SO5 - Plateforme MIS & Jets

Colloc PCMI - 2014.10.30 - Rennes

Plateforme MIS & Jets

Labellisation SO5 by INSU / CSAA in 2012

Goal: Give access to state-of-the-art numerical codes and tools to **prepare** and **interpret** observations in molecular regions

Theoretical services based on reference codes :
- Meudon PDR code
- Paris-Durham Shock Code
- Ramses MHD simulations / Starformat
+ others
- turbulence (TDR)
- …

Scientists: Franck Le Petit, Patrick Hennebelle, Benjamin Godard, Antoine Gusdorf Evelyne Roueff, François Levrier, Sylvie Cabrit, Jacques Le Bourlot, Emeric Bron, Pierre Lesaffre

Software engineers: David Languignon, Nicolas Moreau, Jean-François Rabasse, Carlo-Maria Zwölf

Collaborators: Andréa Ciardi, Edith Falgarone, Maryvonne Gerin, Suzanne Madden, Zakaria Meliani, Guillaume Pineau des Forêts, Chantal Stehlé

The ISM platform services

Downloadable source codes

- PDR Code
- Paris-Durham Shock code

Data bases

- PDR Database
  - Clouds structure
  - Line intensifies / Column densities

- STARFORMAT
  - MHD Simulations / ISM gas dynamics
  - Post-treatment : radiative transfer (RADMC-3D)

- Paris-Durham Shock Models
  - Structure physico-chimique de chocs MHD

Documentations & Support

- Specific code developments asked by users
- Help to use services / codes

Online codes

- Online computing ressources

- Paris-Durham Shock Code
- Meudon PDR Code
- TDR Code
- …

Tools

- Data extractor
- Chemistry analyser

Online services

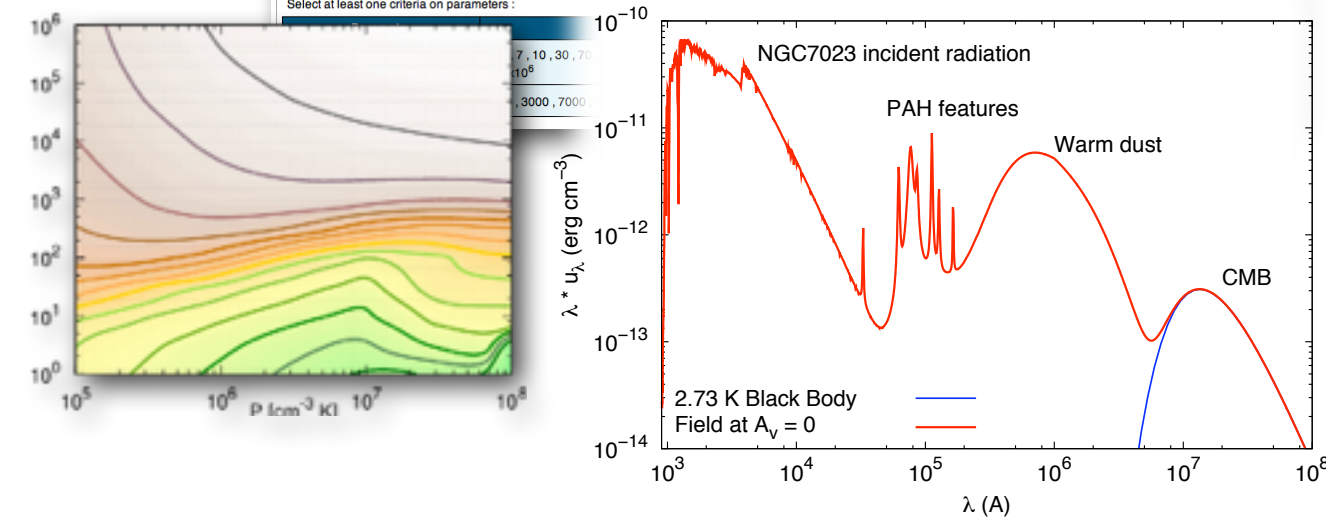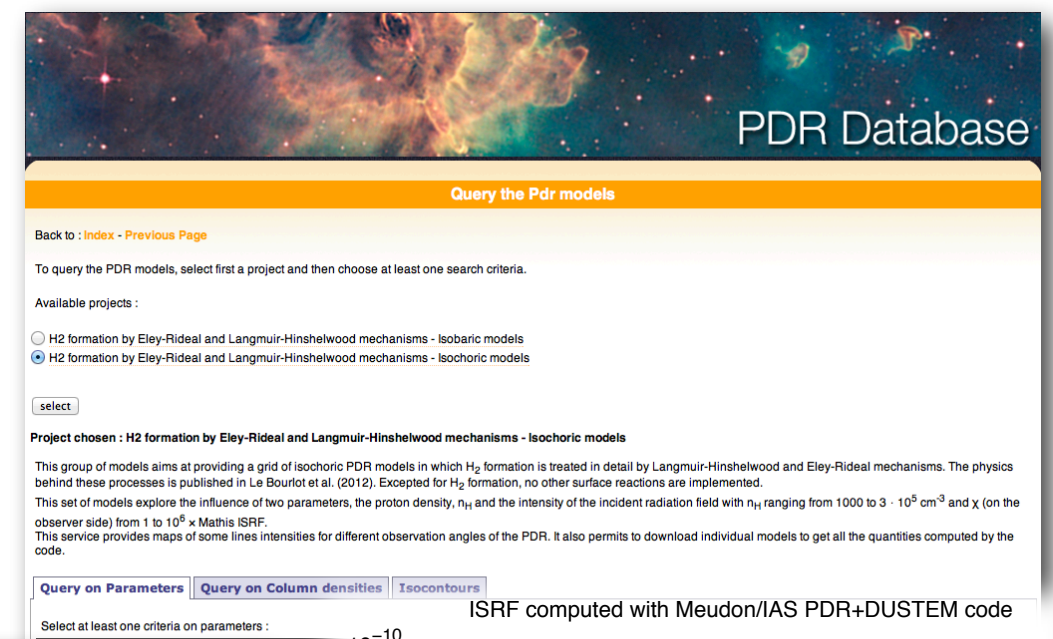- Data mining tools (inverse problems)
- ALMA Simulator

