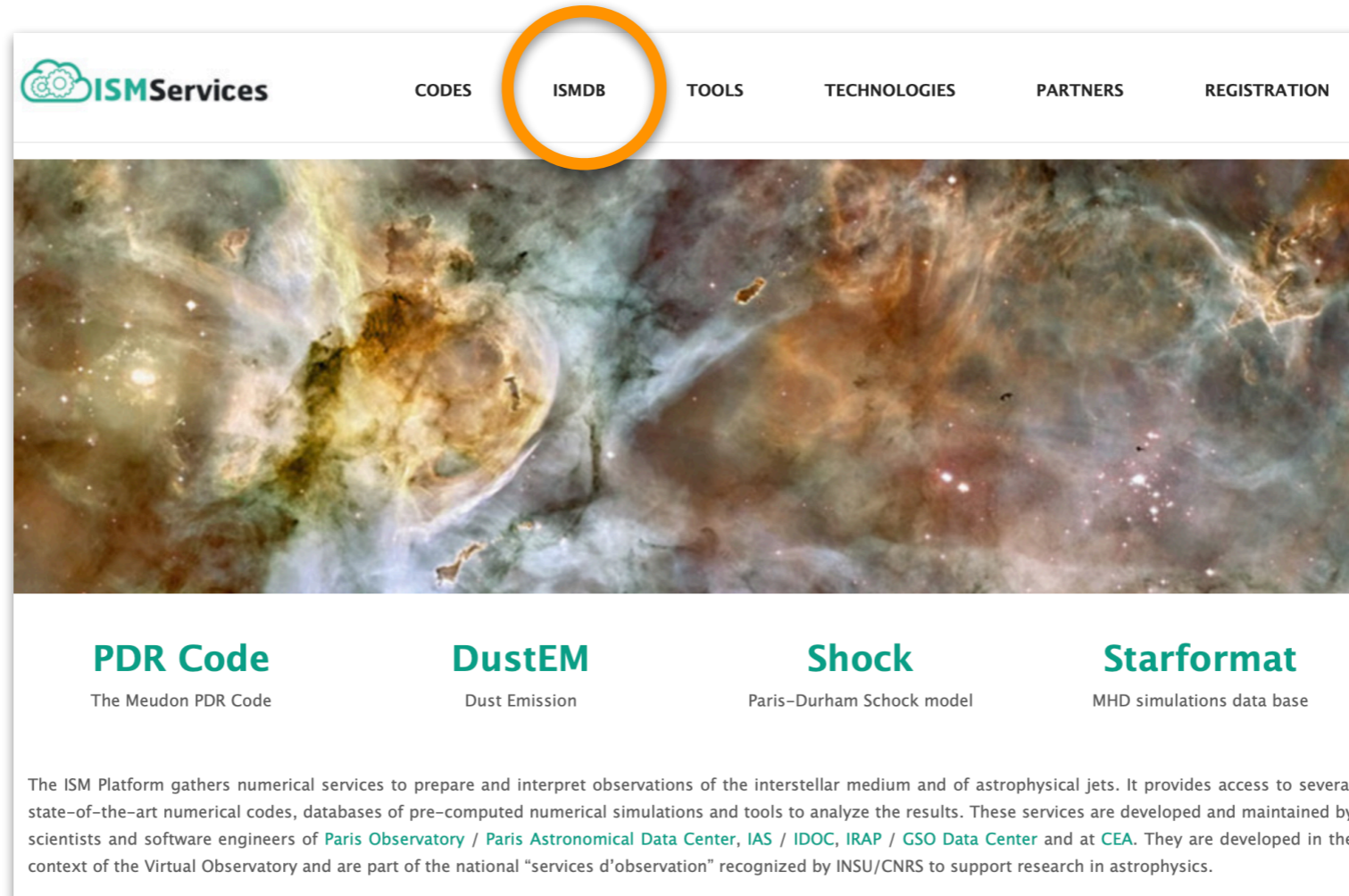


ISMDB

Publication in ISMDB

<http://ism.obspm.fr>

Franck Le Petit, David Languignon, Nicolas Moreau, Emeric Bron



The screenshot shows the ISM Services website. The navigation bar includes 'ISMServices', 'CODES', 'ISMDB' (circled in orange), 'TOOLS', 'TECHNOLOGIES', 'PARTNERS', and 'REGISTRATION'. Below the navigation bar is a large image of a colorful nebula. Underneath the image are four service cards: 'PDR Code' (The Meudon PDR Code), 'DustEM' (Dust Emission), 'Shock' (Paris-Durham Schock model), and 'Starformat' (MHD simulations data base). At the bottom of the screenshot is a paragraph of text describing the ISM Platform's mission and its partners.

The ISM Platform gathers numerical services to prepare and interpret observations of the interstellar medium and of astrophysical jets. It provides access to several state-of-the-art numerical codes, databases of pre-computed numerical simulations and tools to analyze the results. These services are developed and maintained by scientists and software engineers of Paris Observatory / Paris Astronomical Data Center, IAS / IDOC, IRAP / GSO Data Center and at CEA. They are developed in the context of the Virtual Observatory and are part of the national "services d'observation" recognized by INSU/CNRS to support research in astrophysics.

<http://ism.obspm.fr>

Get astrochemistry models to :

prepare observations

- telescope exposure times
- detectability of molecular tracers

interpret observations

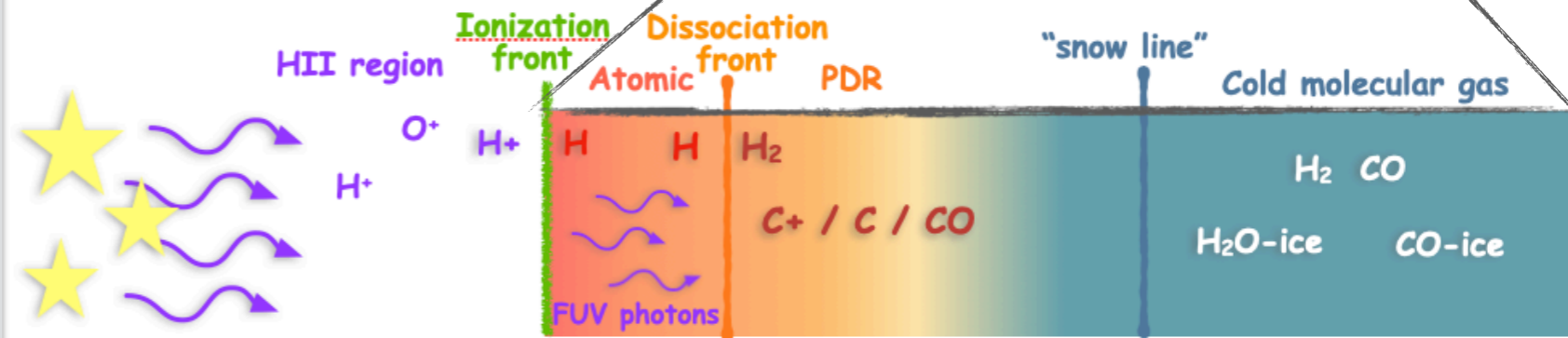
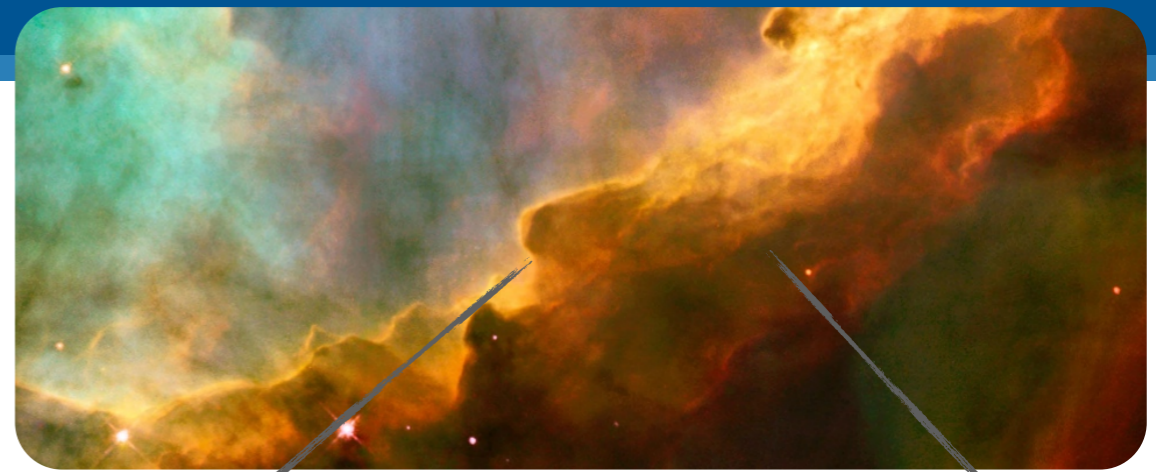
analyse the physics and chemistry in the ISM

PDR code

PDR code:

- computes the atomic and molecular structure of interstellar clouds.
- analysis of physical and chemical processes

- abundances of hundreds species
- excitation in levels
- gas & grains temperatures
- Intensities (H_2 , CO, H_2O , ...)
- Column densities of species

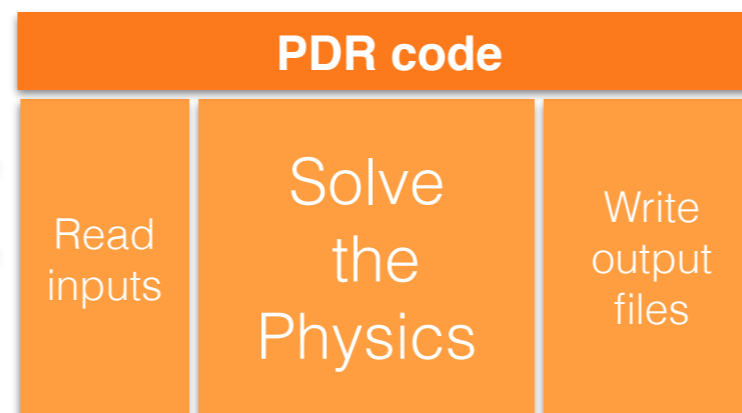


Main parameters:

- UV intensity radiation field
- density, pressure
- metallicity and elemental abundances
- cosmic ray ionisation rate

Atomic & molecular data

- lines
- quantum levels
- collision rates
- chemical reaction rates
- photo-reaction cross sections



- Chemical density profiles
- Gas temperature profile
- Grain temperature profile
- Population in quantum levels
- Chemical reaction rates
- Line intensities
- Column densities
- Spectra

Observation interpretation

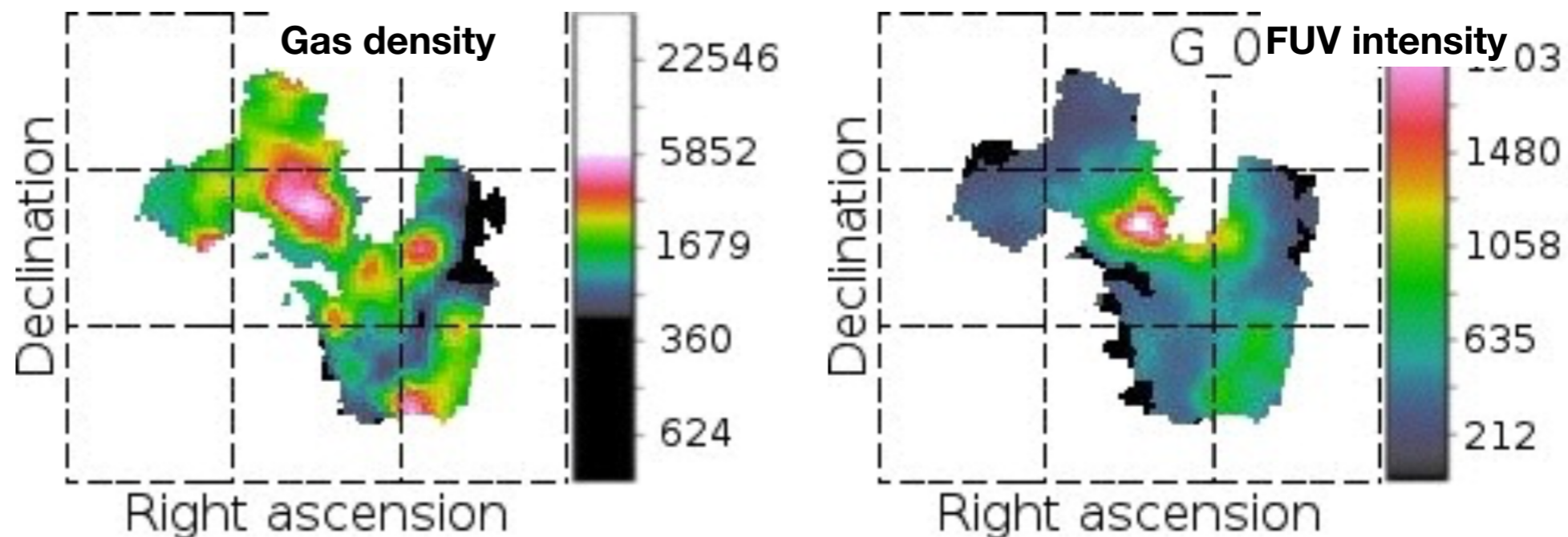
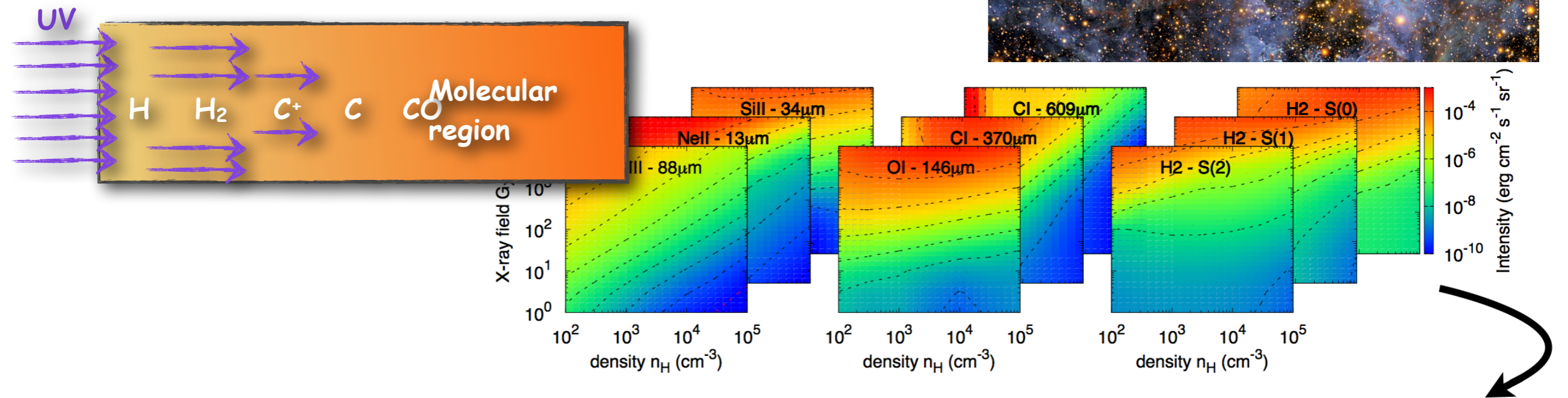
Interpret observations → Grids of models

