Post-processing of MHD simulations with the Meudon PDR code

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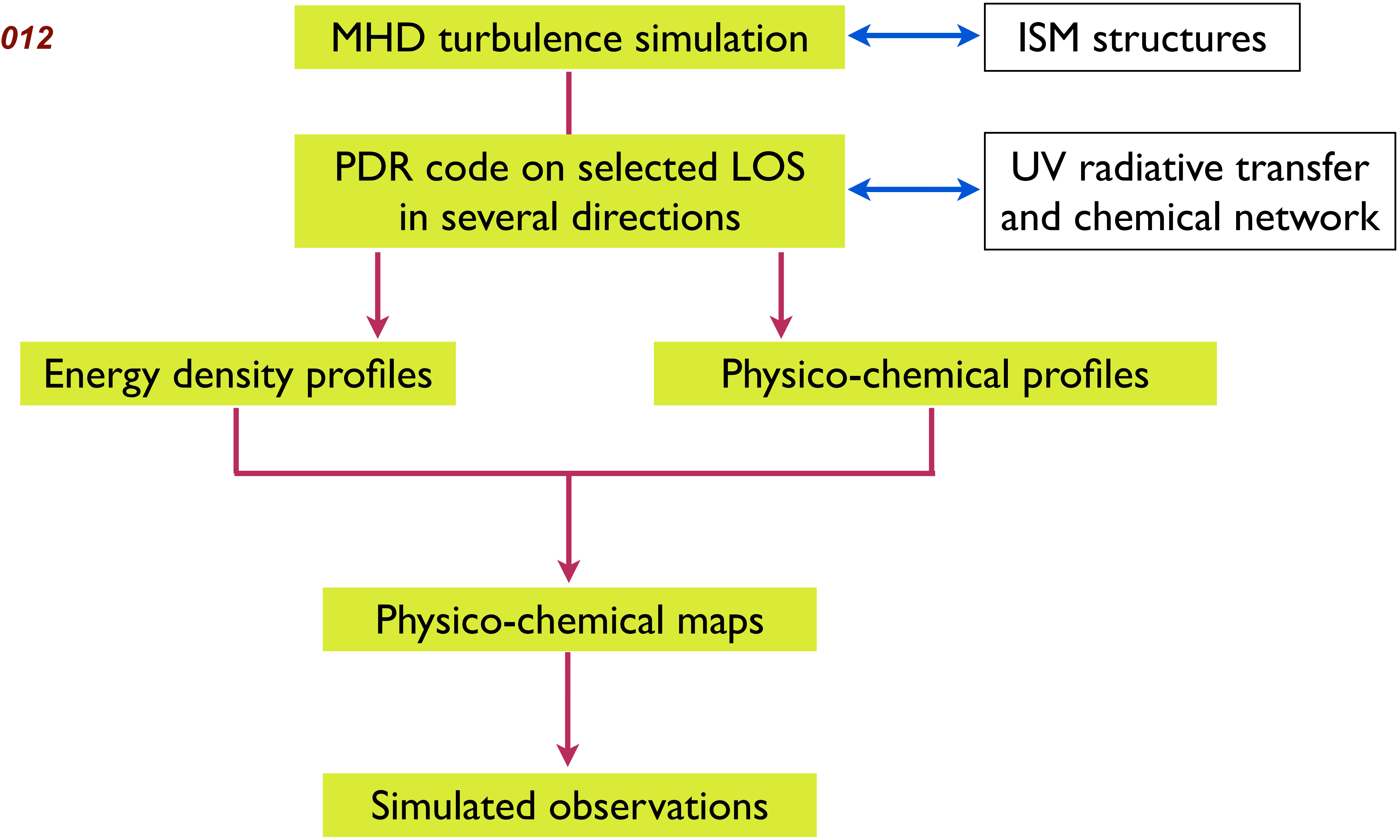
Talk overview

- PDR code on MHD simulations
- “Dark neutral gas”
- H_3^+ chemistry and cosmic ray ionization rate
- Perspectives

UV-driven chemistry of a simulated ISM

Levrier et al. 2012



MHD turbulence simulation

ISM structures

PDR code on selected LOS
in several directions

UV radiative transfer
and chemical network

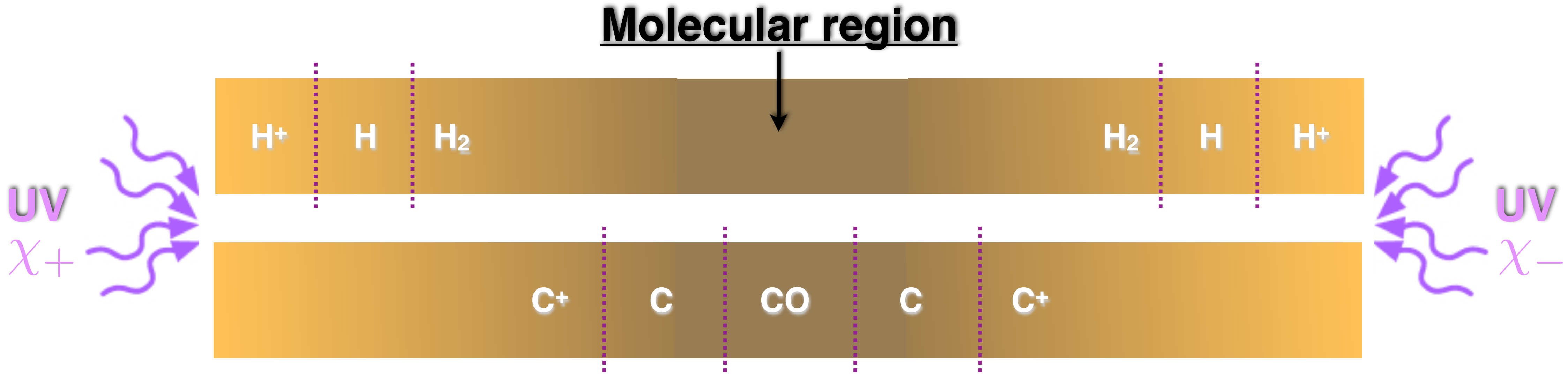
Energy density profiles

Physico-chemical profiles

Physico-chemical maps

Simulated observations

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
  Cosmic ray ionization
- Statistical equilibrium of level populations
  Radiative and collisional excitations and de-excitations
  Photodissociation
- Thermal balance:
  Photoelectric effect
  Chemistry
  Cosmic rays
  Atomic and molecular cooling

$$\boxed{\zeta_0 = 5\ 10^{-17}\ \mathrm{s}^{-1}}$$

Outputs :

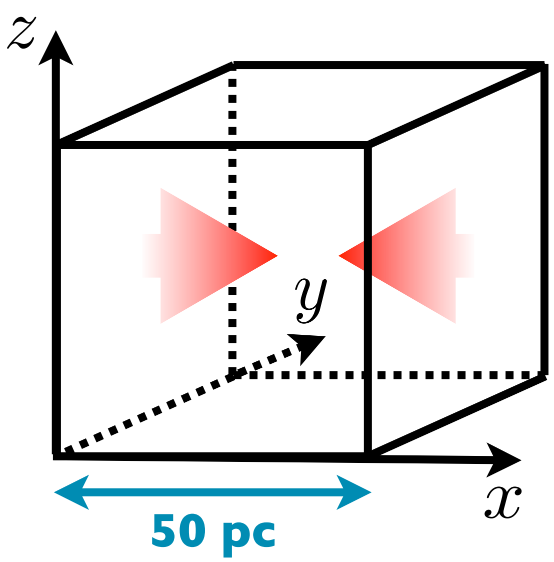
- Local quantities :
  Abundance and excitation of species
  Temperature of gas and duts
  Detailed heating and cooling rates
  Energy density
  Gas and grain temperatures
  Chemical reaction rates
- Integrated quantities on the line of sight :
  Species column densities
  Line intensities
  Absorption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