PDR Database - version 1

Publish large numbers of pre-computed models
- Diffuse gas
- PDRs
- Dark clouds (with surface chemistry)
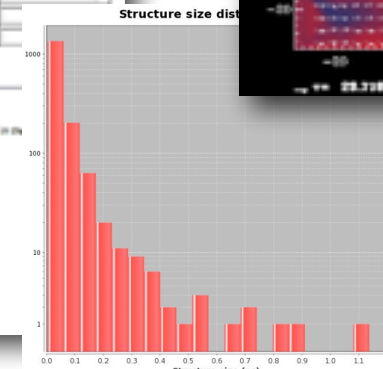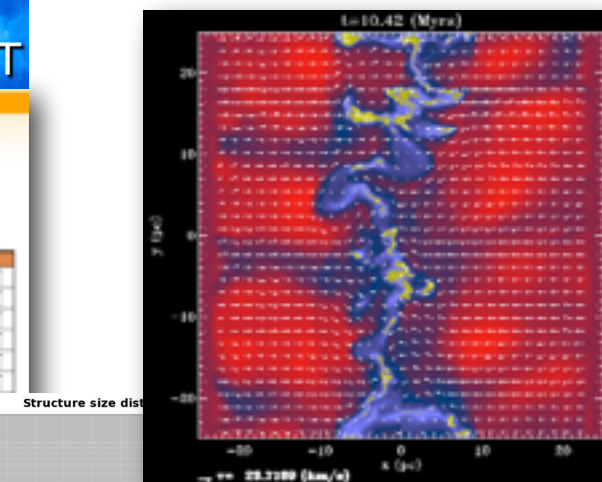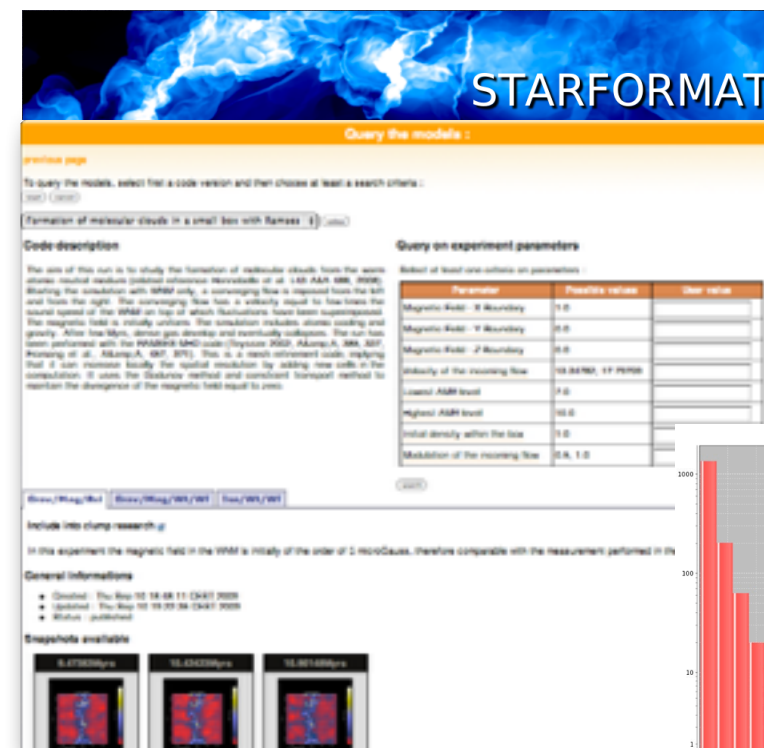- Galactic & Extragalactic ISM

Access to
- column densities & line intensities
- cloud structure (densities, temperature, …)

Starformat (CEA / IRFU - ZAH)

(P. Hennebelle et al.)

- MHD simulations
  - Dense cores & other projects
  - Clumps : Masse distribution, …

- Post-treatment to compute observables
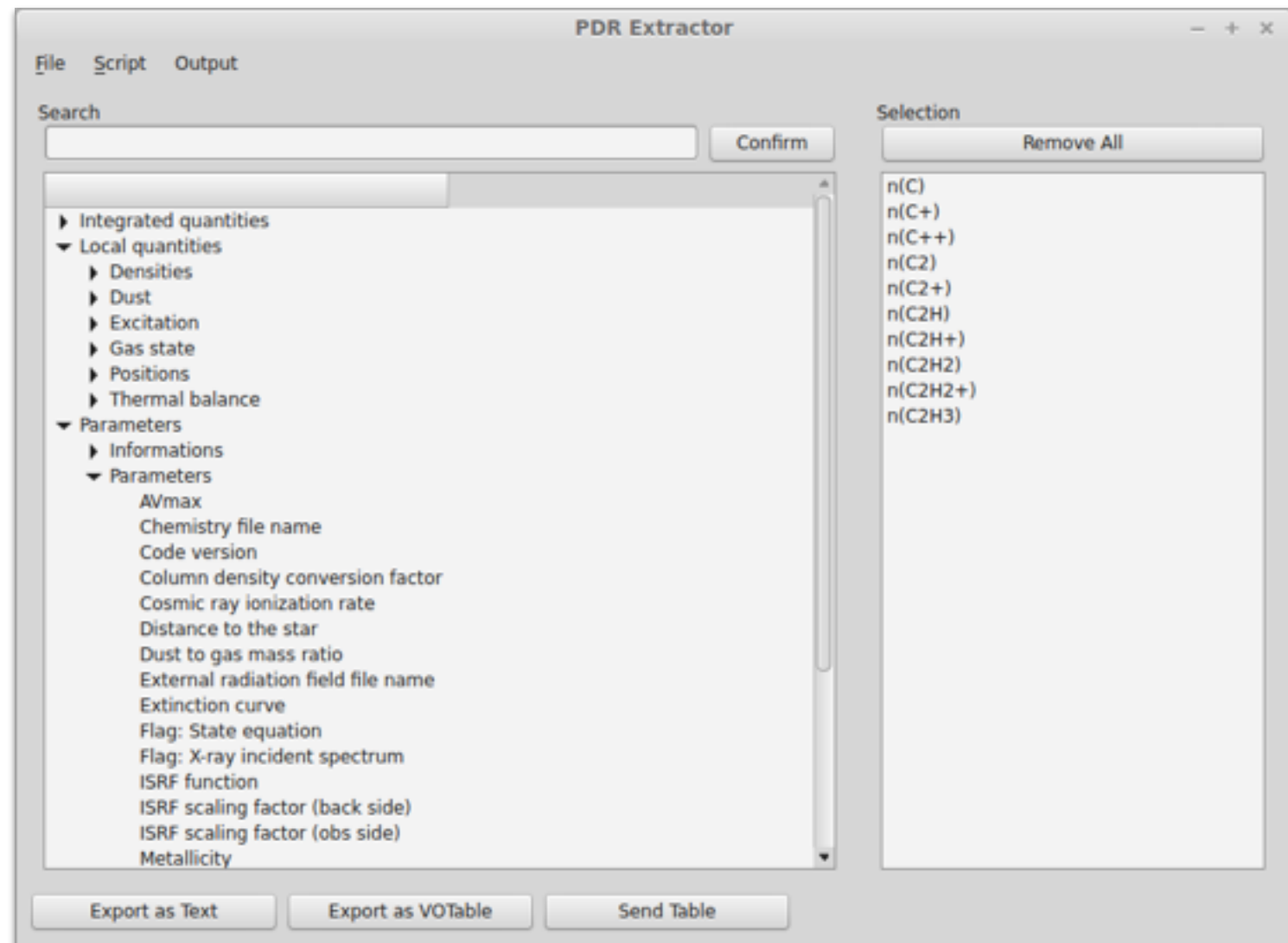 (RADMC-3D)