~ +100 to +1000 models

~ 1 week of computation time

Extract simulated line intensities

Find best models at each position of the observed map



IVOA Standards for Theory

① Simulation Data Model (SimDM)

- Description of simulations
- Meta-model
- Designed to describe most simulations

IVOA Recommendation

International Virtual
Observatory Alliance

IVOA Documents



Simulation Data Model
Version 1.0

IVOA Recommendation 03 May 2012

Interest/Working Group:

<http://www.ivoa.net/twiki/bin/view/IVOA/IvoaTheory>

Author(s):

Gerard Lemson, Laurent Bourges, Miguel Cervino, Claudio Gheller, Norman Gray, Franck LePetit, Mireille Louys, Benjamin Ooghe, Rick Wagner, Herve Wozniak

Editor(s):

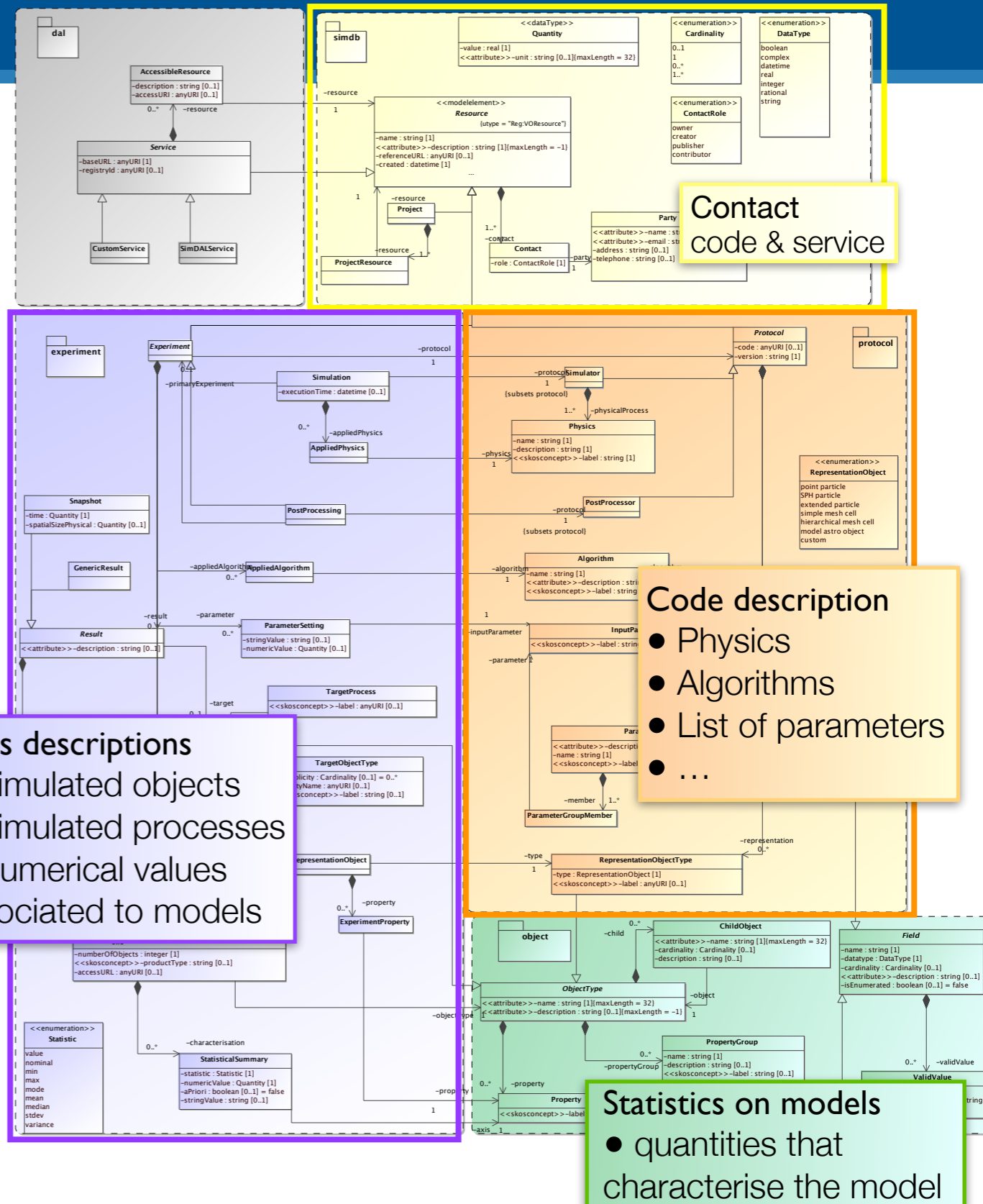
Gerard Lemson, Herve Wozniak

Abstract

In this document and the accompanying documents we describe a data model (Simulation Data Model) describing numerical computer simulations of astrophysical systems. The primary goal of this standard is to support discovery of simulations by describing those aspects of them that scientists might wish to query on, i.e. it is a model for meta-data describing simulations. This document does not propose a protocol for using this model. IVOA protocols are being developed and are supposed to use the model, either in its original form or in a form derived from the model proposed here, but more suited to the particular protocol. The SimDM has been developed in the IVOA Theory Interest Group with assistance of representatives of relevant working groups, in particular DM and Semantics.

Status of this document

This document has been produced by the Theory Interest Group. It has been reviewed by IVOA Members and other interested parties, and has been endorsed by the IVOA Executive Committee as an IVOA Recommendation. It is a stable document and may be used as reference material or cited as a normative reference from another document. IVOA's role in making the Recommendation is to draw attention to the specification and to promote its widespread deployment. This enhances the functionality and interoperability inside the Astronomical Community.



Contact
code & service

Code description

- Physics
- Algorithms
- List of parameters
- ...

Runs descriptions

- Simulated objects
- Simulated processes
- Numerical values associated to models

Statistics on models

- quantities that characterise the model

Use of SimDM in our services :

- learning curve to become experts
- very useful & powerful
- SimDM fulfilled all our requirements



② Simulation Data Access protocol (SimDAL)

- SimDAL Repository
 - SimDAL Search
 - SimDAL Cutout
- allow to discover & retrieve simulations

③ Semantics / SKOS vocabularies

- Algorithms
 - AstronomicalObjects
 - DataObjectTypes
 - PhysicalProcesses
 - PhysicalQuantities
- +300 000 specific ISM concepts (non IVOA) :

⊗ But no standard raw data format

→ a limitation to use the VO

SimDAL bypass this by exchanging VOTables for cutouts

Simulation Data Access Layer Version 1.0

IVOA Recommendation 20 March 2017

Interest/Working Group:

<http://www.ivoa.net/twiki/bin/view/IVOA/IvoaDAL>

Author(s):

David Languignon, Franck Le Petit, Carlos Rodrigo, Gerard Lemson, Marco Molinaro, Hervé Wozniak

Editor(s):

David Languignon, Franck Le Petit

Abstract

The Simulation Data Access Layer protocol (SimDAL) defines a set of resources and associated actions to discover and retrieve simulations and numerical models in the Virtual Observatory. SimDAL and the Simulation Data Model are dedicated to cover the needs for the publication and retrieval of any kind of simulations: N-body or MHD simulations, numerical models of astrophysical objects and processes, theoretical synthetic spectra, etc... SimDAL is divided in three parts. First, SimDAL Repositories store the descriptions of theoretical projects and numerical codes. They can be used by clients to discover theoretical services associated with projects of interest. Second, SimDAL Search services are dedicated to the discovery of precise datasets. Finally, SimDAL Data Access services are dedicated to retrieve the original simulation output data, as plain raw data or formatted datasets cut-outs. To manage any kind of data, eventually large or at high-dimensionality, the SimDAL standard lets publishers choose any underlying implementation technology.

Status of this document

This document has been produced by the Data Access Layer Working Group. It has been reviewed by IVOA Members and other interested parties, and has been endorsed by the IVOA Executive Committee as an IVOA Recommendation. It is a stable document and may be used as reference material or cited as a normative reference from another document. IVOA's role in making the Recommendation is to draw attention to the specification and to promote its widespread deployment. This enhances the functionality and interoperability inside the Astronomical Community.

Home Search concepts Help

This service is dedicated to scientists and VO developers who wish to publish theoretical services described by [the Simulation Data Model](#).

As described in the [IVOA](#) standard, Simulation Data Model, registrations of theoretical services, require to provide several URIs corresponding to semantics keywords describing services and simulations. VO-Theory concepts are based on SKOS description as recommended by [the IVOA Semantic Working Group](#).

Example of a VO-Theory URIs : <http://purl.obspm.fr/vocab/Algorithms/GaussSeidel>

This website is dedicated to the discovery of these URIs. Navigate through the broader, narrower, related terms to discover the most precise concept you wish.

To suggest new concepts or corrections, contact : support.votheory@obspm.fr.

