Astrochemistry in Galaxies

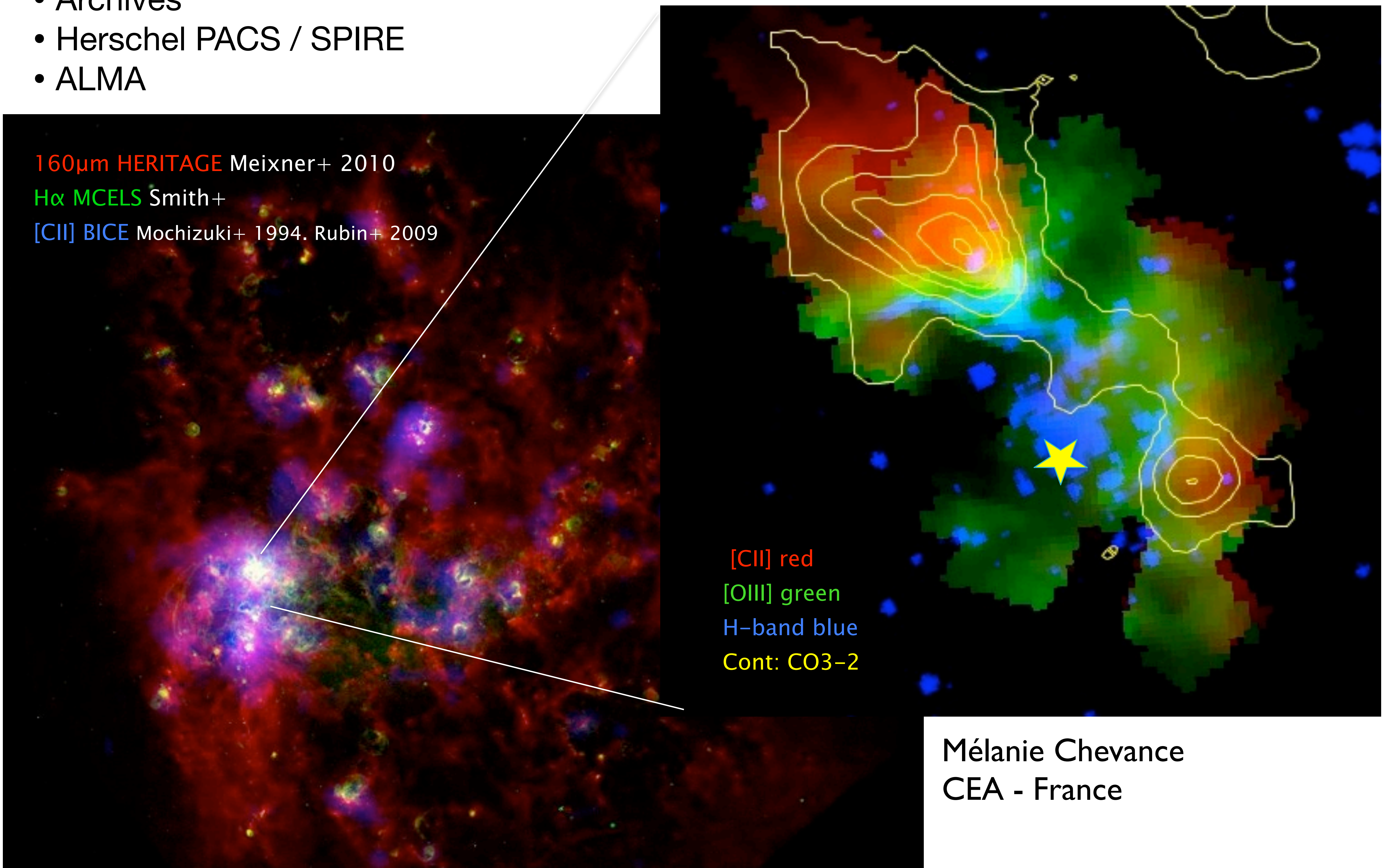
Franck Le Petit

InterOp May 2014 - ESAC

Multi-wavelength observations of ISM in Galaxies

30 Doradus

- Archives
- Herschel PACS / SPIRE
- ALMA



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CEA - France

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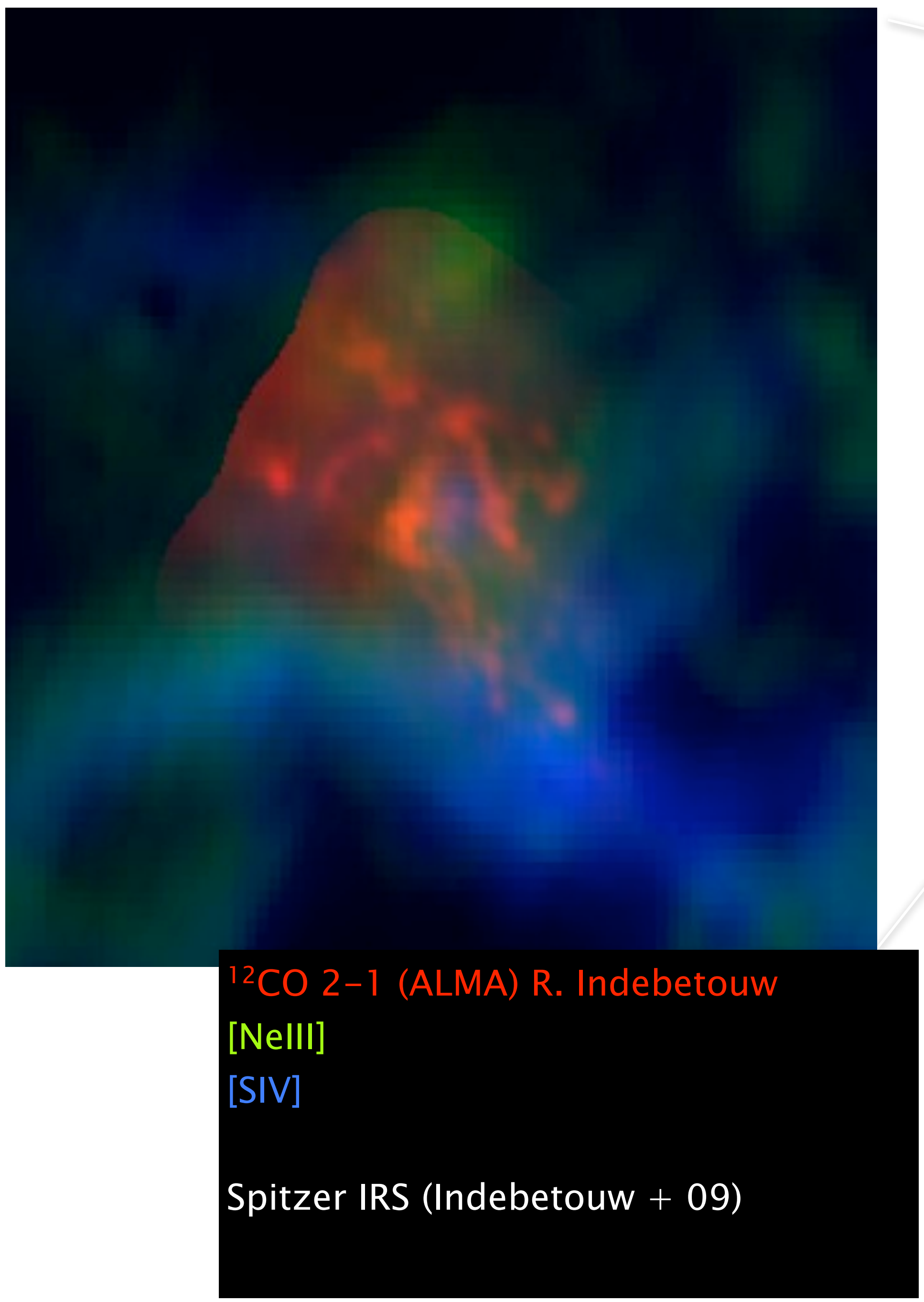

