# PDRDB

VO-Paris Datacentre

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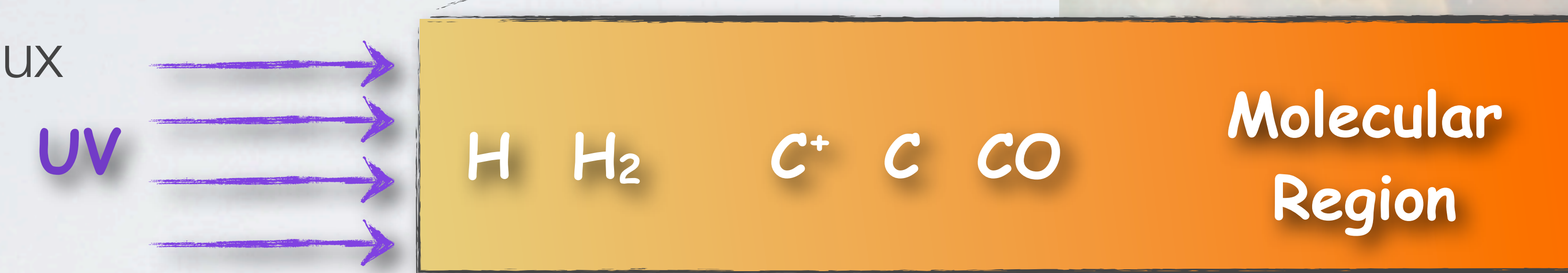
# Interstellar medium & PDR code

PDR : Photo-dissociation regions

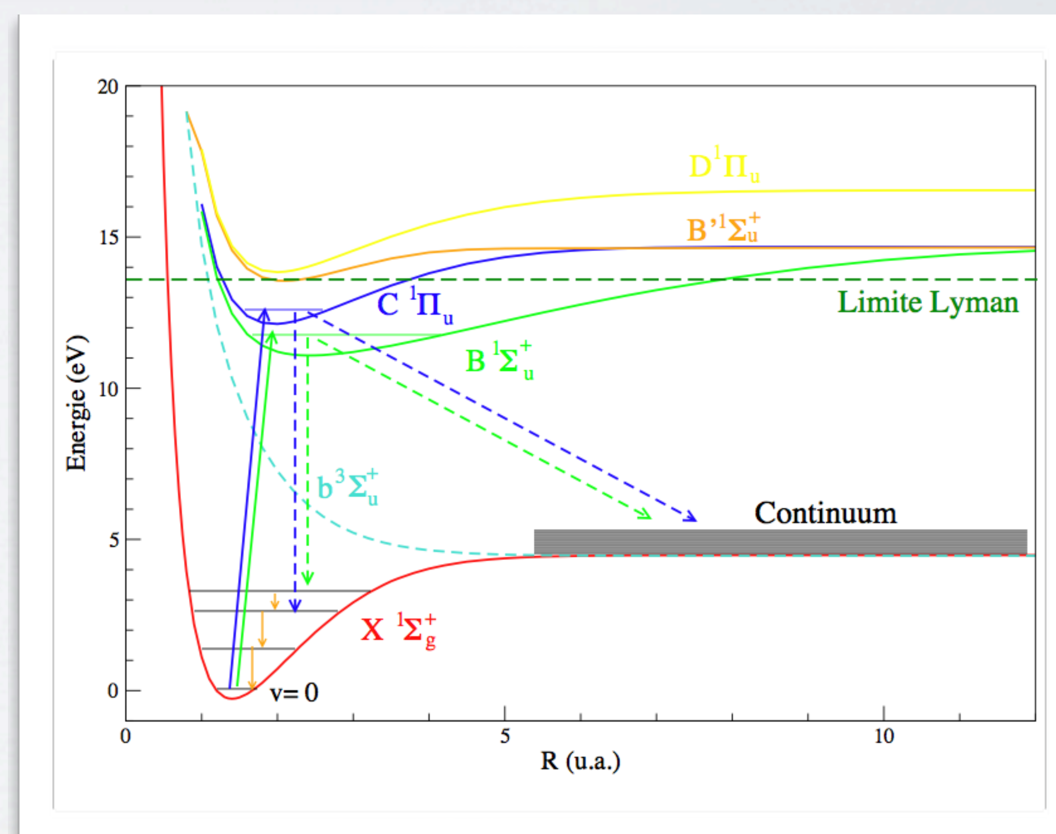
Computes the chemical and thermal structure of interstellar gas

**Input parameters :**
- density
- UV intensity
- Cosmic rays flux
- metallicities
- ...



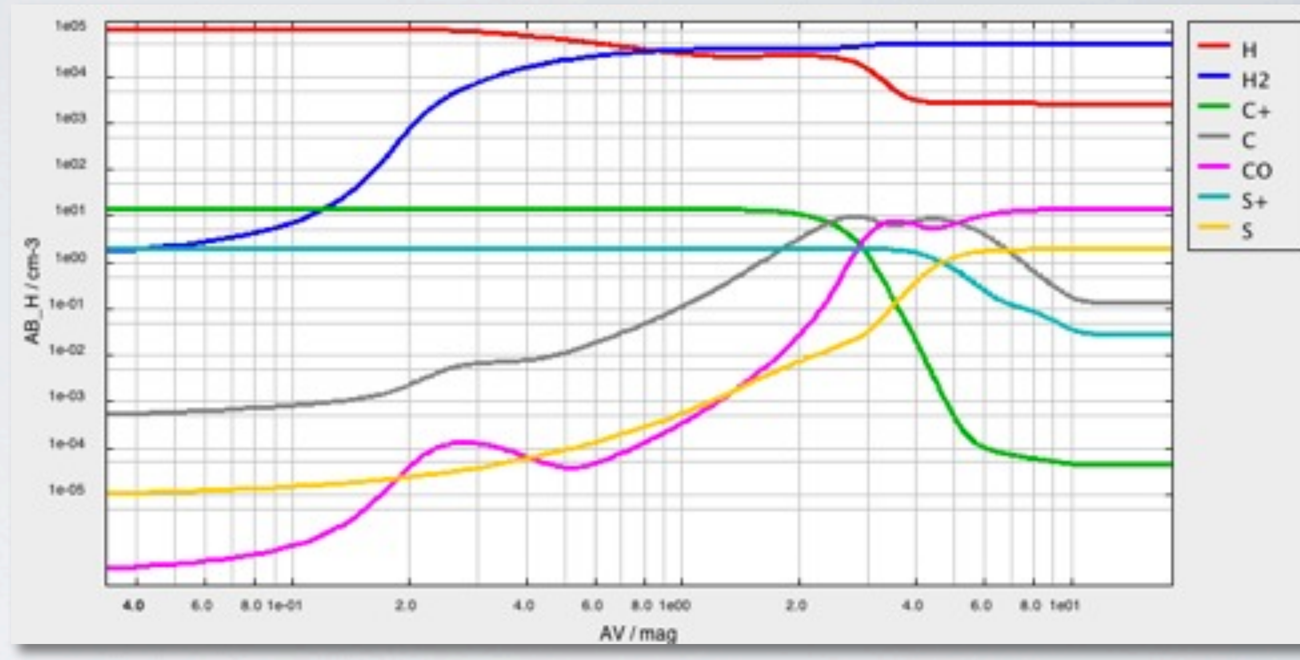

- Atomic & Molecular Data
- Chemical reaction rates

**Physics :**
- Radiative transfer (FUV - sub-mm)
- Chemistry
- Thermal processes
- Statistical equilibrium in levels

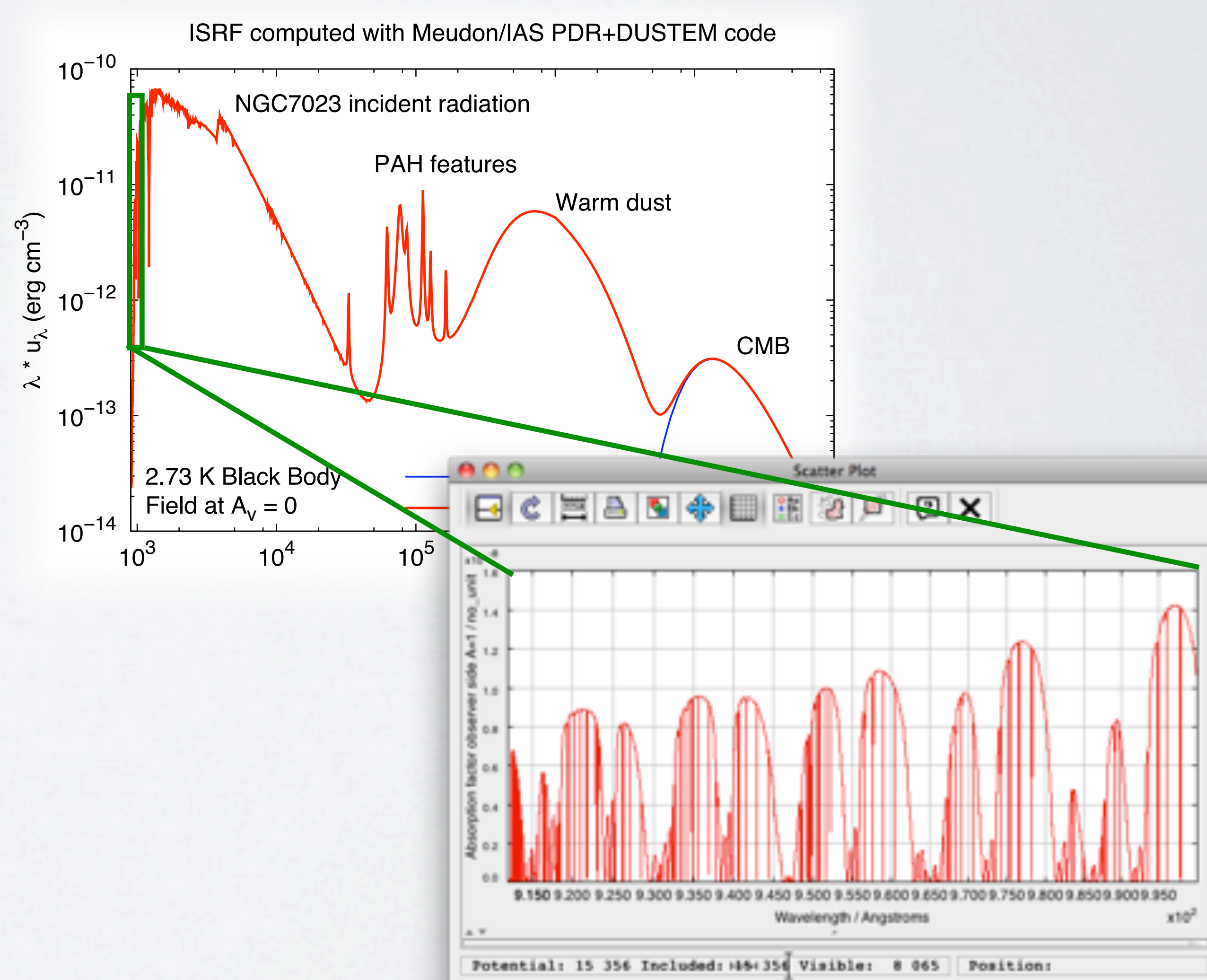


## Outputs

- Local quantities (profiles as a function of Av)
    - Abundances
    - Level excitation ($H_2$, CO, $C^+$, $H_2O$, ...)
    - Temperature
    - Density
    - Heating and cooling rates
    - Local emissivities
    - ...




