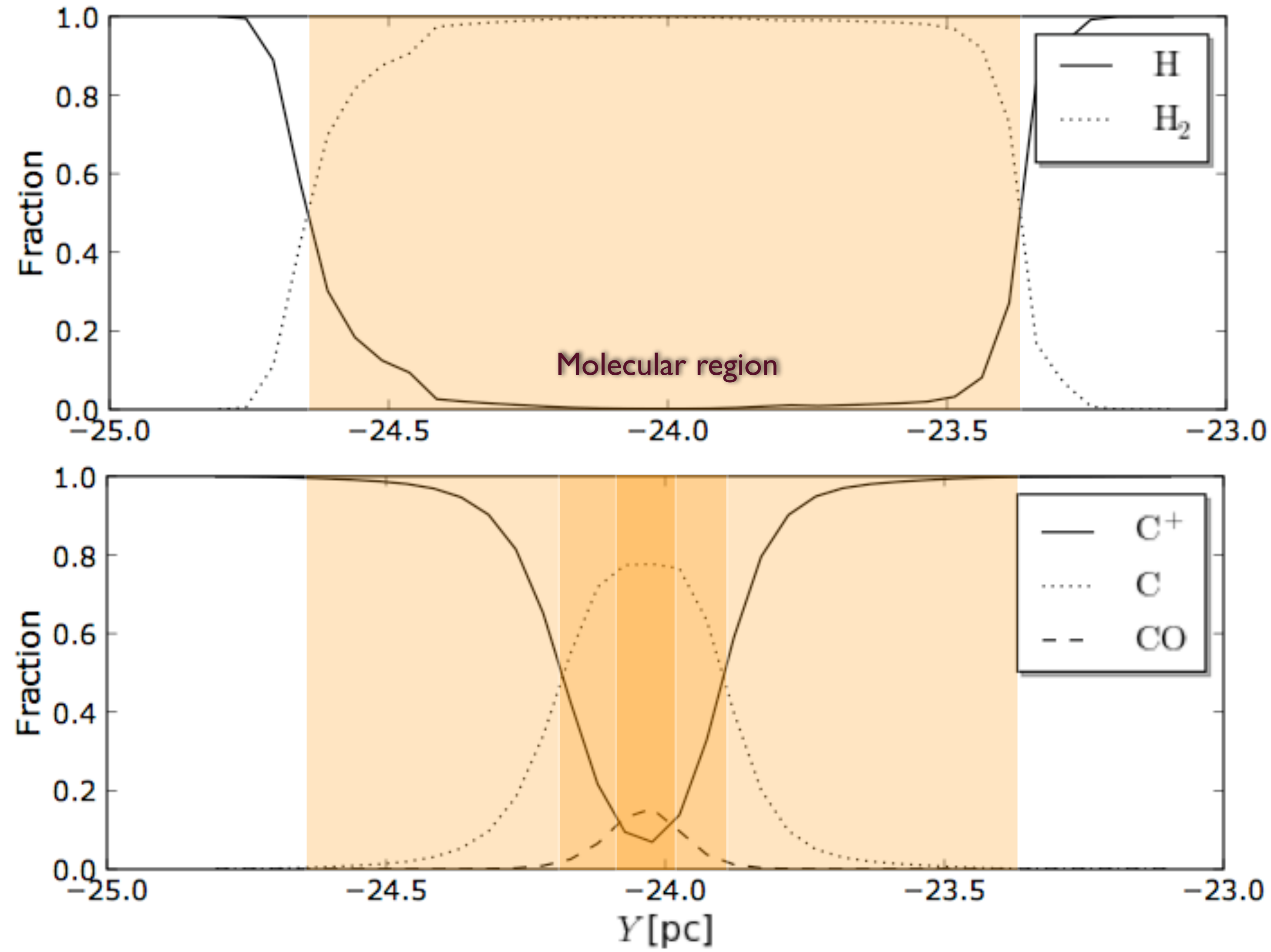
H : $$\frac{n(\mathrm{H})}{2n(\mathrm{H_2}) + n(\mathrm{H})}$$

H_2 : $$\frac{2n(\mathrm{H_2})}{2n(\mathrm{H_2}) + n(\mathrm{H})}$$

C^+ : $$\frac{n(\mathrm{C^+})}{n(\mathrm{C^+}) + n(\mathrm{C}) + n(\mathrm{CO})}$$