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

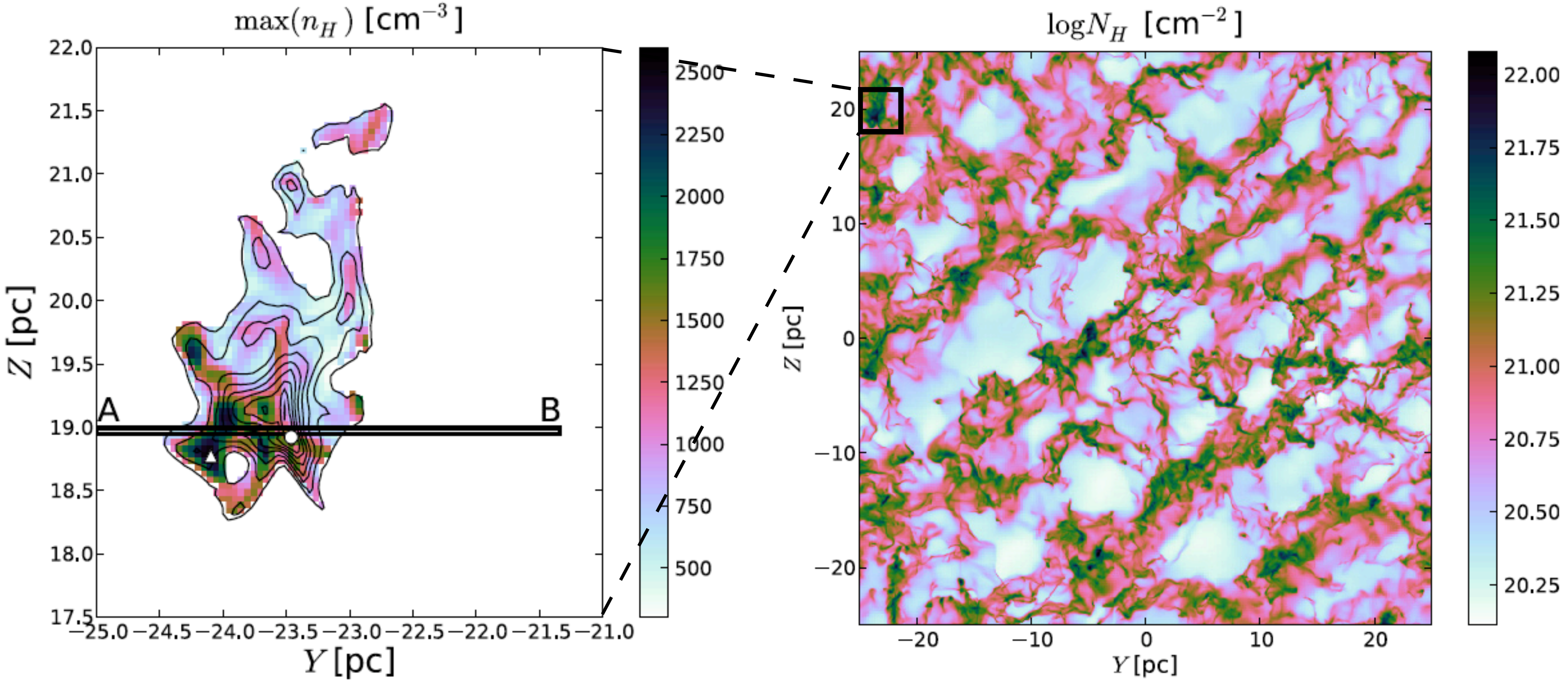
http://pdr.obspm.fr/

Compressible MHD turbulence simulation

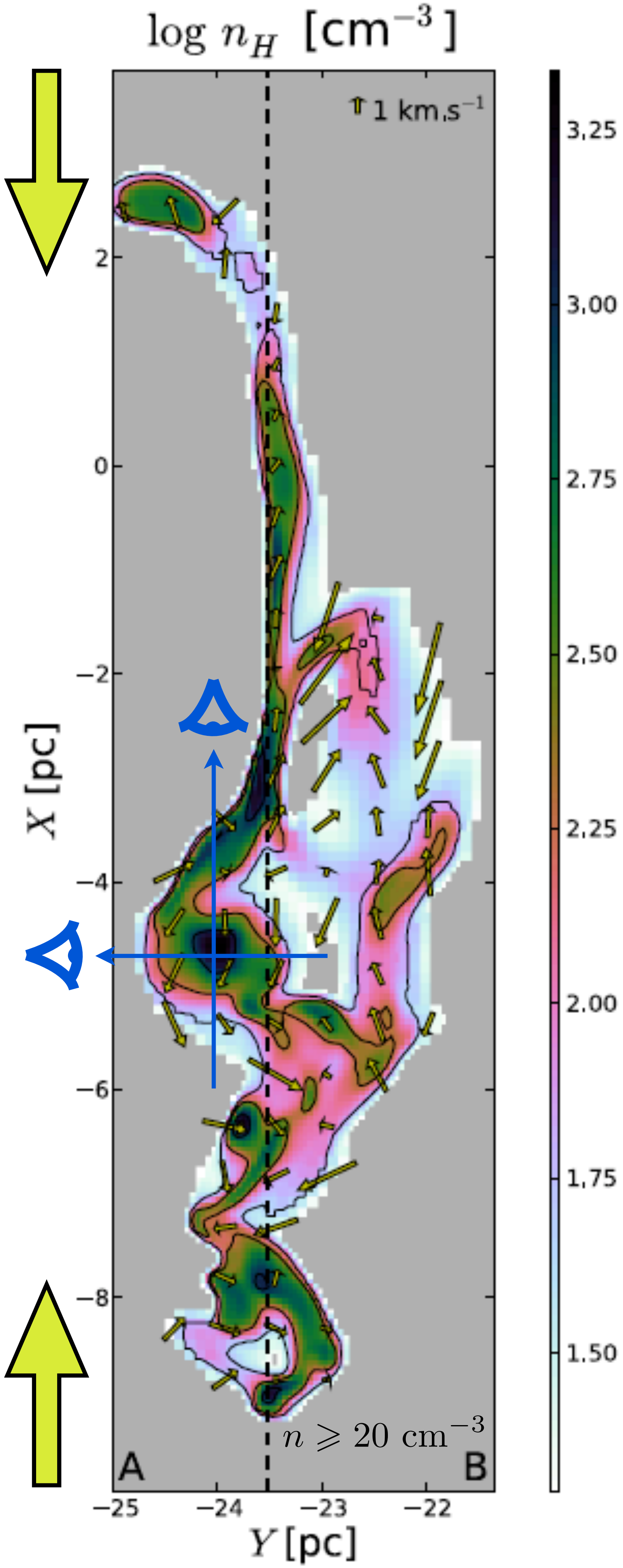
Hennebelle et al. 2008



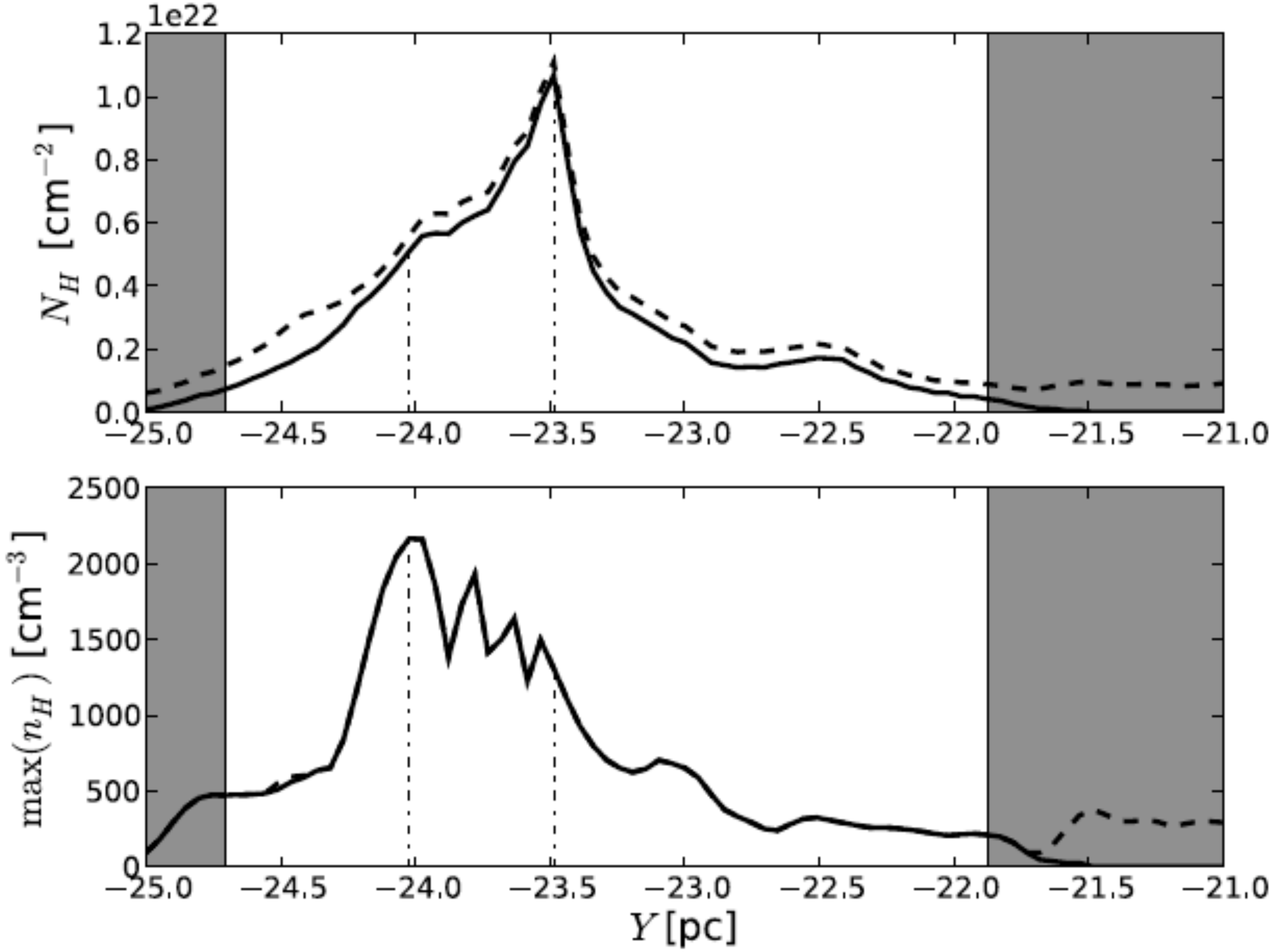
- **RAMSES code (Teysier 2002, Fromang et al. 2006)**
- **Adaptive Mesh Refinement with up to 14 levels**
- **Converging flows of warm (10,000 K) atomic gas**
- **Periodic boundary conditions on remaining 4 sides**
- **Includes magnetic field, atomic cooling and self-gravity consistently**
- **Covers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