Tools

Simplify the analyse/handling of code results

➔ several tools will be developed to manipulate the results of the ISM codes

• New data format : HDF5

• New data extraction tool

• VO compatible (VO-Table & SAMP)

Interpretation of detailed observations (many constraints) requires to launch hundreds models
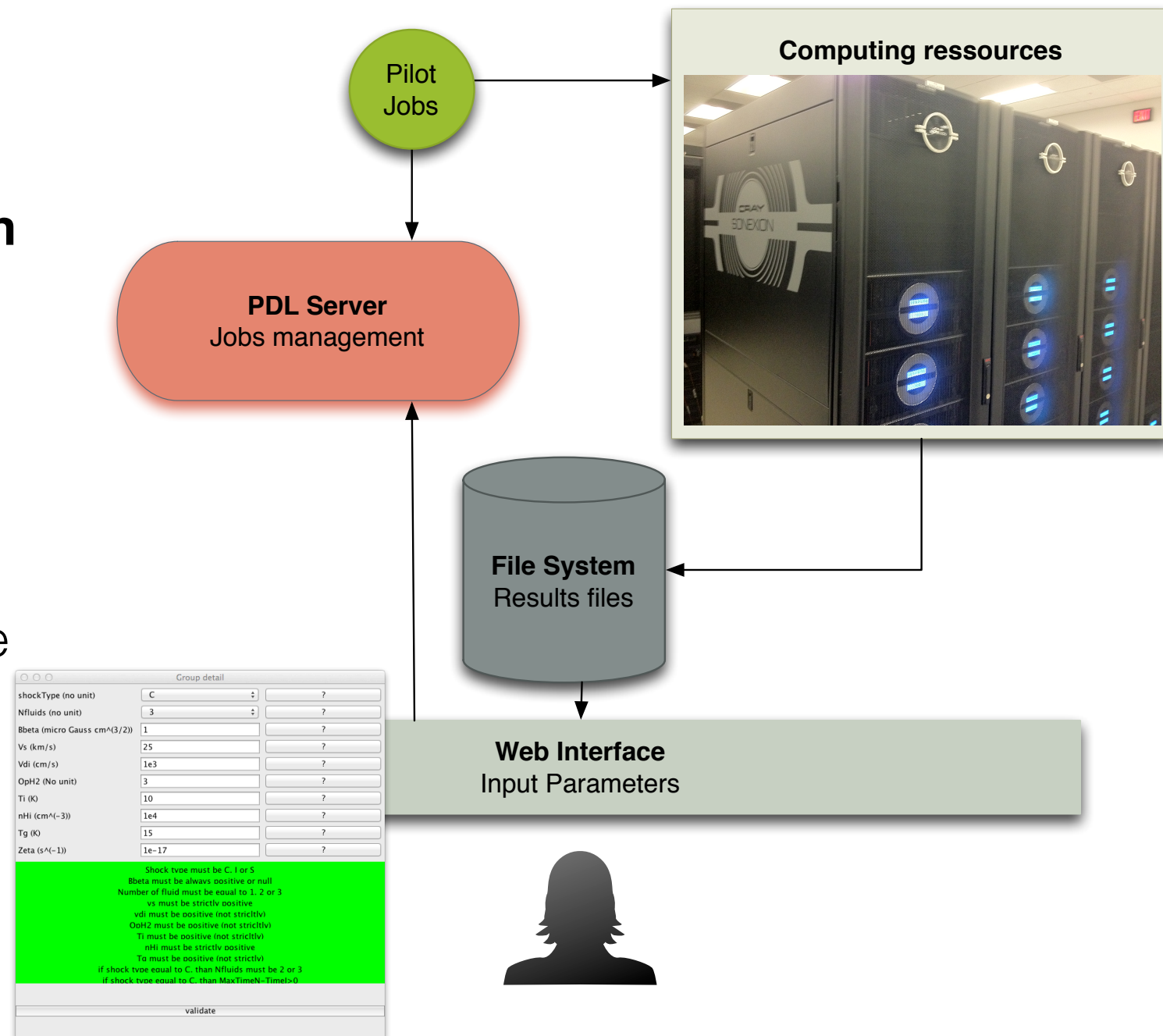PDR code & Shock code may require several tens minutes to several days of computation for 1 run