C : $$\frac{n(\mathrm{C})}{n(\mathrm{C^+}) + n(\mathrm{C}) + n(\mathrm{CO})}$$

CO : $$\frac{n(\mathrm{CO})}{n(\mathrm{C^+}) + n(\mathrm{C}) + n(\mathrm{CO})}$$



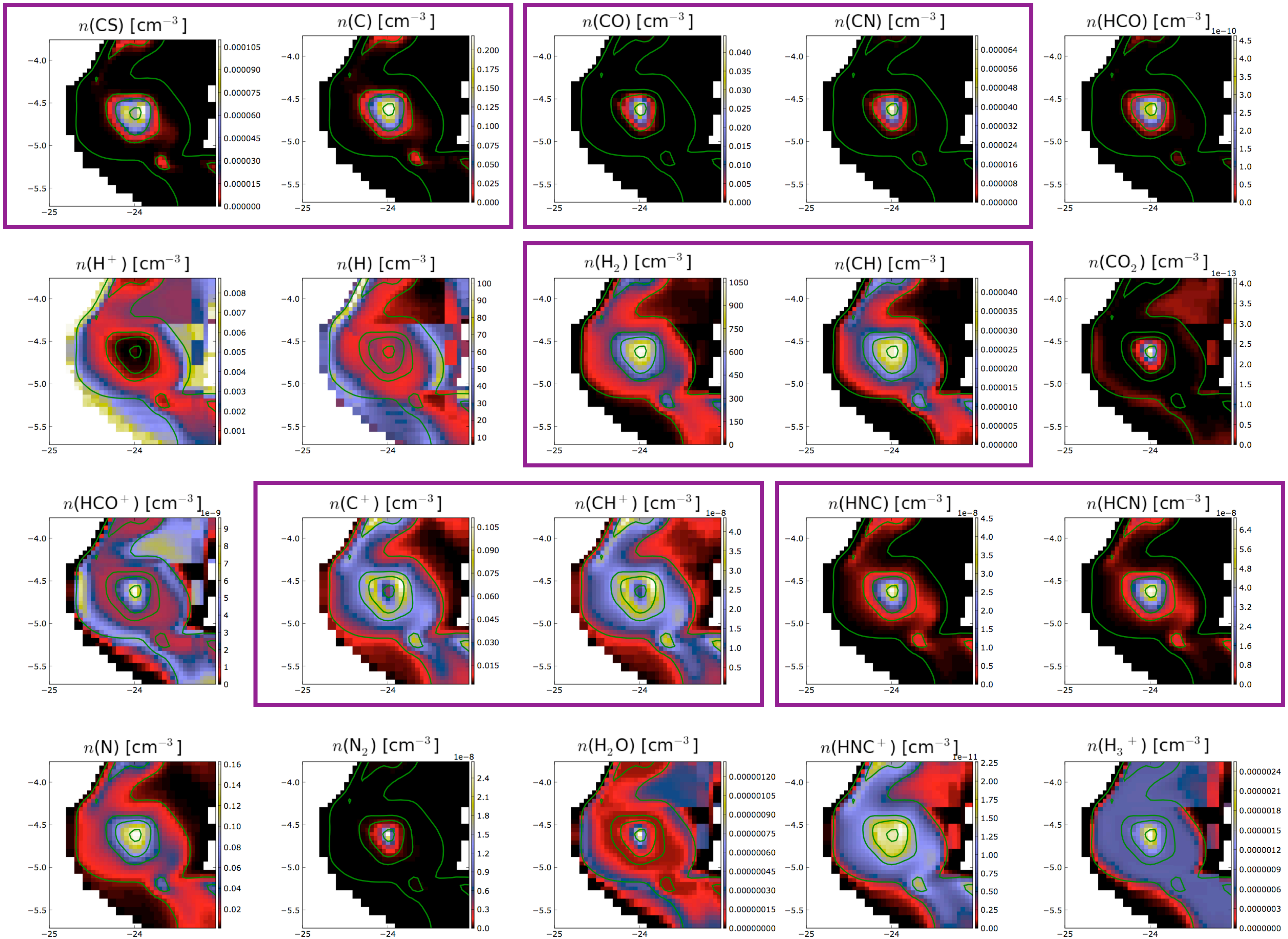
Mass fraction in the molecular region : 98%

... of which traced by C+ : 48%
... of which traced by C : 47%
... of which traced by CO : 5%