Structures along the lines of sight



Central 10 pc cover most of the mass in this 2D slice



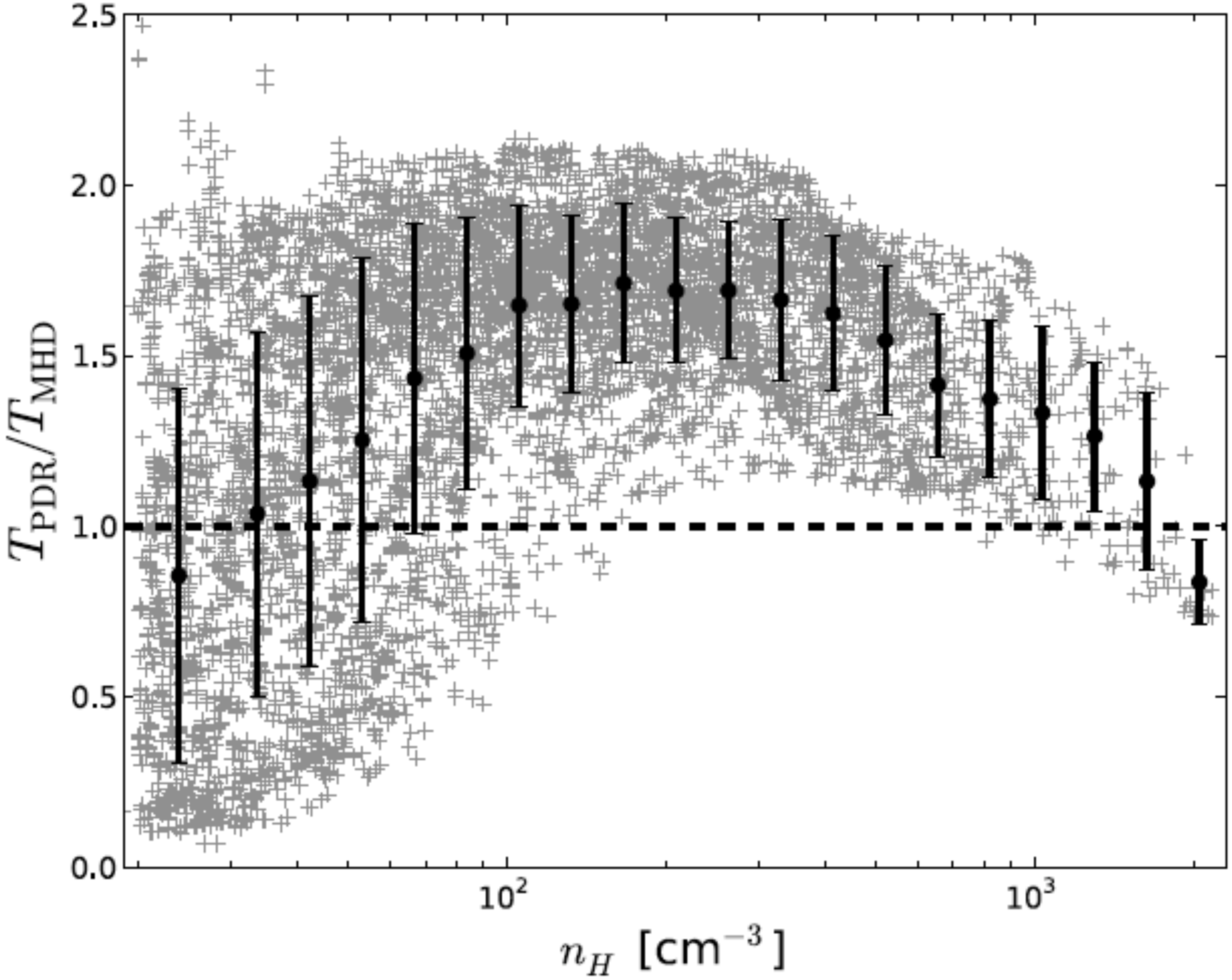
PDR code run on 1D density profiles above 20 cm^{-3} extracted along lines of sight either parallel to X or Y.

→

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

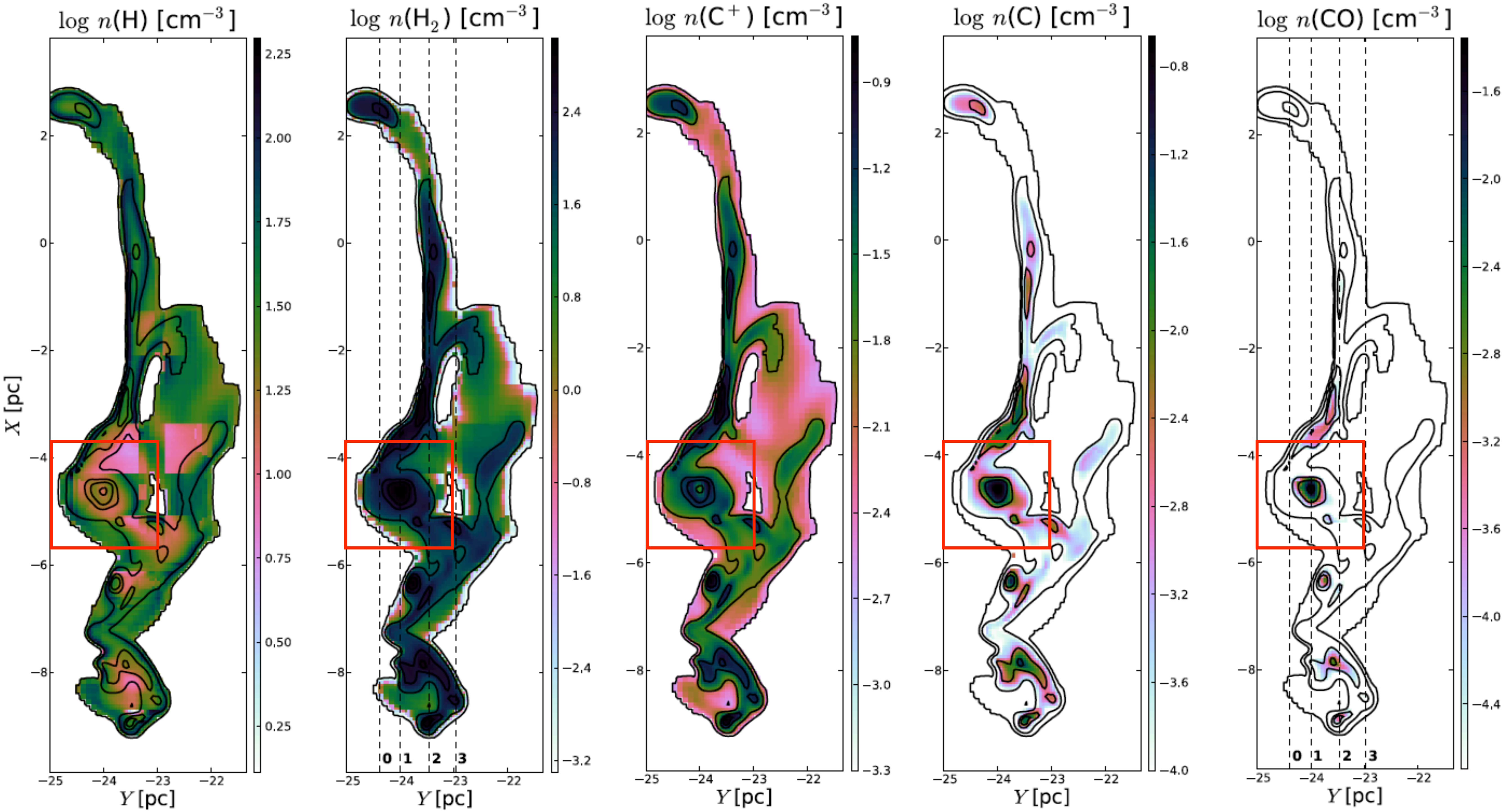


- Different cooling functions
- Steady-state versus dynamical
- 1D versus 3D

and yet...

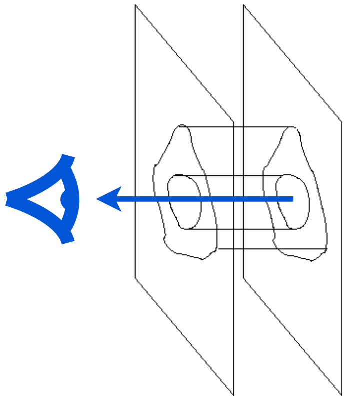
$$0.3 \lesssim \frac{T_{\rm PDR}}{T_{\rm MHD}} \lesssim 2$$