→ Online code service :
• Access to codes & **computing ressources** at Paris Observatory
• Download results - **Turn Key Solution**

Features
• Based on PDL IVOA standard
• System checks consistency of input parameters by users
• Follow evolution of jobs online
• User receive an email when results are ready to download

• Shock code available at http://ism.obspm.fr *(new interface soon)*
• PDR code will follow

Pilot Jobs

Computing ressources

PDL Server
Jobs management

File System
Results files

Web Interface
Input Parameters

shockType (no unit)	C	?
Nfluids (no unit)	3	?
Bbeta (micro Gauss cm^(3/2))	1	?
Vs (km/s)	25	?
Vdi (cm/s)	1e3	?
OpH2 (No unit)	3	?
Ti (K)	10	?
nHi (cm^(-3))	1e4	?
Tg (K)	15	?
Zeta (s^(-1))	1e-17	?

Shock type must be C. I or S
Bbeta must be always positive or null
Number of fluid must be equal to 1. 2 or 3
vs must be strictly positive
vdi must be positive (not strictly)
OpH2 must be positive (not strictly)
Ti must be positive (not strictly)
nHi must be strictly positive
Tg must be positive (not strictly)
if shock type equal to C. than Nfluids must be 2 or 3
if shock type equal to C. than MaxTimeN−Time1>0

validate

New database needs

Yesterday challenge:
Search by model inputs :
What is the CO(15-14) intensity in a cloud of density $n_H = 10^4$ cm^{-3}, $G_0 = 1000$?

Today challenge:
What are the PDR models having I(CO 15-14) ~ 3 10^{-8} W m^{-2} sr^{-1}
(i.e **Search by model outputs**)

Goal of the new PDR Database :
• Publish grids of PDR models
• Solve inverse problems at first order
• **Develop an architecture that can be re-used for other codes** (Ex: Shock Database)
• Combine different models for non spatially resolved observations *(later)*

New database challenges

Technical challenges
- Large number of metadata to manage

NRAO Archives :
- more complex instruments
- Web form has now 23 search parameters

General Search Parameters :

Telescopes ☑All ☐Jansky VLA ☐Historical VLA ☐VLBA ☐GBT

Project Code
GBT:
AGBT12A_055
JVLA: 12A-256

Project Session

Dates From

Observer Name

Archive File ID (partial strings allowed)

To
(2010-06-21 14:20:30)

Position Search :

Target Name

Search Type [SIMBAD or NED ▼]

Min. Exposure (secs)

RA or Longitude (04h33m11.1s or 68.29d)

DEC or Latitude (05d21'15.5" or 5.352d)

Equinox [J2000 ▼]

Search Radius 1.0'
(1d00'00" or 0.2d)

- OR - ☐ Check for automatic VLA field-of-view, freq. dependent. ??

Observing Configurations Search :

Telescope Config ☑All ☐A ☐AB ☐BnA ☐B ☐BC ☐CnB
☐C ☐CD ☐DnC ☐D ☐DA

Observing Bands ☑All ☐4 ☐P ☐L ☐S ☐C
☐X ☐U ☐K ☐Ka ☐Q ☐W

Sub_array ☑All ☐1 ☐2 ☐3 ☐4 ☐5

Frequency Range
(In MHz : 1665.401 - 1720.500)

Polarization [ALL ▼]

Receiver ID [ALL ▼]

Data Type [ALL ▼]

Backend ID [ALL ▼]
((GBT only - select GBT in Telescopes list))

PDR Database
- Version 1 : ~ 10 search parameters
- Version 2 : **+150 000 search parameters !**
  - column densities
  - lines intensities
  - levels populations

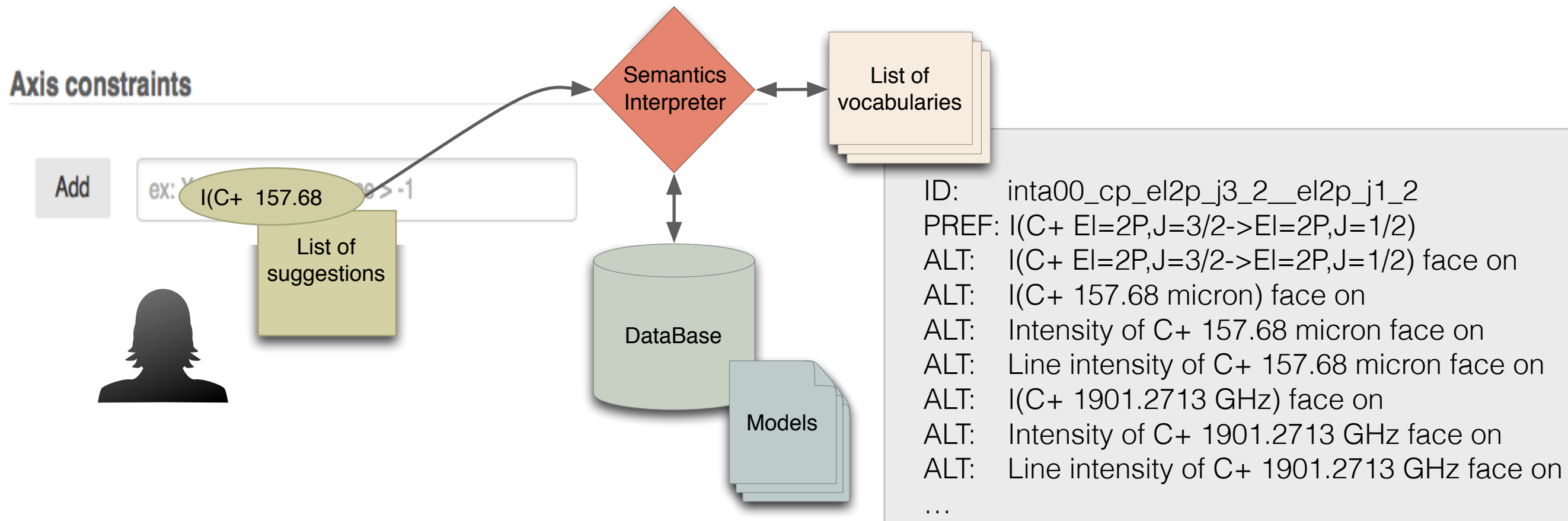➔ New informatics technologies required !