- Integrated quantities (Observables)
    - Column densities
    - Line intensities
    - Spectra



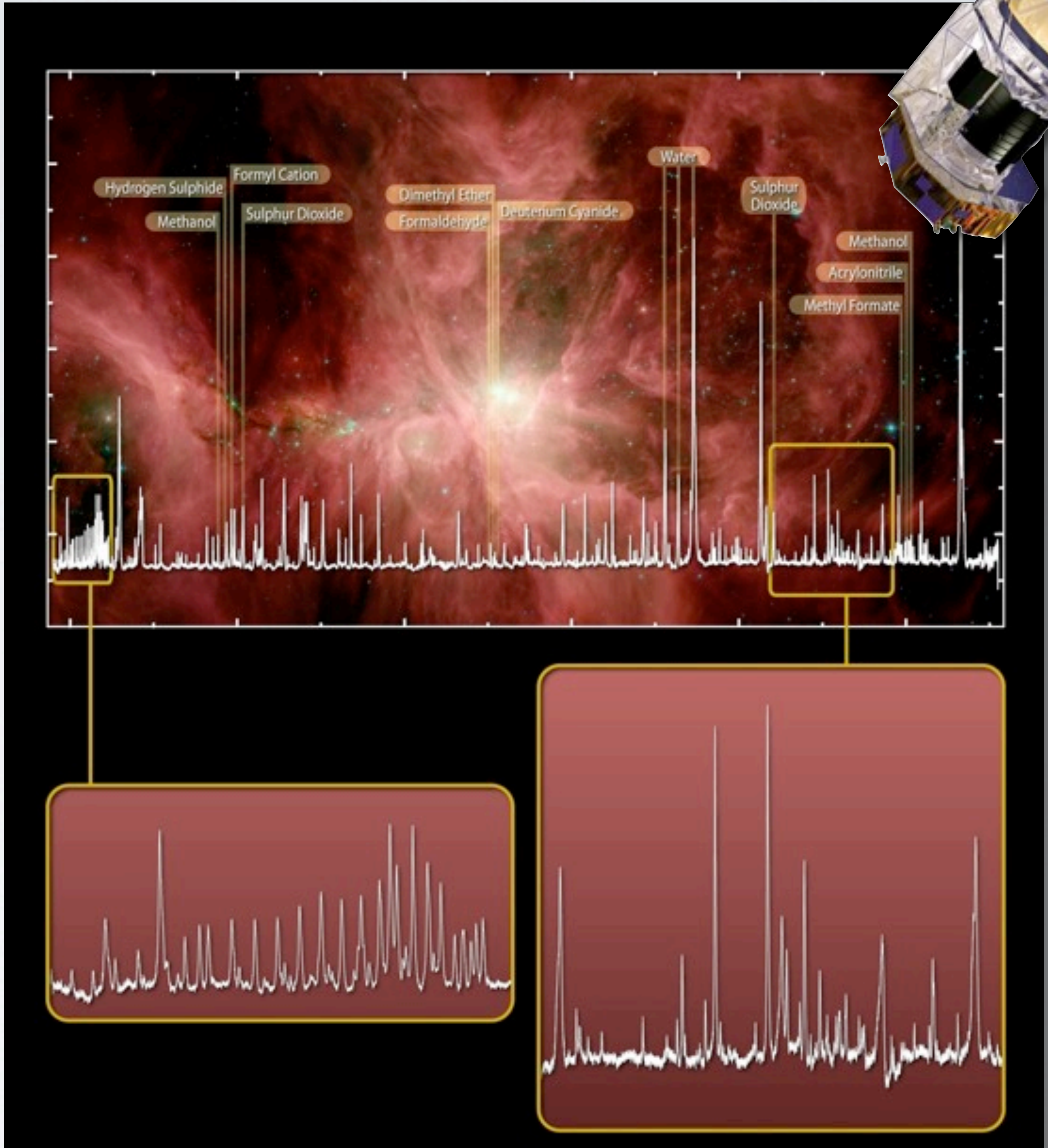
# ☐ Interstellar Medium & PDR code

Motivations

New large equipments

=> share codes and simulation results with the community

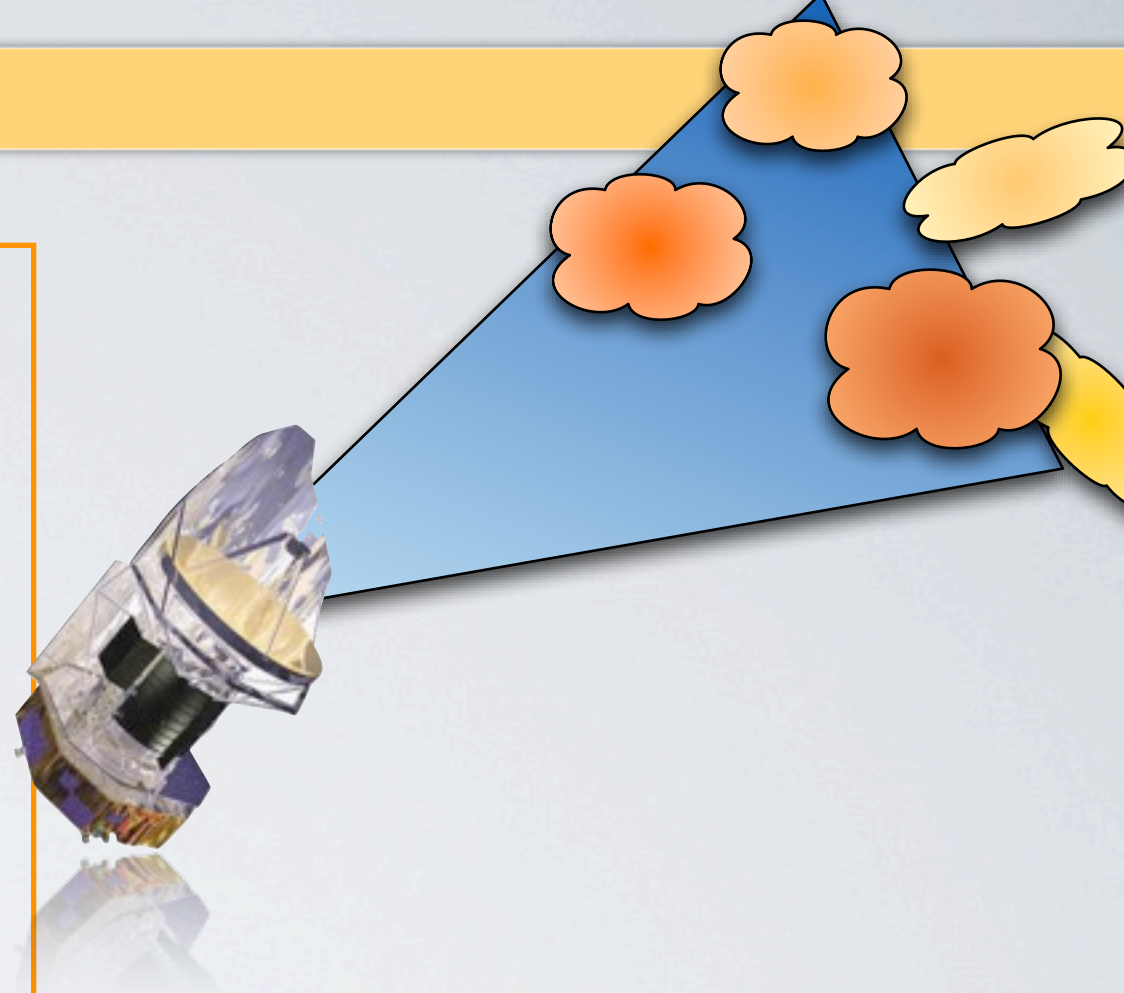
They want :
1) Get the code
2) Get pre-computed results
3) Services to facilitate interpretation of observations
- Lines intensities
- Column densities
- Spectra
- Structure of the cloud
- Physical processes
- Chemistry




HIFI Spectrum of Water and Organics in the Orion Nebula

© ESA, HEXOS and the HIFI consortium E. Bergin

# PDR Database



Objectives :

- Publish PDR simulations in different domains
  - Diffuse clouds
  - Star-formation regions
  - Damped Lyman Alpha systems

- Services :
  - Extract quantities for post-processing
  - Facilitate inverse problems
  - Model easily non-resolved observations

Challenge :

- PDR simulations are complex :
  - Many heterogenous quantities

- PDR codes evolve frequently
  - Computation of new quantities that have to be ingested in the database

## PDR Database

### Implementation

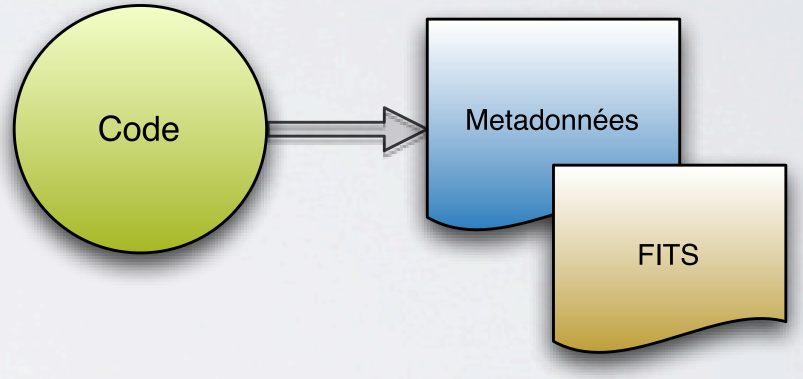
Development of the PDR database in 2 steps :

**1 - Modify code outputs**
- portable data (FITS)
- metadata (XML - VOTable syntax)

**2 - Develop PDRDB**
- Use VO-URP

**Code output metadata (XML - VO-Table) :**

Each quantity has :
- ID
- Name (human readable)
- Description
- Unit
- UCD




- Each quantity is identified by an I.D. (Ex : Temperature)
- Each group of quantities has an I.D. (Ex : Abundance - group of all abundances)