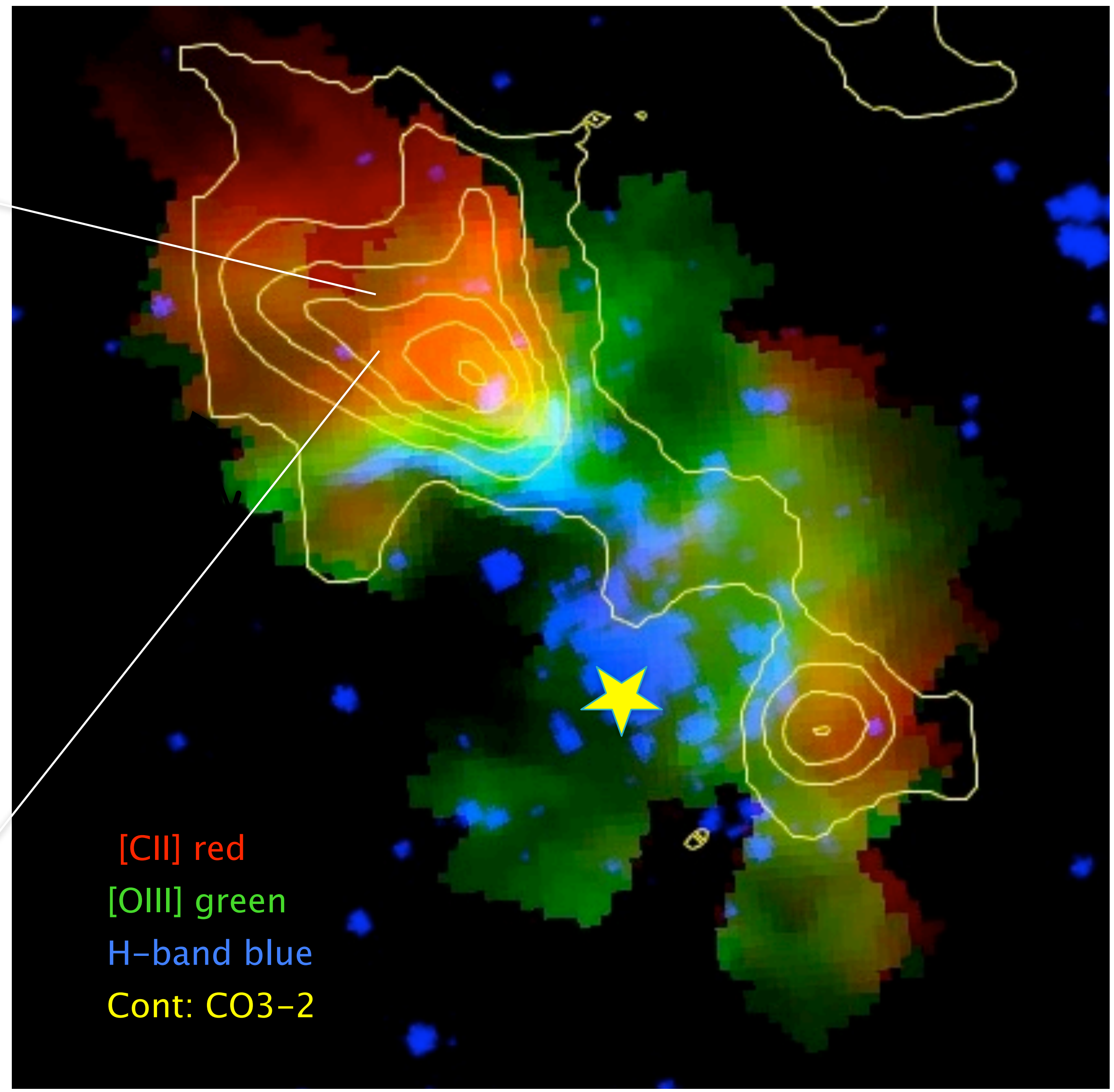

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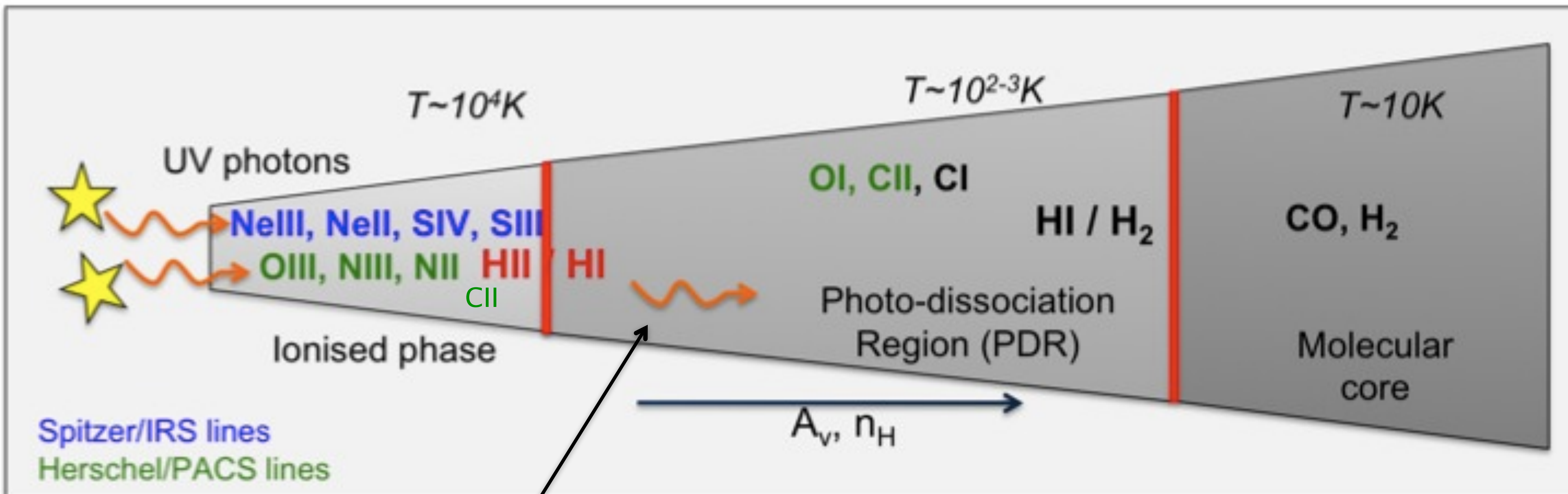
Goal of such observations :

- understand the underlying physical processes
- determine characteristics of observed media

Schema of the transition atoms / molecules



FUV photons between 6 and 13,6 eV

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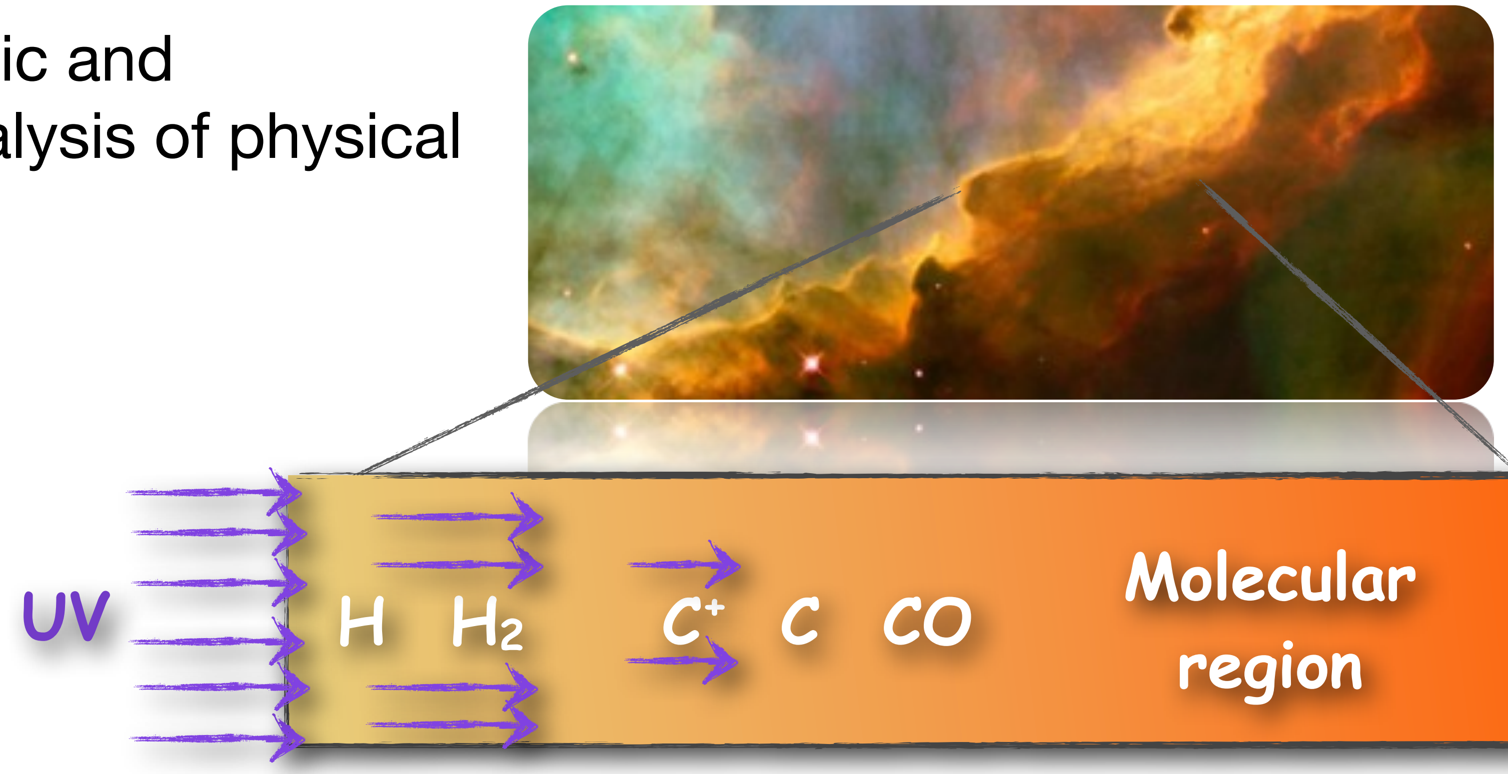
PDR modeling

Le Petit et al. (2006), Gonzalez-Garcia et al. (2008), Le Petit et al. (2009), Le Bourlot et al. (2012)

