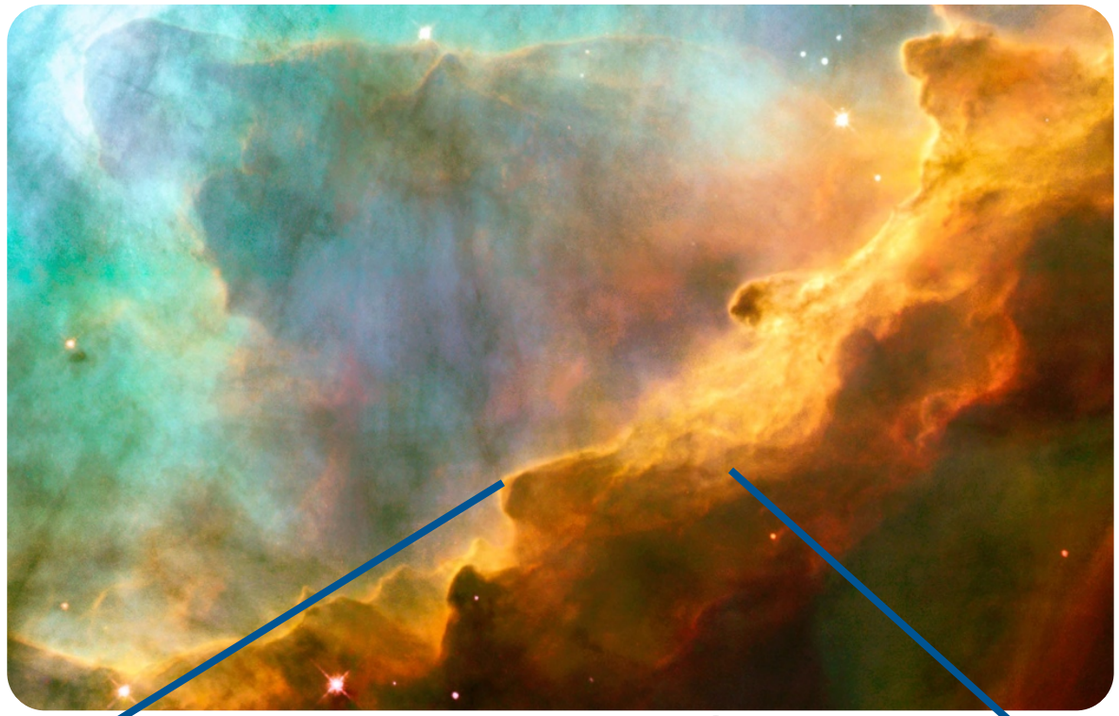
Implementation of SimDB on PDR simulations