Intelligent metadata management

- New database technologies to manage really large number of metadata
- Human friendly interface

➔ Web semantics

Simple form :
- Google bar
- Users enter their query in human-like language
- The system interprets the query and "understands" what it means
- Web semantics / Synonyms

Axis constraints

Add   ex: X ... > -1

I(C+ 157.68)

List of suggestions

Semantics Interpreter

List of vocabularies

DataBase

Models

ID: inta00_cp_el2p_j3_2__el2p_j1_2
PREF: I(C+ El=2P,J=3/2->El=2P,J=1/2)
ALT: I(C+ El=2P,J=3/2->El=2P,J=1/2) face on
ALT: I(C+ 157.68 micron) face on
ALT: Intensity of C+ 157.68 micron face on
ALT: Line intensity of C+ 157.68 micron face on
ALT: I(C+ 1901.2713 GHz) face on
ALT: Intensity of C+ 1901.2713 GHz face on
ALT: Line intensity of C+ 1901.2713 GHz face on
…

Inverse problems service

Example : Interpretation of FUSE Observations towards HD 102065
Nehmé et al. (2008)

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)	$\pm 1.5 (−7)$
$N(C\ I^*_{J=1})/N(C\ I)$	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)	$\pm 0.85 (−6)$
$N(CH)/N(H_2)$	8.4 (−9)	1.85 (−8)	$\pm 0.3 (−8)$
$N(CN)/N(H_2)$	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)	

Observed quantities
- Column densities of H_2, C, CO
- T_{01} with H_2 J=0 and J=1
- Line intensity of C^+ at 158 μm

Inverse problems service

ISMServices   PDR Grid Search

Plot axis

x: nH (input parameter)   ☐ log scale
y: ISRF scaling factor (observer side)   ☐ log scale

Fixed axis

AVmax   0.5

Axis constraints

Add   ex: X-ray power law slope > -1
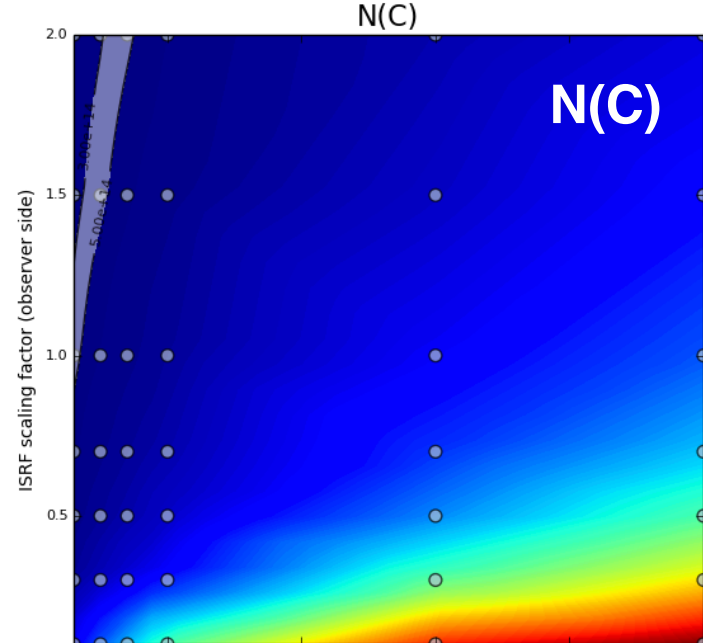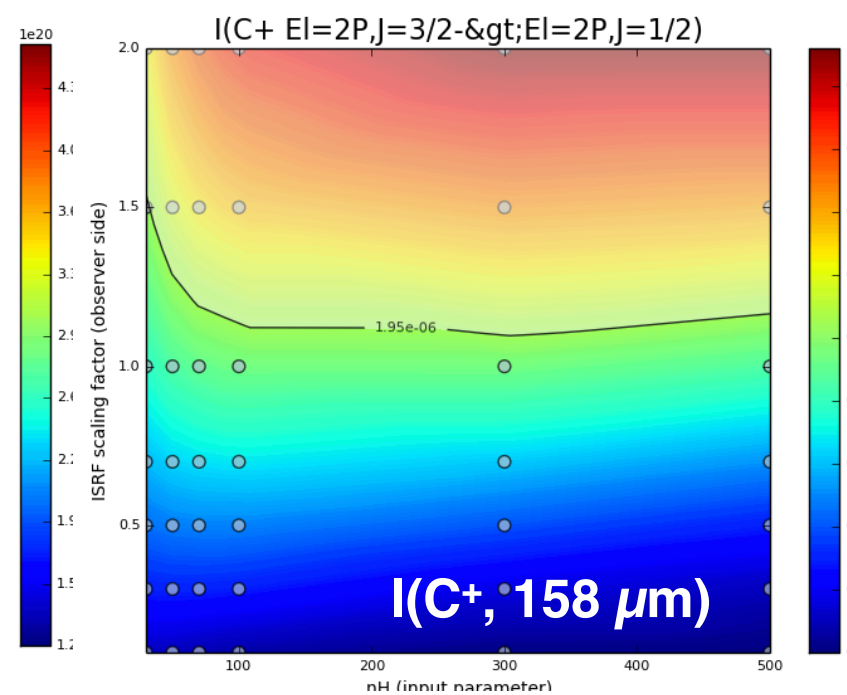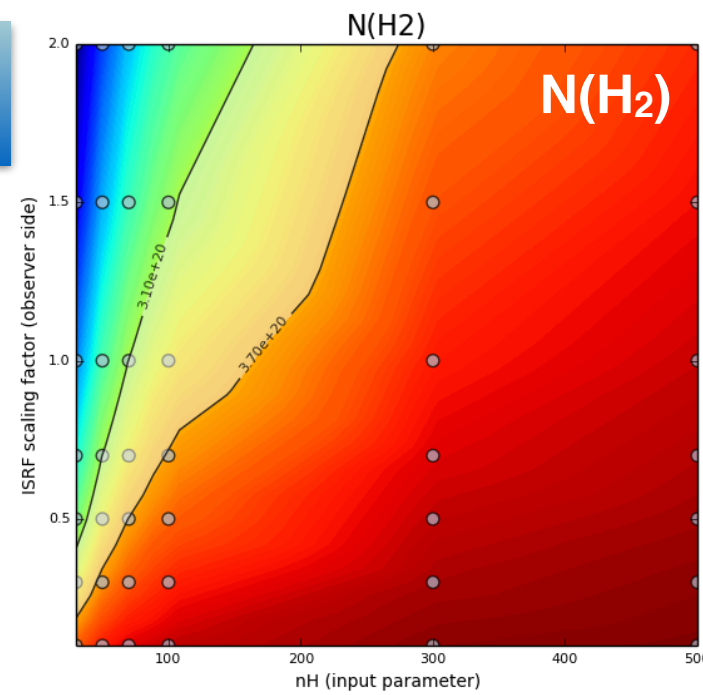
N(H2) > 3.1E20
N(H2) < 3.7E20
N(C) > 3.0E14
N(C) < 5.0E14
I(C+ El=2P,J=3/2->El=2P,J=1/2) > 1.95E-6
I(C+ El=2P,J=3/2->El=2P,J=1/2) < 3.65E-6