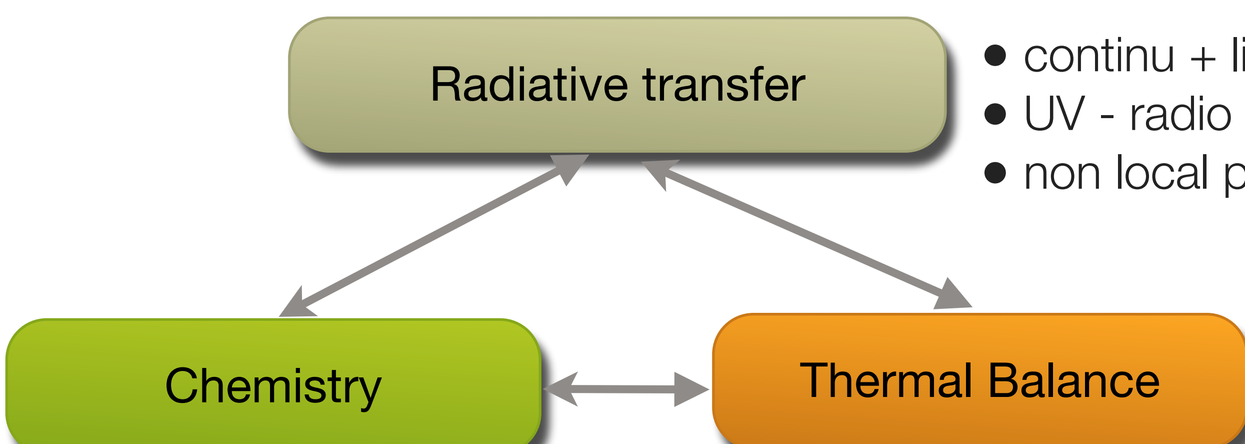
PDR Code : computation of the atomic and molecular structure of clouds and analysis of physical processes

- abundances
- excitation states
- temperatures (gas & grains)

- Intensities (H_2, CO, H_2O, ...)
- Column densities



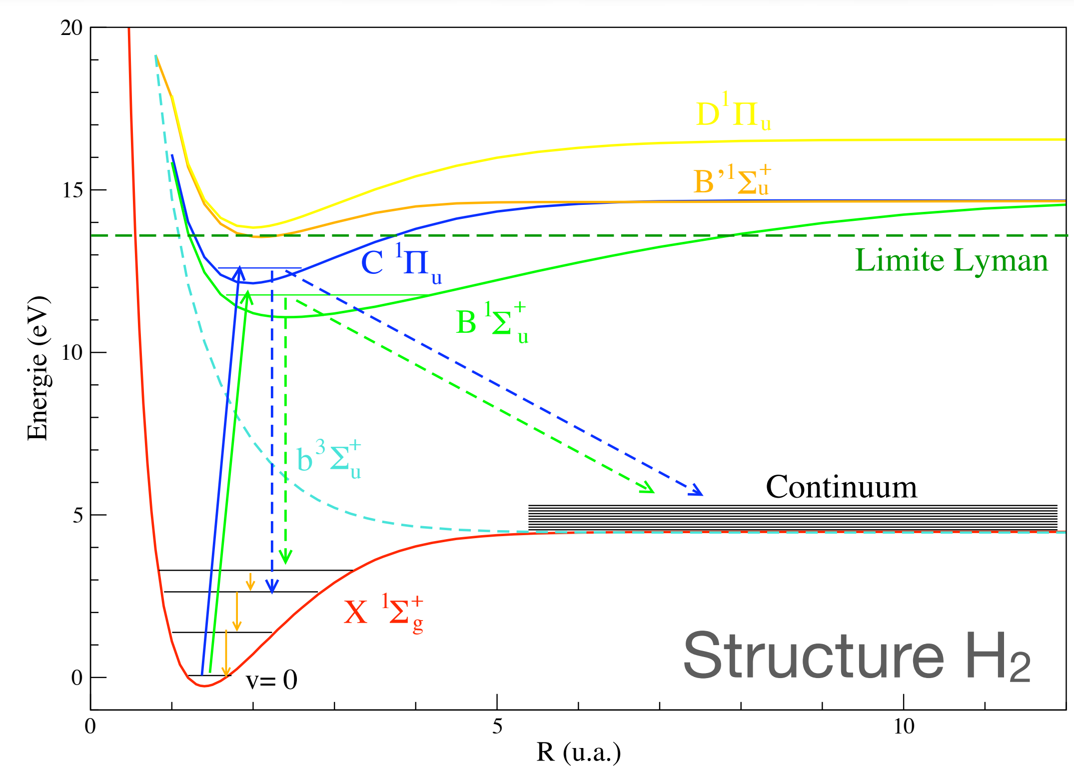
Interpretation of large instruments observations
ALMA, SOFIA, IRAM, HERSCHEL, Spitzer, VLT, HST, FUSE, ...



Radiative transfer:
- continu + lines
- UV - radio
- non local pumpings

Chemistry:
- several hundred species
- thousands reactions

Thermal Balance:
- Non LTE Detailed balance in levels
- Photo-electric effect, cosmic rays, chemistry, ...



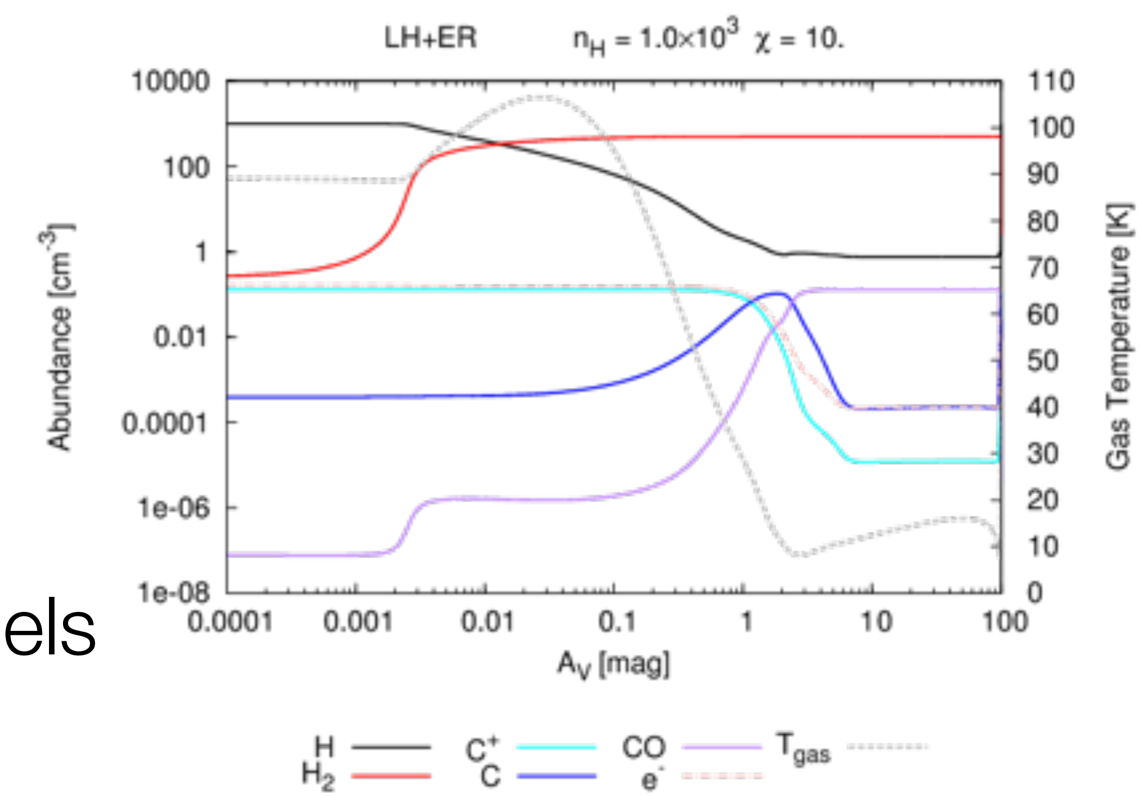
Interpretation of observations

Interpretation of line intensities & column densities requires grids of models
Exploration of :

- density of clouds
- size of clouds
- intensity of radiation field : UV and X-rays
- metallicity
- ...

1 run : 6 hours to several days CPU time
Produce various quantities :

- structure of the cloud
- thousands line intensities
- grains temperature and emission
- spectra



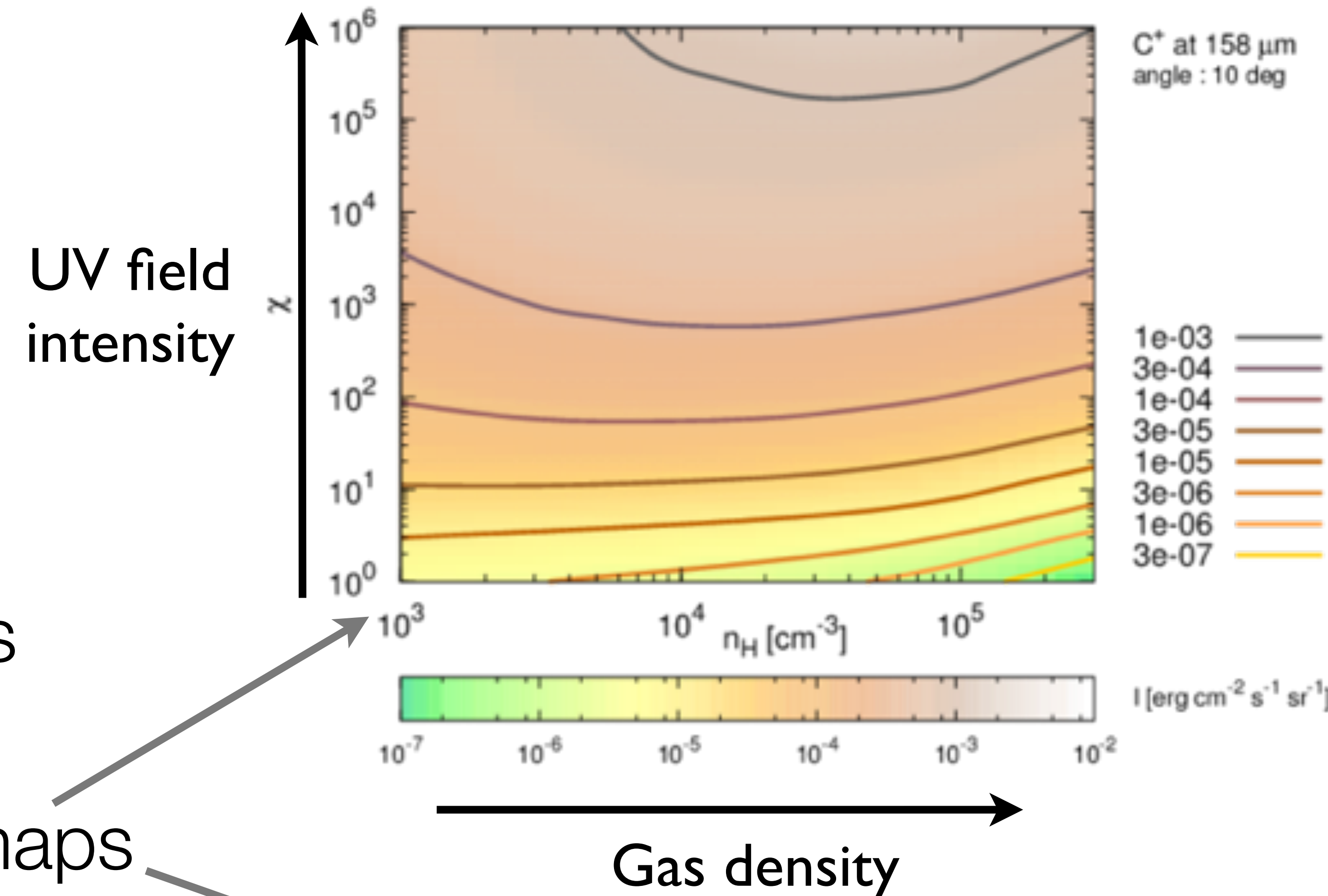
Interpretation requires up to thousands models
➜ weeks or months of work !