Main H and C bearers in the PDR/MHD simulation

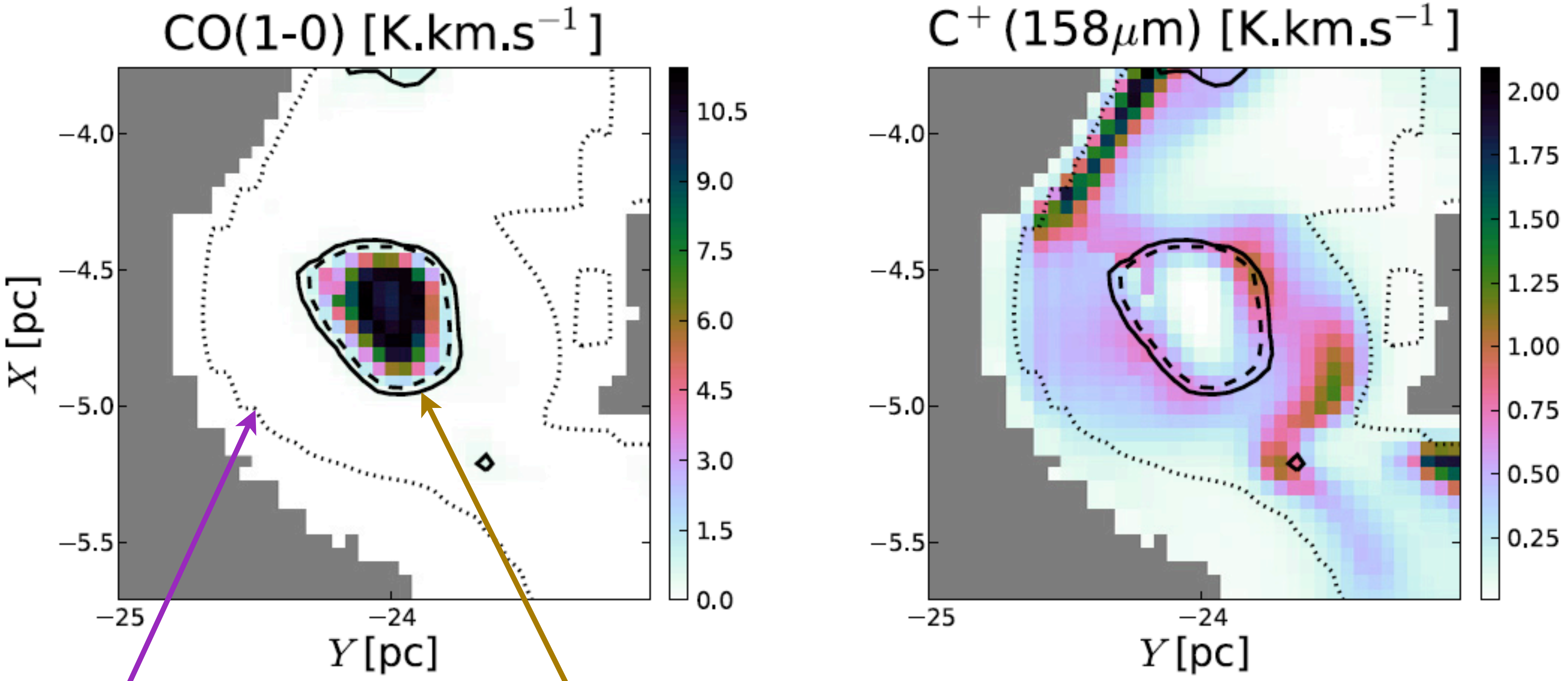


- C^+ closely follows the total gas density, except in the densest regions.
- CO only in the densest regions

Simulated observations in CO and C$^+$



Radiative transfer with RADEX (LVG approximation)



$f_{\mathrm{H_2}} = 1/2$

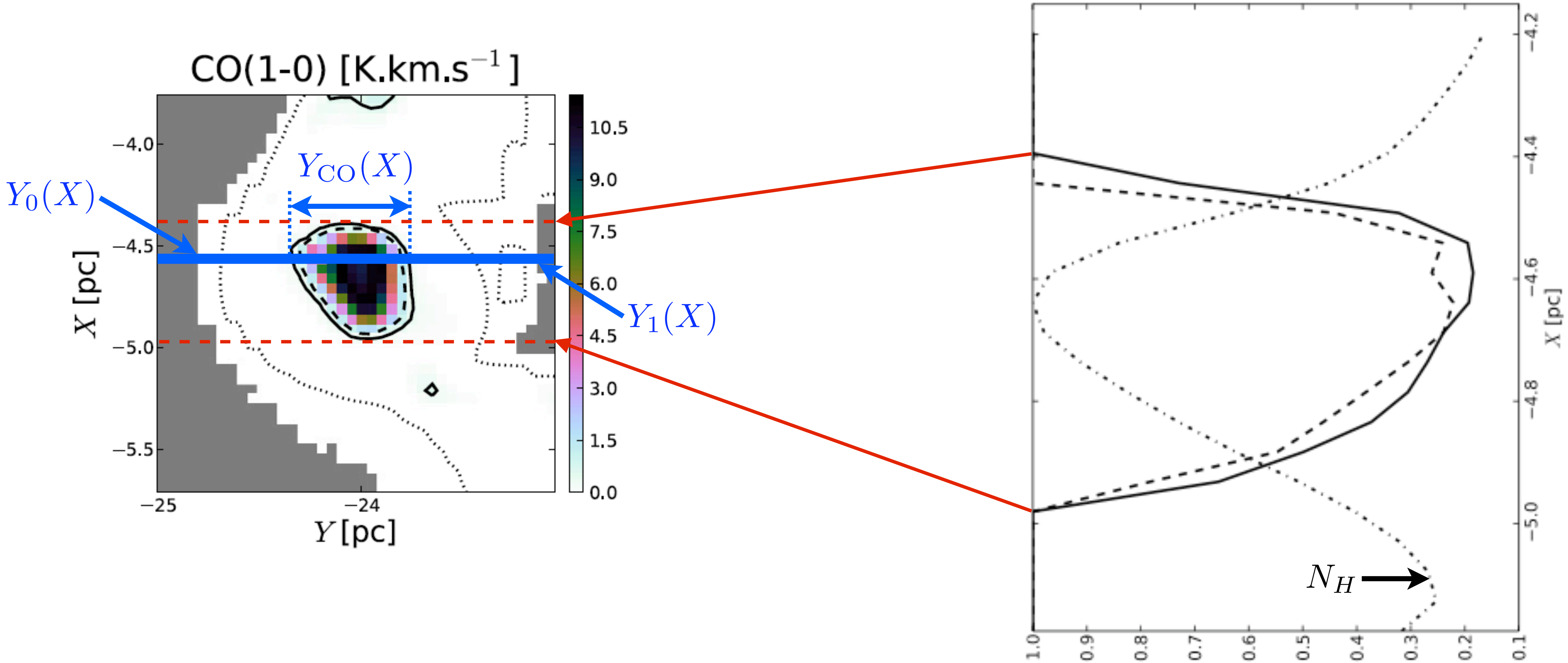
$W_{\mathrm{CO}} = 0.4\ \mathrm{K.km.s}^{-1}$

$\sigma_{\mathrm{CII}} = 0.1 - 0.2\ \mathrm{K.km.s}^{-1}$

Levrier et al. 2012

Velusamy et al. 2010

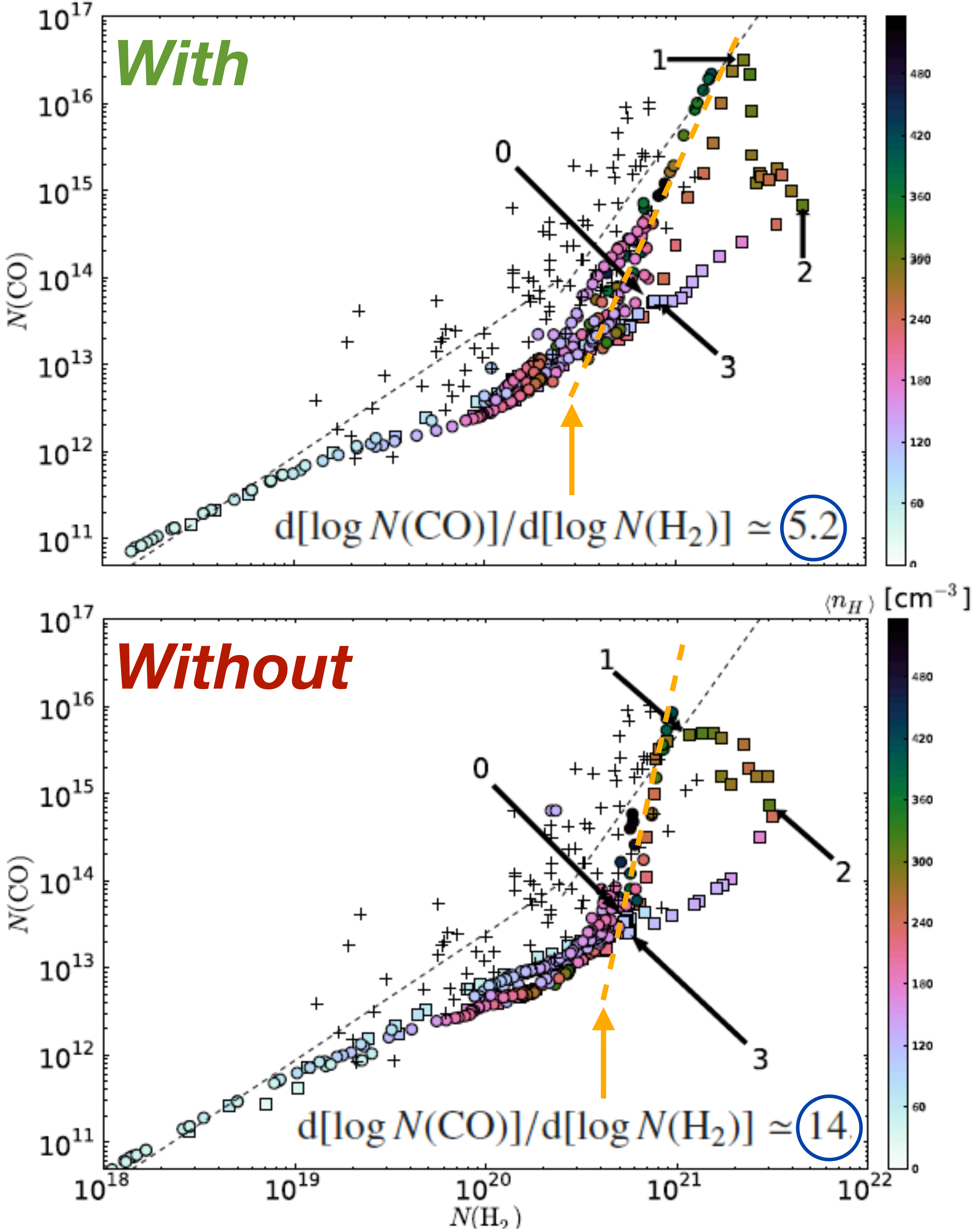
“Dark neutral gas” fraction through the cloudlet



$$f_{DG}(X) = 1 - \frac{\int_{Y_{CO}(X)} n(H_2)\mathrm{d}Y}{\int_{Y_0(X)}^{Y_1(X)} n(H_2)\mathrm{d}Y}$$

- At least 20% of H_2 not traced by CO
- Averaged “dark neutral gas” fraction 0.32
- Somewhat higher than Velusamy et al. 2010, comparable to Wolfire et al. 2010