Plot

Query :
$3.1E20 < N(H_2) < 3.7E20$
$3.0E14 < N(C) < 5.0E14$
$1.9E-6 < I(C+, 158 \mu m) < 3.6E-6$
$62 < T01 < 72$

① select what you are looking for
Example : density & UV radiation field

② fix some quantities
Example : size of the cloud (A_V)

③ Enter the observed quantities

Inverse problems service

ISMServices PDR Grid Search

Plot axis

x: nH (input parameter) ▾   ☐ log scale

y: ISRF scaling factor (observer side) ▾   ☐ log scale

Fixed axis

AVmax ▾   0.5 ▾

Axis constraints

Add   ex: X-ray power law slope > -1

N(H2) > 3.1E20
N(H2) < 3.7E20
N(C) > 3.0E14
N(C) < 5.0E14
I(C+ El=2P,J=3/2->El=2P,J=1/2) > 1.95E-6
I(C+ El=2P,J=3/2->El=2P,J=1/2) < 3.65E-6

Plot

Query :

$$3.1E20 < \quad N(H2) \quad < 3.7E20$$
$$3.0E14 < \quad N(C) \quad < 5.0E14$$
$$1.9E-6 \ < \ I(C+, 158 \ \mu m) \ < 3.6E-6$$
$$62 \ < \quad T01 \quad < 72$$

N(H₂)

I(C⁺, 158 μm)

N(C)

T₀₁

χ²
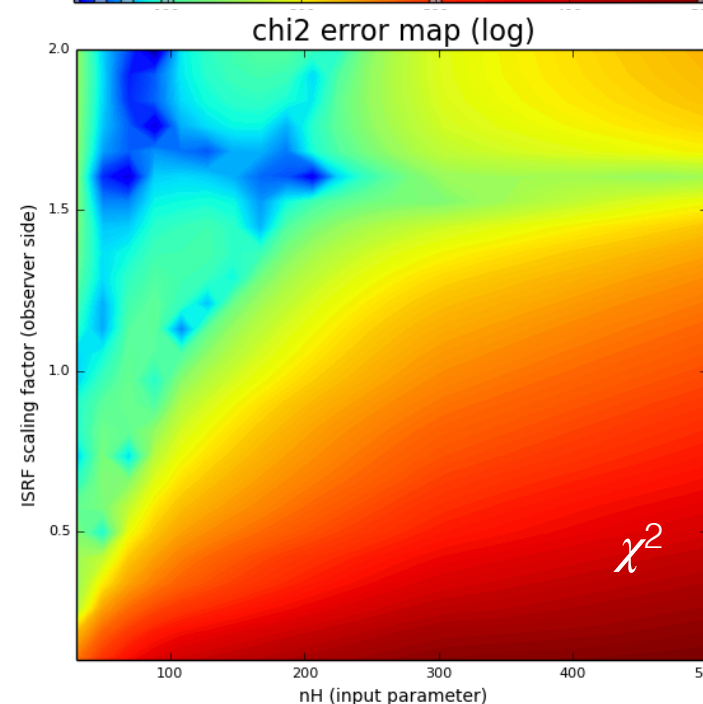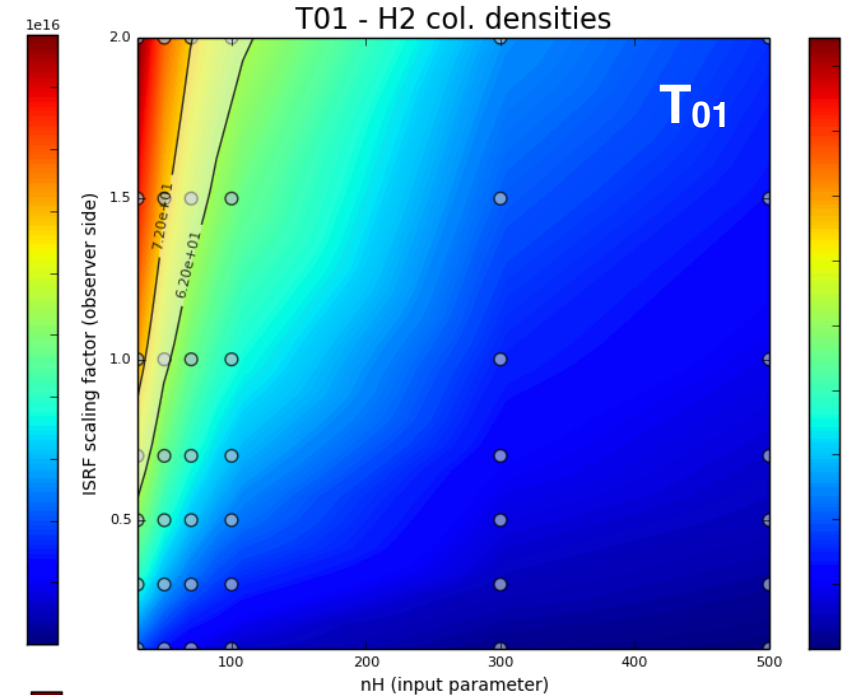
Results :
- $n_H \sim 100$ cm^{-3}
- $G_0 \sim 1.7$ Mathis