How to reduce this work to a few minutes ?

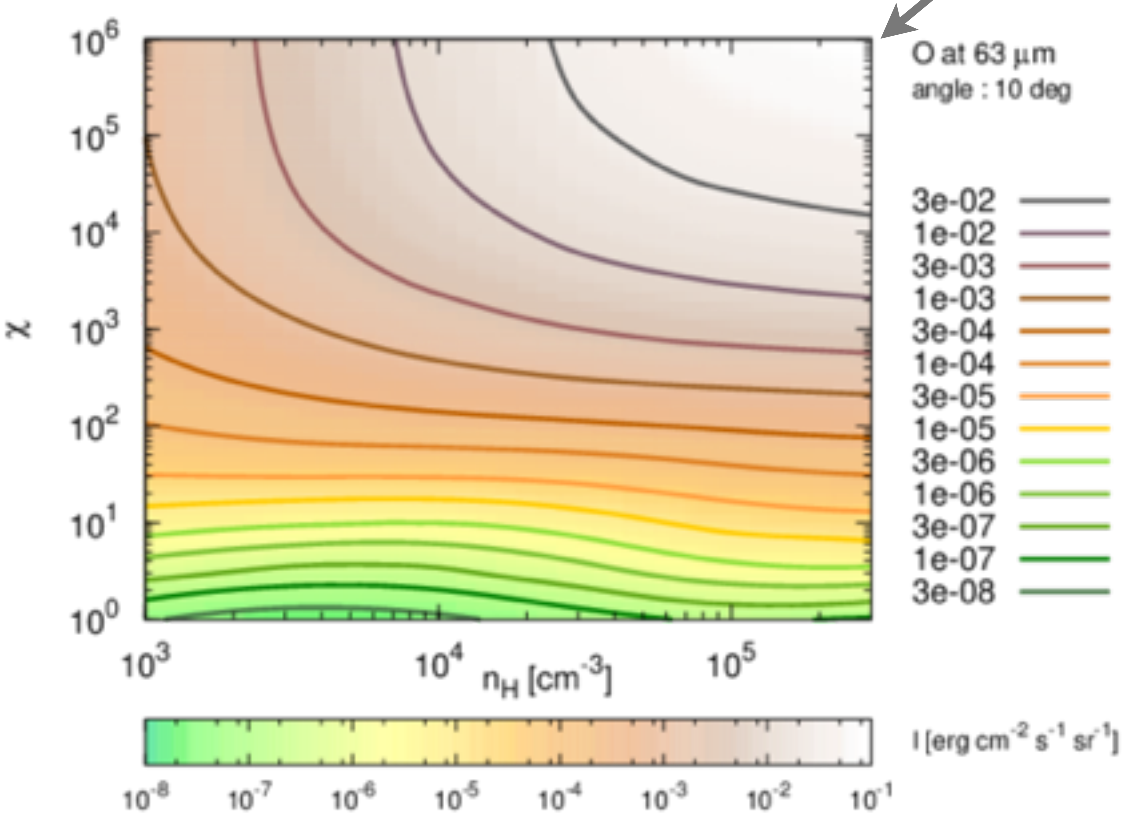
Interpretation of observations : grids of models

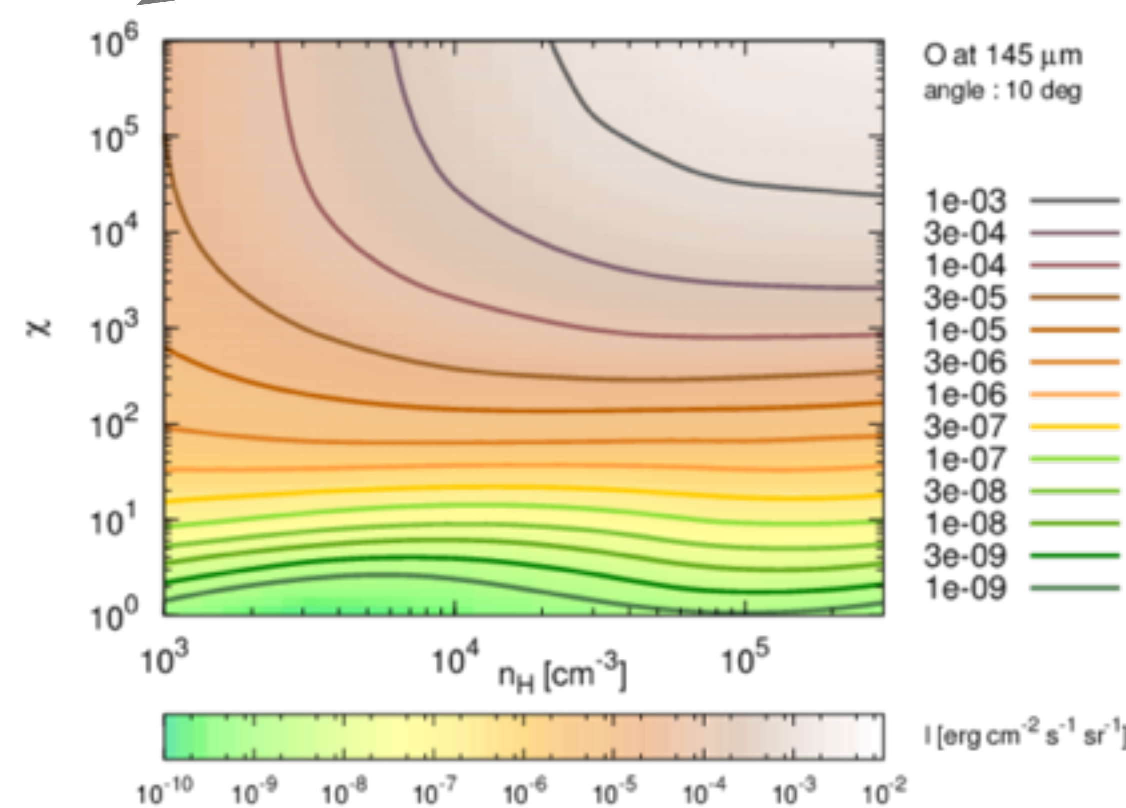
With grids of models, providing line intensities, it is possible to constrain properties of clouds