Franck Le Petit, Laurent Bourgès

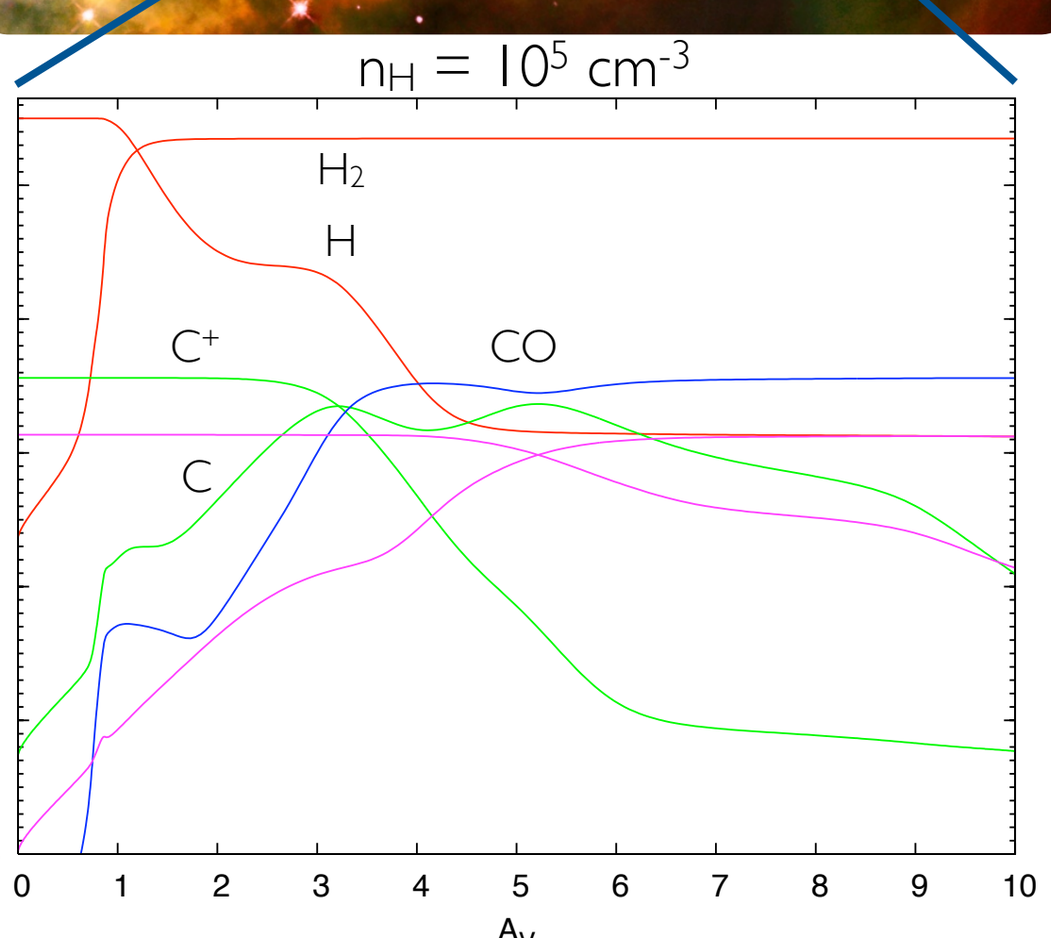
Photodissociation Region simulations

Case:
codes computing the microscopic structure of astrophysical objects

They provide as outputs:
- temperature profile
- chemical abundances
- ionization degree of species
- level excitation
- line emissivities
- heating rates
- cooling rates
- many other quantities



FUV
(13.6 eV - 6eV)
10^5 × ISRF



Observables
- line intensities
- column densities
- spectra

Can SimDB be used to describe PDR simulations ?

Objectives:

- Discover simulations
  - by queries on input parameters
  - by queries on “characterisation”: inverse problem
- Extract quantities for analysis, post-processing, workflows

SimDB :

- cosmology models
- 3 dimensions + time
- snapshots

Meudon PDR code

- Models of microphysics simulations of interstellar clouds
- 1 spatial dimension + no time
- no snapshot

Can SimDB be used to describe PDR simulations ?

Challenges :