Density fluctuations vs. uniform density : CO



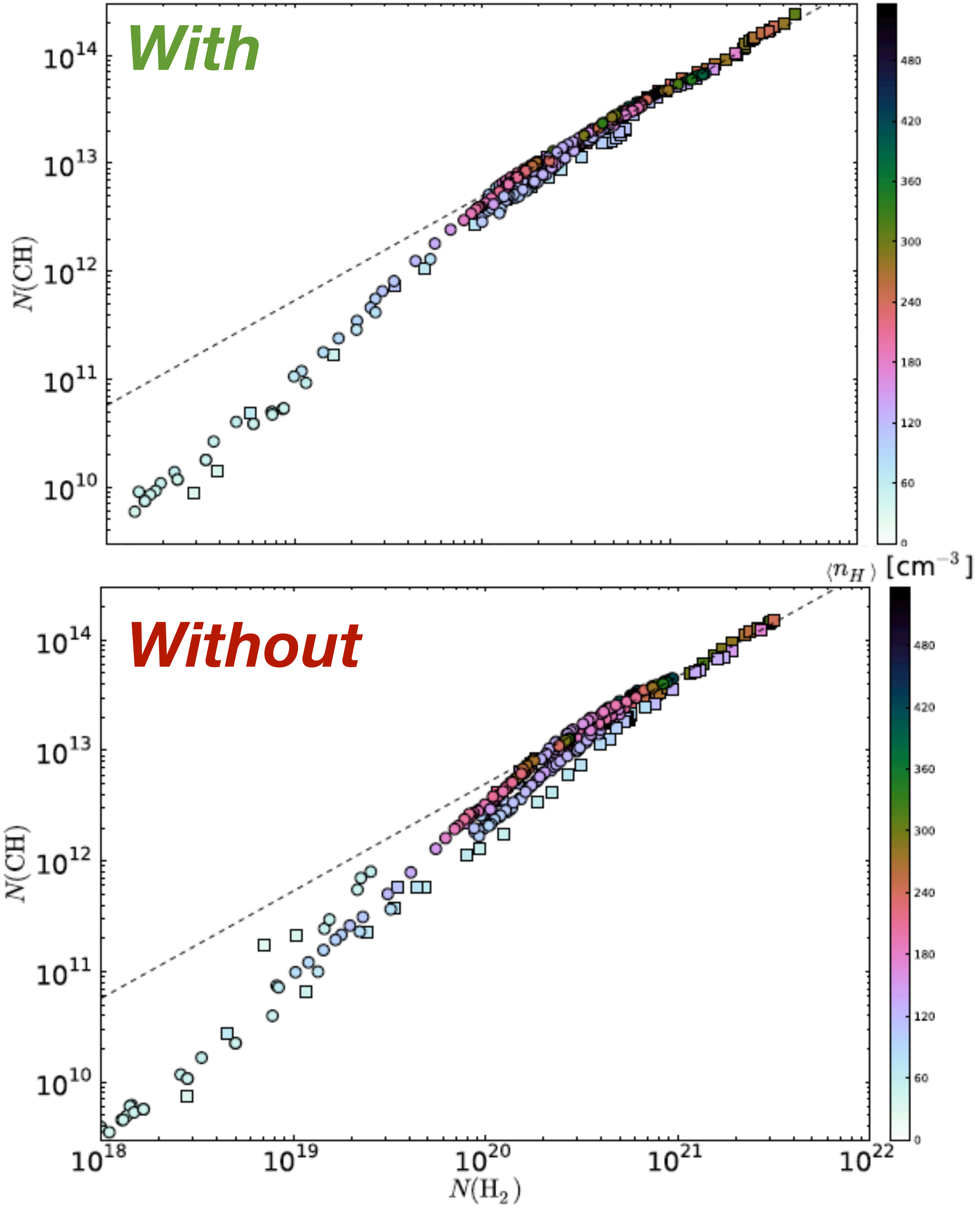
Observational fit

$$d[\log N(\mathrm{CO})]/d[\log N(\mathrm{H_2})] \simeq 3.07 \pm 0.73$$

Sheffer et al. 2008

- Maximum column densities are about 3 times as low in the uniform models
- CO vs H2 column densities correlate better

Density fluctuations vs. uniform density : CH



Observational fit

$$\mathrm{d}\left[\log N\left(\mathrm{CH}\right)\right]/\mathrm{d}\left[\log N\left(\mathrm{H_2}\right)\right] \simeq 1.09 \pm 0.19$$

Sheffer et al. 2008

- Maximum column densities are about twice as low in the uniform models
- CO vs H2 column densities correlation agrees better with observations

H_3^+ chemistry

Indriolo & McCall 2012

FORMATION

$$H_2 + CR \rightarrow H_2^+ + e^- + CR'$$

then

$$H_2 + H_2^+ \rightarrow H_3^+ + H$$

$$\left(\begin{array}{c} H_2^+ + e^- \rightarrow H + H \\ H_2^+ + H \rightarrow H_2 + H^+ \end{array} \right)$$

CR ionization of molecular hydrogen dominates over photoionization (E>15.4 eV)

DESTRUCTION

In diffuse clouds :

$$k_e \left\{ \begin{array}{l} H_3^+ + e^- \rightarrow H_2 + H \\ H_3^+ + e^- \rightarrow H + H + H \end{array} \right.$$

In dense clouds :

$$H_3^+ + CO \rightarrow HCO^+ + H_2$$

$$H_3^+ + CO \rightarrow HOC^+ + H_2$$

$$H_3^+ + O \rightarrow OH^+ + H_2$$

$$H_3^+ + N_2 \rightarrow HN_2^+ + H_2$$

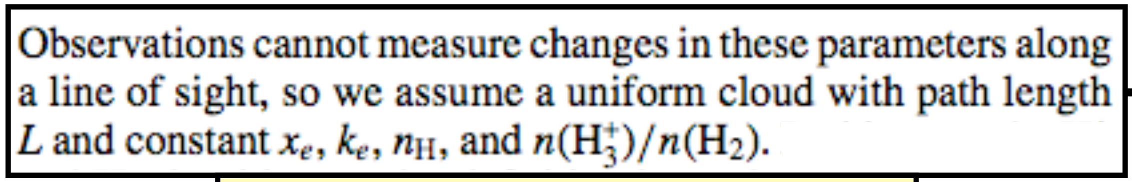
Formation of molecular ions essential to drive more complex chemistry

CR ionization rate from H_3^+ data

Equilibrium in diffuse clouds

$$\zeta_{\rm local} = k_e n(e) \frac{n(\mathrm{H}_3^+)}{n(\mathrm{H}_2)}$$

But data comes integrated on the line of sight…



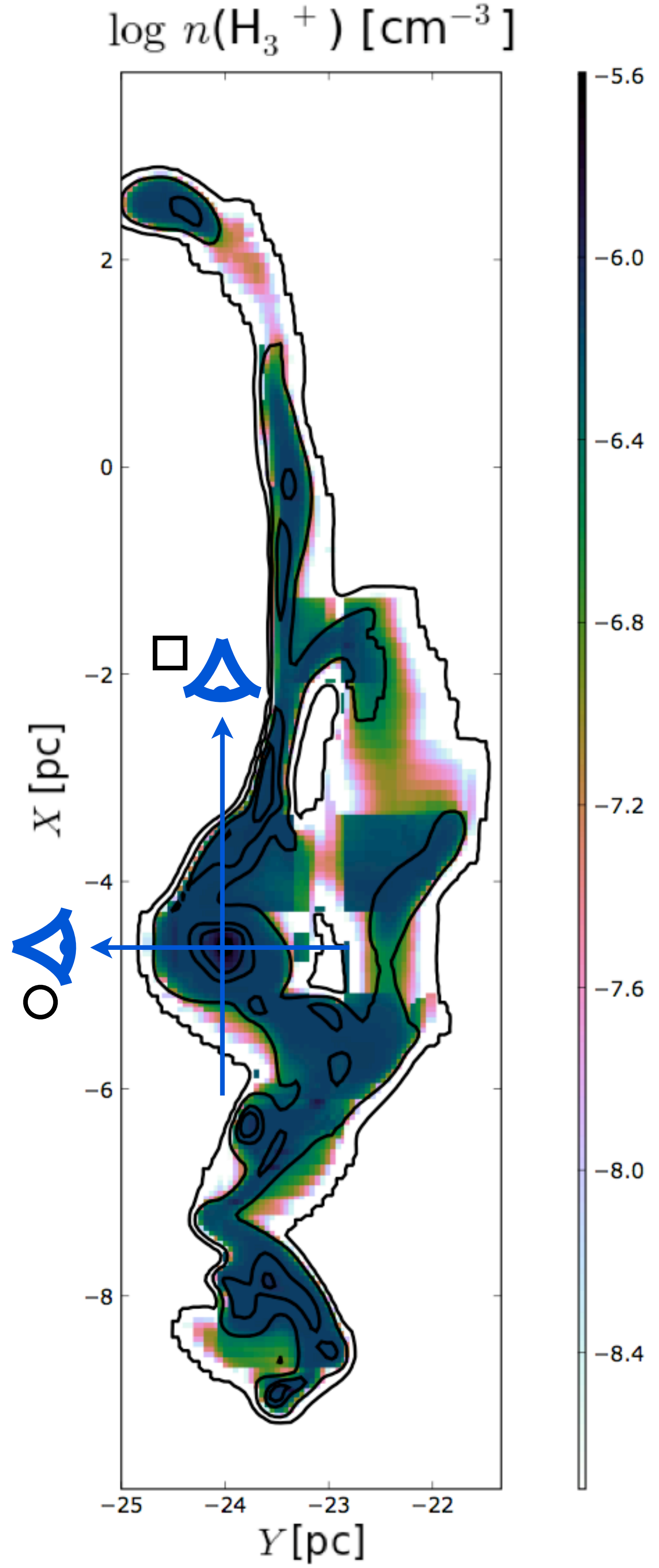
Observations cannot measure changes in these parameters along a line of sight, so we assume a uniform cloud with path length L and constant x_e, k_e, $n_{\rm H}$, and $n(\mathrm{H}_3^+)/n(\mathrm{H}_2)$.