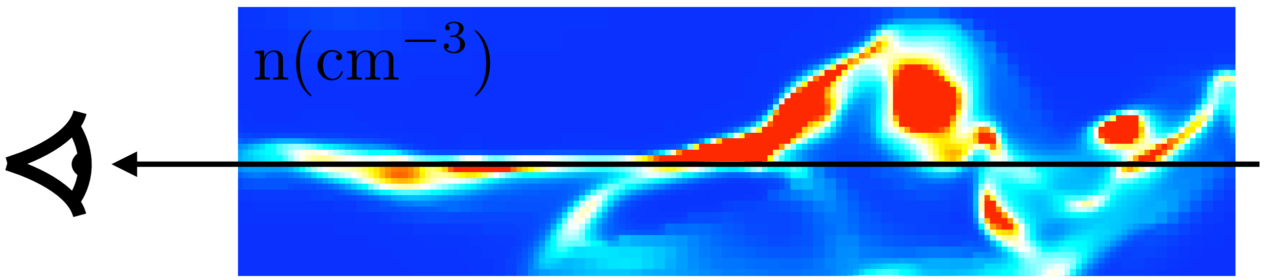
See models by Wolfire et al. 2010

H_2 in H_2/C^+ layers contributes ~30% of the mass of clouds with A_V=8

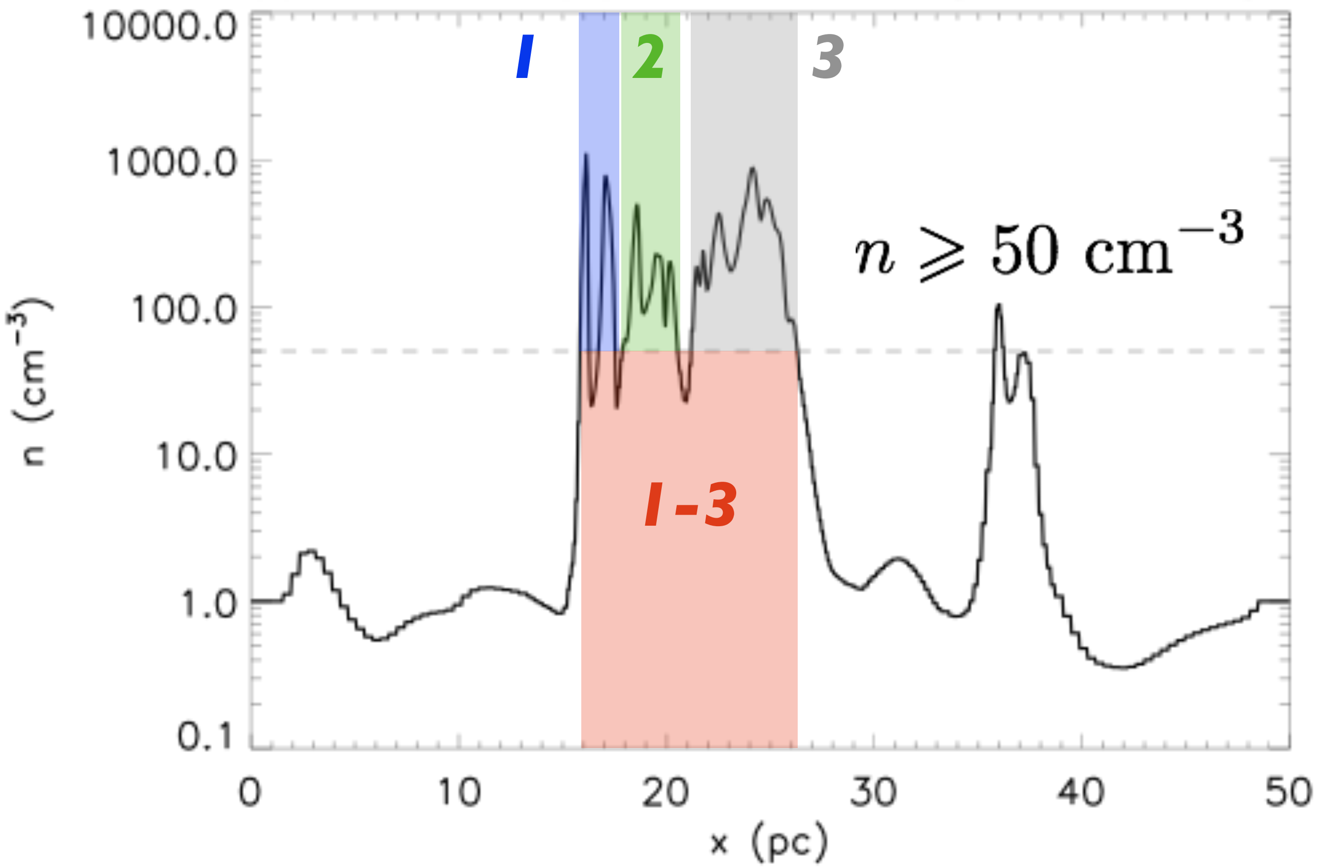
Cloudlet morphology in different tracers