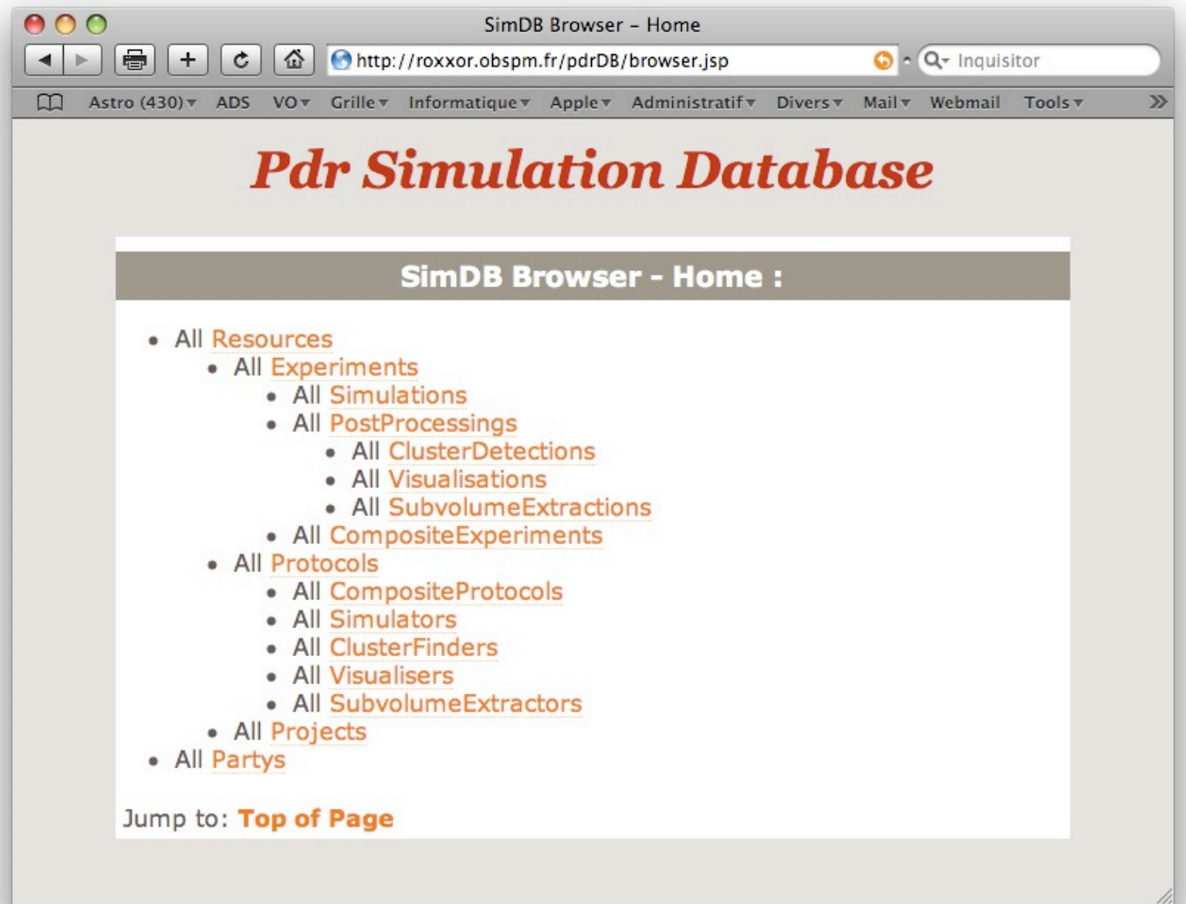
- many input parameters:
  - At least 60 (but about 500 if chemical abundances are considered as parameters)

- many properties (more than 10 000):
  - because a simulation provides abundances as a function of position
    - abundances of several hundreds chemical species
    - abundances in several hundreds of quantum levels for some of them