Publication of grids of models with advanced data mining tools



Line intensities maps



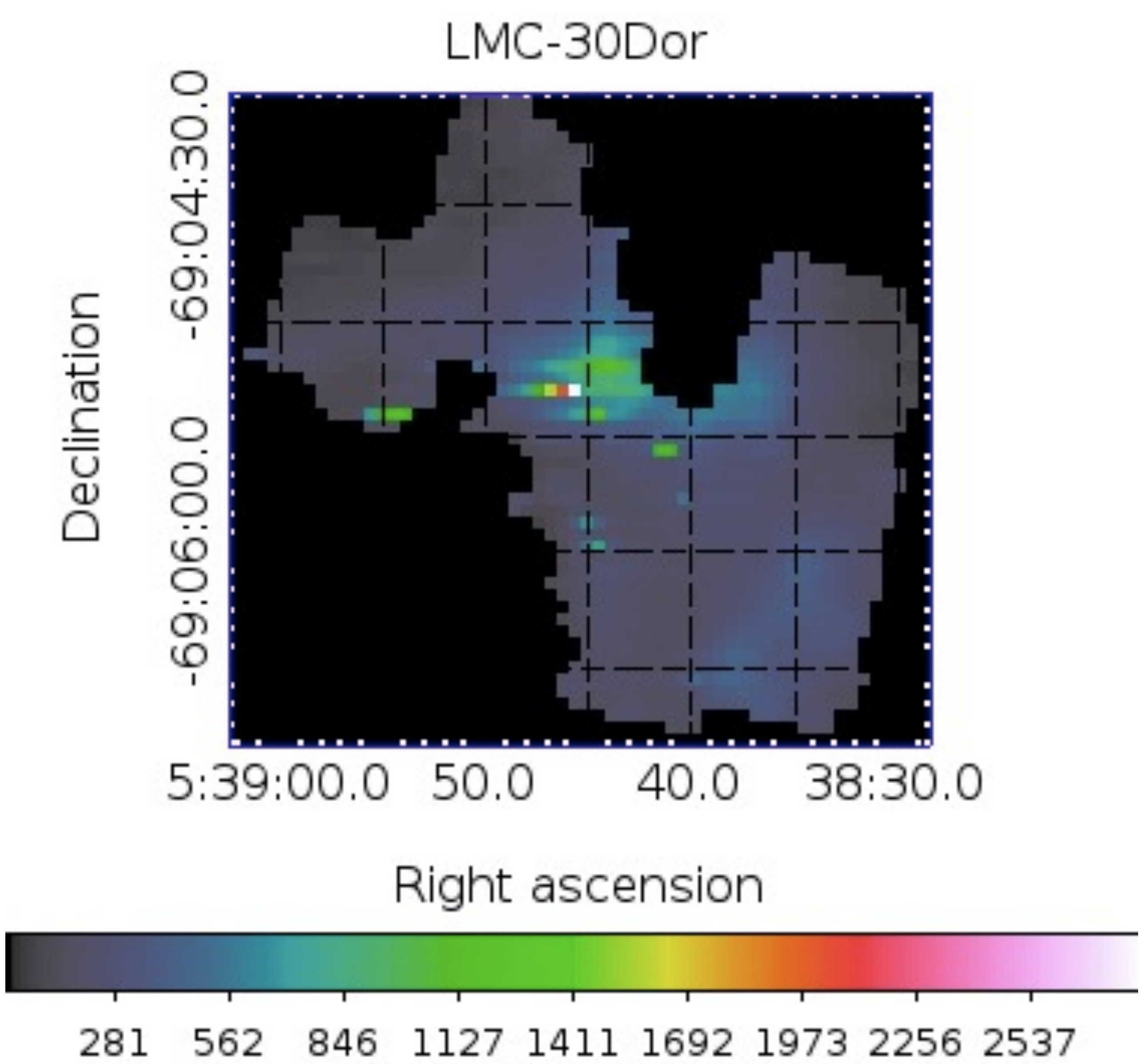


Application to 30 Doradus

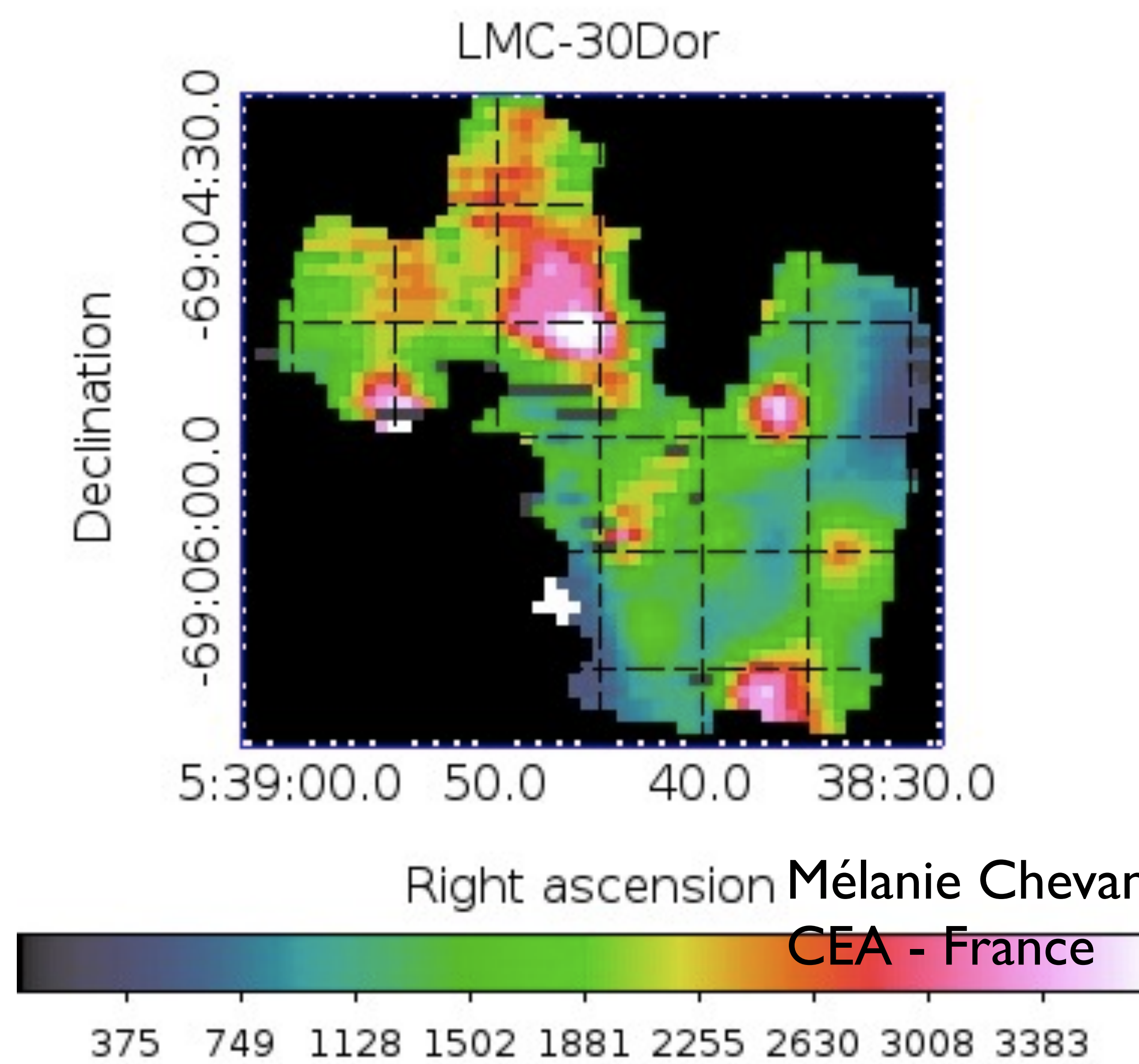
Result of the inversion

- compare observations with line intensities predictions
- chi2 at each pixel using all lines observed
- deduce UV field and gas density

UV Field intensity



Gas density



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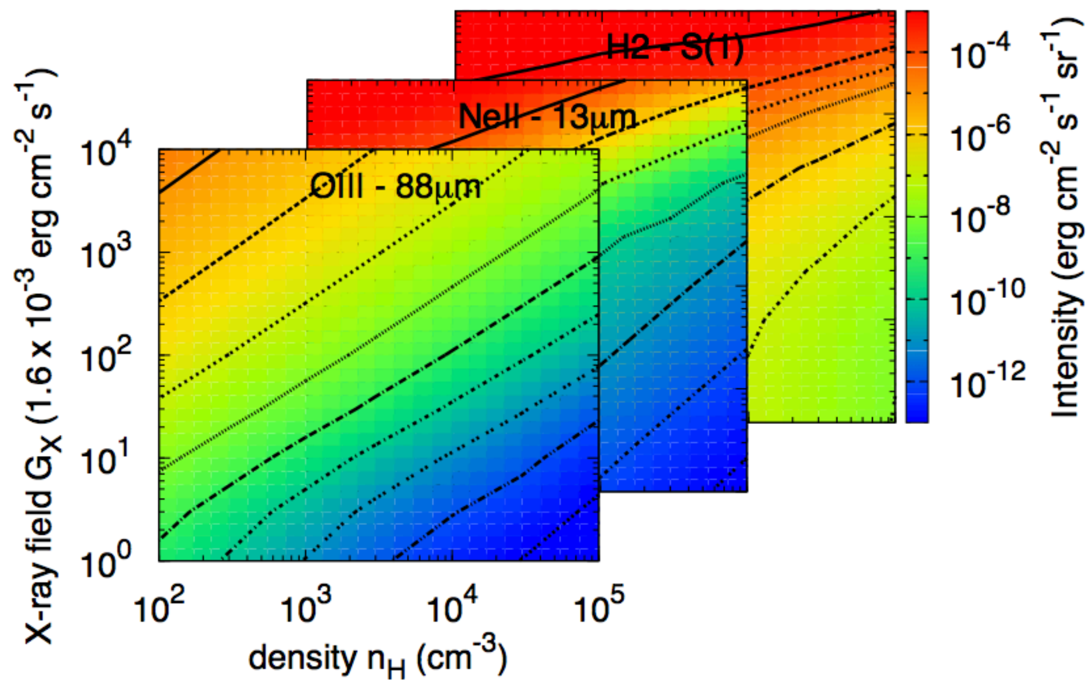
Theory service to interpret observations

1. Run large number of models
2. Characterise models with line intensities
3. Store them in a database
4. Develop a service to browse in the data



Challenges :

Very large number of metadata : +150 000

Large number of models : several thousands

➜ How to manage a so large number of metadata ?