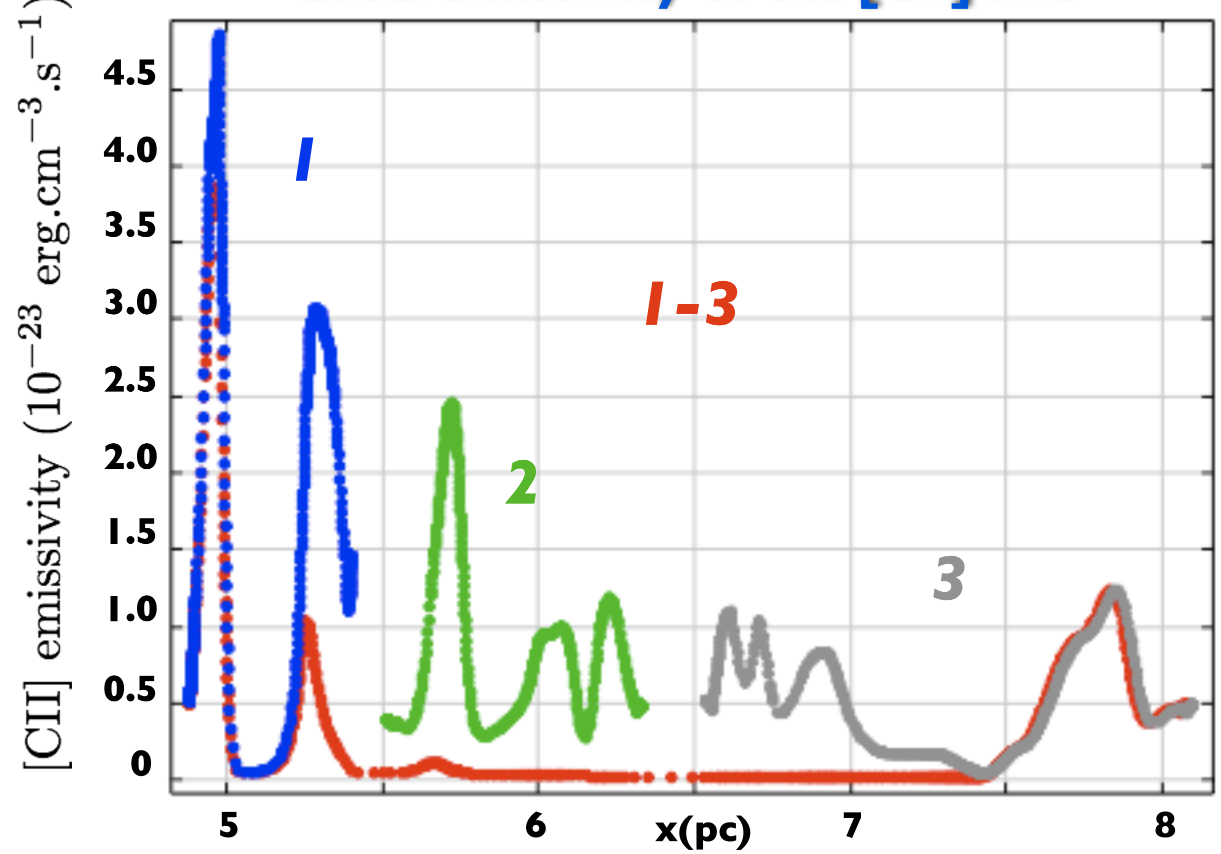
Shadowing effects



Typical density profile of a single line of sight

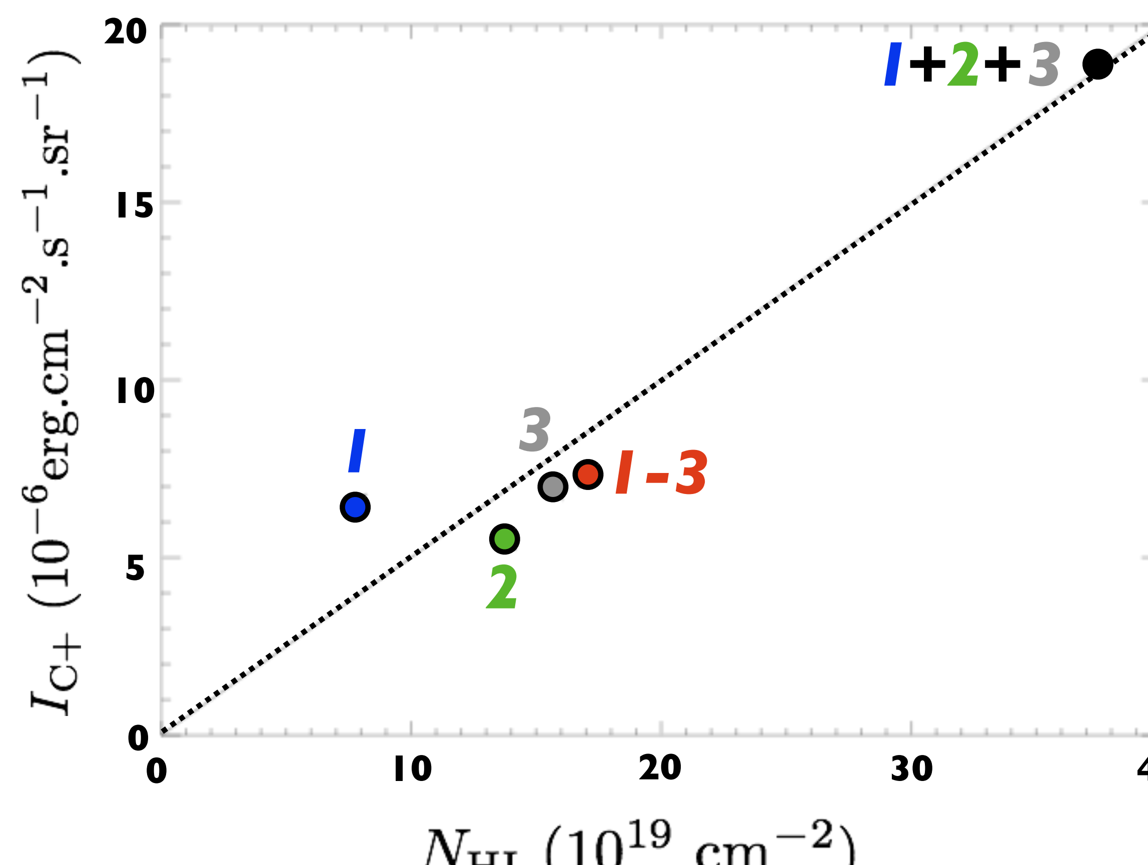


Local emissivity of the [CII] line



$$\frac{I_{C+}}{10^{-6}\mathrm{erg.cm^{-2}.s^{-1}.sr^{-1}}} \simeq 0.5 \times \frac{N_{\mathrm{HI}}}{10^{19}\mathrm{cm^{-2}}}$$

(See Bennett et al. 94)