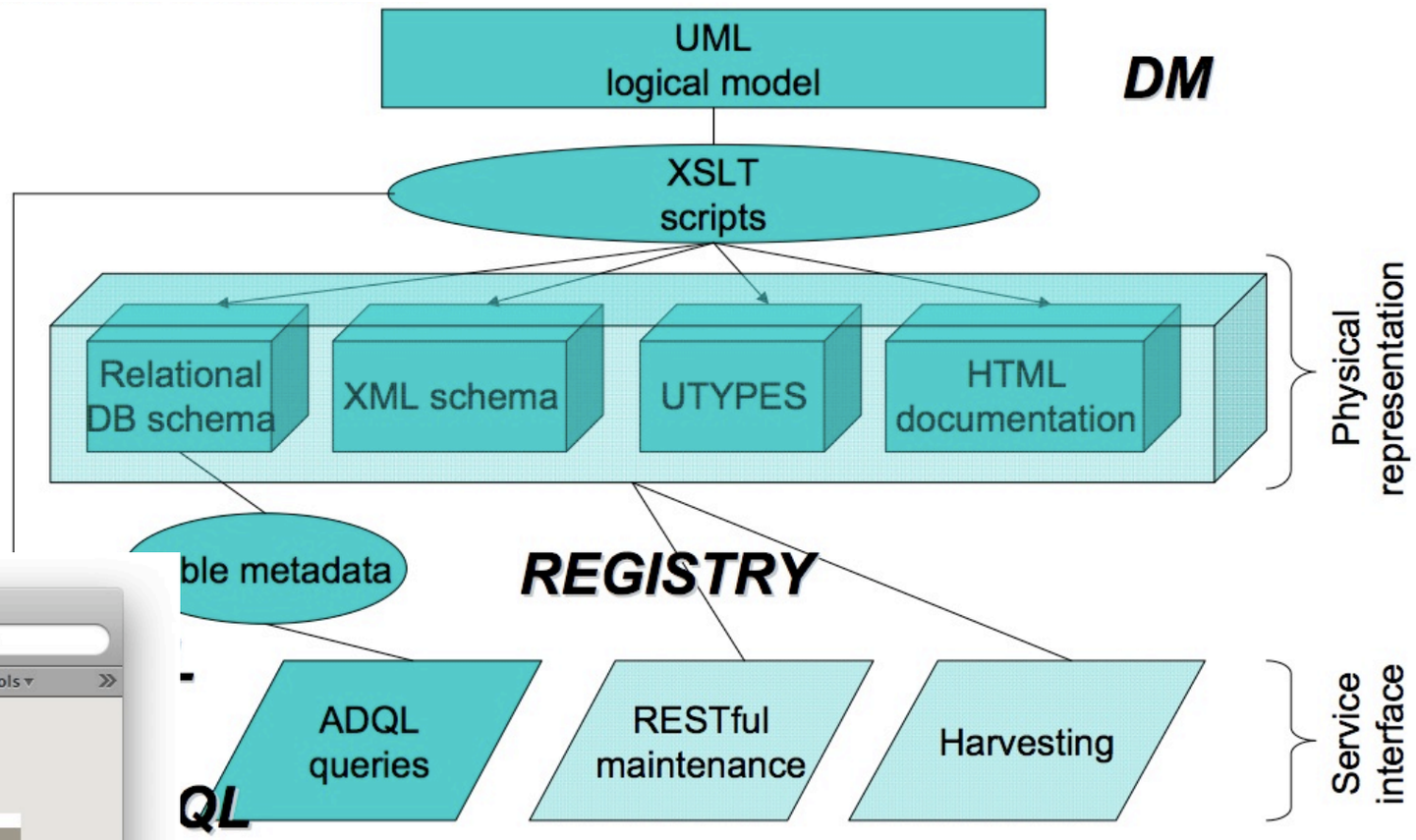
- many different quantities:
  - quantities function of position (ex: abundance, temperature)
  - quantities function of wavelength (ex: absorption spectrum)
  - quantities function of position and wavelength (ex: density of energy)

Implementation of SimDB on PDR simulations

- Use SimDB to:
  - creation of the database *(registry)*
  - Protocol
  - Experiments



SimDB "administrative" browser



Implementation of SimDB on PDR simulations

Protocol

Two challeging parts
1 - protocol definition
2 - parameters
3 - full description of codes

1 - protocol definition

An experiment is produced by :

code version + **chemical network** + **atomic and molecular data**

How to define the chemical networks and atomic and molecular data used ?