Search concepts

3+1 Formalism 8-Wave Scheme Accelerated Lambda Iteration

Adaptive Mesh Refinement Advection Upstream Splitting Method

Algorithm Alternating Direction Implicit BiConjugate Gradient

BiConjugate Gradient Stabilized Block Based AMR

Bulirsch-Stoer Cell Based AMR Cell Centred

Central Difference Scheme Chebyshev Iteration

Conjugate Gradient Method Conjugate Gradient Squared Method

Constrained Transport Coupled Escaped Probability

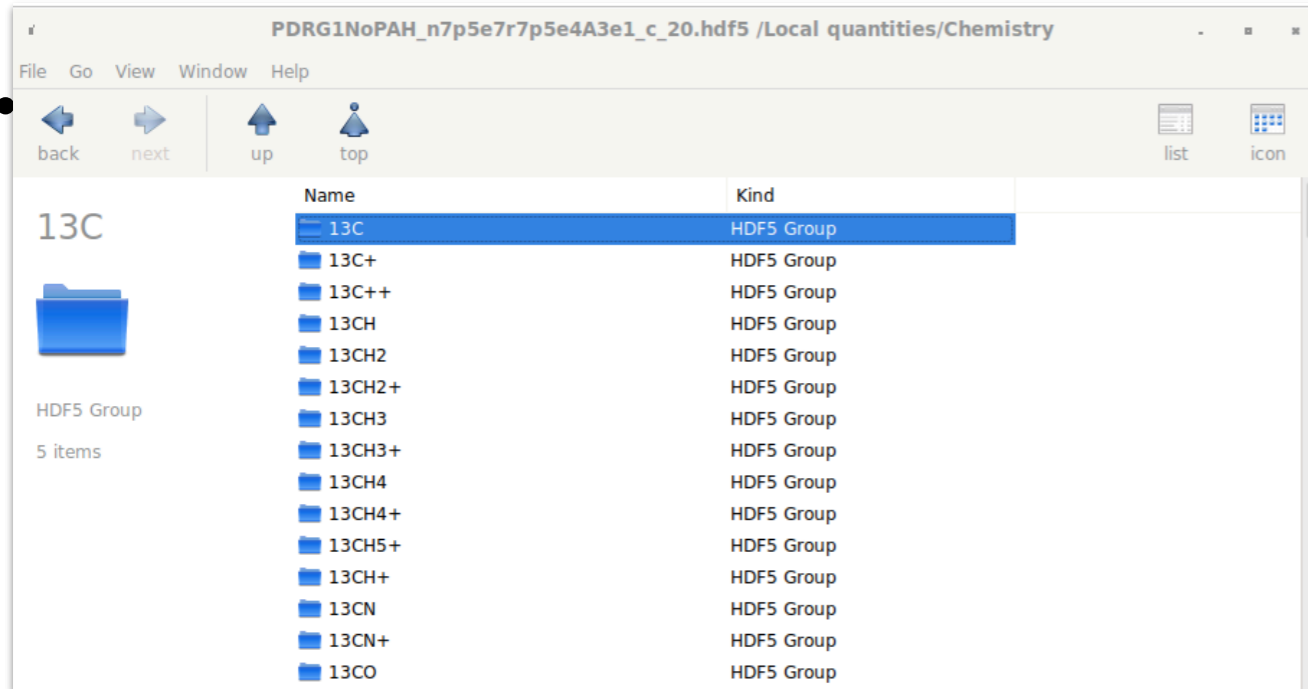
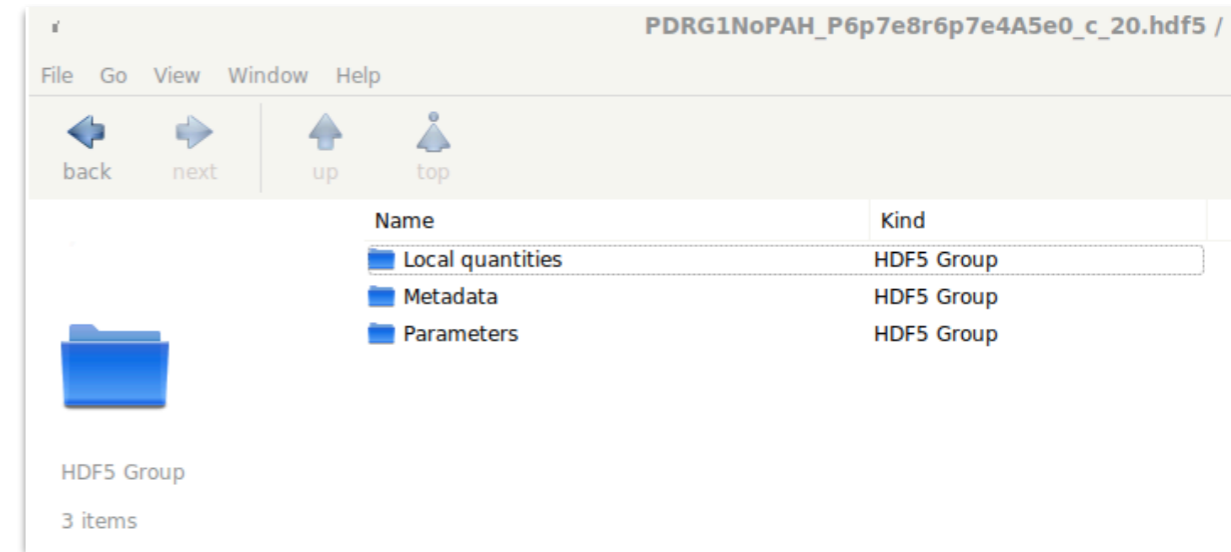
Crank-Nicolson Discontinuous Galerkin

Discontinuous Galerkin methods Escape Probability Euler

Output files & metadata

Output data produced by the PDR
Include SimDM metadata

- **HDF5 with a metadata table**
 - raw data (all quantities computed by the code)
 - metadata : datatype, utype, unit, SKOS concept, ...



The screenshot shows a metadata table with columns 0 through 7. The table contains 16 rows of data, each representing a different chemical species and its associated density and spectral data.

0	1	2	3	4	5	6	7	
Chemistry/13C_180	Densities 13C_180	0	dens_spec_13c_180	n(13C_180)	real	cm-3	http://purl.or	
Chemistry/13C	Densities 13C	0	dens_spec_13c	n(13C)	real	cm-3	http://purl.or	
Chemistry/13CH2	Densities 13CH2	0	dens_spec_13ch2	n(13CH2)	real	cm-3	http://purl.or	
Chemistry/13CH2+	Densities 13CH2+	0	dens_spec_13ch2p	n(13CH2+)	real	cm-3	http://purl.or	
Chemistry/13CH3	Densities 13CH3	0	dens_spec_13ch3	n(13CH3)	real	cm-3	http://purl.or	
Chemistry/13CH3+	Densities 13CH3+	0	dens_spec_13ch3p	n(13CH3+)	real	cm-3	http://purl.or	
Chemistry/13CH4	Densities 13CH4	0	dens_spec_13ch4	n(13CH4)	real	cm-3	http://purl.or	
Chemistry/13CH4+	Densities 13CH4+	0	dens_spec_13ch4p	n(13CH4+)	real	cm-3	http://purl.or	
Chemistry/13CH5+	Densities 13CH5+	0	dens_spec_13ch5p	n(13CH5+)	real	cm-3	http://purl.or	
9	/Local quantities/Chemistry/13CH	Densities 13CH	0	dens_spec_13ch	n(13CH)	real	cm-3	http://purl.or
10	/Local quantities/Chemistry/13CH+	Densities 13CH+	0	dens_spec_13chp	n(13CH+)	real	cm-3	http://purl.or
11	/Local quantities/Chemistry/13CN	Densities 13CN	0	dens_spec_13cn	n(13CN)	real	cm-3	http://purl.or
12	/Local quantities/Chemistry/13CN+	Densities 13CN+	0	dens_spec_13cnp	n(13CN+)	real	cm-3	http://purl.or
13	/Local quantities/Chemistry/13CO2+	Densities 13CO2+	0	dens_spec_13co2p	n(13CO2+)	real	cm-3	http://purl.or
14	/Local quantities/Chemistry/13CO	Densities 13CO	0	dens_spec_13co	n(13CO)	real	cm-3	http://purl.or
15	/Local quantities/Chemistry/13CO+	Densities 13CO+	0	dens_spec_13cop	n(13CO+)	real	cm-3	http://purl.or



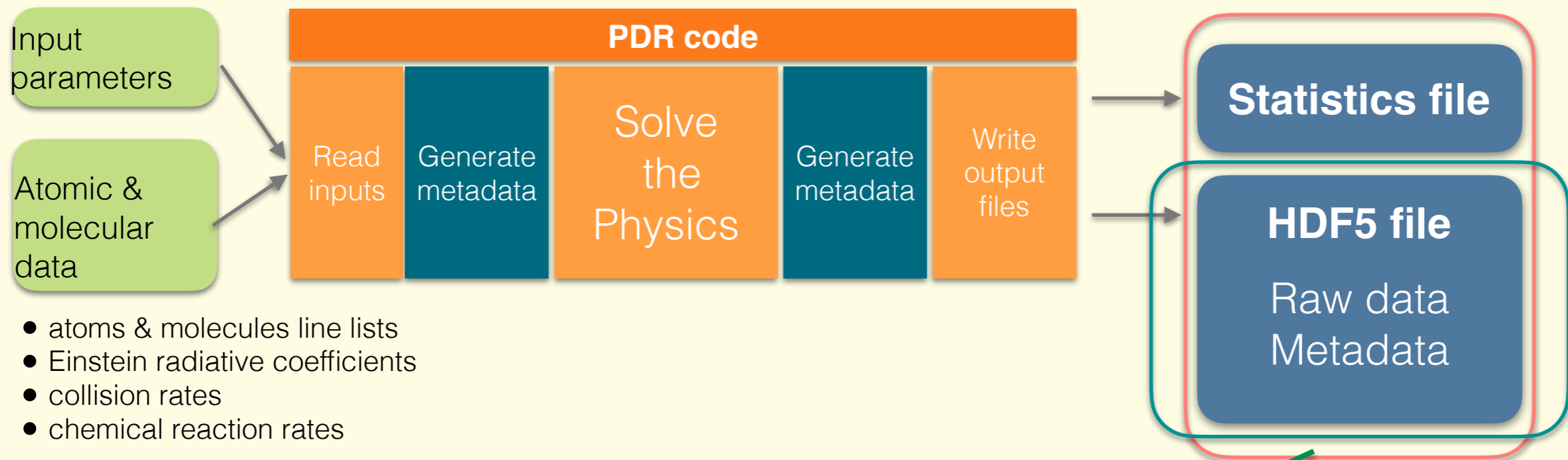
SimDM attributes

HDF5 : structure is not standardised

→ Worthwhile to have a discussion on the topic in the IVOA Theory I.G.

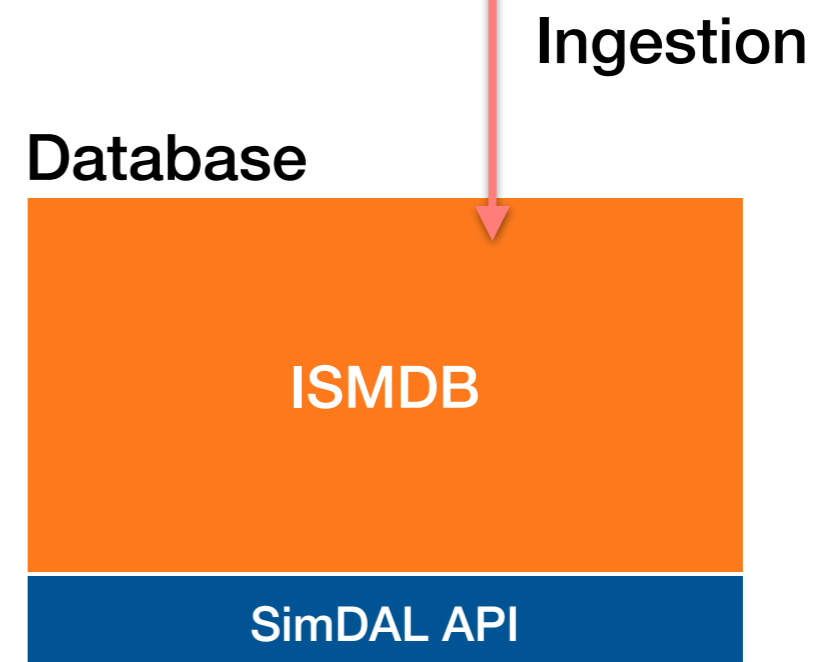
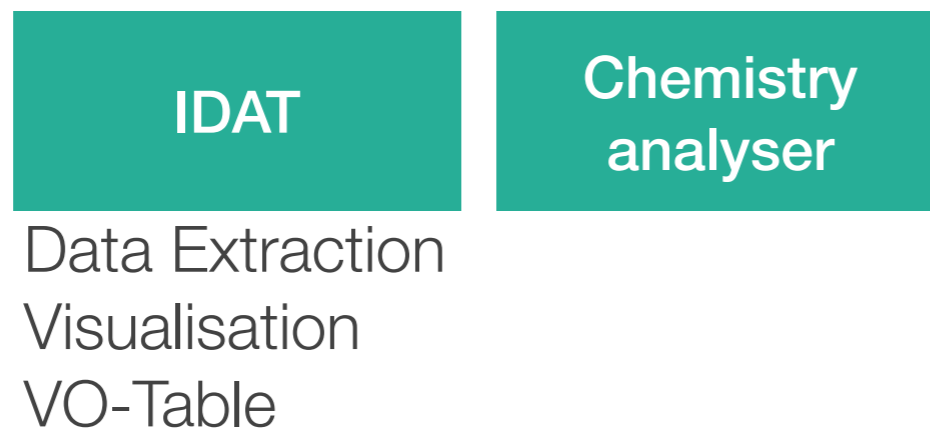
Mapping of PDR models on SimDM

The production of metadata for VO compatibility is **integrated inside the code**



Data produced by the code are complex

→ need to provide tools to read and manipulate the outputs

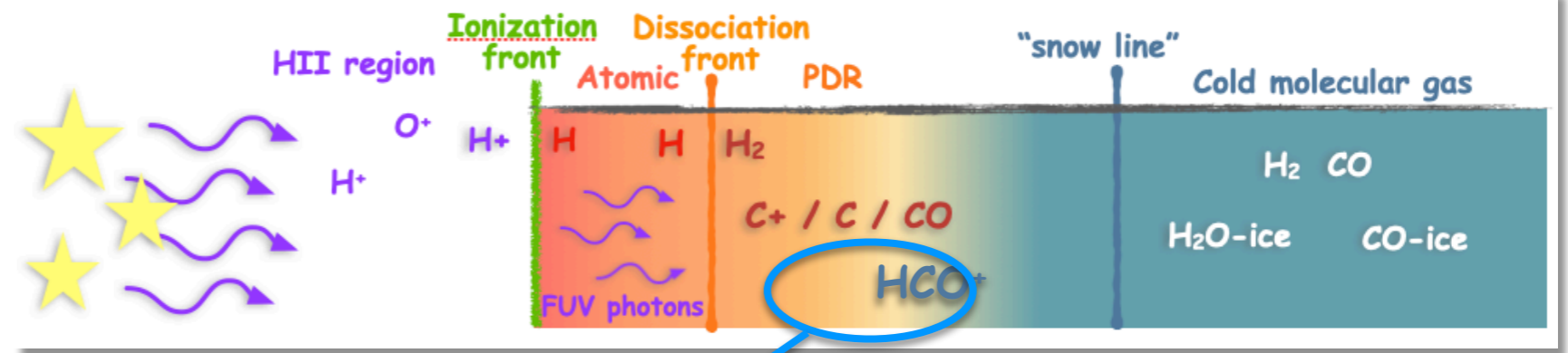


Tools : Chemistry Analyser

Tools : IDAT & Chemistry analyser

Web technologies

- Easier to maintain
- less compatibility problem between operating systems
- ISMPy : python virtual environment to facilitate installation