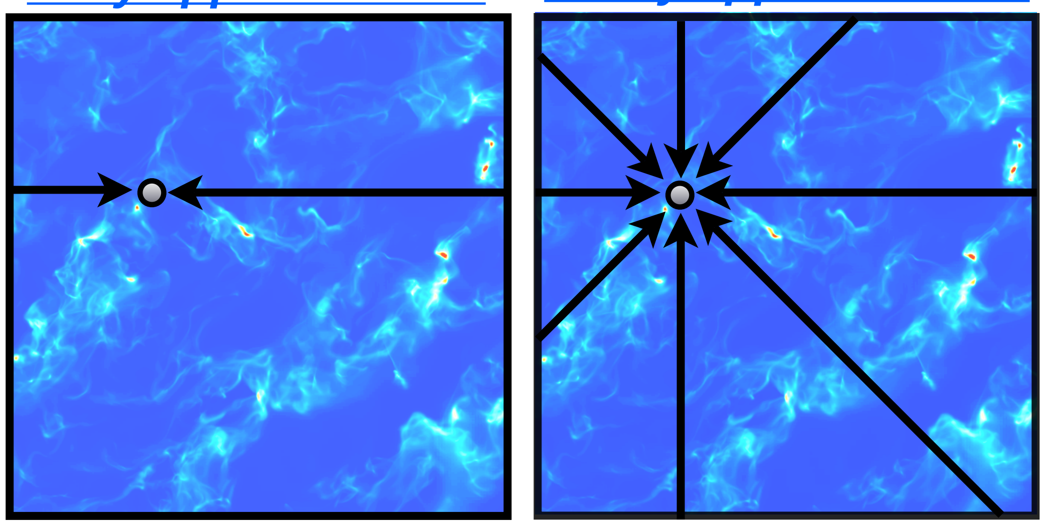


Beyond the 1D PDR code

Compute local UV field from extinctions in many directions

$$\chi \propto \langle \exp\left(-\alpha A_v\right)\rangle$$

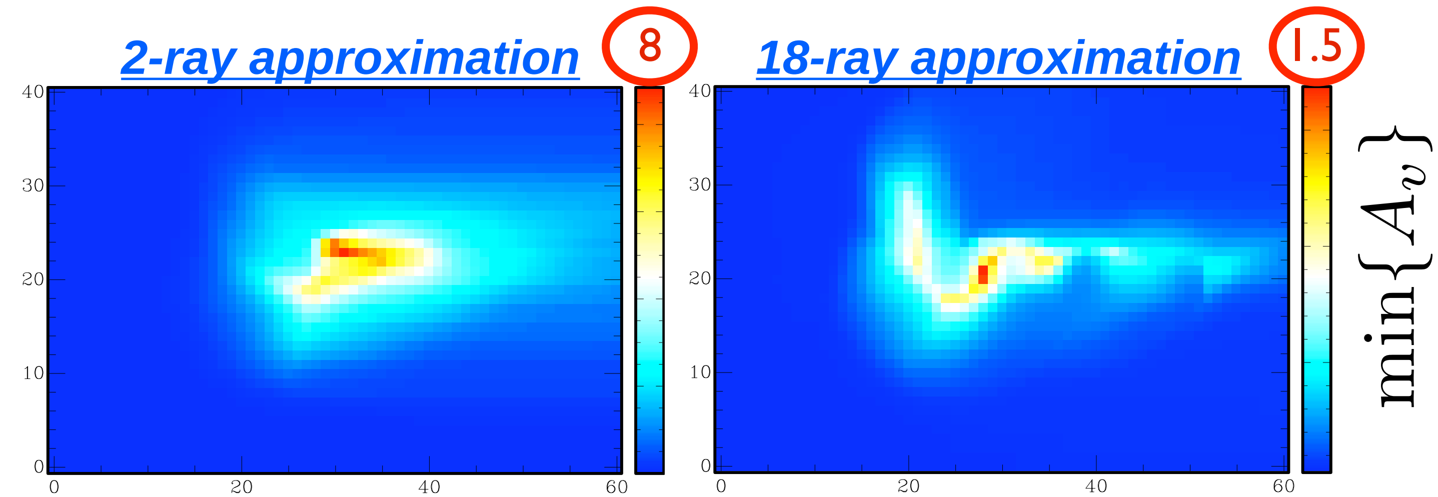
2-ray approximation *18-ray approximation*

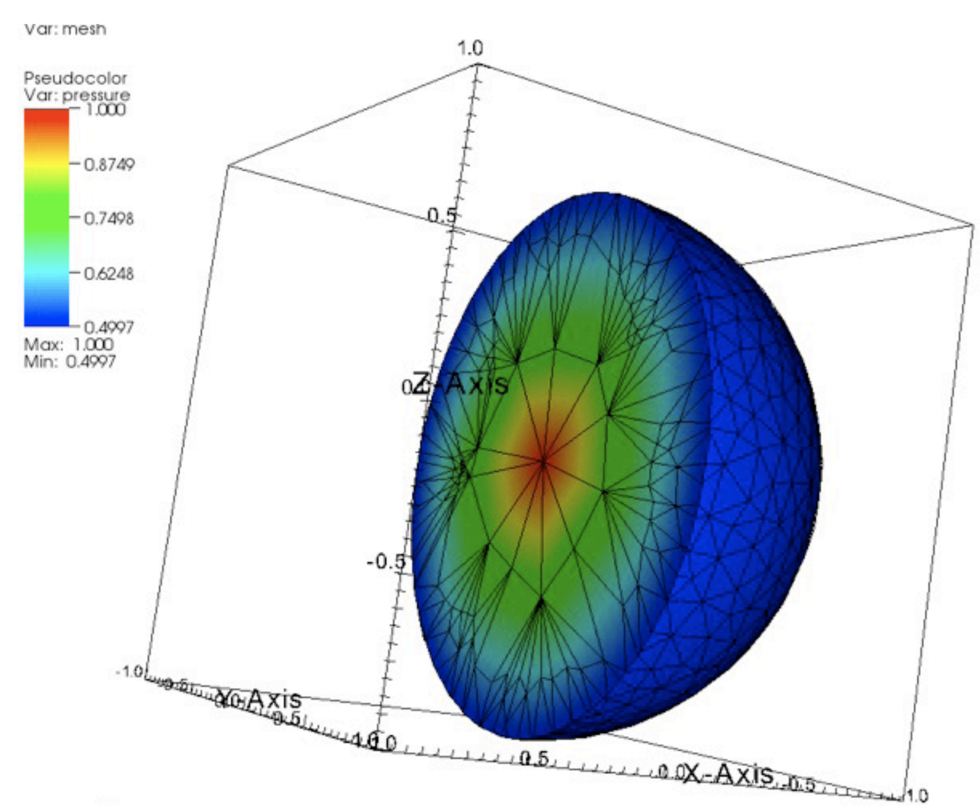


(1D : same as PDR code) *(in each of XY, XZ, YZ planes)*

- "Fractal" nature of ISM clouds and simulated density structures
- Each point may be illuminated from many directions
- Illumination computed as post-processing or "on-the-fly"
- May be used for incoming UV field in the PDR code