- Data base challenge (performance)
- Size of the metadata description in the communication client / server
- UI : - cannot have 150 000 buttons
  - users cannot learn a 150 000 quantities vocabulary

SimDAL prototype

- Google Bar interface

- Simple multiple queries :

$$2.4\ 10^{20} < N(H2) < 4.4\ 10^{20}\ cm^{-2}$$

and

$$3.0\ 10^{14} < N(C) < 5\ 10^{14}\ cm^{-2}$$

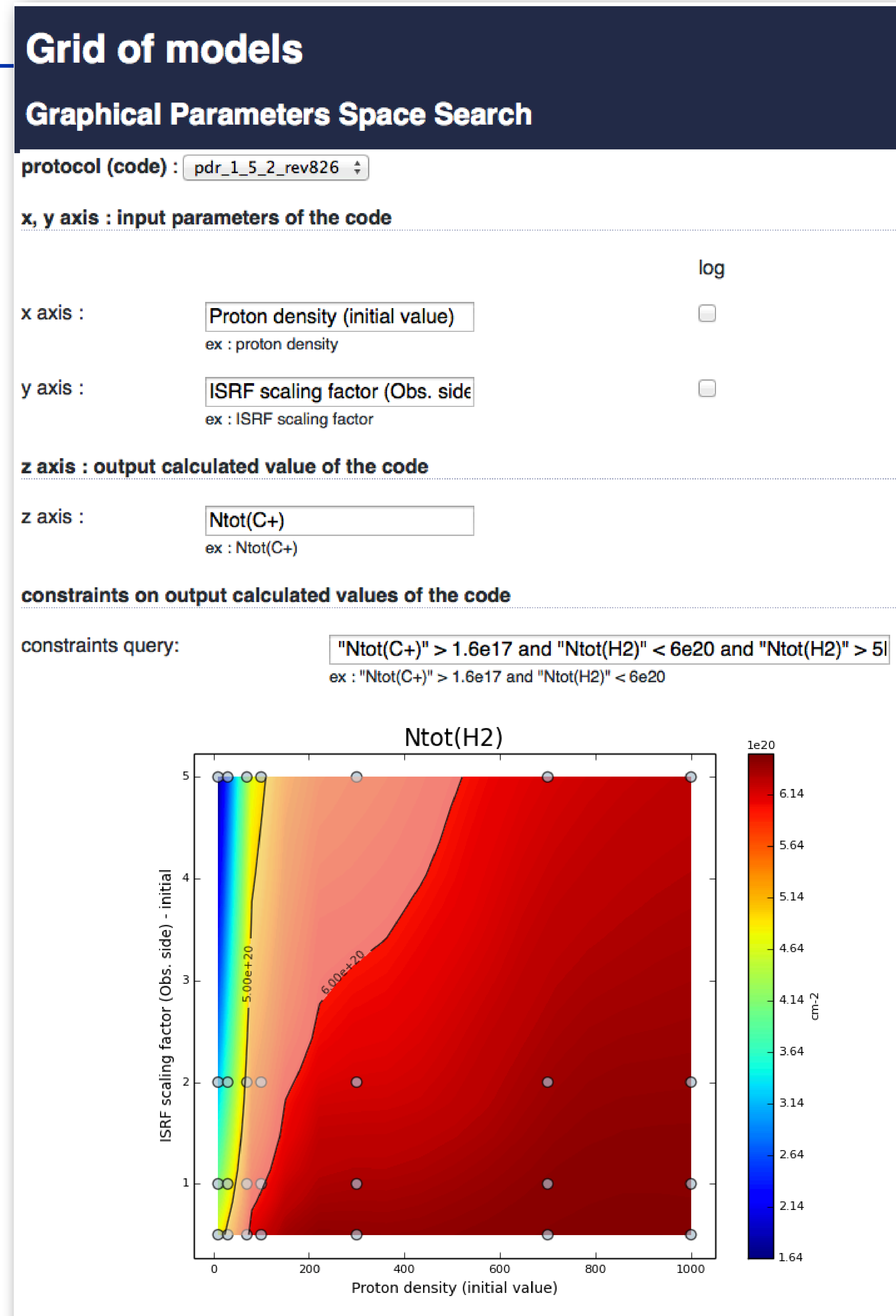
and

$$N(CO) < 1.0\ 10^{14}\ cm^{-2}$$

and

$$2.0\ 10^{-6} < I(C+,\ 158\ \mu m) < 4\ 10^{-6}\ erg\ s^{-1}\ cm^{-2}\ sr^{-1}$$

- Fast answers



Example of applications : HD 102065

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Astronomy & Astrophysics

Modeling of diffuse molecular gas applied to HD 102065 observations

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ABSTRACT

Aims. We model a diffuse molecular cloud present along the line of sight to the star HD 102065. We compare our modeling with observations to test our understanding of physical conditions and chemistry in diffuse molecular clouds.

Methods. We analyze an extensive set of spectroscopic observations which characterize the diffuse molecular cloud observed toward HD 102065. Absorption observations provide the extinction curve, H_2, C I, CO, CH, and CH^+ column densities and excitation. These data are complemented by observations of C^+, CO and dust emission. Physical conditions are determined using the Meudon PDR model of UV illuminated gas.

Results. We find that all observational results, except column densities of CH, CH^+ and H_2 in its excited ($J \geq 2$) levels, are consistent with a cloud model implying a Galactic radiation field ($G \sim 0.4$ in Draine's unit), a density of 80 cm^{-3} and a temperature (60–80 K) set by the equilibrium between heating and cooling processes. To account for excited ($J \geq 2$) H_2 levels column densities, an additional component of warm (~250 K) and dense ($n_H \geq 10^4$ cm^{-3}) gas within 0.03 pc of the star would be required. This solution reproduces the observations only if the ortho-to-para H_2 ratio at formation is ~1. In view of the extreme physical conditions and the unsupported requirement on the ortho-to-para ratio, we conclude that H_2 excitation is most likely to be accounted for by the presence of warm molecular gas within the diffuse cloud heated by the local dissipation of turbulent kinetic energy. This warm H_2 is required to account for the CH^+ column density. It could also contribute to the CH abundance and explain the inhomogeneity of the CO abundance indicated by the comparison of absorption and emission spectra.

Key words. astrochemistry – ISM: clouds – ISM: molecules – ISM: structure – ISM: individual objects: Chamaeleon clouds – stars: individual: HD 102065

1. Introduction

Since the pioneering work of Black & Dalgarno (1977), observations of diffuse molecular clouds continue to motivate and challenge efforts to model the thermal balance and chemistry of interstellar gas illuminated by UV photons. Models allow observers to determine physical conditions from their data and observations contribute to models by quantifying physical processes of general relevance to studies of matter in space such as H_2 formation, photo-electric heating, and cosmic ray ionization.

Many models of well characterized lines of sight have been presented (e.g. in the last years: Zsargó & Federman 2003; Le Petit et al. 2004; Shaw et al. 2006). They are successful in reproducing many observables apart from some molecular abundances, most conspicuously CH^+, which points to out-of-equilibrium chemistry. This molecular ion, and several of the molecular species commonly observed in diffuse molecular clouds such as CH, OH and HCO^+ may be produced by MHD shocks (Draine & Katz 1986; Pineau des Forêts et al. 1986; Flower & Pineau des Forêts 1998), and small scale vortices (Joulain et al. 1998; Falgarone et al. 2006) where H_2 is heated by the localized dissipation of the gas turbulent kinetic energy. Turbulent transport between the cold and warm neutral medium may also significantly impact the chemistry of diffuse clouds (Lesaffre et al. 2007).

Independently of gas chemistry, the presence of H_2 at higher temperatures than that set by UV and cosmic-rays heating of diffuse molecular clouds, may be probed through observations of the H_2 level populations (Cecchi-Pestellini et al. 2006). A correlation between CH^+ and rotationally excited H_2 was found by Lambert & Danks (1986) using Copernicus observations. Falgarone et al. (2005) reported the detection of the S(0) to S(3) H_2 lines in a line of sight towards the inner Galaxy away from star forming regions. They interpret their observation as evidence for traces of warm molecular gas in the diffuse interstellar medium. But the interpretation of the wealth of H_2 observations provided by the FUSE satellite is still a matter of debate. Gry et al. (2002) modeled FUSE H_2 observations of three stars in Chamaeleon using the Meudon Photon Dominated Regions (PDR) model (Le Bourlot et al. 1993). They show that the model cannot account for H_2 column densities in rotational states with $J > 2$. A larger sample of H_2 FUSE observations (Tumlinson et al. 2002; Gillmon et al. 2005; Wakker 2006), including 2 of the 3 Chamaeleon lines of sight of Gry et al. (2002), have been analyzed on the basis of model calculations presented by Browning et al. (2003). Their model, like other PDR models, takes into

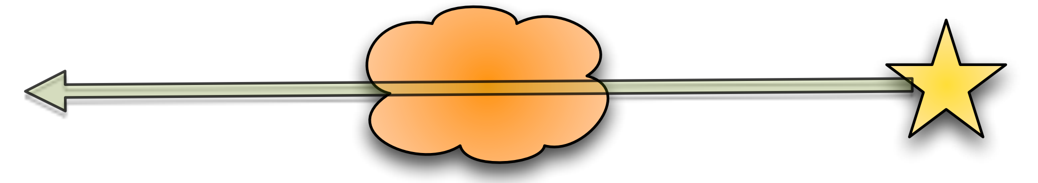


Table 1. Observational constraints and best model results. Upper part are constraints used in Fig. 2, lower part compares unconstrained observations and results. Number in parentheses are powers of 10.