Profile installation

OrBarJ18_BestMod_c_20.hdf5



Temperature n(HCO+)

AV (mag)

1.0970813

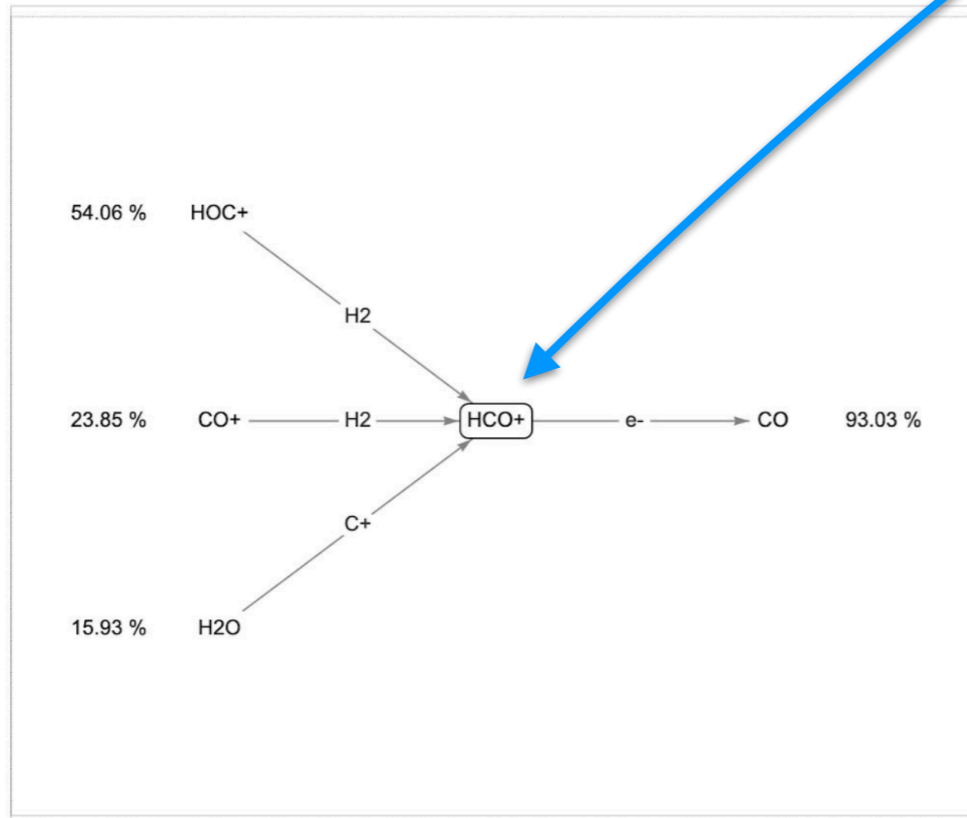
Species

n(HCO+) 3.62e-2 cm-3

HCO+ back

Quantities

Gas Grains



Gas conditions

ng(e-) 6.05e+1 cm-3
 nd(e-) -1.62e-3 cm-3
 nH 7.65e+5 cm-3
 Tg 5.39e+2 K
 UV 2.09e+11 cm-2 s-1
 zeta 5.00e-17 s-1 / H2

Formation of HCO+			Total formation rate 3.86e-7 cm-3 s-1		
A + B → C + D	n(A) (cm-3)	n(B) (cm-3)	k	rate (cm-3 s-1)	proportion
H ₂ + HOC ⁺ → H ₂ + HCO ⁺	3.22e+5	1.71e-3	3.80e-10	2.09e-7	54.06 %
H ₂ + CO ⁺ → H + HCO ⁺	3.22e+5	3.81e-4	7.49e-10	9.20e-8	23.85 %
H ₂ O + C ⁺ → H + HCO ⁺	2.61e+0	4.51e+1	5.22e-10	6.14e-8	15.93 %

Destruction of HCO+			Total destruction rate 3.86e-7 cm-3 s-1		
A + B → C + D	n(A) (cm-3)	n(B) (cm-3)	k	rate (cm-3 s-1)	proportion
HCO ⁺ + e ⁻ → H + CO	3.62e-2	6.05e+1	1.64e-7	3.59e-7	93.03 %

Web technologies :

- local installation
- integration as applications above ISMDB

ISMDB: Project browser & Search model by input parameters

2020 :

- Robustness of ISMDB code
- integration of various components in ISMDB

Project browser

ISMDB – Projects portal

Isobaric PDR 1.5.4 models June 18, 2020
Code: PDR 1.5.4 (2065), Project ID: PDRG1NoPAH_P_200618

Produced by Meudon ISM team

Explored parameters	min	max
AVmax	1	40 mag
Pressure	1e+05	1e+09 cm ⁻³ K
chi front	1	1e+05 ISRF

Description
This grid of isobaric PDR 1.5.4 models (revision 2065) covers photo-dominated regions conditions. Explored parameters are gas thermal pressure, UV field intensity and size of the clouds. The full grid contains 2129 2-side models where the back side of the cloud is submitted to the ISRF. The chemistry takes into account 239 species, including C and O isotopes, linked by 7700 chemical reaction. No surface reactions are considered excepted for H₂. H₂ formation model takes into account Eley-Rideal and Langmuir-Hinshelwood mechanisms as described in Le Bourlot et al. (2012). These models give access to all quantities computed by PDR 1.5.4 (line intensities, column densities, densities, temperature of gas and grains, ...).

Produced by Meudon ISM team

Explored parameters	min	max
AVmax	1	30 mag

Search models by input parameters :

Example :

- n_H or pressure
- G_0
- A_V

Search models by input parameters

1. Select parameters

At each selection, the unauthorized combinations are grayed out. To deselect a value, click the button again.

2. Click on submit

The button "Get model" is not available as long as more than 1 model is found.

AVmax (mag)

1	2	5	7	10
20	25	30	35	40

Pressure (cm⁻³ K)

1.0e+5	3.5e+5	1.0e+6	3.5e+6	1.0e+7
1.9e+7	3.5e+7	6.7e+7	1.0e+8	1.9e+8
3.5e+8	6.7e+8	1.0e+9		

chi front (ISRF)

1	3.5	10	35	100
190	350	670	1.0e+3	1.9e+3
3.5e+3	6.7e+3	1.0e+4	1.9e+4	3.5e+4
6.7e+4	1.0e+5			

Get model

Found 11 models

ISMDB: Inverse search

inta00_cp_el2p_j3_2_el2p_j1_2

I(C+ 157.68 micron)

I(C+ 1901.2713 GHz)

I(C+ El=2P,J=3/2->El=2P,J=1/2)

Line intensity of C+ 157.68 micron

Intensity of C+ 157.68 micron

...

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
 ...

"I(CO v=0,J=7->v=0,J=6 angle 00 deg)" > 3E-5
 "I(CO v=0,J=7->v=0,J=6 angle 00 deg)" < 8E-5
 "I(H2 2-1 S(1)) face on" > 1E-5
 "I(H2 v=2,J=3->v=1,J=1 angle 00 deg)" < 2E-5
 "Intensity of C+ 157.68 micron face on" > 3E-4
 "I(C+ El=2P,J=3/2->El=2P,J=1/2 angle 00 deg)" < 6E-4

Info
 Start typing a quantity among auto-completes. Then, click "Use" to add constraints list below.

Info
 You can do operations on quantities. The syntax is:
 (op "quantity1" "quantity2")
 The available operators are +, -, /, *
 For example:
 (/ "I(H2 2-1 S(1)) face on" "I(H2 1-

Semantics
 No need to know the name of quantities in the database

ISMDB: Inverse search

ISMServices CODES

Projects > PDRG1NoPAH_P_200618

ISMDB – Inverse Search

isobaric PDR 1.5.4 models

Date: June 18, 2020 Code: PDR 1.5.4 (2065), Project ID: PDRG1

1 – Search among two parameters

x Pressure (cm⁻³ K)

y chi front (ISRF)

2 – Fix all the other parameters

AVmax (mag)

3 – Observational constraints

Quantity search bar

Intensity of C+ 157.68 micron face on

"(C+ EI=2P,J=3/2->EI=2P,J=1/2 angle 00 deg)"