Solution 1: consider the chemical network as an input parameter (string for the file name)
- A single parameter for the name of chemistry file: string
- A list of parameters for each chemical rate: +10 000 new parameters

Solution 2: a protocol is a **code** + **chemical network** + **atomic and molecular data**
- name: PDR1.2_chemistry08

Implementation of SimDB on PDR simulations

Protocol

Detail of Simulator : 1 :

Back to : **Index** - **Previous Page**

Data Model serialization : XML

Property	Value
id	1
identity	[1]
name	Pdr1.2_chimie08-test
description	First test protocol
referenceURL	http://aristote.obspm.fr/MIS
publisherDID	Pdr1.2_chimie08_TEST
created	Fri Oct 17 18:11:05 CEST 2008
updated	Fri Oct 17 18:11:05 CEST 2008
status	private
code	http://aristote.obspm.fr/MIS
version	1.2

Similar to another problem :

How to describe in SimDB modular codes ?
Example: Ramses

- core code
- some plugins can be added to Ramses to control various processes :
  - MHD
  - forcing terms
  - ...

Best solution : to define a new protocol for each “code + plugins” ?

Implementation of SimDB on PDR simulations

Protocol

2 - Parameters

Input Parameters of Meudon PDR code can fit in SimDB

Large number of parameters
- ParameterGroup are very usefull to structure parameters
- But difficulties to **use** the DM when the number of parameters is large

No vocabulary for all parameters
- Semantic Group's vocabularies cover most of the parameters
- But some specific notions are not covered

Example:
The intensity of the flux illuminating an interstellar cloud is given as a multiplicative factor of
- G or chi : for Habing or Draine's units

- Need precise definition of those quantities
- This can only be done community by community

Implementation of SimDB on PDR simulations

Protocol

Detail of Simulator : 1

http://roxxor.obspm.fr/pdrDB/Show.do?entity=Simulator&id=1

Inquisitor

Astro (430) ADS VO Grille Informatique Apple Administratif Divers Mail Webmail Tools Others Program GAMS

parameter

[324 - xmlId: DU_MODPARAM_S.FD_SRCNAME]	External source name	STRING
[308 - xmlId: DU_MODPARAM_I.FD_IFEQTH]	ifeqth	INT
[327 - xmlId: DU_MODPARAM_R.FD_TINIT]	tg_init	DOUBLE
[290 - xmlId: DU_MODPARAM_I.FD_IFISOB]	ifisob	INT
[277 - xmlId: DU_MODPARAM_R.FD_PRESSE]	presse	DOUBLE
[299 - xmlId: DU_MODPARAM_S.FD_PROFNAME]	nH - Temp profile file name	STRING
[318 - xmlId: DU_MODPARAM_R.FD_FMRC]	fmrc	DOUBLE
[322 - xmlId: DU_MODPARAM_R.FD_VTURB]	vturb	DOUBLE
[273 - xmlId: DU_MODPARAM_S.FD_CHEMNAME]	Chemistry file name	STRING
[271 - xmlId: DU_MODPARAM_R.FD_METAL_He]	MetallicityHe/H	DOUBLE
[301 - xmlId: DU_MODPARAM_R.FD_METAL_C]	MetallicityC/H	DOUBLE
[321 - xmlId: DU_MODPARAM_R.FD_METAL_N]	MetallicityN/H	DOUBLE
[320 - xmlId: DU_MODPARAM_R.FD_METAL_O]	MetallicityO/H	DOUBLE
[286 - xmlId: DU_MODPARAM_R.FD_METAL_D]	MetallicityD/H	DOUBLE
[315 - xmlId: DU_MODPARAM_R.FD_METAL_C13]	MetallicityC13/H	DOUBLE
[309 - xmlId: DU_MODPARAM_R.FD_METAL_N15]	MetallicityN15/H	DOUBLE
[304 - xmlId: DU_MODPARAM_R.FD_METAL_O18]	MetallicityO18/H	DOUBLE
[288 - xmlId: DU_MODPARAM_R.FD_METAL_PAH]	MetallicityPAH/H	DOUBLE
[319 - xmlId: DU_MODPARAM_R.FD_METAL_F]		
[272 - xmlId: DU_MODPARAM_R.FD_METAL_Na]		
[316 - xmlId: DU_MODPARAM_R.FD_METAL_Mg]		
[283 - xmlId: DU_MODPARAM_R.FD_METAL_Al]		
[270 - xmlId: DU_MODPARAM_R.FD_METAL_Si]		
[312 - xmlId: DU_MODPARAM_R.FD_METAL_P]		
[307 - xmlId: DU_MODPARAM_R.FD_METAL_S]		
[276 - xmlId: DU_MODPARAM_R.FD_METAL_Cl]		
[293 - xmlId: DU_MODPARAM_R.FD_METAL_Ca]		
[296 - xmlId: DU_MODPARAM_R.FD_METAL_Fe]		