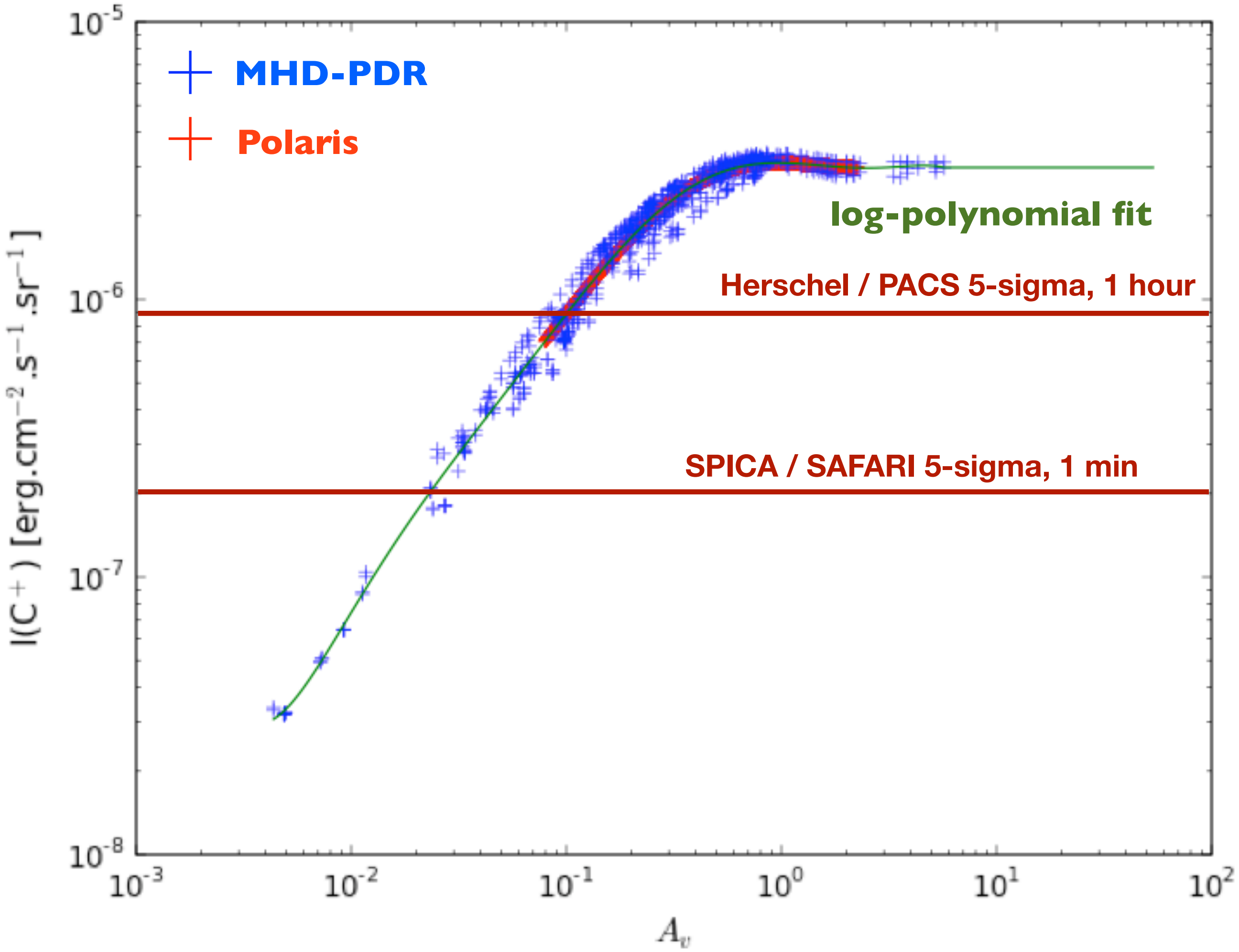
Example on a 2D cut



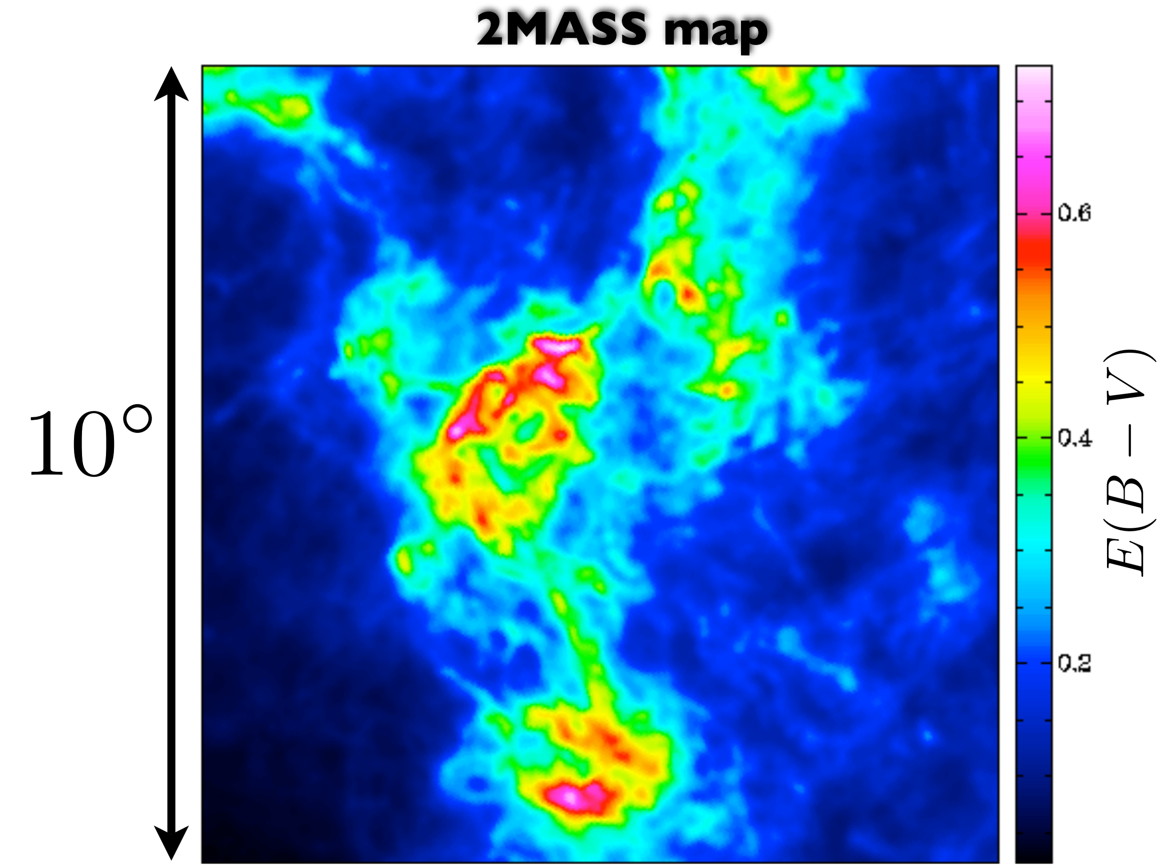


Also in the works : development of a 3D PDR code (Cecilia Pinto)