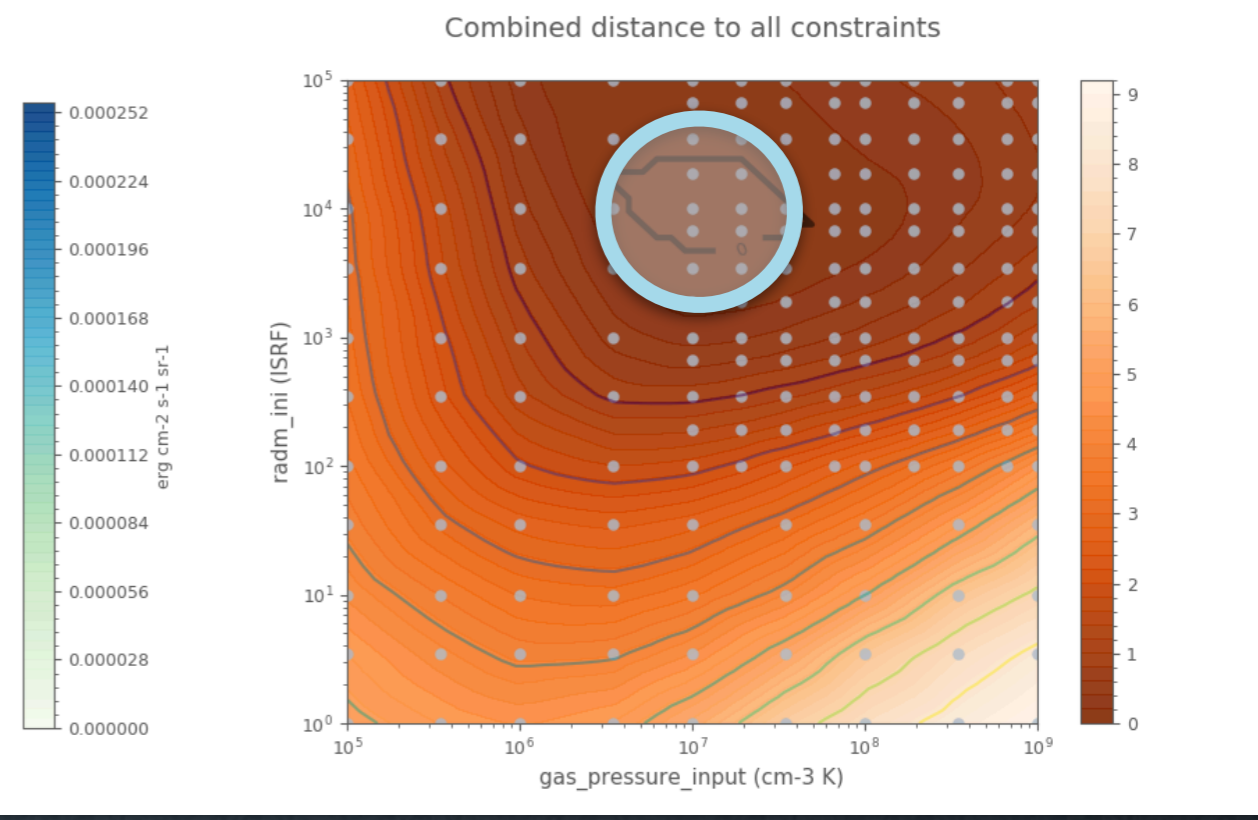
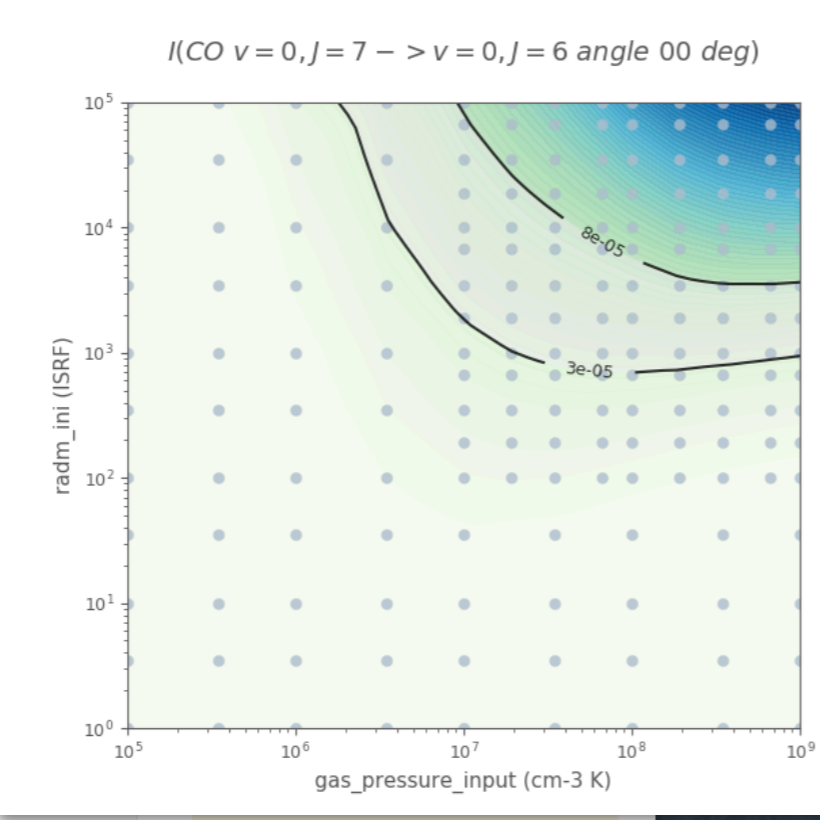
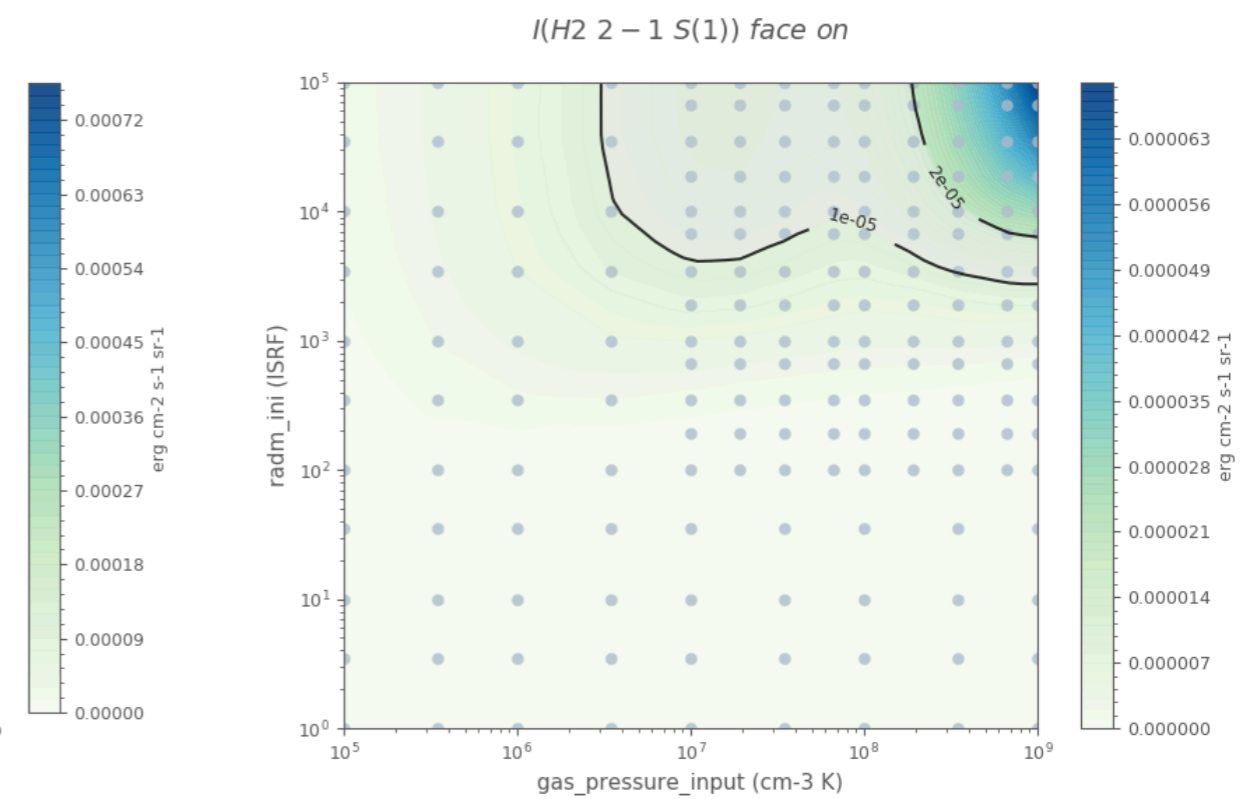
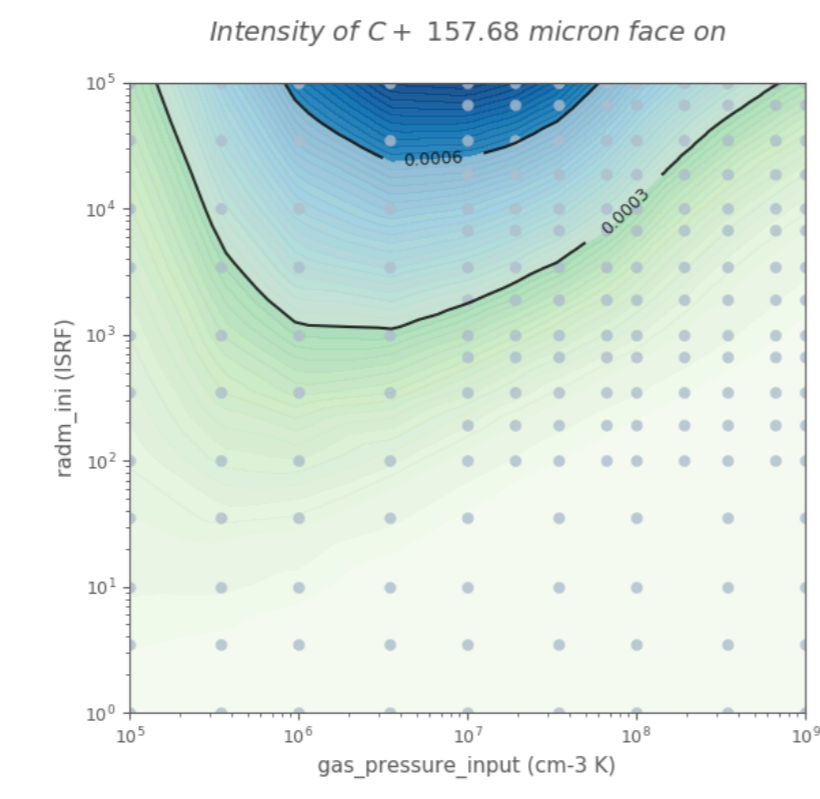
Line intensity integrated over line profile and for a specific angle between the PDR and the line of sight

Unit	Min value	Max
erg cm ⁻² s ⁻¹ sr ⁻¹	2e-12	0.00

Selected observational constraints

- "I(CO v=0,J=7->v=0,J=6 angle 00 deg)" > 3E-5
- "I(CO v=0,J=7->v=0,J=6 angle 00 deg)" < 8E-5
- "I(H2 2-1 S(1)) face on" > 1E-5
- "I(H2 2-1 S(1)) face on" < 2E-5
- "Intensity of C+ 157.68 micron face on" > 3E-4
- "Intensity of C+ 157.68 micron face on" < 6E-4

Search



The available operators are +, -, /, *

For example:

(/ "I(H2 2-1 S(1)) face on" "I(H2 1-

Model viewer

ISMServices
CODES
ISMDB
PARTNERS
REGISTRATION

Projects > PDRG1NoPAH_P_200618 > PDRG1NoPAH_P1p9e8r1p9e4A3e1

ISMDB – Model viewer

Model PDRG1NoPAH_P1p9e8r1p9e4A3e1 June 18, 2020
Code: PDR 1.5.4 (2065), Project id: PDRG1NoPAH_P_200618

Produced by Meudon ISM team
ISMServices

Parameters ([toggle all parameters](#))

Main parameters		
chi front	1.9e+04	ISRF
AVmax	30	mag
Pressure	1.9e+08	cm ⁻³ K

Other		
zeta	1e-16	s ⁻¹ per H2
Z	1	

Algorithms		
Rad. transfer algo.	0	

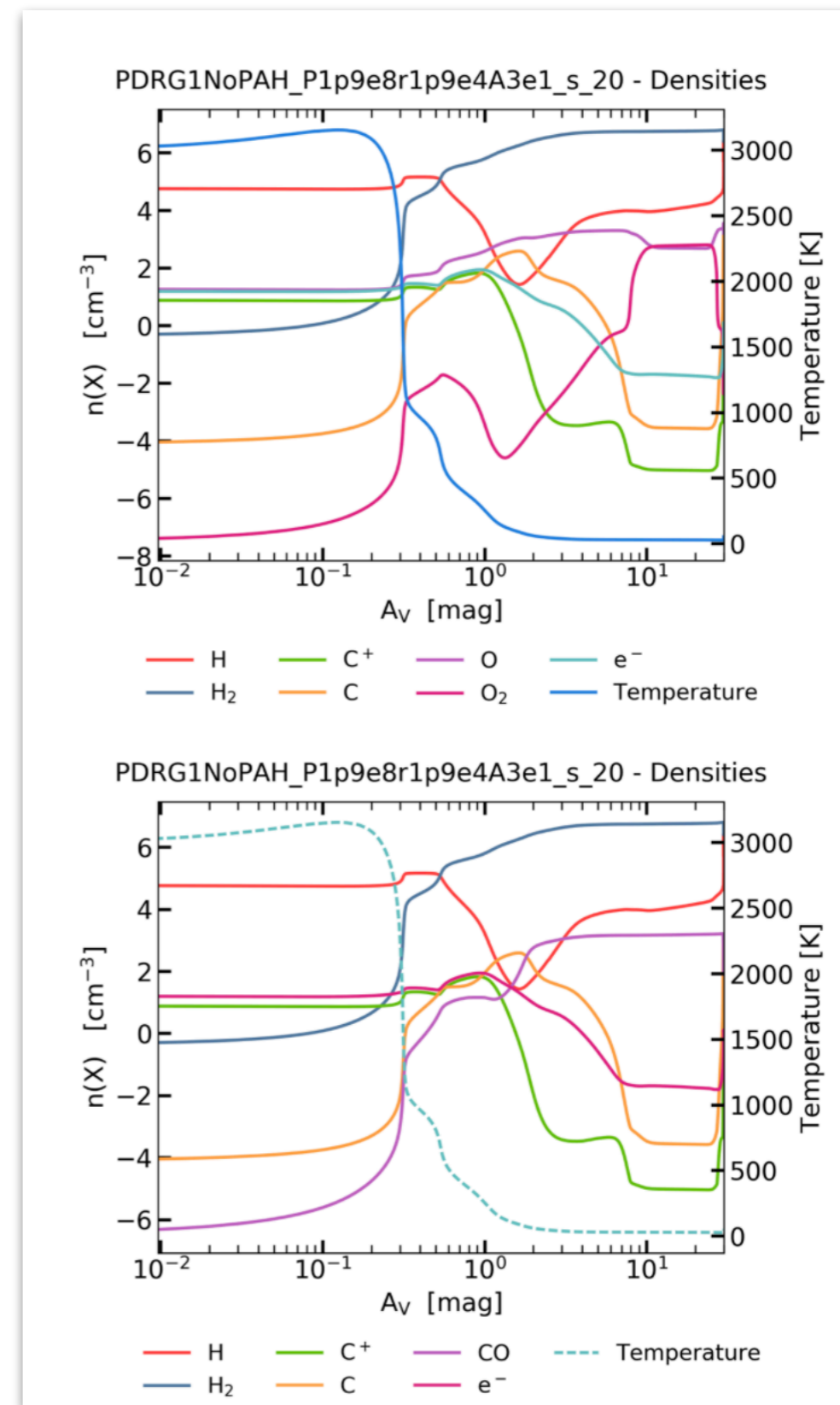
Grain properties		
Extinction curve	Galaxy	
RV	3.1	
NH/E(B-V)	5.8e+21	cm ⁻² mag ⁻¹
m(dust)/m(gas)	0.01	
m(PAH)/m(dust)	0	
Grains distrib. slope	3.5	
Grains min radius	1e-07	cm
Grains max radius	3e-05	cm

Online analysis

online analysis with IDAT

Download

- [Source code](#)
- [Chemistry file](#)
- [Main output](#)
- [Chemistry analysis output](#)
- [Emissivity output](#)



Model viewer

ISMServices
CODES
ISMDB
PARTNERS
REGISTRATION

Projects > PDRG1NoPAH_P_200618 > PDRG1NoPAH_P1p9e8r1p9e4A3e1

ISMDB – Model viewer

Model PDRG1NoPAH_P1p9e8r1p9e4A3e1 June 18, 2020
Code: PDR 1.5.4 (2065), Project id: PDRG1NoPAH_P_200618

Produced by Meudon ISM team
ISMServices

Parameters ([toggle all parameters](#))