Inverse problems service

Get results in a few minutes instead of weeks / months of work
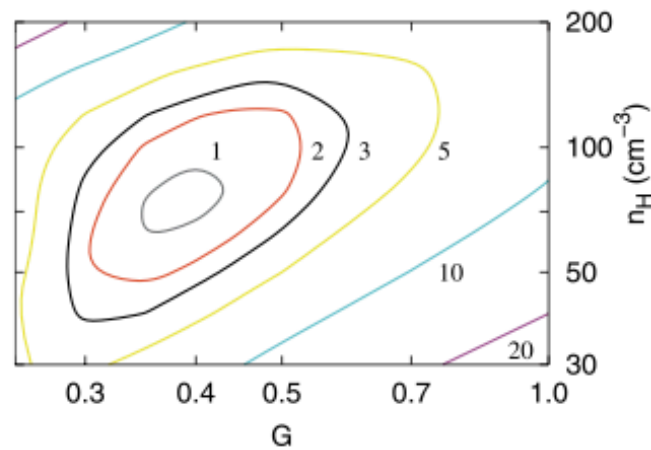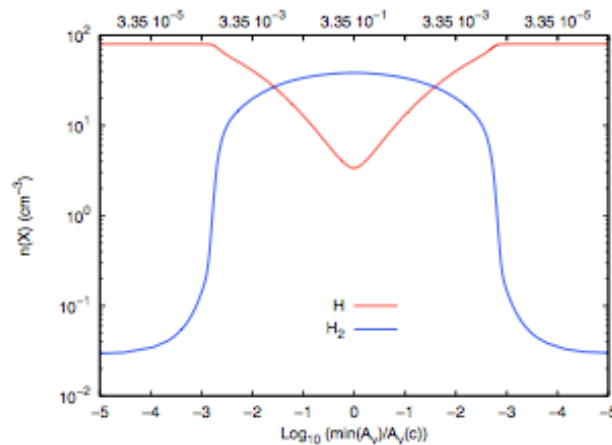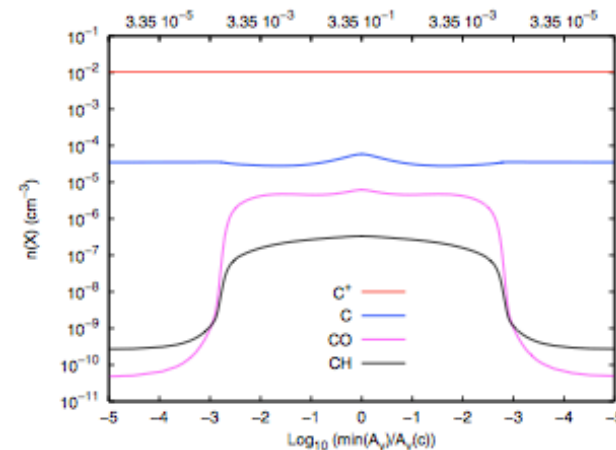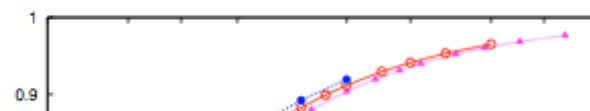
Once one / several models are found :

Functionalities on each model
- Download all models results
- Extraction of some quantities
  - Abundance profiles
  - Temperature profiles
  - Line intensities
  - Column densities
  - Spectra
  - …

Pôle thématique national

Evolution towards a Pôle thematique national SO5 (asked by INSU)
- Plateforme MIS & Jets
- Service DustEM

Pole thématique national de diffusion des modèles de référence pour la matière interstellaire

Plateforme MIS & Jets

Service DustEM

PDR | Shock | Starformat | …
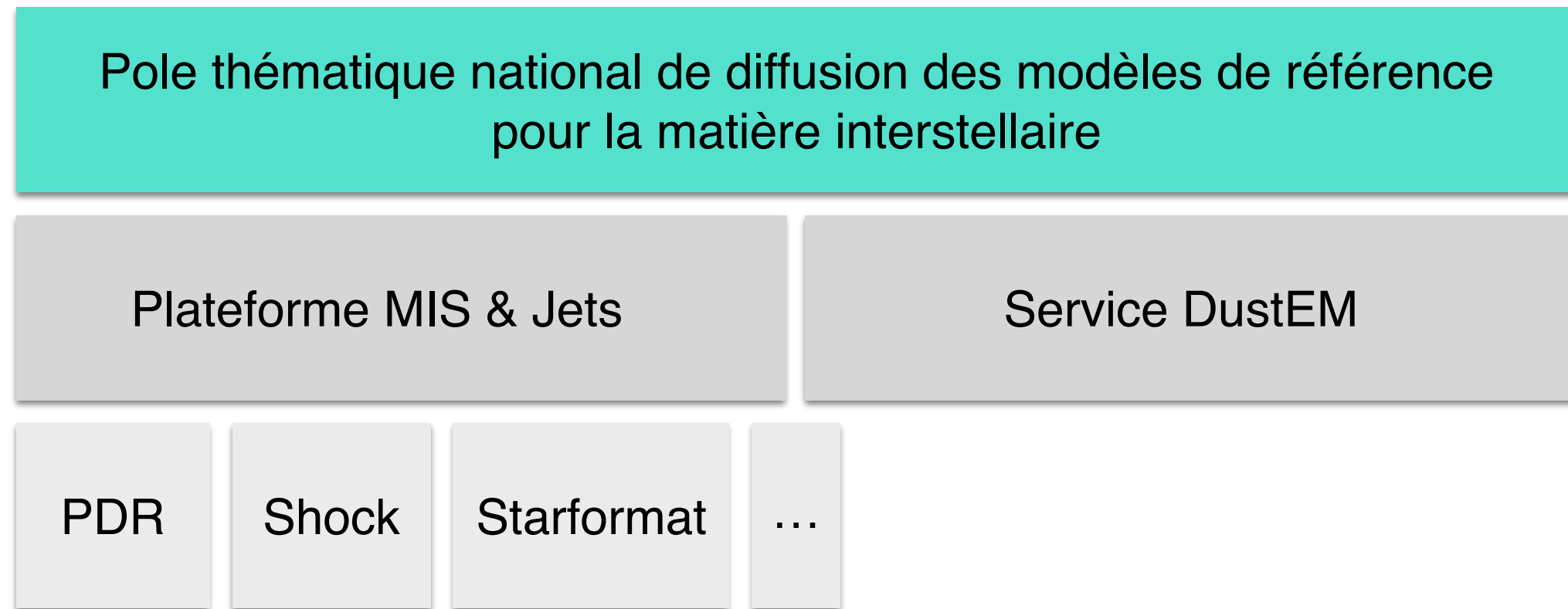
National programs
- PCMI
- PNCG
- PNPS