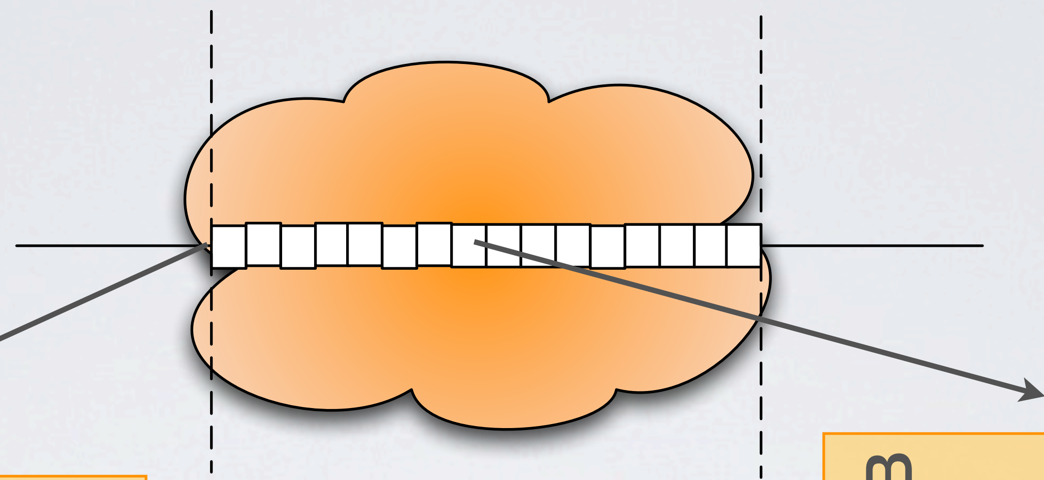
Ingestion pipeline searches the quantities or group of quantities to ingest in the DB
- Evolution of the code implies very few (none) modifications to be compatible with PDRDB
- Very easy to add new properties in PDRDB

# PDR Database

```
<FIELD name="Mass grain / Mass of gas"   ID="DU_MODPARAM_R.FD_GRATIO"   datatype="double"
       unit="no unit"     ucd=""         utype=""  >
       <DESCRIPTION> <![CDATA[ <b>m_grain / m_gas</b> <br>
                     Dust on grain mass ratio.<br>  <i>Typical value: 0.01</i>]]>
       </DESCRIPTION>
</FIELD>
<FIELD name="Grains albedo"              ID="DU_MODPARAM_R.FD_ALBEDO"   datatype="double"
       unit="no unit"     ucd=""         utype=""                                    >
       <DESCRIPTION> <![CDATA[<b>Dust albedo</b><br>
                     <i>Typical value: 0.42</i><br><i>Ref: Mathis ApJ, 472, 643, 1996.</i>]]>
       </DESCRIPTION>
</FIELD>
<FIELD name="Grains anisotropy factor"    ID="DU_MODPARAM_R.FD_GG"      datatype="double"
       unit="no unit      ucd="»         utype=""                                    >
       <DESCRIPTION> <![CDATA[<b>Anisotropy factor of grains</b><br><i>Typical value: 0.6 </i><br>
                     <i>Ref: Weingartner et Draine, ApJ 548, 296, 2001</i>]]>
       </DESCRIPTION>
</FIELD>
```

# PDR Database

## Implementation



Integrated quantities

- **Column densities H, H2, ...**
- **Lines intensities**
- Spectra

Local quantities

SimDB

- **Temperature**
- **Density**
- **Abundances H, H2, ...**

File System

- Level populations
- Heating rates
- Cooling rates
- Lines emissivities
- ...

Too many quantities to implement in SimDB

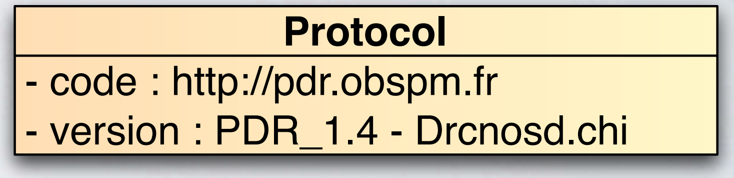
**Objectives : discover simulations**

1) only **the most important quantities are stored in SimDB** as metadata
2) **other quantities are stored in the FileSystem** and can be extracted by services

## Implementation

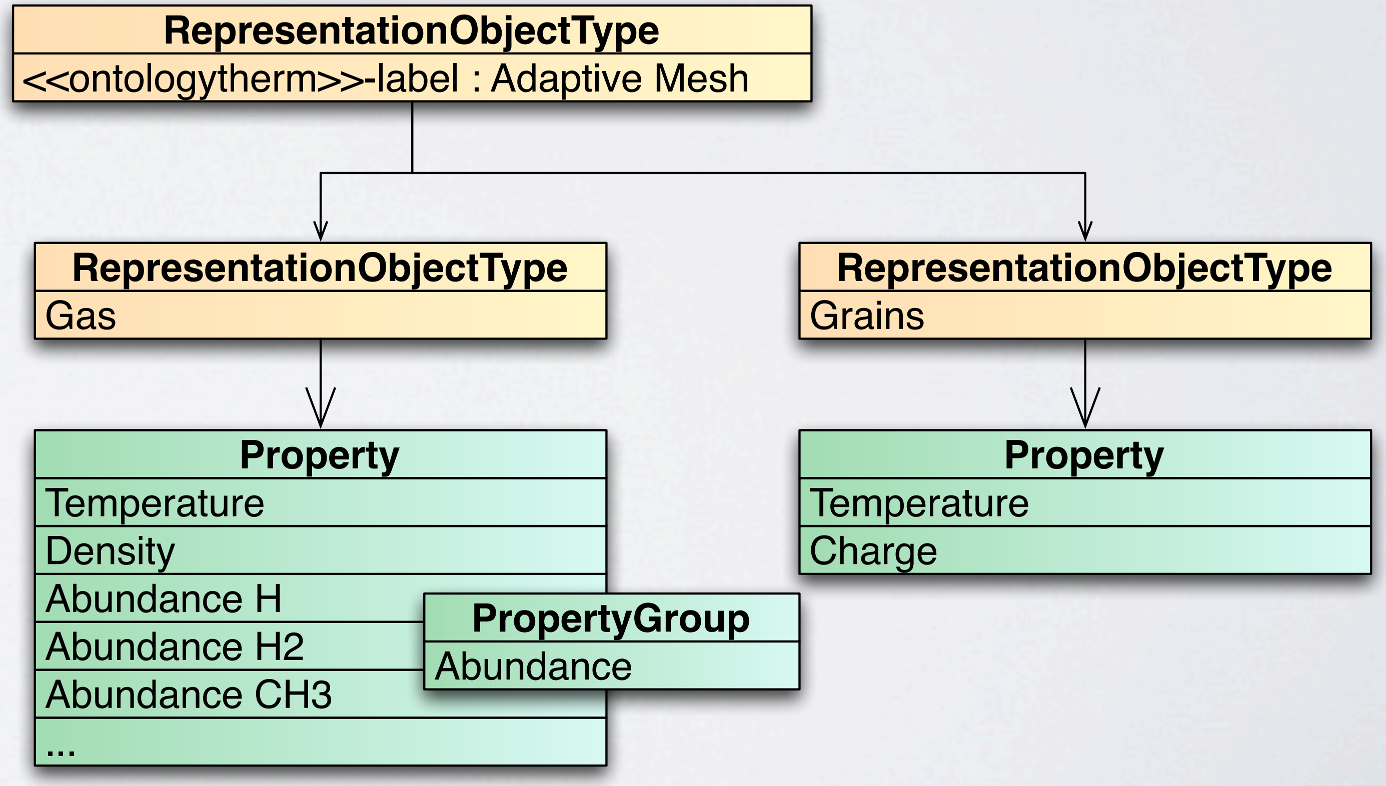
- Protocol

  - Protocol : **Code + Atomic and Molecular Data + Chemistry**
  - Physical processes : **Radiative transfer, ...**
  - Algorithms : not useful for such codes



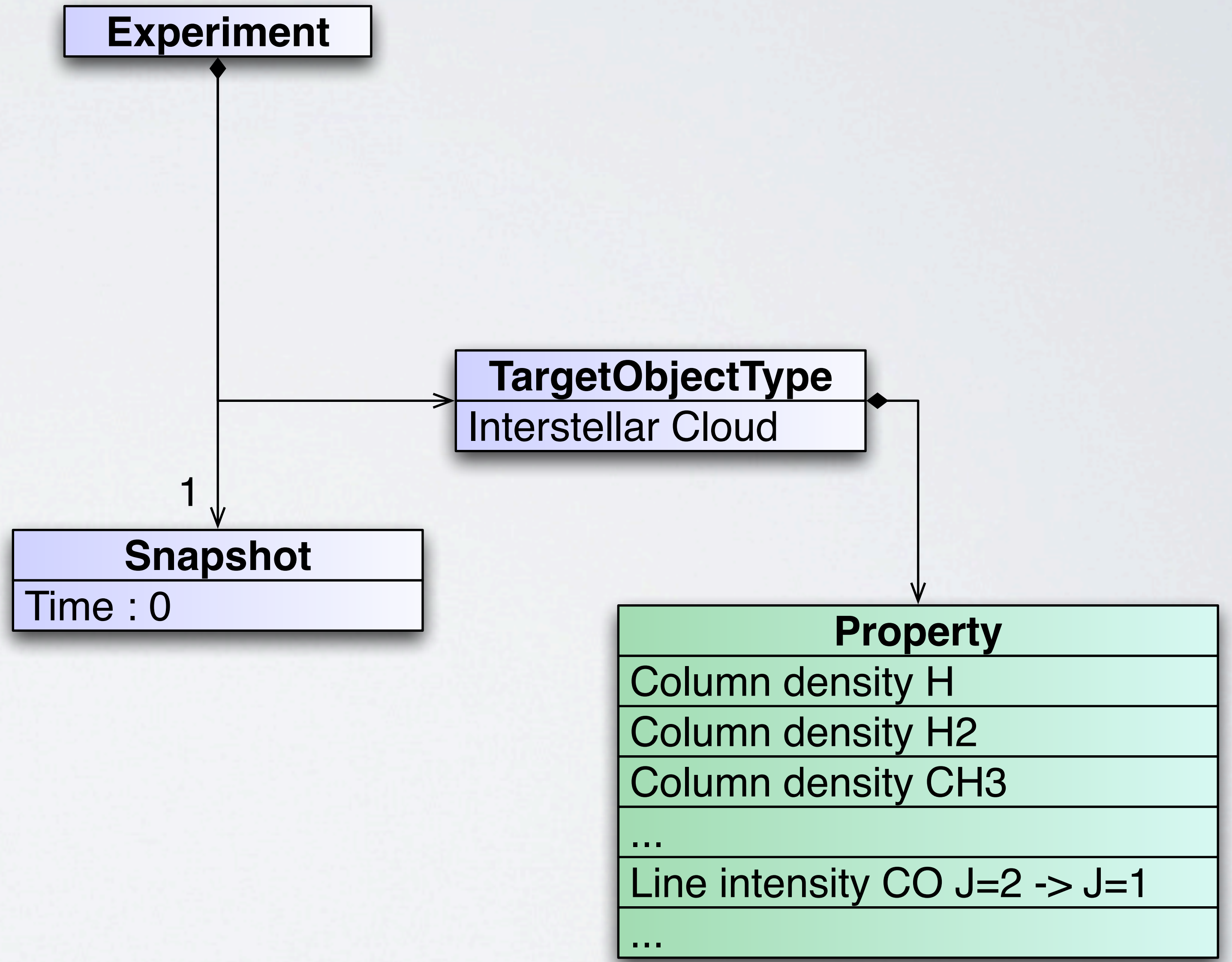

- RepresentationObjectType

  - Gas and Grains
  - Properties :
    - Temperature
    - Density
    - Ionization degree
    - Abundances H, H2, C+, ...
    - ...