Main parameters

chi front	1.9e+04	ISRF
AVmax	30	mag
Pressure	1.9e+08	cm ⁻³ K

Other

zeta	1e-16	s ⁻¹ per H2
Z	1	

Algorithms

Rad. transfer algo.	0
---------------------	---

Grain properties

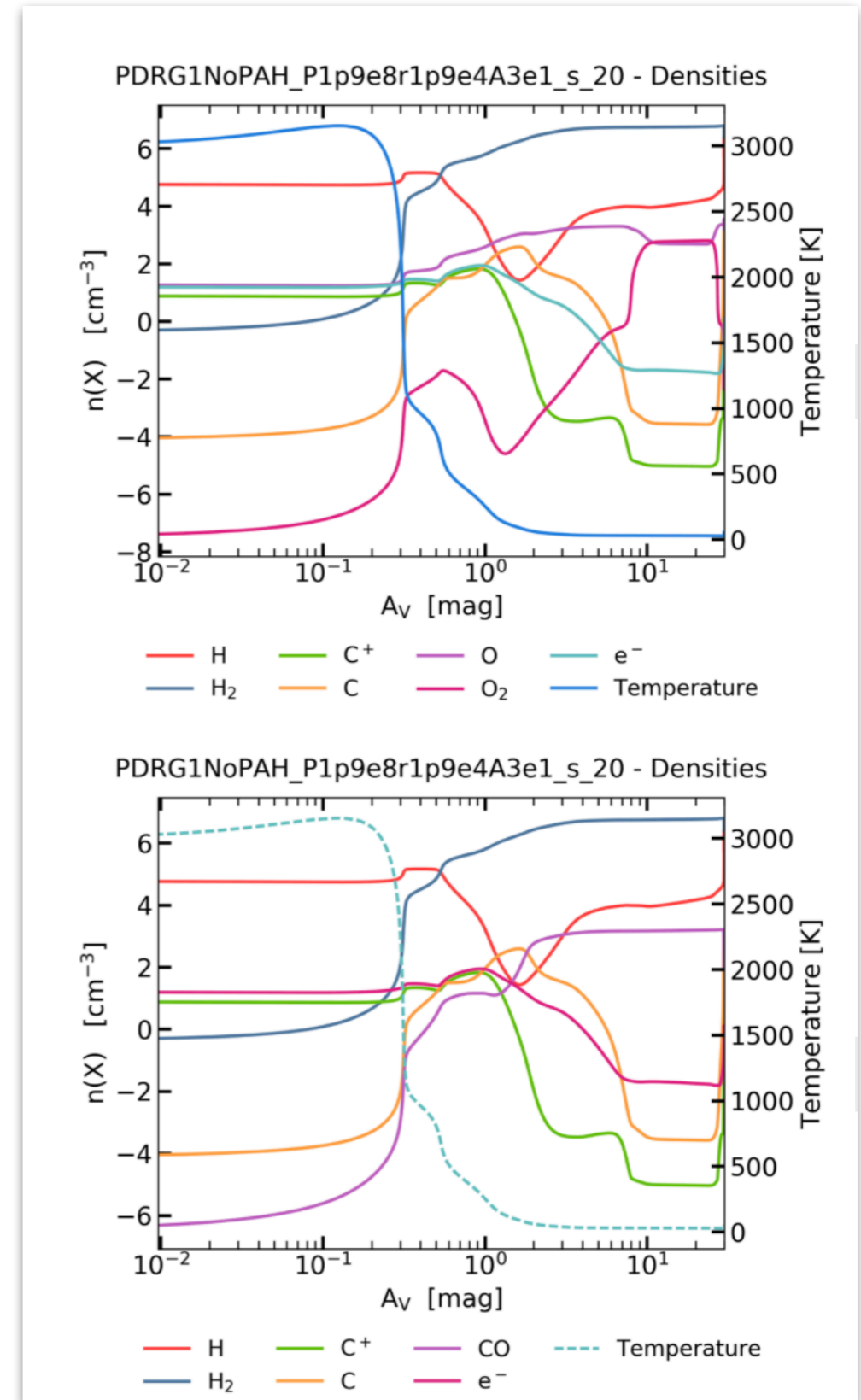
Extinction curve	Galaxy	
RV	3.1	
NH/E(B-V)	5.8e+21	cm ⁻² mag ⁻¹
m(dust)/m(gas)	0.01	
m(PAH)/m(dust)	0	
Grains distrib. slope	3.5	
Grains min radius	1e-07	cm
Grains max radius	3e-05	cm

Online analysis

online analysis with IDAT

Download

- [Source code](#)
- [Chemistry file](#)
- [Main output](#)
- [Chemistry analysis output](#)
- [Emissivity output](#)



Browse the content of a model

IDAT: Data analysis

Local version

Opened model: OrBarJ18_BestMod_s_20.hdf5

This tool allows to extract data produced by the ISM platform codes (as text files) and to plot the results.

- Search among the computed quantities with the search bar or in the data tree listing all available quantities.
- The quantities you select will appear in the boxes of section 2.
- If you already know the quantity names, you can also directly type or paste them into the boxes.
- Export as text files or plot the data with our interactive plot tool using the corresponding buttons.

1. Select quantities to extract or plot

Find quantities computed by the code with the search bar

Find quantities in the data tree

- Integrated quantities
- Local quantities
 - Auxiliary
 - Densities
 - Column densities
 - Densities
 - Dust
 - Gas state
 - Positions
 - Parameters

n(a-C3H4) n(a-C3H4+) n(Ar) n(Ar+) n(ArH+) n(C) n(C+) n(C++) n(c-C3H) n(c-C3H2)
 n(c-C3H2+) n(c-C3H3+) n(C2) n(C2+) n(C2H) n(C2H+) n(C2H2) n(C2H2+) n(C2H3) n(C2H3+)
 n(C2H3O+) n(C2H4) n(C2H4+) n(C2H5+) n(C2HO+) n(C2N+) n(C2S) n(C2S+) n(C3) n(C3+)
 n(C3H) n(C3H+) n(C3H2+) n(C3H3) n(C3H3+) n(C3H5+) n(C4) n(C4+) n(C4H) n(C4H+)
 n(C4H2) n(C4H2+) n(C4H3+) n(CH) n(CH+) n(CH2) n(CH2+) n(CH3) n(CH3+) n(CH3OH)
 n(CH3OH+) n(CH4) n(CH4+) n(CH5+) n(CH5O+) n(CN) n(CN+) n(CNC+) n(CO) n(CO+) n(CO2)
 n(CO2+) n(CS) n(CS+) n(e-) n(Fe) n(Fe+) n(Fe++) n(H) n(H+) n(H2) n(H2+) n(H2:)
 n(H2C3) n(H2CO) n(H2CO+) n(H2CS) n(H2CS+) n(H2NC+) n(H2O) n(H2O+) n(H2O2) n(H2S)
 n(H2S+) n(H3+) n(H3CO) n(H3CO+) n(H3CS+) n(H3O+) n(H3S+) n(H:) n(H::) n(HCN) n(HCN+)

Next step >>

Clear all selection

2. List of selected quantities

Extract the chosen quantities as datafiles or plot them with our interactive plot tool.
Direct cut/paste into this box is possible. You can also manually add and delete quantities.

The selected quantities are divided between local quantities (functions of the position) on the left, and global quantities (taking one single value for the whole model) such as integrated quantities and model parameters on the right.

Local quantities (position dependant)

AV
Distance
nH
Temperature
n(H2)
n(H)
n(CO)
n(C+)

Actions

Export as ASCII file

Export as VOTable

Plot

Integrated quantities or parameters

Actions

Export as ASCII file

Export as VOTable

Download data

Visualize data

3. Plot selected quantities

graph

Title

x axis

Quantity Label log

Min Max

Min auto

y1 axis

Label log Min Max

<input checked="" type="checkbox"/>	n(H2)	cm-3	n(H2)
<input checked="" type="checkbox"/>	n(H)		n(H)
<input checked="" type="checkbox"/>	n(CO)	cm-3	n(CO)
<input checked="" type="checkbox"/>	n(C+)	cm-3	n(C+)
<input checked="" type="checkbox"/>	n(C)	cm-3	n(C)

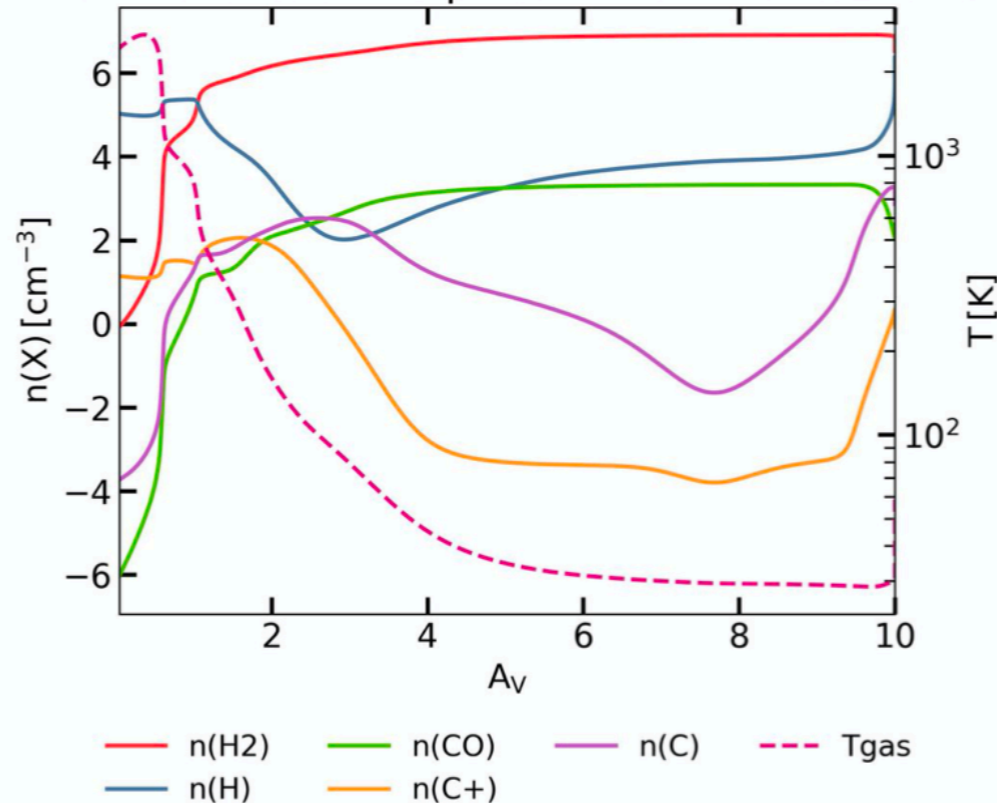
y2 axis

Label log Min Max

<input type="checkbox"/>	AV	mag	AV
<input type="checkbox"/>	Distance	cm	Distance
<input type="checkbox"/>	nH		nH
<input checked="" type="checkbox"/>	Tgas	K	Temperature
<input type="checkbox"/>	n(H2)	cm-3	n(H2)

Plot

Chemical abundance profile in the Orion Bar PDR



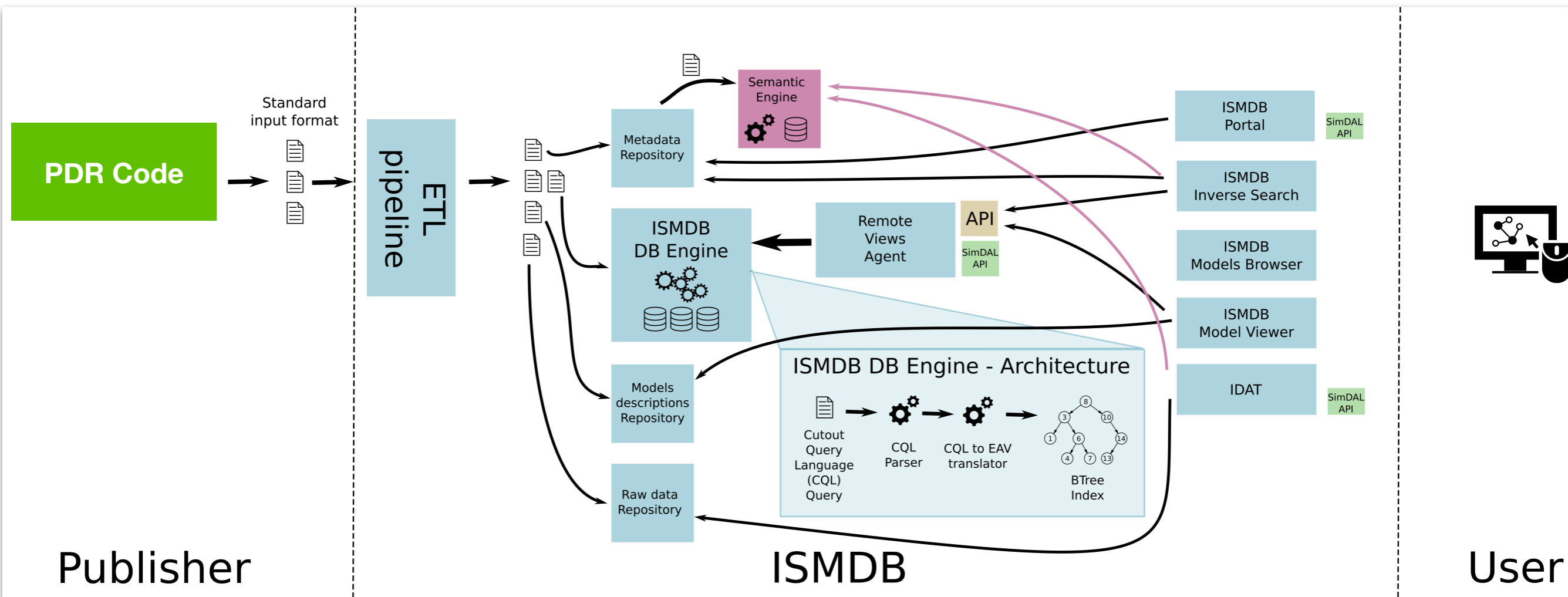
To save the figure: right click and select Save