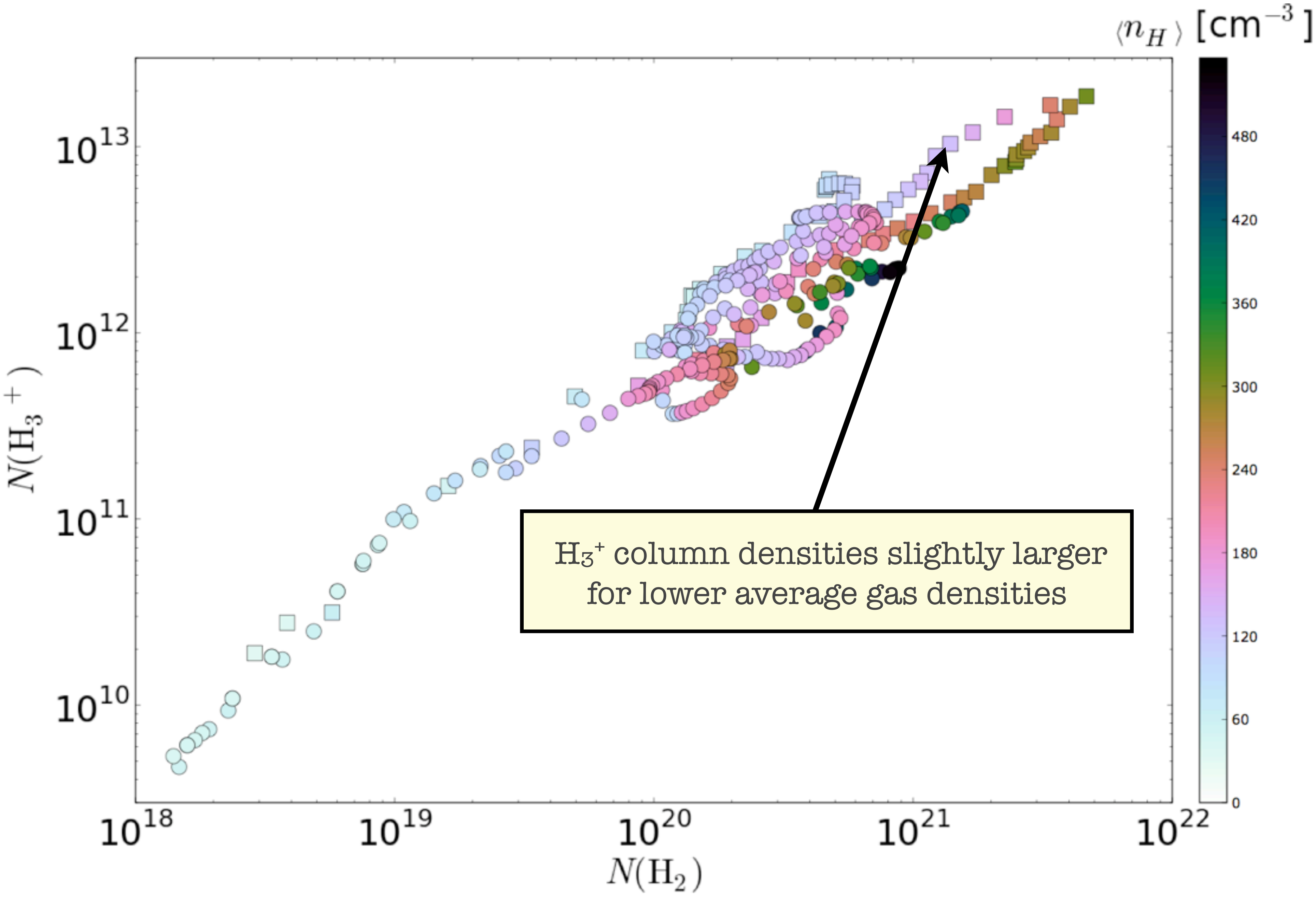
Indriolo & McCall 2012

$$\zeta_{\rm LOS} = \langle k_e \rangle \langle n(e) \rangle \frac{N(\mathrm{H}_3^+)}{N(\mathrm{H}_2)}$$

$$\boxed{\zeta_{\rm local} \overset{?}{=} \zeta_{\rm LOS}}$$

H_3^+ diagnostics





H_3^+ column densities slightly larger for lower average gas densities

Local CR ionization rate

Dissociative recombination speed constant

$$k_e = -1.3\ 10^{-8} + 1.27\ 10^{-6} T_e^{-0.48} \quad \mathrm{cm^3.s^{-1}}$$

(Indriolo & McCall 2012)

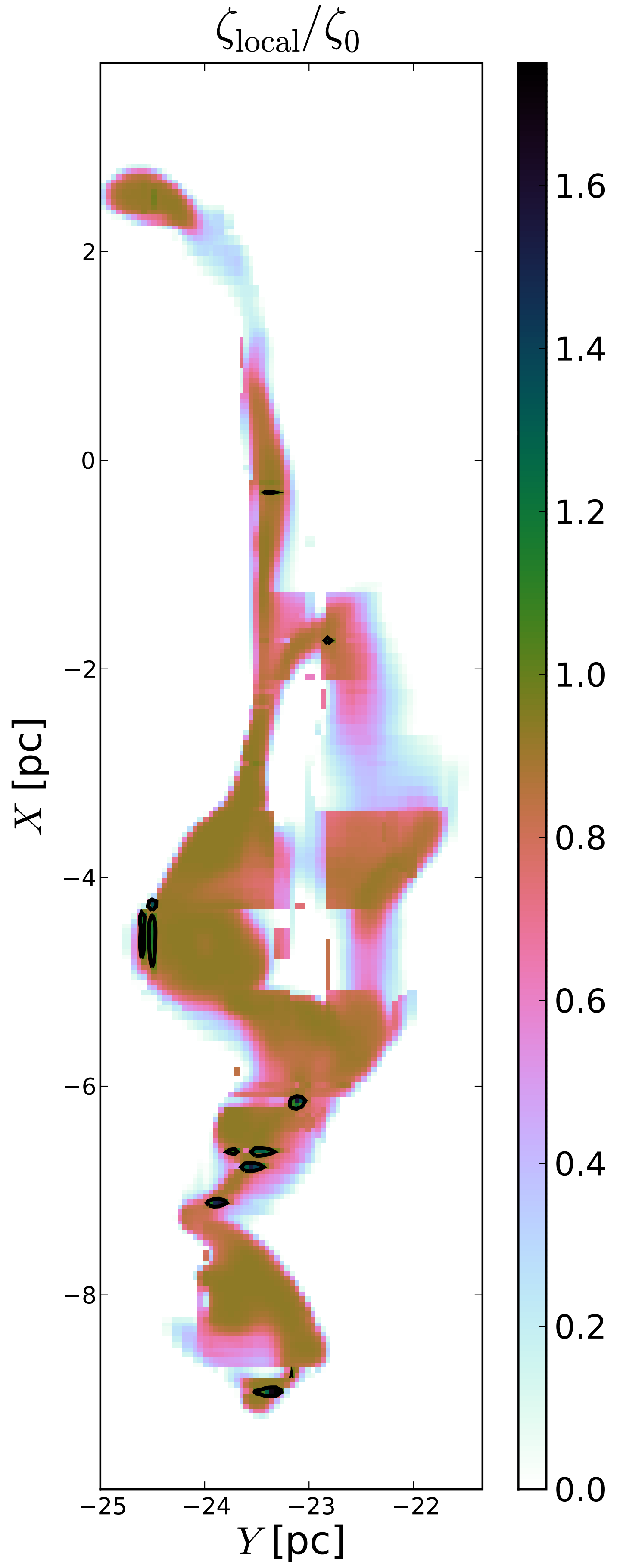
$$k_e = 6.8\ 10^{-8} \left(\frac{T_e}{300}\right)^{-0.5} \mathrm{cm^3.s^{-1}} \qquad (T_e = T)$$

(PDR code)

$$\Rightarrow \quad \zeta_{\mathrm{local}} = k_e n(e) \frac{n(\mathrm{H_3^+})}{n(\mathrm{H_2})}$$