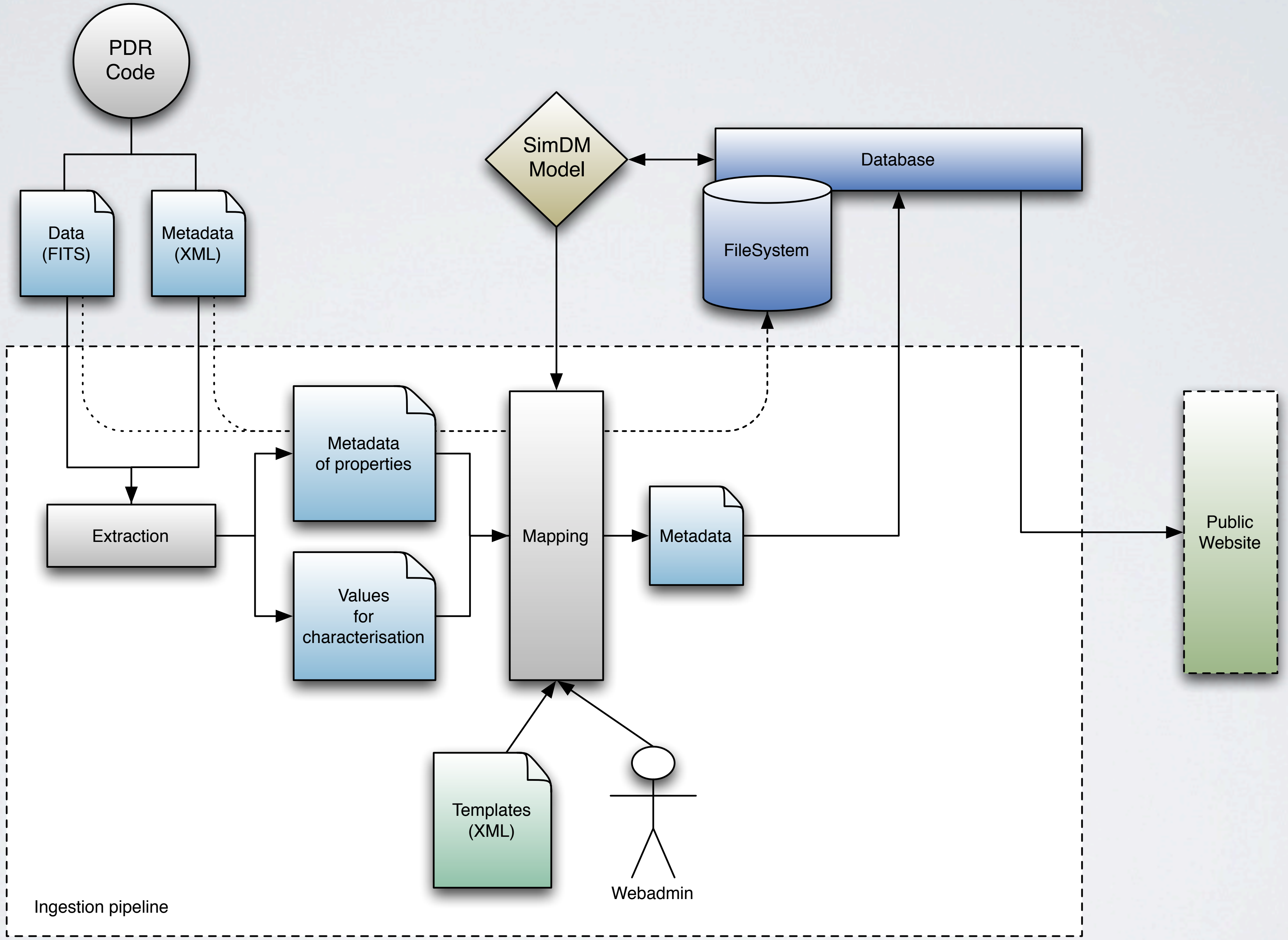
- Experiment

  - Snapshot : **Stationnary Code** => only one snapshot per experiment
  - TargetObjectType : Interstellar Cloud
  - Properties : Integrated quantities
    - Column densities
    - Most useful line intensities



# PDR Database

Ingestion pipeline
- Use VO-URP (developed by Gerard Lemson and Laurent Bourgès)




Code Metadata + VO-URP = Easy to maintain
- If the code evolves : the new quantities are automatically ingested in PDRDB
- To add new properties in PDRDB just add its ID in the Template file

# PDR Database

International
Virtual
Observatory
Alliance

## Implementation of the Simulation Data Model for theoretical databases

## Version 0.1

### *IVOA Note 2010 May 15*

**This version:**
Version 0.1-20100515
**Latest version:**
http://www.ivoa.net/Documents/latest/latest-version-name
**Previous version(s):**

**Author(s):**
Franck Le Petit
Benjamin Ooghe-Tabanou
Nicolas Moreau
Jonathan Normand
Laurent Bourgès

#### 2.2.1 Snapshot

The Meudon PDR code is a stationary 1D code. We do not have snapshots with the meaning it can have in the context of cosmological simulations for instance. In the SimDB implementation, we consider that for each experiment we have a single snapshot that corresponds to the output of the code, the stationary state.

#### 2.2.2 TargetObject

TargetObjects represents the astrophysical object that has been simulated. For PDRDB, most of the time this is «Interstellar Cloud». That could also be «disks» when a model has been run to simulate a protoplanetary disk.

### 2.3 Object

This part is a heritage of the protocol and of the experiment parts. We describe first, the ObjectType and Properties for the protocol, then for the experiment.

#### 2.3.1 – RepresentationObjectType and Properties for the protocol

At each position of the grid, the code computes several quantities for the gas and the grains. We consider two ObjectTypes : gas and grains with the attribute Mesh Cell.

The properties of the RepresentationObjectType are all the quantities computed locally. In the Meudon PDR code, we have several thousands of these properties. Only the most important ones to search models in the database are implemented.

Examples for the RepresentationObjectType, gas, with in bold face, those that are stored in the database
- **gas temperature, proton density, and ionization degree**
- **abundances of H, $H_2$, $C^+$, C, CO, ...**
- levels populations of CO in J=0, J=1, ... of $H_2$ in v=0 J=0, ...
- local line emissivity (erg $cm^{-3}$ $s^{-1}$ $Ang^{-1}$ $std^{-1}$) of $H_2$ from v=0 J= 2 to v=0 J=0
- heating rate by photoelectric effect, by cosmic rays, ...
- density of energy per bin of wavelength
- ...

Examples for the RepresentationObjectType : grains
- **size of grains**
- **temperature of grains**
- **charge of grains**

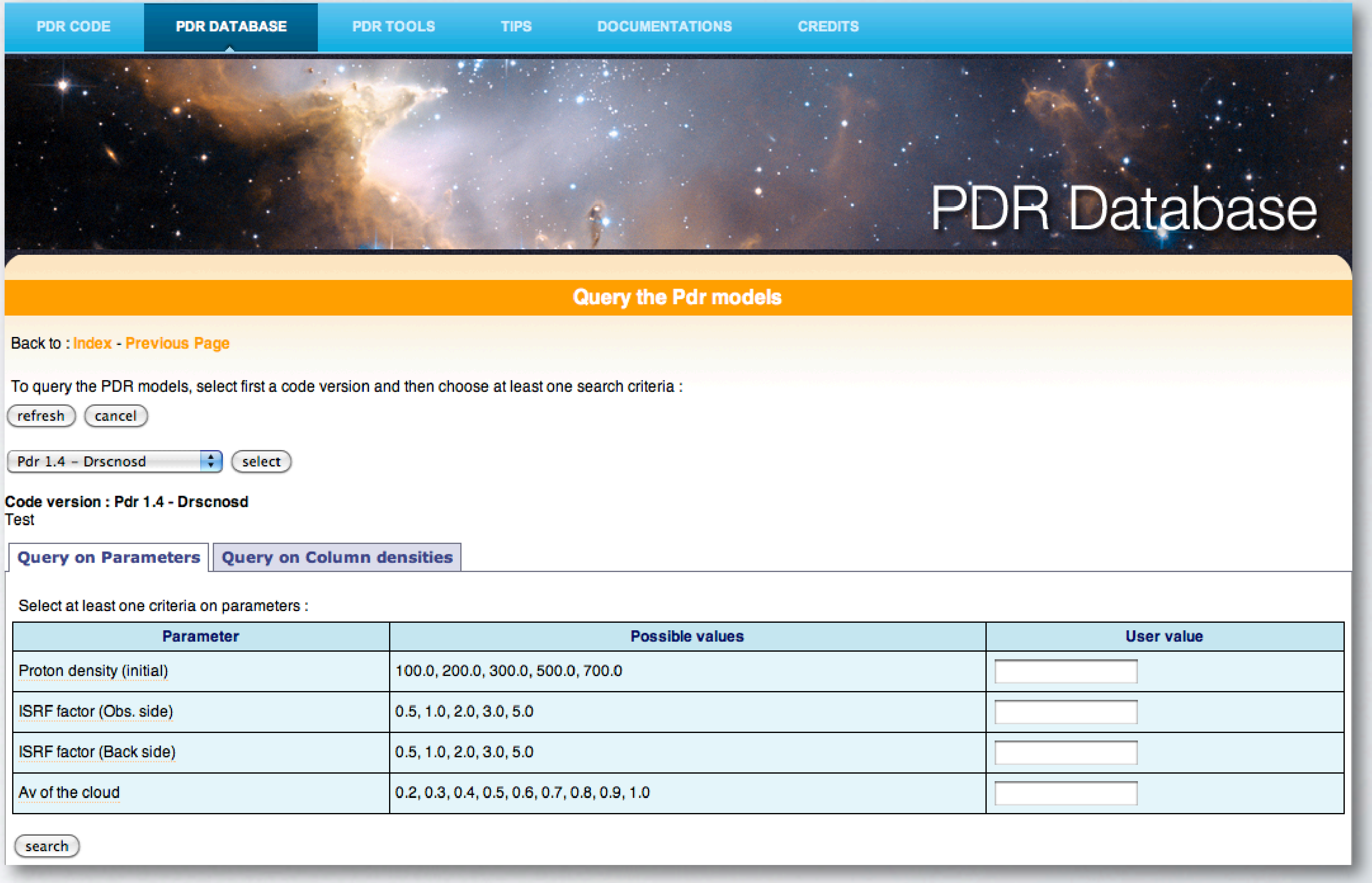
# ☐ PDR Database - N. Moreau & B. Ooghe

PDR Database is developped as a **SimDB** service

**Project : Diffuse clouds**
225 models (700 days CPU)
Parameters space :
- Density 100 to 700 cm-3
- Radiation field 0.5 - 5 ISRF
- Size 0.2 to 1 mag