	X^{mod}	X^{obs}	σ_{obs}
$N(CO)/N(H_2)$	1.5 (−7)	1.6 (−7)	$\pm^{0.2(-7)}_{0.15(-7)}$
$N(C\,I)/N_H$	5.8 (−7)	6.0 (−7)	±1.5 (−7)
$N(C\,I^*_{J=1})/N(C\,I)$	0.17	0.16	±0.07
$N(C\,I^{**}_{J=2})/N(C\,I)$	0.03	0.024	±0.01
$f_{H_2} = \frac{2N(H_2)}{N(H)+2N(H_2)}$	0.9	0.69	±0.12
$N(H_2^o)/N(H_2^p)$	0.73	0.7	±0.12
$I(C^+)$ (erg/s cm^2 sr)	2.0 (−6)	2.8 (−6)	±0.85 (−6)
$N(CH)/N(H_2)$	8.4 (−9)	1.85 (−8)	±0.3 (−8)
$N(CN)/N(H_2)$	1.2 (−10)	<1.5 (−9)	
$N(C_2)/N(H_2)$	3.6 (−8)	<3.5 (−8)	
$N(CO_{J=0})/N(H_2)$	9.0 (−8)	9.6 (−8)	$\pm^{1.4(-8)}_{1.7(-8)}$
$N(CO_{J=1})/N(H_2)$	5.1 (−8)	6.2 (−8)	$\pm^{1.5(-8)}_{1.2(-8)}$
$N(CO_{J=2})/N(H_2)$	3.7 (−9)	<7.3 (−9)	

Quantités observées :

- Densité de colonne de H_2, C, CO
- Populations états quantiques de H_2
- Intensité de C^+ à 158 μm

Example of applications : HD 102065

Grid of models using the PDR code version 1.5.2 rev814

date of the runs : 2012-12-24

PDR 1.5.2 is the version of the PDR code released in 2013. In this version, Langmuir-Hinshelwood and Eley-Rideal mechanisms are implemented for H_2 formation on grains. Several atomic and molecular data have been updated (collision rates of O, photo-reactions cross sections, ...). The chemical network has also been updated from different references. Level excitation and line intensities of CH^+ and OH have been introduced for comparison to observations.
See Le Bourlot et al. (2011) for more informations.

protocol (code) : pdr_1_5_2_rev826

x, y axis : input parameters of the code

log

x axis : Proton density (initial value) ☑
ex : proton density

y axis : ISRF scaling factor (Obs. side ☑
ex : ISRF scaling factor

z axis : output calculated value of the code

z axis : Ntot(H2)
ex : Ntot(C+)

constraints on output calculated values of the code

constraints query: "Ntot(H2) " > 2.4E20 and "Ntot(H2) " < 4.4E
ex : "Ntot(C+)" > 1.6e17 and "Ntot(H2)" < 6e20

Query :

```
    "N(H2)"    > 2.4E20 and "N(H2)"    < 4.4E20
and "Ntot(C)"  > 3.0E14 and "Ntot(C) " < 5.0E14
and "Ntot(CO)" < 1.0E14
and "C+ 158 microns" > 2.0E-6
and "C+ 158 microns" < 3.6E-6
```

Constraints on:

- Column densities of H_2, C, CO
- Line intensity of C^+

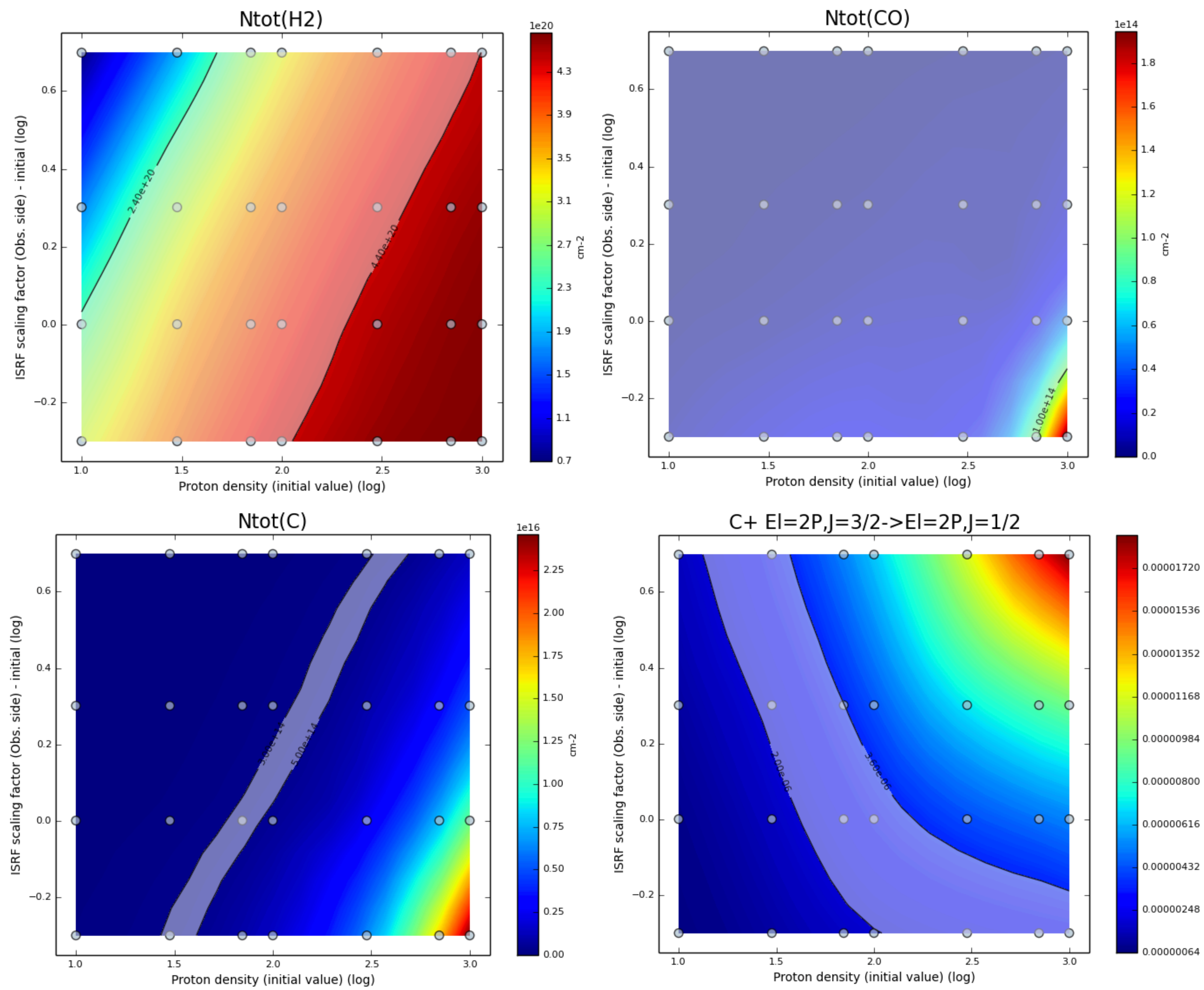
Example of applications : HD 102065

Results:
Visualization in the space parameters of matching models

constraints on output calculated values of the code

constraints query: "Ntot(H2) " > 2.4E20 and "Ntot(H2) " < 4.4E

ex : "Ntot(C+)" > 1.6e17 and "Ntot(H2)" < 6e20



Services:

- Download of models
- Extraction of data
- Visualization of other quantities

Example of applications : HD 102065

simdal api client | Home | About | Contact

Simdal (SimDB) search interface

cd_tot_h2 < 4.4E20 and cd_tot_h2 > 2.5E20 and cd_tot_c > 3E14 and cd_tot_c < 5E

matching objects

*protocol:***[pdr_1_5_2_rev814]**
experiment: tdiff_n3e1r5m1r5m1z1e1a5m1_20_20121223111158

*protocol:***[pdr_1_5_2_rev814]**
experiment: tdiff_n3e1r5m1r5m1z5a5m1_20_20121220113124

*protocol:***[pdr_1_5_2_rev814]**
experiment: tdiff_n7e1r1r1z1e1a5m1_20_20121223112439

*protocol:***[pdr_1_5_2_rev814]**
experiment: tdiff_n7e1r1r1z5a5m1_20_20121223112931

Cutout

matching objects

*protocol:***[pdr_1_5_2_rev814]**
experiment: tdiff_n1e1r5m1r5m1z1e1a7m1_20_20121223102
cumulated error: 11.445 %

cd_tot_h2 3
cd_tot_c 10.21

*protocol:***[pdr_1_5_2_rev814]**
experiment: tdiff_n1e2r1r1z1e1a5m1_20_201212201026
cumulated error: 23.226 %