[Download figure](#)

[Save plot configuration file](#)

ISMDB : Architecture

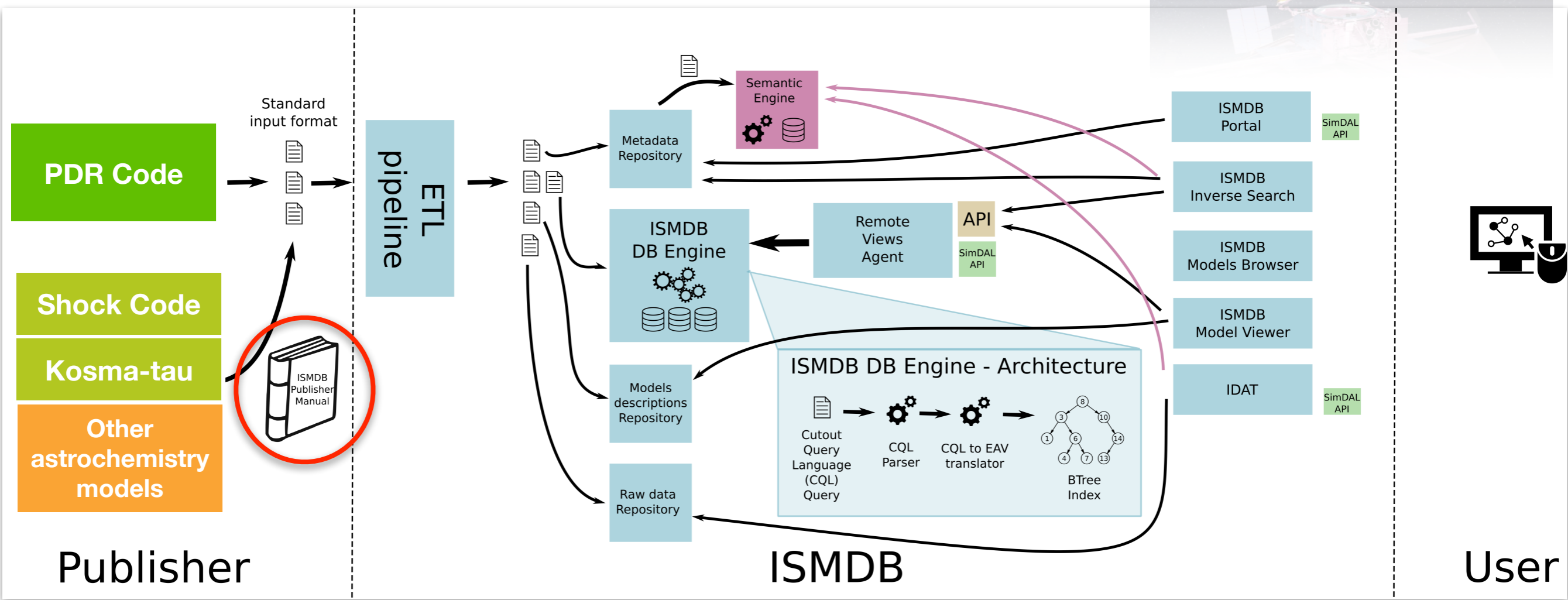
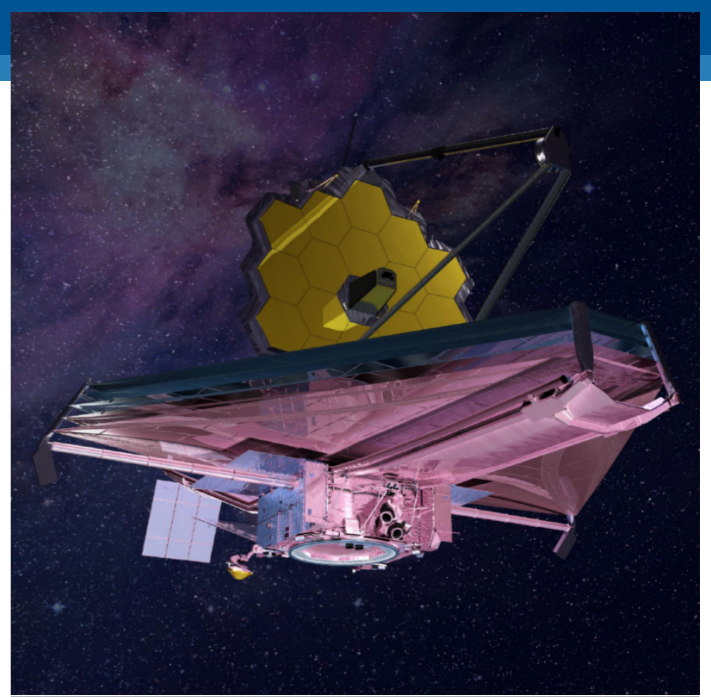
- high dimension database - we had to invent our own solutions to manage such data
- VO-based (SimDM & SimDAL)
- heavy to develop & maintain
- could contain any astrochemical modes



ISMDB : Publication of models of other teams

Several groups want to publish their models in ISMDB

- JWST context
 - they are scientists and not VO experts
- can be complex for them to understand SimDM





DOCUMENTATION

ISMDB Publisher Manual

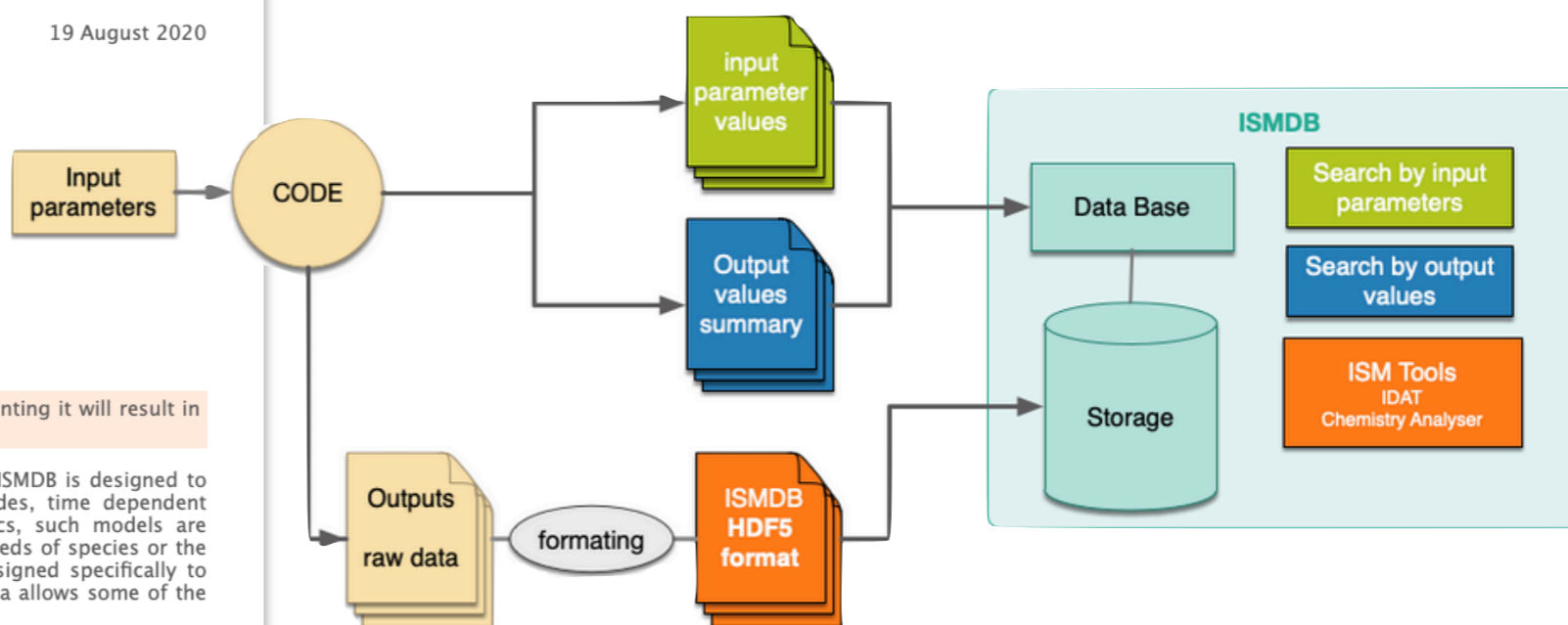
19 August 2020

Table of content

- The code description file
- The project description file
- The input parameters files
- The output files

This documentation has been formatted as an HTML page meant to be read in a web browser. Printing it will result in cutting out part of the tables and example files.

This note explains how to publish grids of models in the Interstellar Medium Data Base, ISMDB. ISMDB is designed to publish astrochemical model grids produced by various types of codes (radiative transfer codes, time dependent astrochemical codes, PDR codes, shock codes, etc.). Compared to other codes in astrophysics, such models are characterised by the large number of quantities they can compute, such as the densities of hundreds of species or the integrated line intensities of tens of thousands of lines. The structure of ISMDB has been designed specifically to handle such high dimensional datasets. This ability to store and manipulate high dimensional data allows some of the advanced usages proposed in ISMDB.



Case	Input parameters values	Output values summary	output raw data in ISMDB HDF5 format	ISMDB feature
1	✓			Search by input parameters
2	✓	✓		Search by input parameters + inverse search
3	✓	✓	✓	Search by input parameters + inverse search + ISM Tools (IDAT, ...)
4	✓		✓	Search by input parameters + ISM Tools (IDAT, ...)

Publication in ISMDB

2.2. Second part - input parameter description

After these general informations, the `<codeID>_code.yaml` file must contain a description of the input parameters of the code. All input parameters are listed, one per line, with information about each parameter, one per line. In yaml format, this table must be written between brackets as in the example below (the commented header line gives the meaning of each column):

```
#      parameterID      ,name      ,datatype ,unit      ,rvalmin ,rvalmax ,groupID      , OrderInGroup ,absolute_order ,UCD ,SKOS
code/parameters: [
  [ proton_density_input ,nH      ,real      , cm-3      ,1.0      ,1.0E6      ,Grp_General      ,1      ,2      ,''      ,http://purl.obspm.org/terms/ontology/parameters/proton_density_input
  [ radm_ini      ,G0 front side ,real      , Habing      ,0.0      ,1E7      ,Grp_General      ,2      ,4      ,''      ,''
  [ chemistry_file      ,Chemistry      ,string      , ''      ,''      ,''      ,Grp_Chemistry      ,1      ,5      ,''      ,''
]
```

The informations to provide for each input parameter are described below. Some of these informations are actually not used by ISMDB but are used by other services of the ISM Platform (ex: online code).

field	doc
ParameterID	This is a unique ID to identify the input parameter
Name	Name of the input parameter as it should appear on a web page to a human reader
datatype	Must be one of <code>real</code> , <code>integer</code> , <code>string</code>
Unit	Unit of the parameter. Use <i>no unit</i> if the parameter has no unit. This should be a string
rval. min/max	Recommended minimum and maximum value allowed by the code for the input parameter. Only used by "Online Code service", not ISMDB. Can be "" to provide no values.
GroupID, orders	Used to group and sort the input parameters. See explanations below
UCD and SKOS	Tags used by the Virtual Observatory to add semantics to the input parameters. Use "" to not provide semantics. Or search for the proper tag in the UCD list and the IVOA SKOS concepts vocabularies. If a choice has to be made, prefer to fill the SKOS field rather than the UCD field. The list of SKOS tags can be found here: SKOS vocabularies for Theoretical Data in the Virtual Observatory .
Description	Text description of the parameter. This field can contain HTML code.