**Project : PDRs**
120 models
Parameters space :
- Density 1000 to 1E6 cm-3
- Radiation field 100 - 7E5 ISRF

Queries on :
- input parameters
- outputs as column densitie


PDR CODE | PDR DATABASE | PDR TOOLS | TIPS | DOCUMENTATIONS | CREDITS

PDR Database

Query the Pdr models

Back to : Index - Previous Page

To query the PDR models, select first a code version and then choose at least one search criteria :

refresh cancel

Pdr 1.4 – Drscnosd select

**Code version : Pdr 1.4 - Drscnosd**
Test

Query on Parameters | Query on Column densities

Select at least one criteria on parameters :

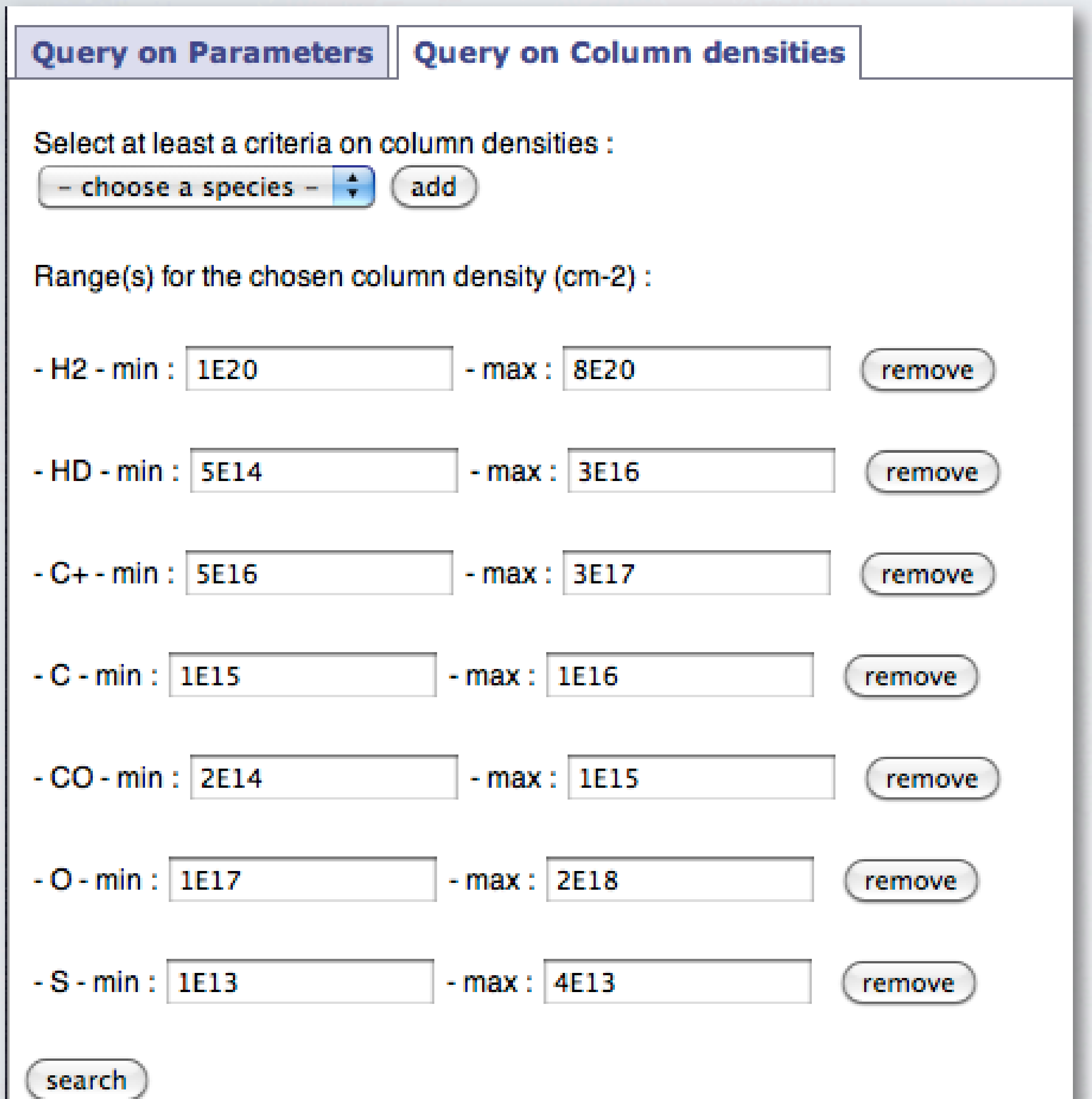
| Parameter | Possible values | User value |
|---|---|---|
| Proton density (initial) | 100.0, 200.0, 300.0, 500.0, 700.0 | |
| ISRF factor (Obs. side) | 0.5, 1.0, 2.0, 3.0, 5.0 | |
| ISRF factor (Back side) | 0.5, 1.0, 2.0, 3.0, 5.0 | |
| Av of the cloud | 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 | |

search

Next set of models :
- Extra-galactic medium
- ...

# PDR Database

## Queries on column densities




**Queries on column densities :** functionnal
**Queries on line intensities :** coming soon

| **Species** | min | max |
|---|---|---|
| H | 5.7 (20) | 7.1 (20) |
| $H_2$ | 3.2 (20) | 7.1 (20) |
| HD | 2.0 (15) | 1.1 (16) |
| $C^+$ | 1.8 (17) | |
| C | 2.9 (15) | 3.6 (15) |
| CO | 5.4 (14) | |
| CH | 1.9 (13) | 2.0 (13) |
| CH+ | 3.5 (12) | |
| C2 | 1.6 (13) | 2.2 (13) |
| C3 | 1.0 (12) | |
| CN | 2.7 (12) | 3.3 (12) |
| NH | 9.0 (11) | |
| O | 0.2 (18) | 1.0 (18) |
| OH | 4.0 (13) | |
| H3+ | 8.0 (13) | |
| S+ | 1.7 (16) | 2.3 (16) |
| S | 1.5 (13) | 2.2 (13) |
| Si+ | 2.8 (16) | 6.6 (16) |
| H2 (J=0) | 2.2 (20) | 4.8 (20) |
| H2 (J=1) | 1.0 (20) | 2.3 (20) |
| H2 (J=2) | 1.1 (18) | 2.4 (18) |
| H2 (J=3) | 2.0 (16) | 9.6 (16) |
| H2 (J=4) | 1.1 (15) | 2.0 (15) |
| H2 (J=5) | 2.3 (14) | 2.8 (14) |

Column densities [cm$^{-2}$] towards Zeta Perseus

# PDR Database

Results :

Input parameters
- description of all parameters

PDR CODE | PDR DATABASE | PDR TOOLS | TIPS | DOCUMENTATIONS | CREDITS


**Model : n1e2r5m1r5m1J4A9m1_10**

Back to : Index - Previous Page

**Model : n1e2r5m1r5m1J4A9m1_10**
Description :
Test
Download full simulation for the PDR analyzer

Model | Structure | Plot | Column densities | Line intensities

| Cloud parameters | |
|---|---|
| Av of the cloud | 9.000E-01 mag |
| Proton density (initial) | 1.000E02 cm-3 |
| Flag : 1 or 2 side(s) model | 0 |
| ISRF factor (Obs. side) | 5.000E-01 |
| ISRF factor (Back side) | 5.000E-01 |
| Distance of the point UV source | 0 pc |
| External source name | |
| Flag : Thermal balance | 1 |
| Gas temperature (initial) | 7.000E01 K |
| Flag: State equation | 0 |
| Gas pressure | 7.000E03 cm-3 K |
| Density-Temperature profile file name | |
| Flux of cosmic rays | 5.000E00 1E-17 s-1 |
| Micro-turbulent velocity | 2.000E05 cm s-1 |

| Line of sight parameters | |
|---|---|
| Line of sight dust extinction curve | Galaxy |
| C = NH / E(B-V) | 5.800E21 cm-2 mag-1 |
| Rv | 3.100E00 |

| Algorithm parameters | |
|---|---|
| Number of global iterations | 10 |
| Flag: Algorithm for line self-shielding | 2 |
| J limit for H2 exact self-shielding | 4 |
| Code version | 10VII08_JLB_and_Co |

| Grains parameters | |
|---|---|
| Mass grain / Mass of gas | 1.000E-02 |
| Grains minimal radius | 3.000E-07 cm |
| Grains maximum radius | 3.000E-05 cm |
| Grains albedo | 4.200E-01 |
| Grains anisotropy factor | 6.000E-01 |
| Grains volumic mass | 2.590E00 g cm-3 |
| Index of grains size distribution | 3.500E00 |

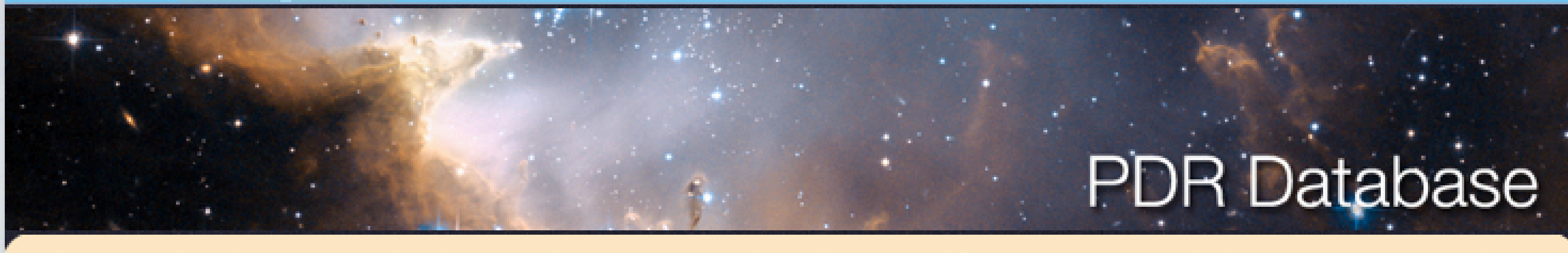
| Chemistry parameters | |
|---|---|
| Chemistry file name | Drcnosd.chi |
| He / H | 1.000E-01 |
| C / H | 1.320E-04 |
| N / H | 7.500E-05 |
| O / H | 3.190E-04 |
| D / H | 1.500E-05 |
| C13 / H | 0 |
| N15 / H | 0 |
| O18 / H | 0 |
| PAH / H | 0 |
| F / H | 0 |
| Na / H | 2.100E-07 |
| Mg / H | 0 |
| Al / H | 0 |
| Si / H | 8.200E-07 |
| P / H | 9.000E-10 |
| S / H | 1.860E-05 |
| Cl / H | 0 |
| Ca / H | 0 |
| Fe / H | 1.500E-08 |
| H2 excitation model after formation on grains | 0 |
| Model for H + H2 collision rates | 2 |
| Model for atoms sticking on dust | 4 |

| Information | |
|---|---|
| ISRF factor (Obs. side) - edge of the cloud | 3.083E-01 |
| ISRF factor (back side) - edge of the cloud | 3.083E-01 |
| ISRF scaling factor (Obs. side) in Habing units | 3.871E-01 |
| ISRF scaling factor (back side) in Habing units | 3.871E-01 phot cm-2 s-1 |
| Flux of secondary photons | 5.000E03 s-1 |
| Relative abundance of grains | 1.777E-09 |
| Mean number of adsorption sites per grain | 1.338E-05 |
| Mean grains cross section | 2.261E-21 cm2 |
| Distance between adsorption sites | 2.600E-08 cm |
| Total grain surface | 9.046E-21 |