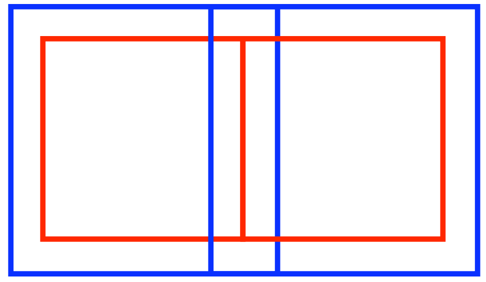
[CII] emission and visual extinction



Polaris : a tenuous non-star forming region of the ISM

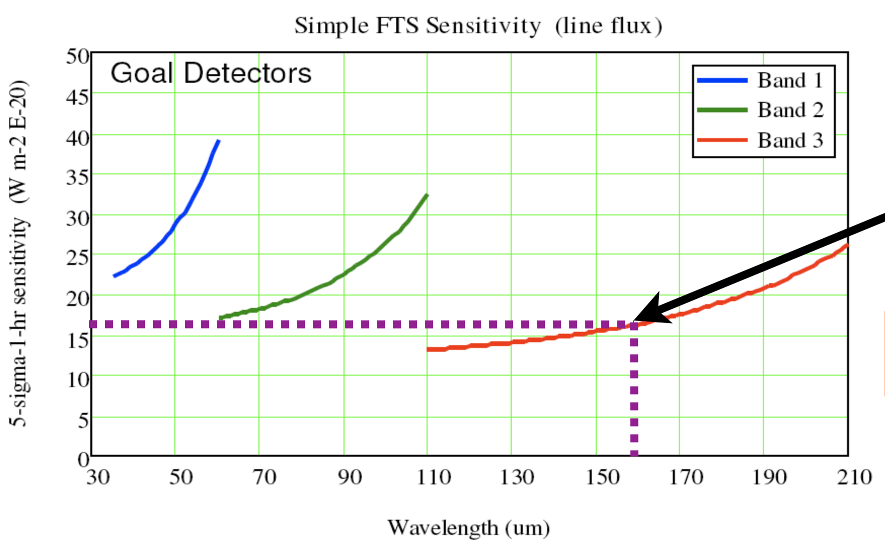


$$A_V = R_V \times E(B-V) \Rightarrow I_{[CII]} \Rightarrow S_p = \frac{I_{[CII]} \times \Omega_{\rm 2MASS}}{(20 \times 20)\ \text{FPA pixels}}$$



2MASS pixel : 1.5' x 1.5'

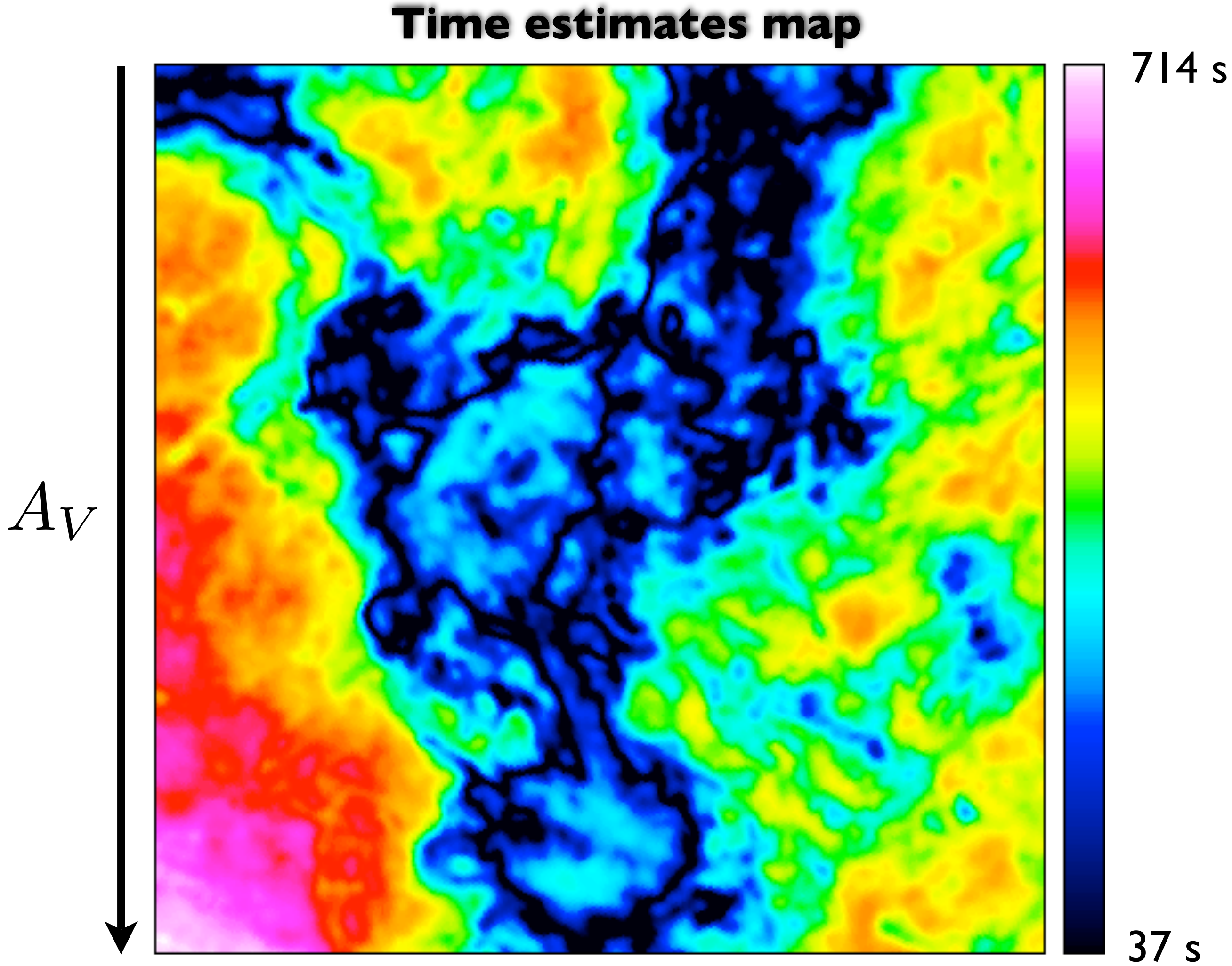
SAFARI FoV : 2' x 2'