Need to set up an executive committee
- Participation of representatives of PN
- Responsible of services
- Users
- …

ISM platform access

http://ism.obspm.fr
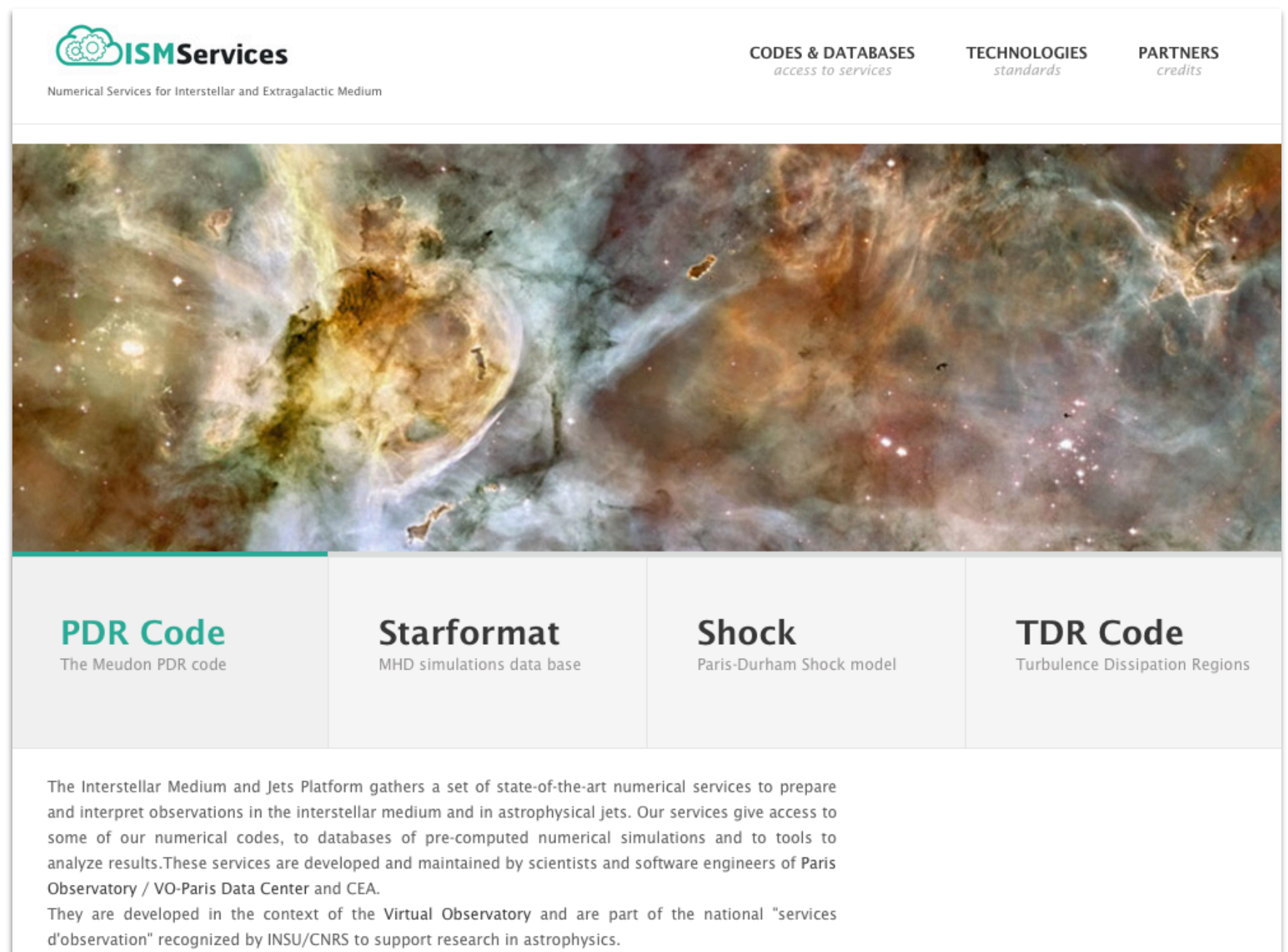
Replace progressively old websites like pdr.obspm.fr

Access to:
- PDR source code
- PDR Light source code
- PDR database (v1)
- Starformat
- Shock code online
- Documentations
- **Registration to mailing list**

Soon
- PDR Database with data mining
- New Shock interface

ANNEXE

Interoperability

Developed following VO standards & integrated in a single platform
- Interoperability between services

Levrier et al. (2012)