# PDR Database

## Column densities

PDR CODE | PDR DATABASE | PDR TOOLS | TIPS | DOCUMENTATIONS | CREDITS




Mod

Back to : Index - Previous Page

**Model : n1e2r5m1r5m1J4A9m1_10**
Description :
Test
Download full simulation for the PDR analyzer

Model | Structure | Plot | Column densities | Line intensitie

Column densities of chemical species in cm-2

| Species | Column density [cm-2] |
|---|---|
| H+ | 1.830E16 |
| D+ | 2.048E10 |
| H2+ | 3.818E11 |
| HD+ | 1.067E07 |
| H3+ | 1.412E13 |
| H2D+ | 4.158E09 |
| He+ | 5.085E14 |
| C+ | 2.180E17 |
| CH+ | 2.380E10 |
| CD+ | 1.999E06 |
| CH2+ | 1.642E11 |
| CHD+ | 3.949E06 |
| CH3+ | 2.490E11 |
| CH2D+ | 3.492E07 |
| CH4+ | 8.791E04 |
| CH3D+ | 6.285E00 |
| CH5+ | 7.010E06 |
| CH4D+ | 5.152E02 |
| O+ | 6.183E10 |
| O2+ | 1.194E08 |
| OH+ | 7.958E10 |
| OD+ | 8.441E05 |
| H2O+ | 7.409E10 |
| HDO+ | 3.618E05 |

## Line intensities

- Main lines
- Face-on cloud

**Model : n1e2r5m1r5m1J4A9m1_10**

Back to : Index - Previous Page

**Model : n1e2r5m1r5m1J4A9m1_10**
Description :
Test
Download full simulation for the PDR analyzer

Model | Structure | Plot | Column densities | Line intensities

Line intensities for a face-on cloud *To get line intensities for other angles or other lines, download the simulation in PDR Analyzer*

| [C I] Line Intensities | |
|---|---|
| 3P_J=1, 3P_J=0, 609.75 micron | 1.235E-08 |
| 3P_J=2, 3P_J=1, 370.37 micron | 1.120E-08 |

| [O I] Line Intensities | |
|---|---|
| 3P_J=0, 3P_J=1, 145.53 micron | 2.242E-09 |
| 3P_J=1, 3P_J=2, 63.19 micron | 7.793E-08 |

| [C II] Line Intensities | |
|---|---|
| 2P_J=3/2, 2P_J=1/2, 157.68 micron | 2.106E-06 |

| H2 Line Intensities | |
|---|---|
| 1 2 0 0 1- 0 S( 0), 2.2232 micrometres | 4.904E-09 |
| 1 3 0 1 1- 0 S( 1), 2.1217 micrometres | 3.867E-09 |
| 1 4 0 2 1- 0 S( 2), 2.0337 micrometres | 3.659E-09 |
| 1 5 0 3 1- 0 S( 3), 1.9575 micrometres | 1.460E-09 |
| 2 4 1 2 2- 1 S( 2), 2.1541 micrometres | 1.747E-09 |
| 2 5 1 3 2- 1 S( 3), 2.0734 micrometres | 6.484E-10 |

| CO Line Intensities | |
|---|---|
| 1 0 115.268 GHz | 6.666E-11 |
| 2 1 230.537 GHz | 1.571E-10 |
| 3 2 345.805 GHz | 8.186E-11 |
| 6 5 691.485 GHz | 2.517E-13 |
| 15 14 1726.587 GHz | 2.859E-14 |

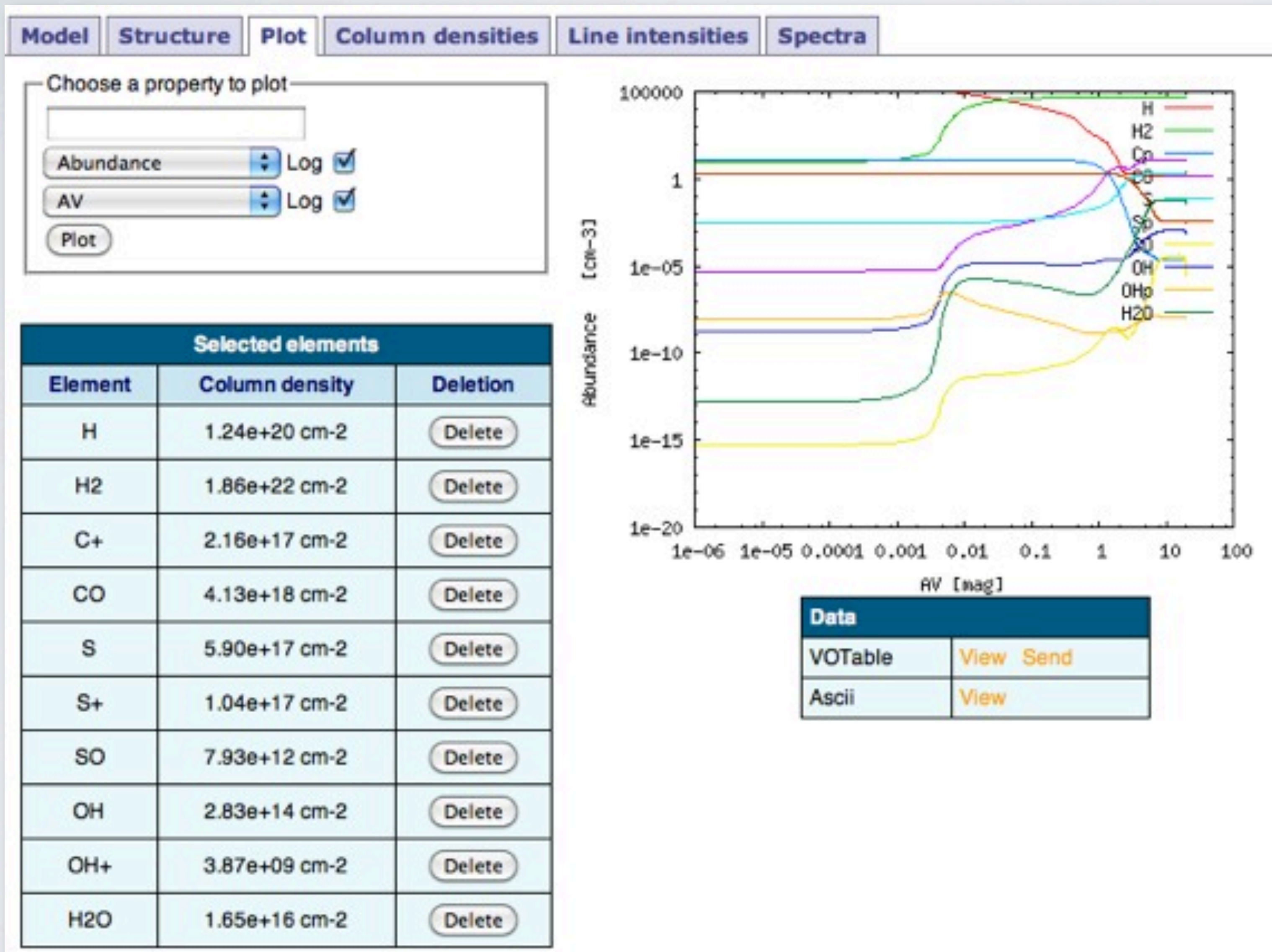
| HD Line Intensities | |
|---|---|
| 0 1 0 0 0- 0 R( 0), 112.0707 micrometres | 7.009E-09 |
| 0 2 0 1 0- 0 R( 1), 56.2283 micrometres | 3.708E-11 |