Detail of InputParameter : 323 :

Back to : **Index** - **Previous Page**

Data Model serialization : XML

Property	Value
id	323
identity	[323 - xmlId: DU_MODPARAM_R.FD_RADM_INI]
name	radm_ini
datatype	DOUBLE
cardinality	ONE
description	Scaling factor to Draine radiation field on the observer side of the cloud in the entrance parameters. The corresponding radiation field corresponds to the one seen from a position far from the cloud.
isEnumerated	
label	
Collection	**Value**
validValue	

Jump to: **Top of Page**

Implementation of SimDB on PDR simulations

Protocol

3 - Description of physics covered by the code

Requirements: need to describe in details the physical processes in the code

Example: Rollig et al., A&A, 2007 :

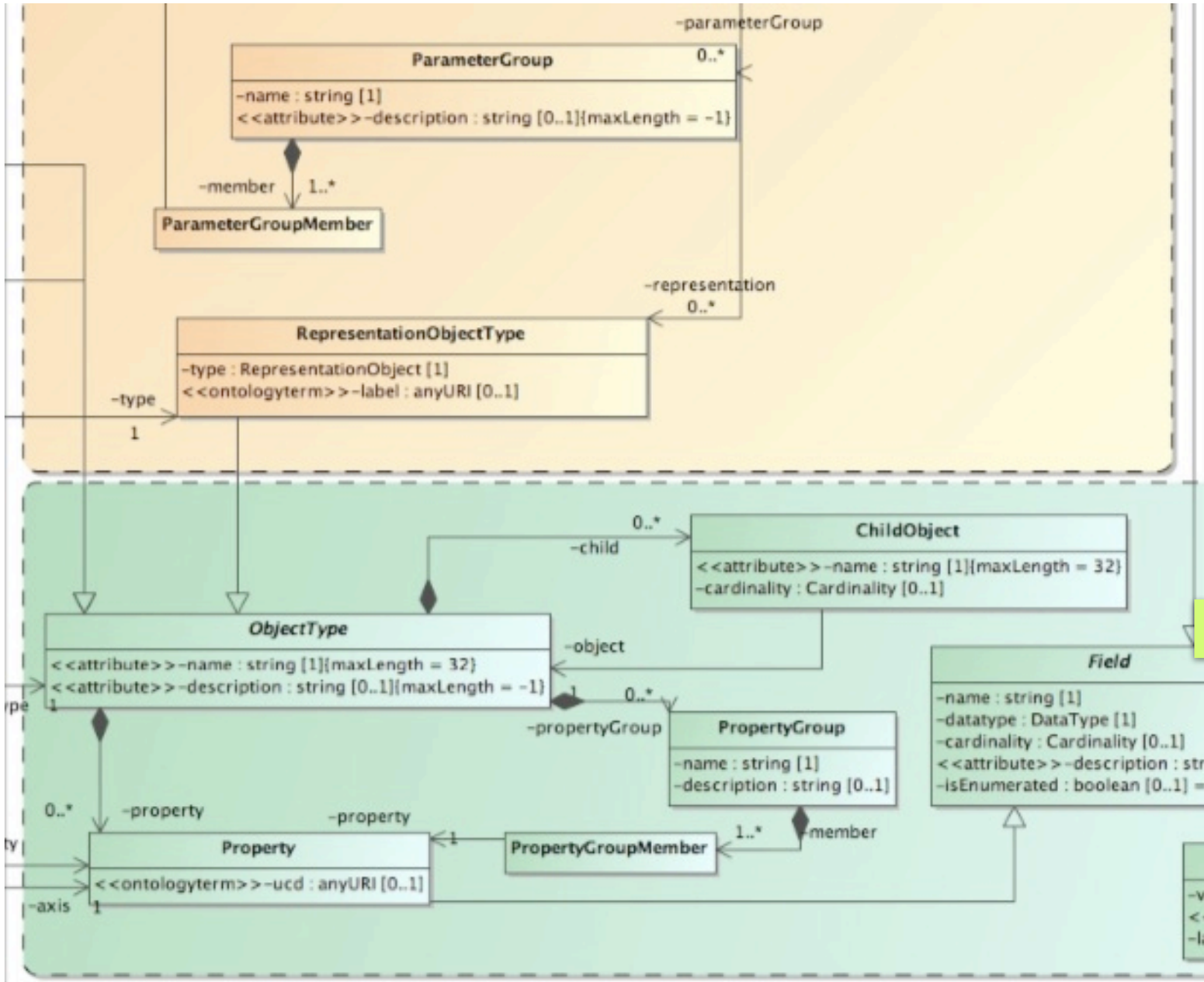
	Cloudy	COSTAR	Meudon	UCL_PDR	HTBKW	KOSMA-τ	Aikawa	Leiden	Lee96mod	Sternberg	Meijerink
solved self-consistently	x	x	x	x	x	x		x		x	x
simple exponential attenuation	x	x	x	x	x	x	x	x	x	x	x
bi-exponential attenuation		x								x	
full RT in lines			x					x			
DUST											
treatment of rad. transfer	x		x		x	x		x		x	x
grain size distribution	x		x	x		x					
extinction/scattering law	x	x	x	x	x	x	x	x	x	x	
albedo	x		x	x				x			x
scattering law	x		x					x			
H_2 SHIELDING											
shielding factors	x	x			x		x		x	x	x
single line	x			x							x
detailed solution	x		x			x		x			
CO SHIELDING											
shielding factors	x	x		x	x	x	x	x	x	x	x
single line	x							x			x
detailed solution			x					x			
isotope selective photodissociation			x			x		x			x
UV PROFILE FUNCTION											
Gaussian				x	x						
Voigt	x		x					x		x	x
Box											
other											