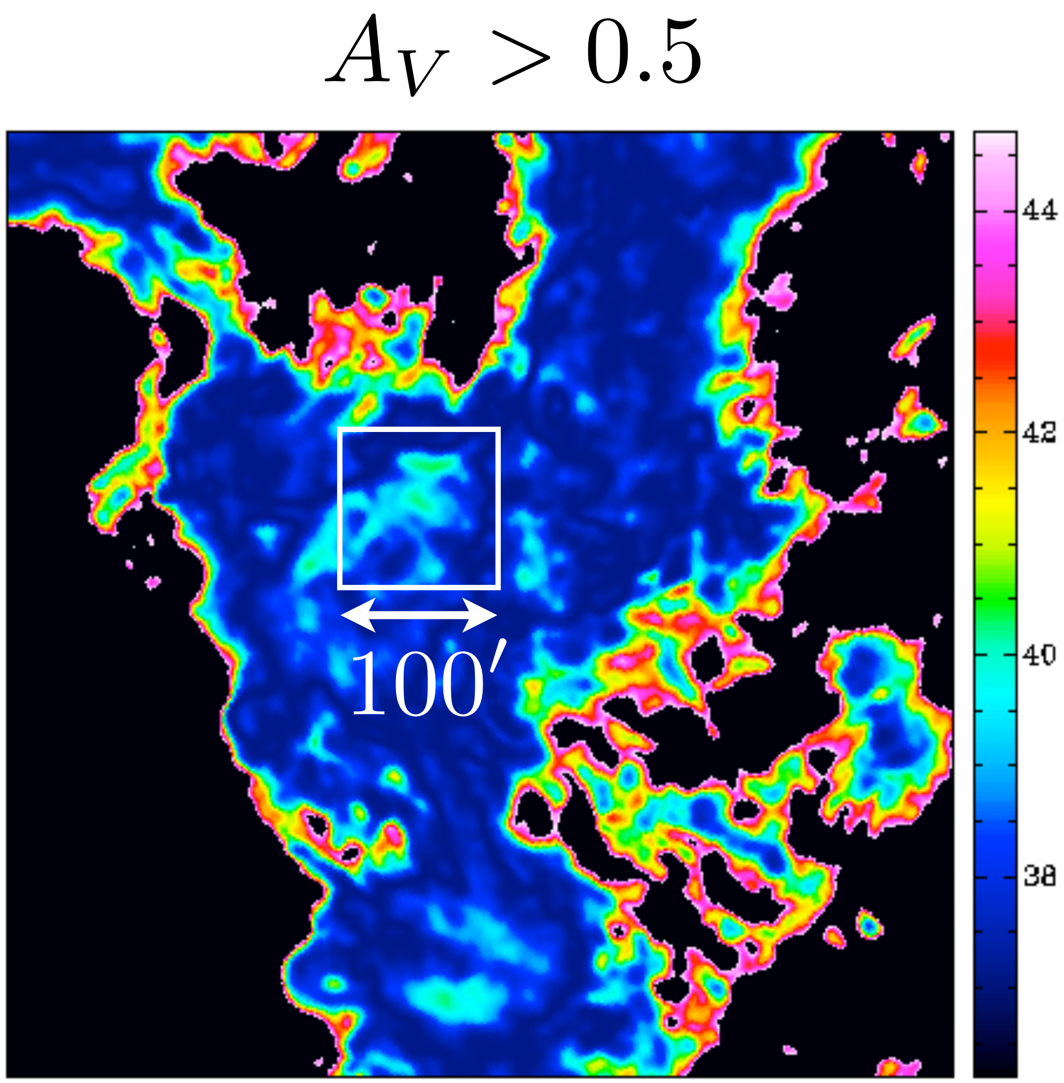


$$S_0 = 1.6\ 10^{-19}\ \text{W.m}^{-2}$$

Use 2μ filter for the [CII] line

Time estimates for mapping Polaris





$$\Delta t = (1 \text{ hour}) \times \left(\frac{S_0}{S_p}\right)^2$$

$$\langle \Delta t \rangle_{\text{pointing}} \sim 1 \text{ min}$$

- **Relax FoV overlapping**
- **100' x 100' field**
- **Minimum extinction 0.5**

$T \sim 28$ hours

To open up...

Cosmic rays ionisation rate $\zeta_{\rm CR} = 5\ 10^{-17}\ {\rm s}^{-1}$

Do we need to change this ? As a function of column density ?

[CII] from WIM $I_{\rm WIM}(C+) = 6.67\ 10^{-7}{\rm erg.cm}^{-2}{\rm .s}^{-1}{\rm .sr}^{-1}$

(Reynolds 92)

Towards more realistic simulations

Steady state post-processed vs dynamically coupled chemistry
Energy inputs : PDR vs TDR
Clumpy ISM : 3D PDR code vs pseudo-3D