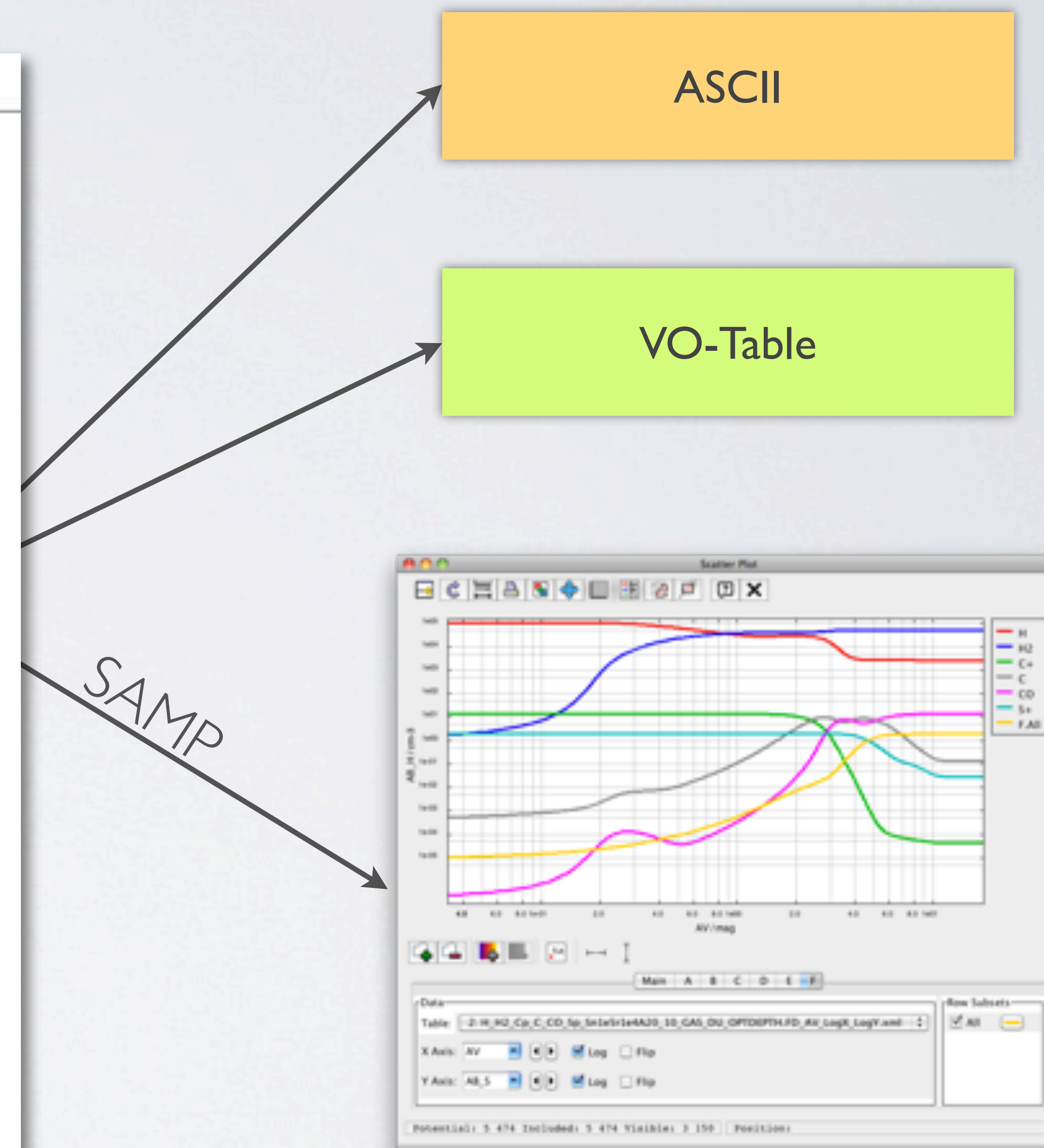
| H2O Line Intensities | |
|---|---|
| 2 2 1 1 1 0 92.5263 cm-1 | 5.619E-14 |
| 3 0 3 2 1 2 57.2630 cm-1 | 9.813E-14 |
| 2 1 2 1 0 1 55.6999 cm-1 | 6.952E-13 |
| 2 2 1 2 1 2 55.4032 cm-1 | 3.107E-14 |
| 1 1 0 1 0 1 18.5768 cm-1 | 1.286E-13 |
| 3 1 2 2 2 1 38.4624 cm-1 | 1.546E-14 |
| 3 1 2 3 0 3 36.6025 cm-1 | 1.981E-14 |
| 2 2 0 1 1 1 99.0225 cm-1 | 2.389E-14 |
| 1 1 1 0 0 0 37.1356 cm-1 | 4.811E-13 |
| 2 0 2 1 1 1 32.9524 cm-1 | 1.260E-13 |
| 2 1 1 2 0 2 25.0842 cm-1 | -1.524E-14 |

# PDR Database

Exportation :

- **Extraction** from web interface
  - ASCII / VO-Table
  - SAMP towards VO-Tools



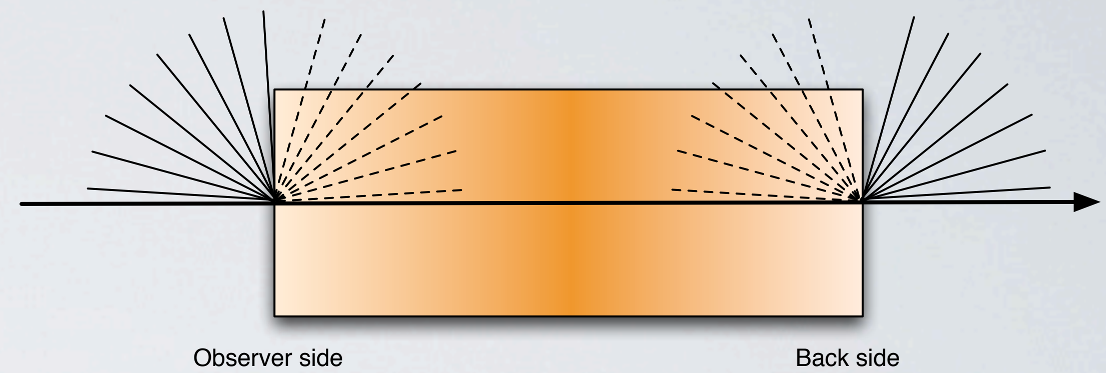




- **Download** the full result
  - Usable in PDR Analyser
  - Restart new model with small changed in input parameters

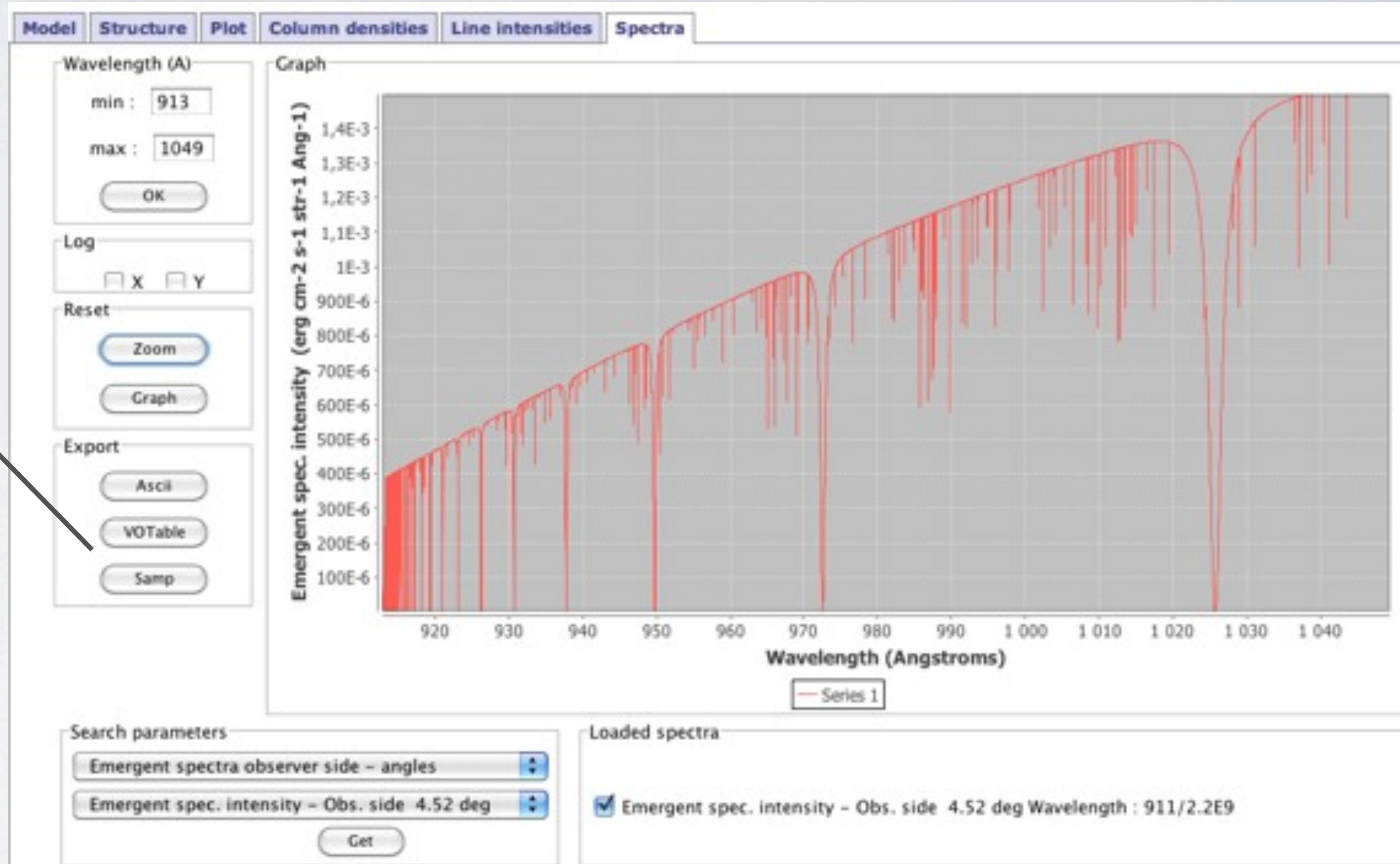
# PDR Database

## Spectra

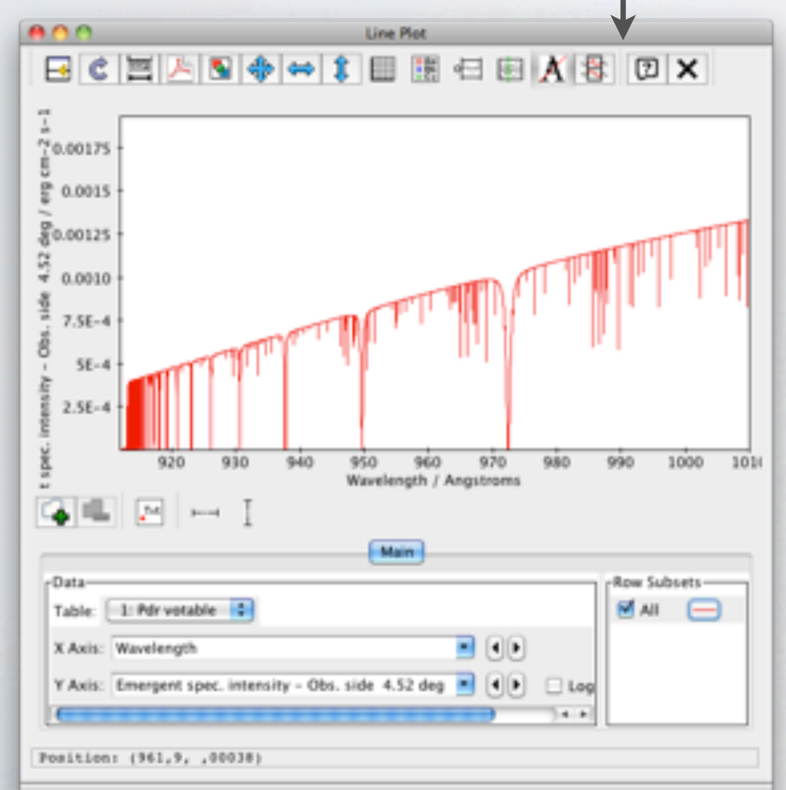
- Incident spectra [erg cm$^{-2}$ s$^{-1}$ str$^{-1}$ Ang$^{-1}$]
- Emergent spectra [erg cm$^{-2}$ s$^{-1}$ str$^{-1}$ Ang$^{-1}$] sampled for about 10 angles




- Absorption spectrum [no unit]