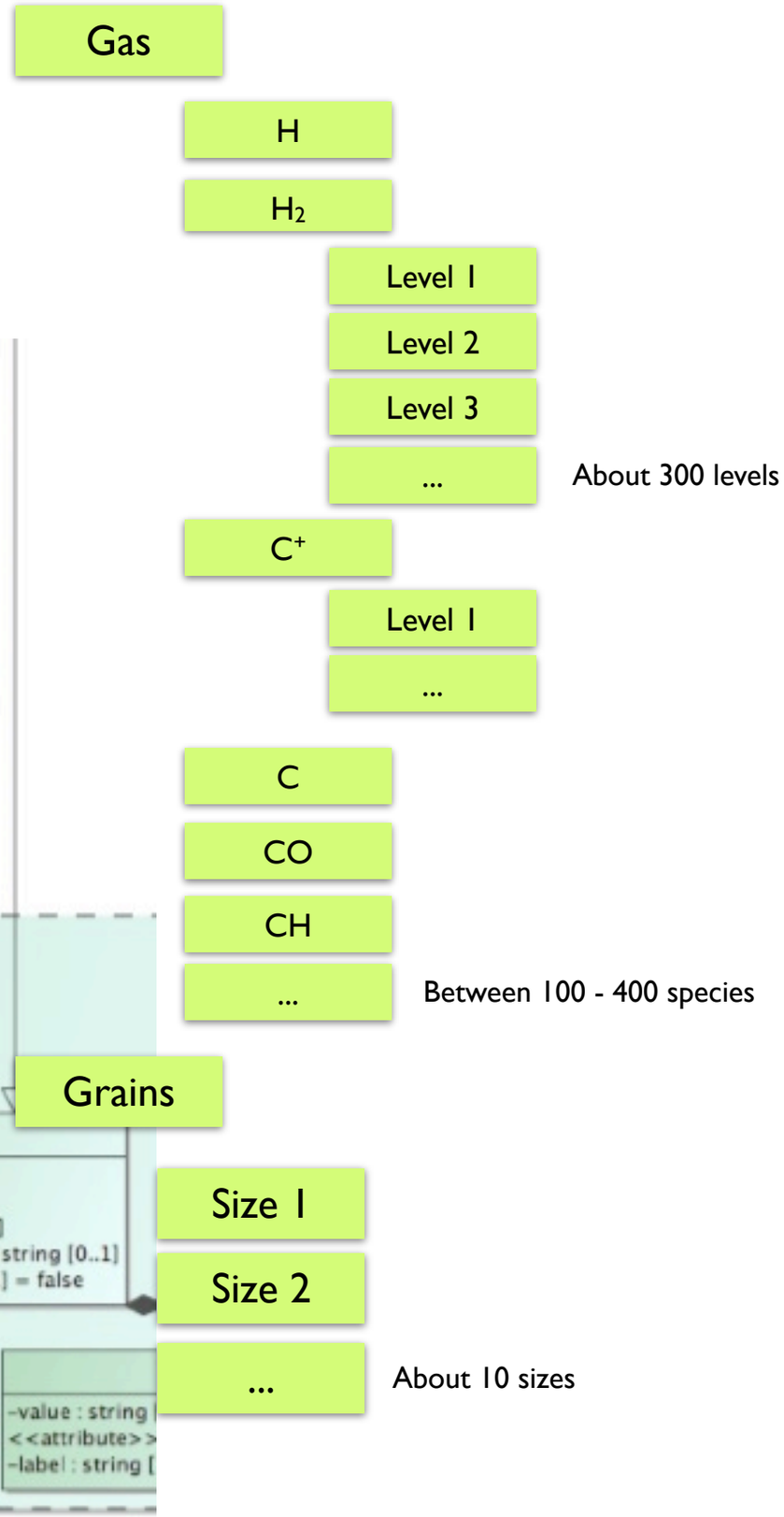
- Effort by PDR modelers community to characterize codes
- Such description not possible in SimDB
- Can wait SimDB 2.0