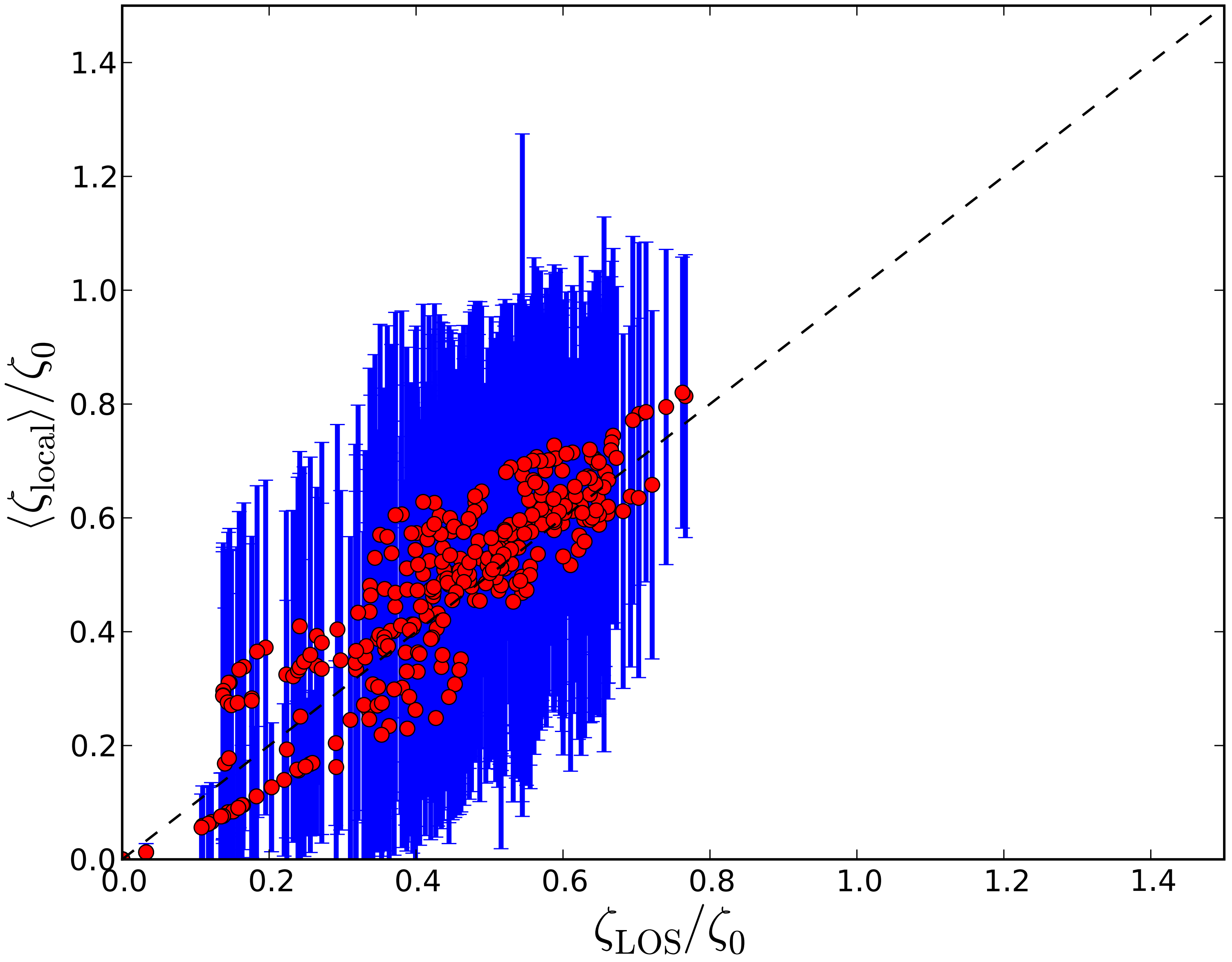
Dense : $\zeta_{\mathrm{local}}/\zeta_0 \simeq 0.8 - 1$

Diffuse : $\zeta_{\mathrm{local}}/\zeta_0 \simeq 0.2 - 0.5$



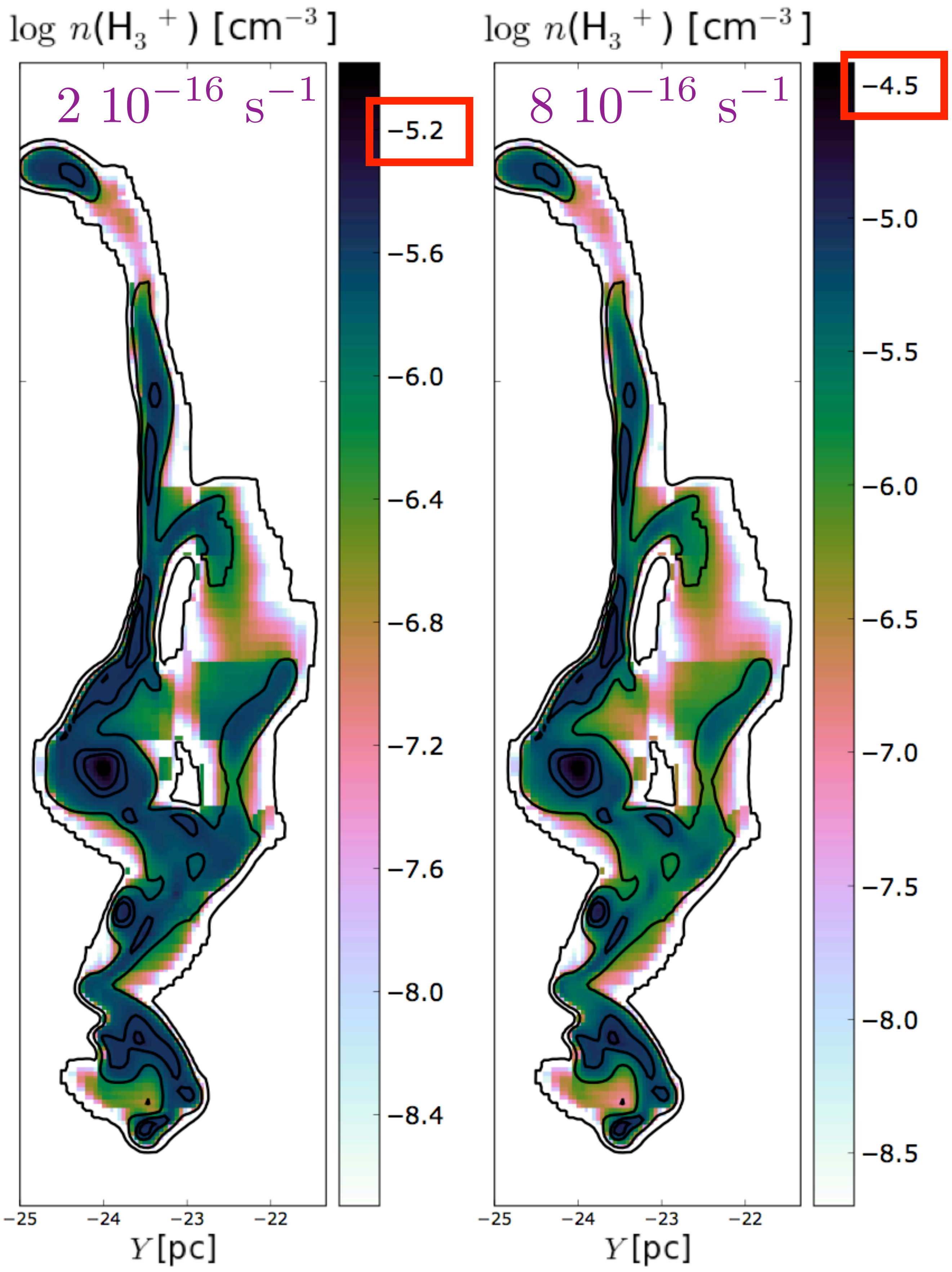
Local vs. line-of-sight CR ionization rate

On each LOS, compute mean and standard deviation of the local CR ionization rate



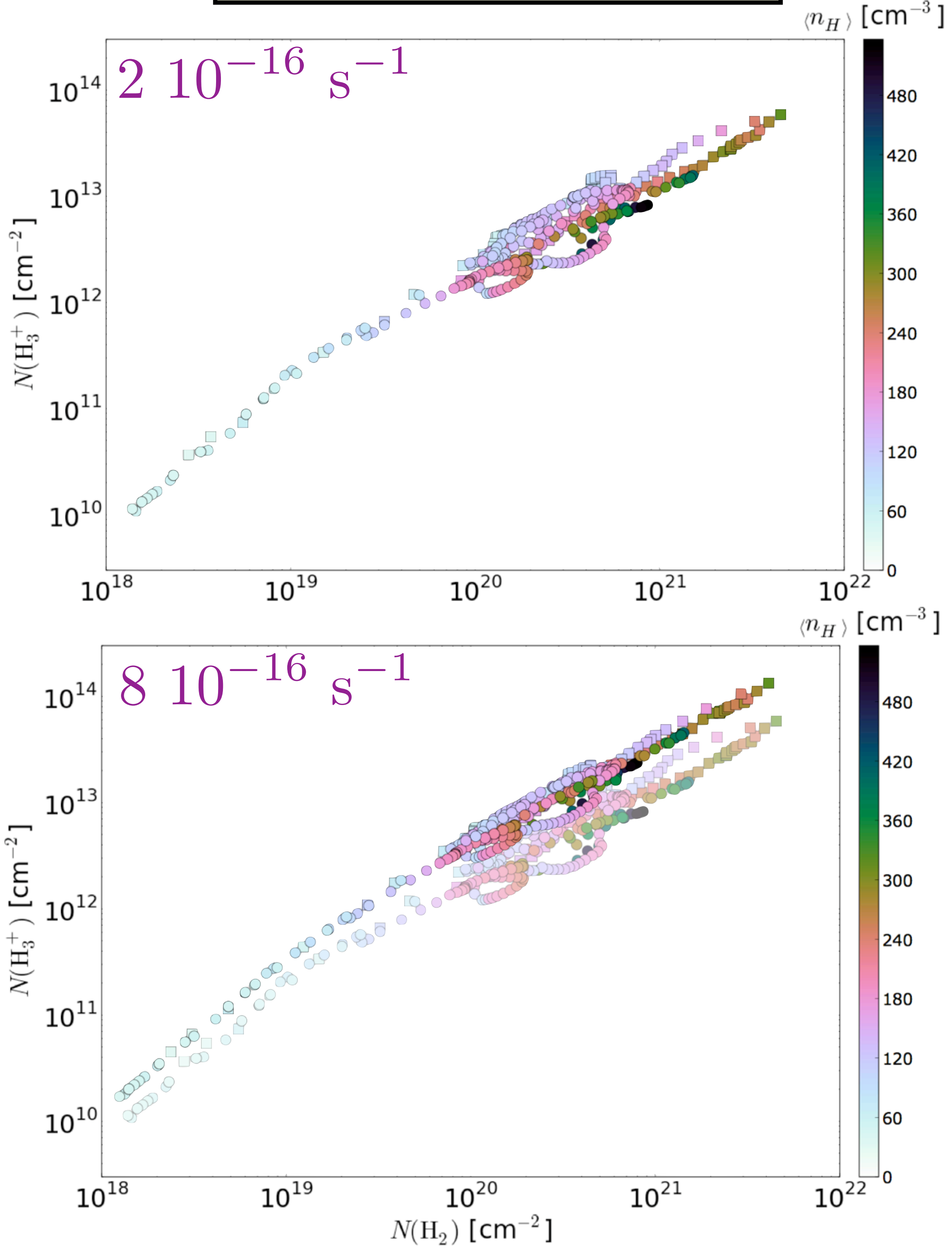
- Average local values follow the LOS integrated estimates
- Large scatter around the mean
- Systematic underestimation with respect to input CR ionization rate