VO-Paris SAMP connector

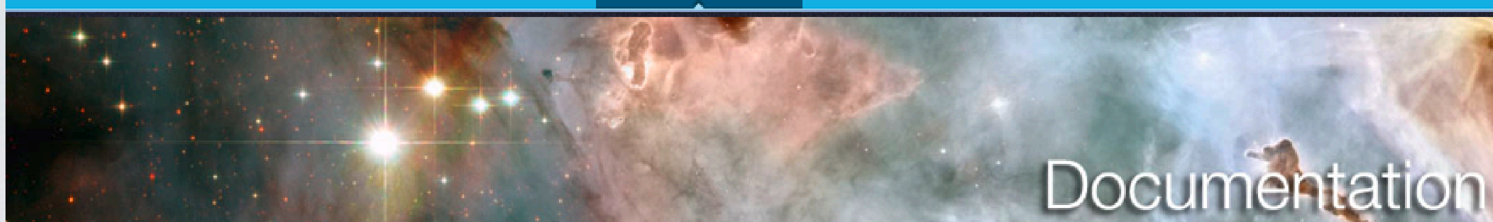


# PDR Database

Feedbacks of the observers :

- Theoretical services difficult to use
- Need :
    - Documentations
    - User friendly interfaces
    - Help desk

PDR CODE | PDR DATABASE | PDR TOOLS | TIPS | DOCUMENTATIONS | CREDITS




**Documentations**

**User documentations**

**PDR code description**
Main description of the physics implemented in the Meudon PDR code

**Quick UserGuide**
Provides the main informations to run quickly a model

**PDR code installation guide**
Describe how to instal the code on a local computer

**PDR analyser documentation**
PDR analyser is a java tool to navigate in the code outputs

**PDR online**
Describe how to run the code online on Paris Observatory dedicated server

**Publications**

- Radiative transfer revisited for emission lines in photon dominated regions
  *Manuel Gonzalez-Garcia et al., A&A ,2008*
- The penetration of Far-UV radiation into molecular clouds
  *Javier Goicoechea and Jacques Le Bourlot, A&A, 2007*
- A Model for atomic and molecular interstellar gas: The Meudon PDR Code
  *Franck Le Petit et al., ApJ Supp., 2006*

**Technical documentations** (VO-service developpers)

**Registration of codes in Astrogrid**
How to register a code in Astrogrid

**SimDB implementation**
Example of the impletation of SimDB on the PDR database

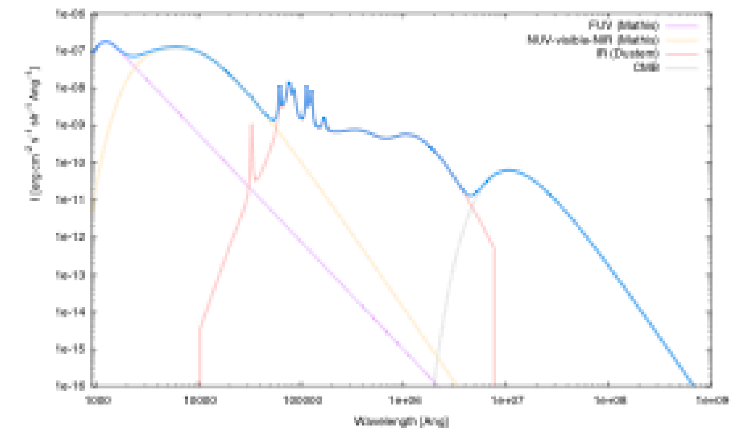
top of page

**Semi-infinite cloud** : to model a semi-infinite cloud, no radiation field should be added on the back side of the cloud (i.e. set radp to 0 and d_sour <= 0).

## Interstellar Standard Radiation Field (ISRF)

The ISRF used in the Meudon PDR code goes from Far-UV to submillimeter. It is the sum of 4 components :

- Far-UV to Near-UV
- Near-UV - Visible - Near IR
- Dust emission (IR)
- CMB



*Specific intensity in erg $cm^{-2}$ $s^{-1}$ $Ang^{-1}$ $str^{-1}$ used in the Meudon PDR code.*

**Far UV to Near UV**

The expression of the UV radiation field based on Mathis et al. 1983 and Black 1994 and fitted by Jacques Le Bourlot is :

$$\lambda \leq 8000\mathring{A}, \quad I(\lambda) = \left[tanh(4.07 \cdot 10^{-3} * \lambda - 4.5991) + 1.0\right] * 107.192 * \lambda^{-2.89}$$
$$\lambda > 8000\mathring{A}, \quad I(\lambda) = 2 * 107.192 * \lambda^{-2.89}$$

In this expression, the wavelength is in Angstroms and the specific intensity in erg $cm^{-2}$ $s^{-1}$ $Ang^{-1}$ $str^{-1}$.

The intensity of this component can be scaled by the radm and radp parameters in the input data file.

**Near UV to near IR**

The expression of the radiation field form near UV to near IR is the sum of 3 black bodies. Data comes from Mathis et al. (1983) and Black (1994). They have been fitted by Jacques Le Bourlot.

$$\begin{aligned} I(\lambda) &= 1.05 \cdot 10^{-14} \times \frac{2 \times h \times c^2 \times 1 \cdot 10^{32}}{\lambda^5 \times e^{\frac{hc10^8}{k\lambda 7127}}} \\ &+ 1.25 \cdot 10^{-13} \times \frac{2 \times h \times c^2 \times 1 \cdot 10^{32}}{\lambda^5 \times e^{\frac{hc10^8}{k\lambda 4043}}} \\ &+ 3.30 \cdot 10^{-13} \times \frac{2 \times h \times c^2 \times 1 \cdot 10^{32}}{\lambda^5 \times e^{\frac{hc10^8}{k\lambda 2930}}} \end{aligned}$$

**Dust emission (IR)**

The I.R. component produced by dust has been estimated by the code DUSTEM. The resulting specific intensity is the sum of the emission by PAHs, very small grains and big grains. Data are provided in the file : `data/Astrodata/IR_field_dustem.dat` .

# ☐ Conclusion

- PDR database
  - Application of SimDM / SimDB

    SimDM can be used to publish micro-physics simulations as PDR models

  - Fulfill most of our requirements (from user's wishes) :
    - Search on input parameters
    - Seach on most important outputs

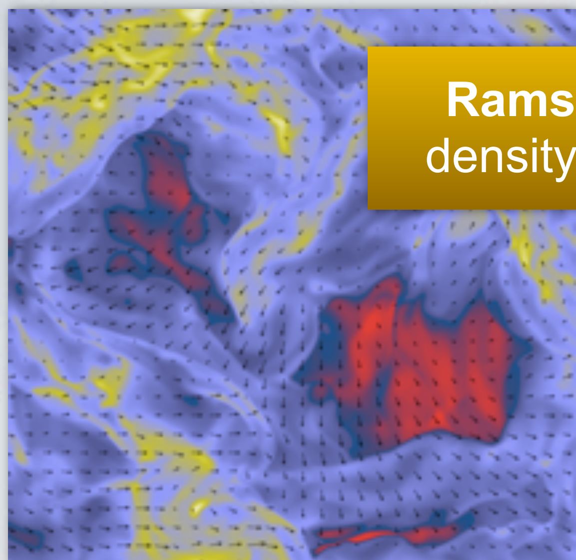
Future evolutions :

- Polish to finalize the service

- Interoperability
  - BUT need :
    - extraction protocol / TAP layer
    - vocabulary / semantics

- Need to define some quantities as lines
  - Wait for VAMDC results

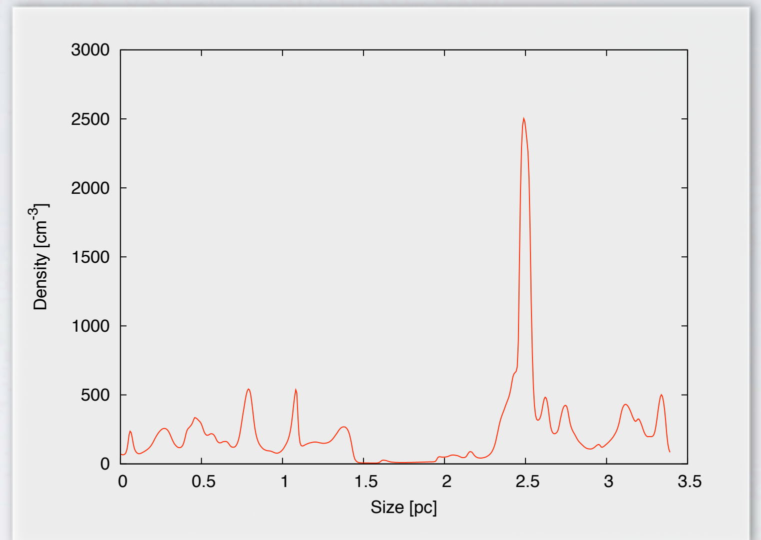
# Interstellar Medium Platform

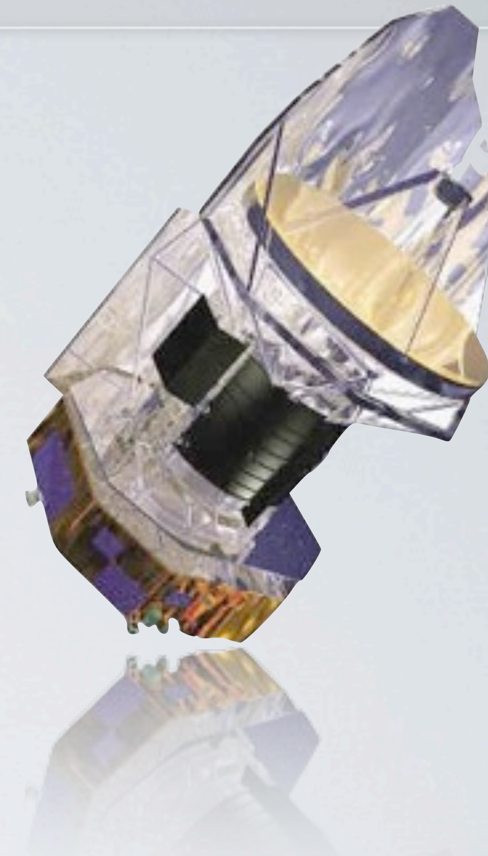


**Ramses-MHD database**
density & velocity structure

SimDAP

Density profile on a line of sight (3.5 pc)



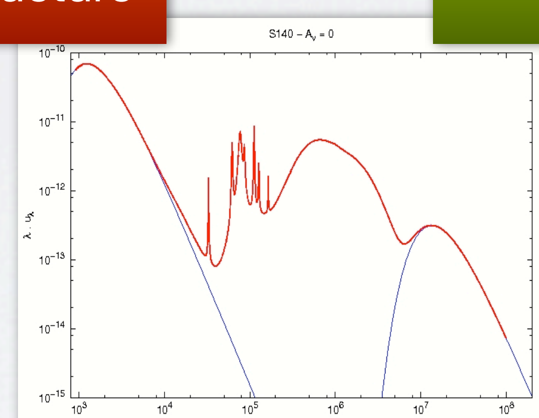



**Meudon PDR code**
Chemical & thermal structure

SimDAP

**Radiative transfer code**
Molecules excitations

Line intensity



**DUSTEM**
Grains emission / temperature

*SLAP*

*SLAP*

**Atomic & Molecular Databases**
**(VAMDC)**