Data providers have only to produce

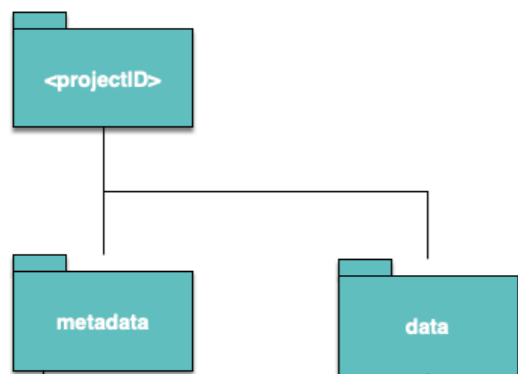
- simple yaml files
- ASCII files

```
!Model ID      # Parameter ID      # Value      # Comment (used here for unit)
!-----
PDR_n_A3e1n1e3r1e1 # proton_density_input # 1000      # cm-3
PDR_n_A3e1n1e3r1e1 # radm_ini      # 1.0E+01      # Habing
PDR_n_A3e1n1e3r1e1 # avmax      # 3.0E+01      # mag
PDR_n_A3e1n1e3r1e1 # chemistry_file      # ch1901.chi      # no unit
PDR_n_A3e1n1e3r1e1 # rv      # 3.1E+00      # no unit
PDR_n_A3e1n1e3r1e1 # metal      # 1.0E+00      # no unit
```

Output files

```
---
#      Name,      Type,      Link
experiment/links: [
  ["Source code",      data,      "https://ism.obspm.fr/?page_id=1466"],
  ["Main output",      data,      "https://appdev.ism.obspm.fr/files/ismdb/{project}/raw/{experiment}/{experiment}_s_20.hdf5"],
  ["Chemistry analysis output",      data,      "https://appdev.ism.obspm.fr/files/ismdb/{project}/raw/{experiment}/{experiment}_c_20.hdf5"],
  ["Emissivity output",      data,      "https://appdev.ism.obspm.fr/files/ismdb/{project}/raw/{experiment}/{experiment}_a_20.hdf5"],
  ["online analysis with IDAT",      service,      "http://koratta.obspm.fr/ismdb/idat/index.html?project={project}&model={experiment}"],
]
```

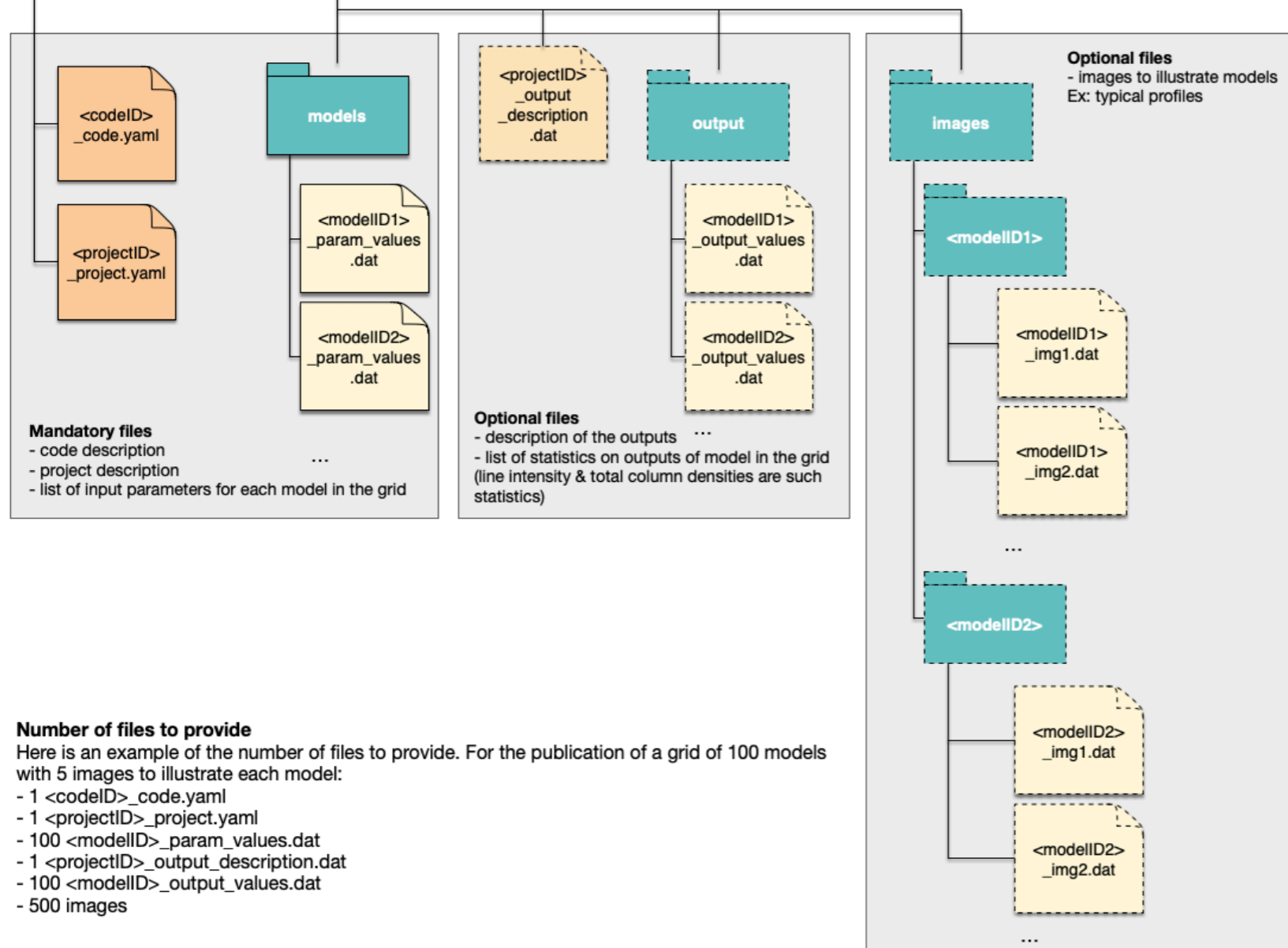
Publication in ISMDB



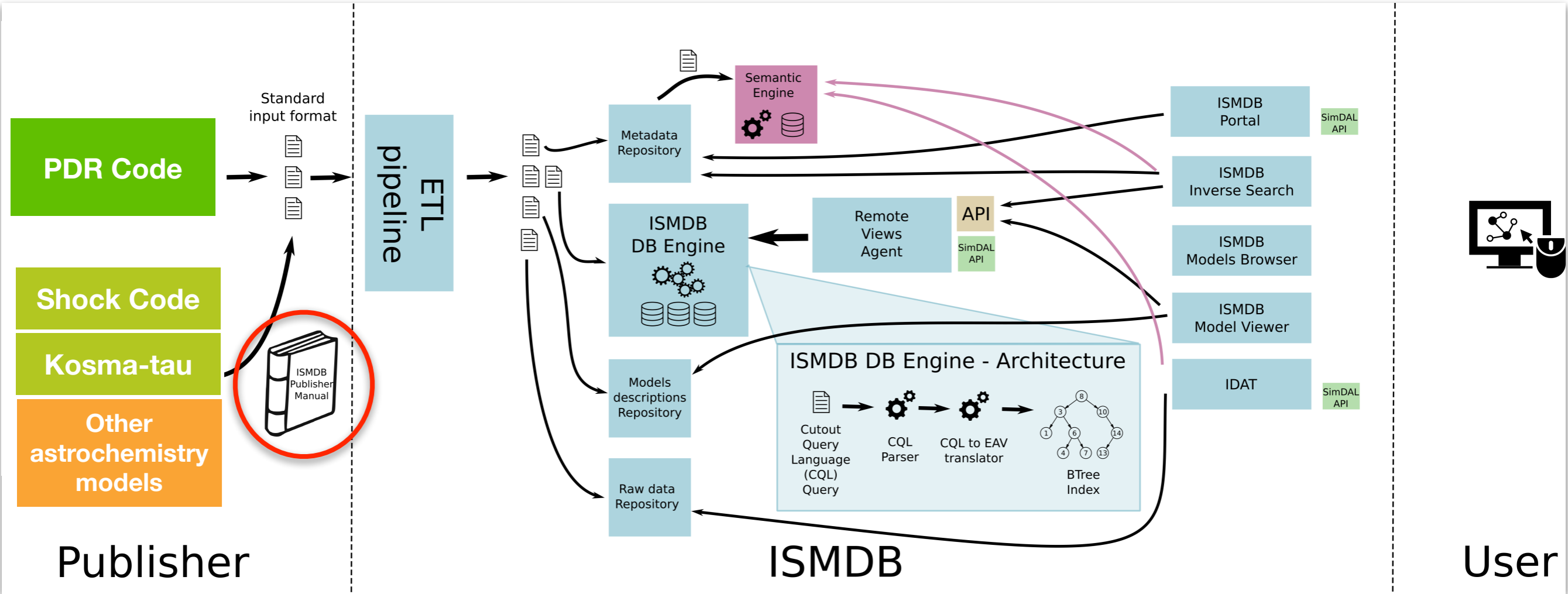
```

code/ident:      pdr154
code/name:       PDR 1.5.4
code/family:     meudon_pdr154
code/version:    1579
code/created:    20200530
code/contacts:
  - {name: "Jacques Le Bourlot", role: "owner", mail: "Jacques.LeBourlot@obspm.fr"}
  - {name: "Franck Le Petit", role: "owner", mail: "Franck.LePetit@obspm.fr"}
code/url:        https://pdr.obspm.fr
code/doc: >
code/publisher:  ism.obspm
  
```

Few lines to describe the code.
A full documentation could be on the web site above.



Conclusion



Conclusion

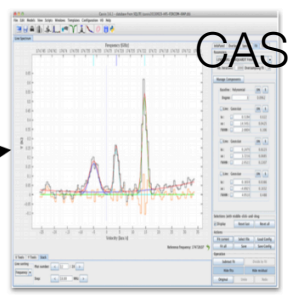
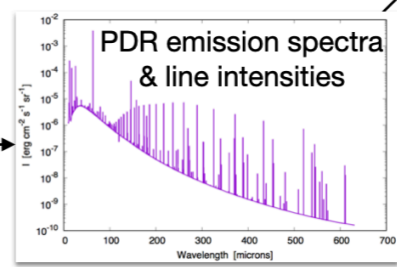
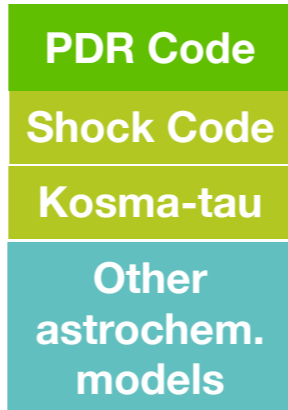
Next version of ISMDB is ready

- discover astrochemical models by input parameters
- solve inverse problems
- online tools to analyse problems

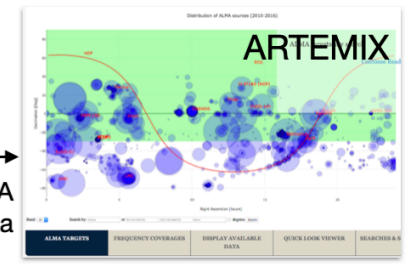
Possibility to publish models from other teams

- Meudon PDR code
- Paris-Durham shock code
- Kosma-tau models
- Time dependent chemistry models
- ...

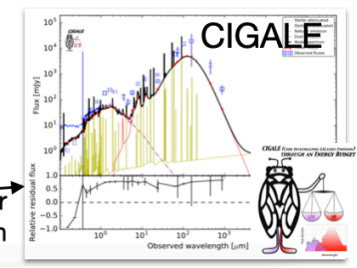
→ Services & VO compatibility



Interpret ISM spectra

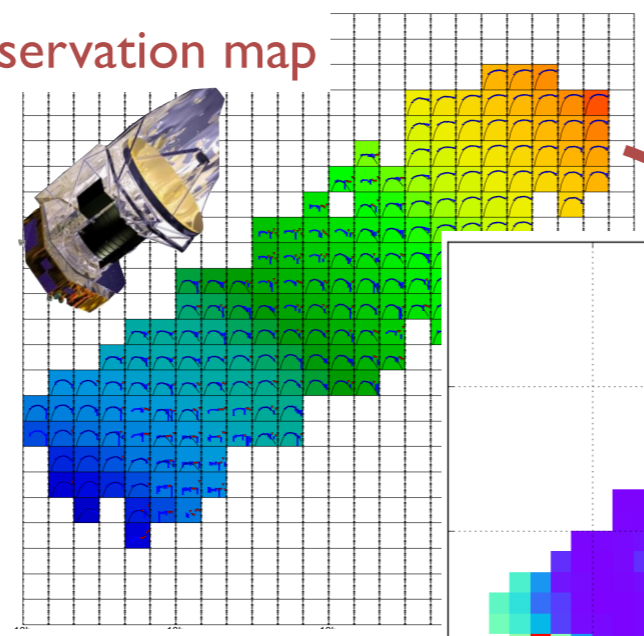


Interpret ALMA archive data

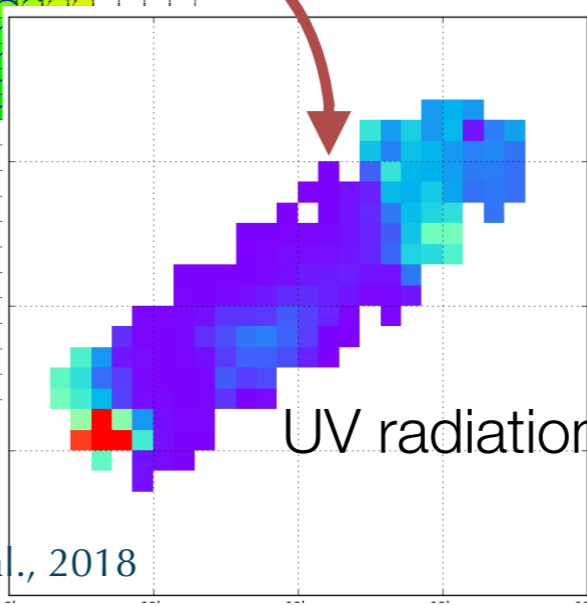


Analyse galaxies molecular emission

Observation map



Map of physical parameters



UV radiation field

Next steps

- coupling to other services
- interpretation of maps
- DOI on datasets