Changing the input CR ionization rate



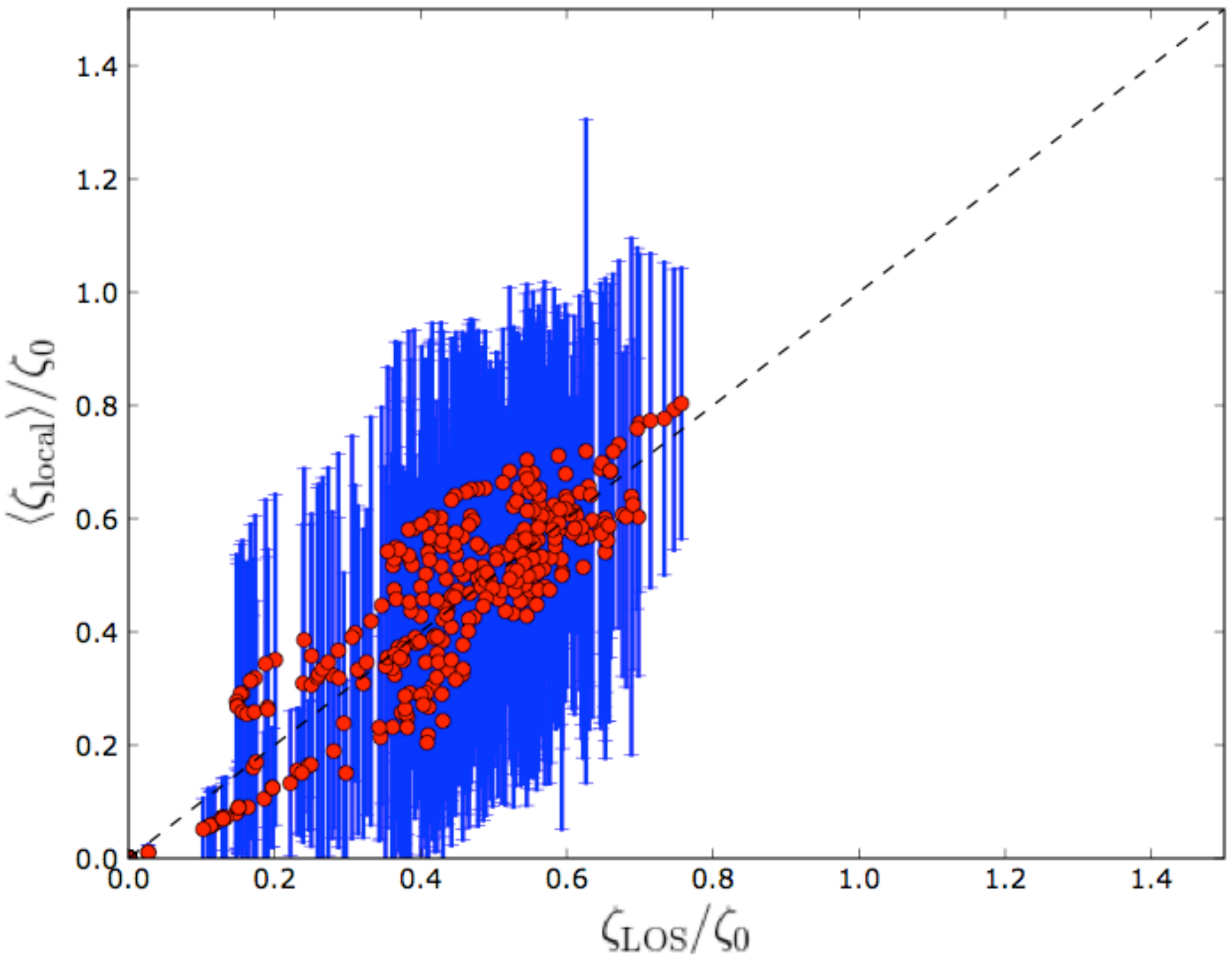
$$\zeta = 3.5^{+5.3}_{-3.0}\ 10^{-16}\ \mathrm{s}^{-1}$$

Indriolo & McCall 2012

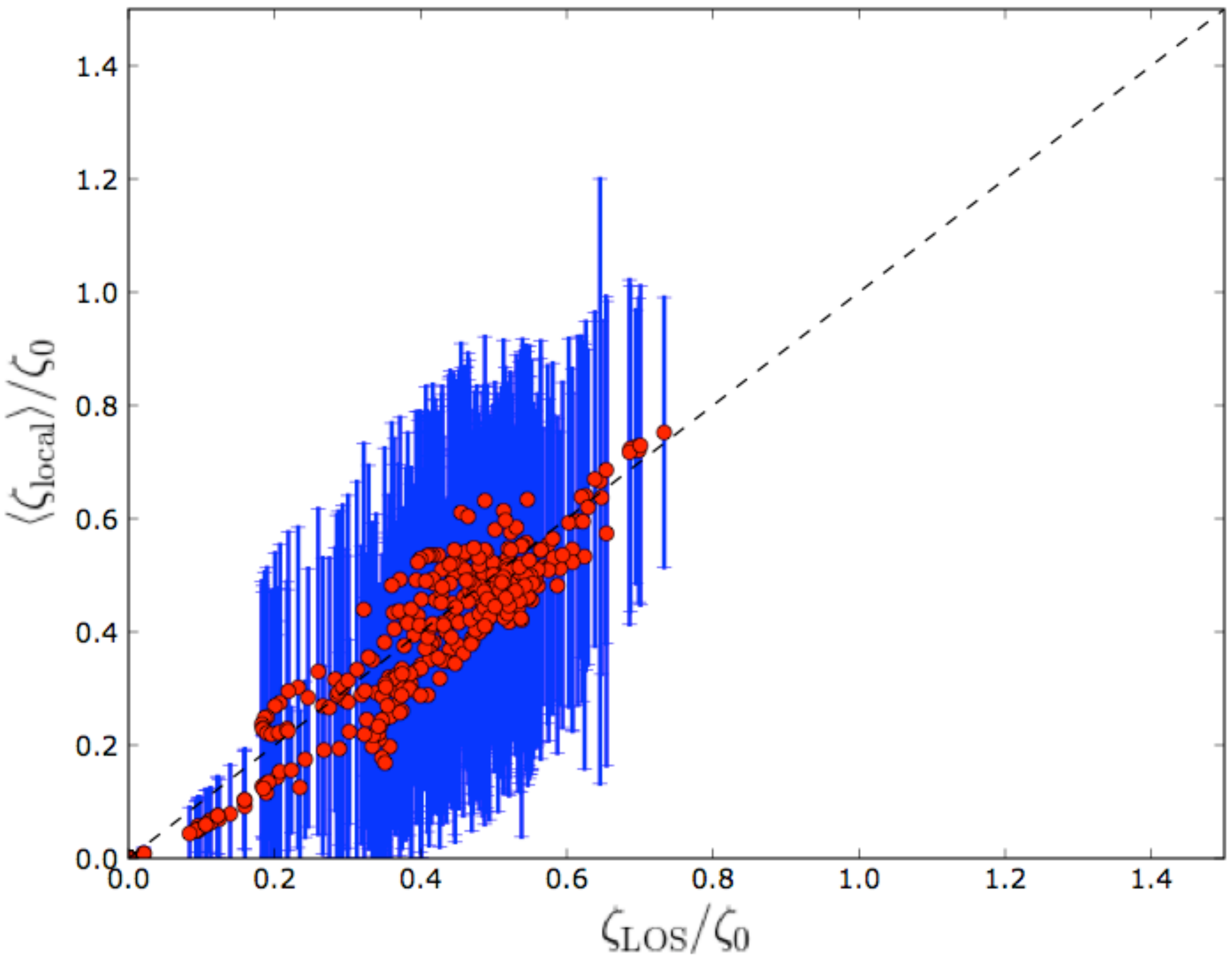


Changing the input CR ionization rate

$\zeta_0 = 2\ 10^{-16}\ \mathrm{s}^{-1}$



$\zeta_0 = 8\ 10^{-16}\ \mathrm{s}^{-1}$



- H3+ abundances globally enhanced by CR ionization rate enhancement
- Local vs. line-of-sight averaged CR ionization rate correlation remains unchanged

Summary and perspectives

- Observational column density scalings better reproduced when including density fluctuations
- "Dark neutral gas" fraction agrees with Herschel observations and independent PDR models
- LOS-integrated CR ionization rate agrees with local estimates
- Large scatter from different physical conditions : large sample required
- CR ionization rate systematically lower than input value, especially at low densities

……

- Simple chemistry for H_3^+ ideal for coupled dynamical and chemical 3D simulations (Lesaffre)
- Illumination effects : on-the-fly shadowing in RAMSES (Valdivia)
- Additional energy inputs : TDR/MHD (Godard) and shock models (Lesaffre)
- CR propagation through a fractal medium (Padovani)