cd_tot_h2
cd_tot_c -23.23

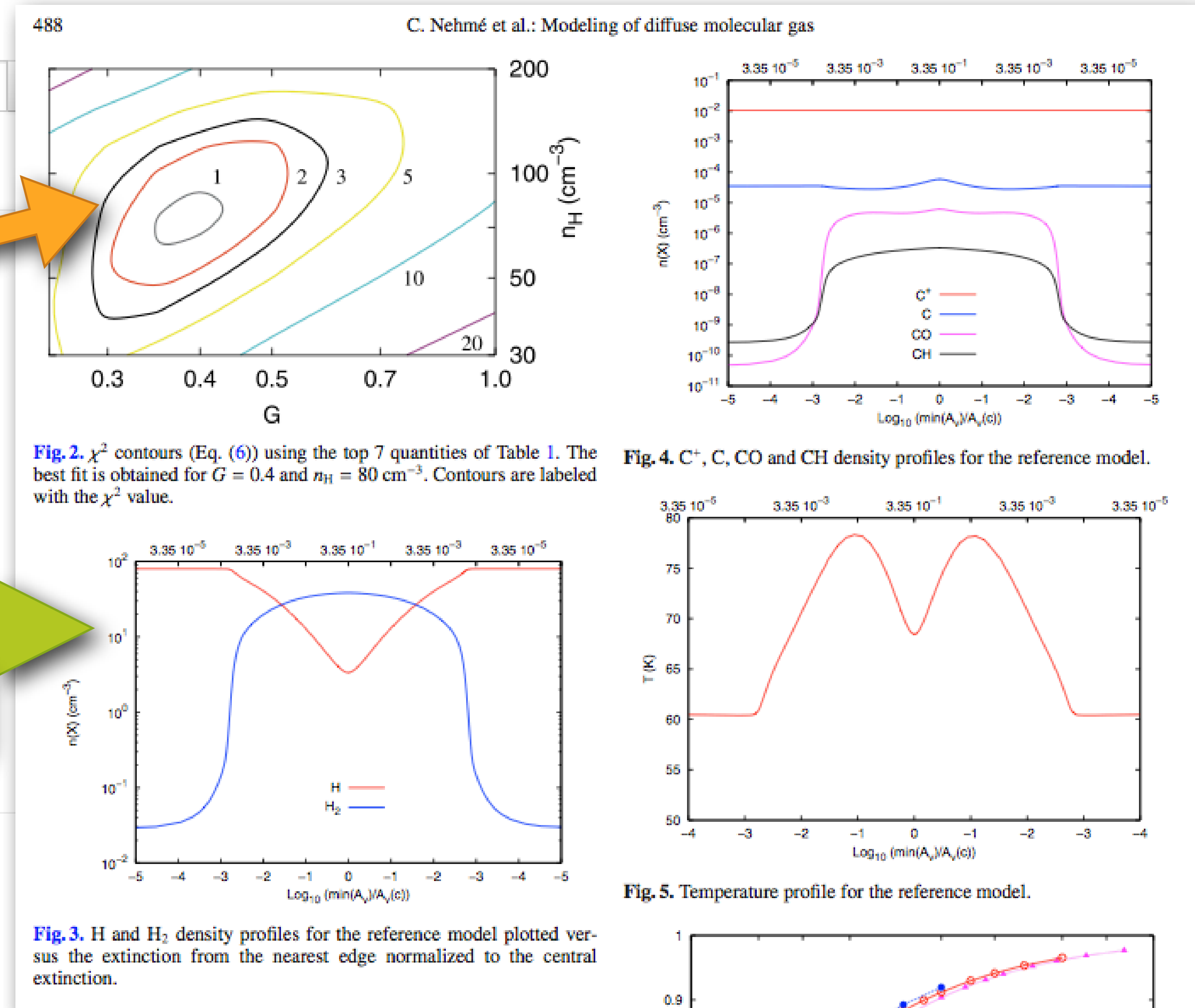


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Fig. 2. χ^2 contours (Eq. (6)) using the top 7 quantities of Table 1. The best fit is obtained for $G = 0.4$ and $n_H = 80$ cm^{-3}. Contours are labeled with the χ^2 value.

Fig. 4. C^+, C, CO and CH density profiles for the reference model.

Fig. 3. H and H_2 density profiles for the reference model plotted versus the extinction from the nearest edge normalized to the central extinction.

Fig. 5. Temperature profile for the reference model.

Within a few minutes we get the results of the paper.

Why do we need interoperability ?

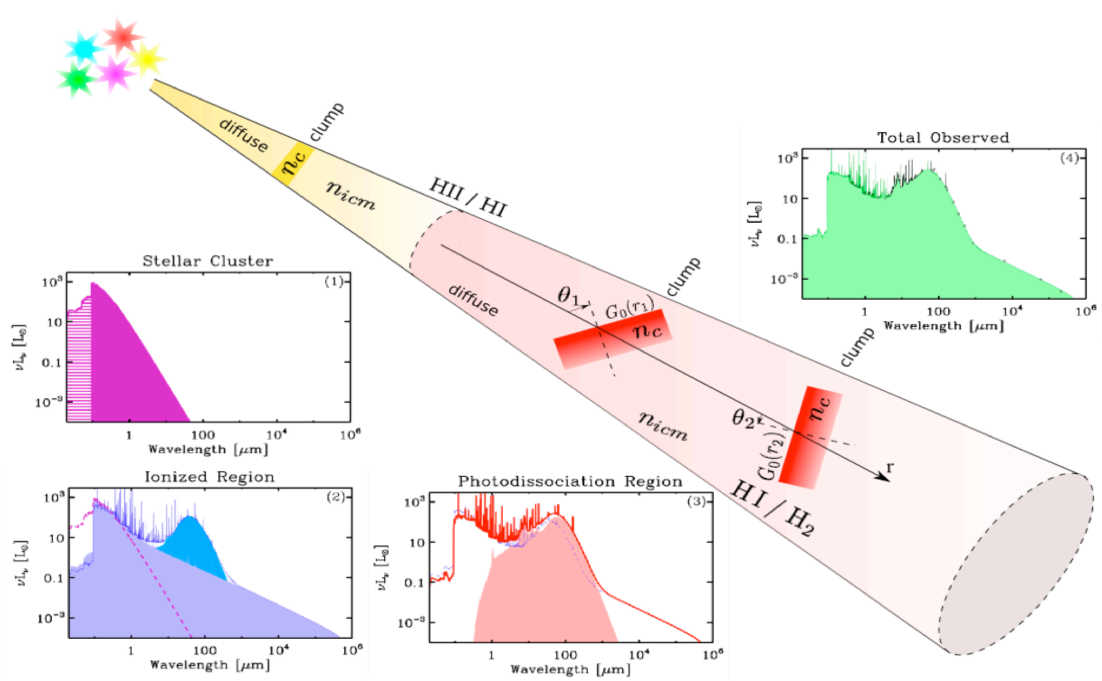
Several reasons. One of them :

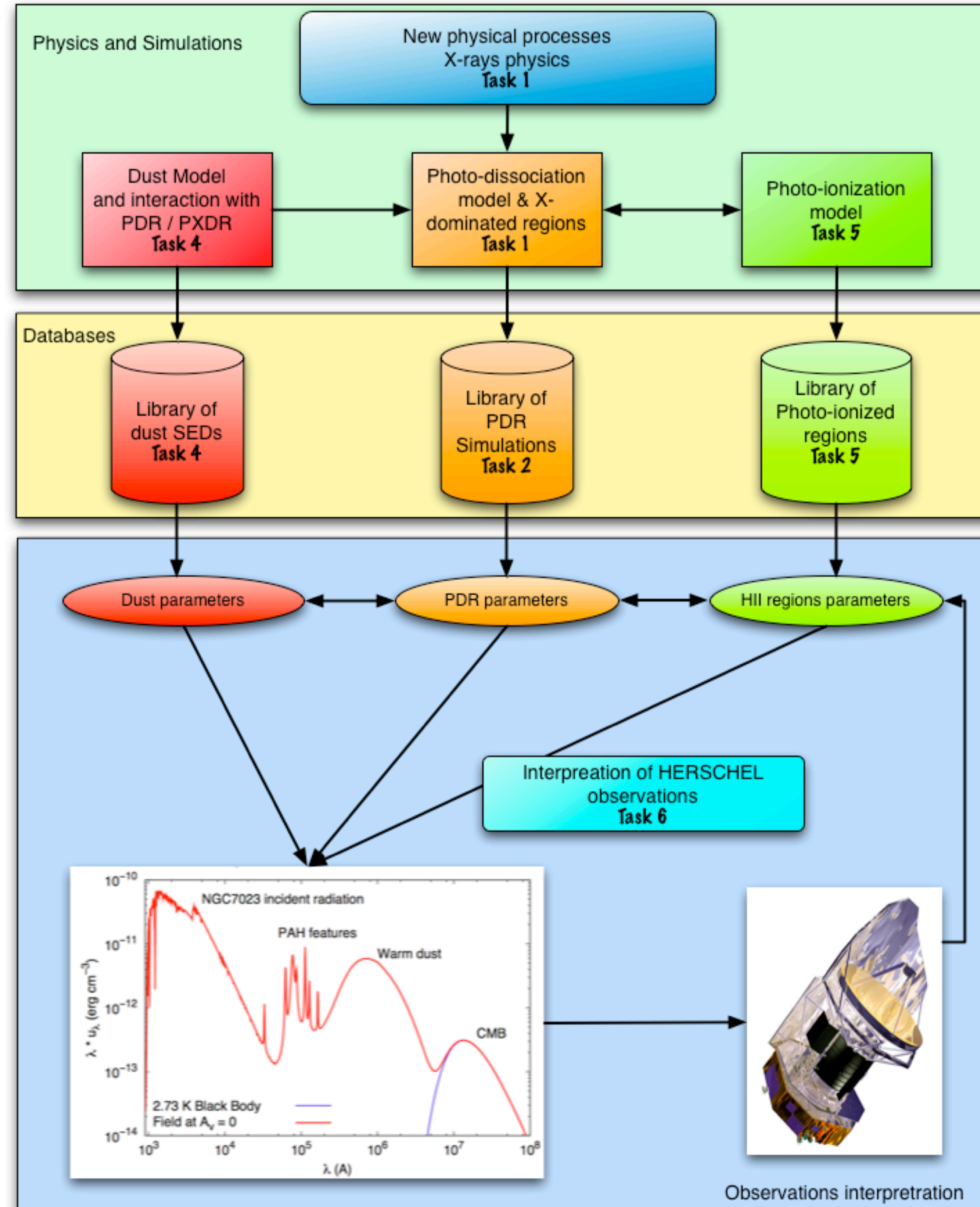
Gas emission in galaxies comes from :

- PDRs (clouds)
- Shocks
- H II regions

Unresolved observations

Need to combine results of different codes





➜ interoperability between services required