Implementation of SimDB on PDR simulations

Experiments

- RepresentationObject
- Properties
- Characterisation





Implementation of SimDB on PDR simulations

Experiments

Adaptative Mesh cells

We can describe the content of the simulation **BUT**
Not obvious to choose between RepresentationObjects and Properties

Two solutions to describe the simulations:

- Solution 1 :
  - Object is : gas
  - Properties are : Temperature, density, abundance of H, H_2, C^+, C, CO, ...

- Solution 2 :
  - Objects are : gas, H, H_2, C^+, C, CO, ...
  - Properties are : temperature, density, abundance

- **No obvious choice**
- All PDR simulations in the VO should do it in the same way
- **Best choice will be the one that simplify queries**

Many properties (or objects depending on choosen solution):
- ObjectGroup & PropertyGroup
are usefull

Try to use SimDB for PDR simulations

Experiments

Second difficulty: **Vocabulary**

Semantic Group's vocabulary cover some of the requirements:
- temperature, density, pressure, abundance, ...

But we also need to define by vocabulary (or DM ?):
1- Name for all molecules (included isotops), Ex: CH_3COOH, $CH_3C^{18}OOH$

2- quantum levels for quantities as : "Abundance of H_2 in level v=0, J=3"

3- Need to define precisely properties as "emissivity of CO J=6->5"

4- How to define a quantity as "Abundance of H_2 sticked on silicates of size 0.1 nm" ?

Atomic and Molecular Line Data Model should help for 2 and 3
=> need to define quantities through SimDB and AMLDM

Try to use SimDB for PDR simulations

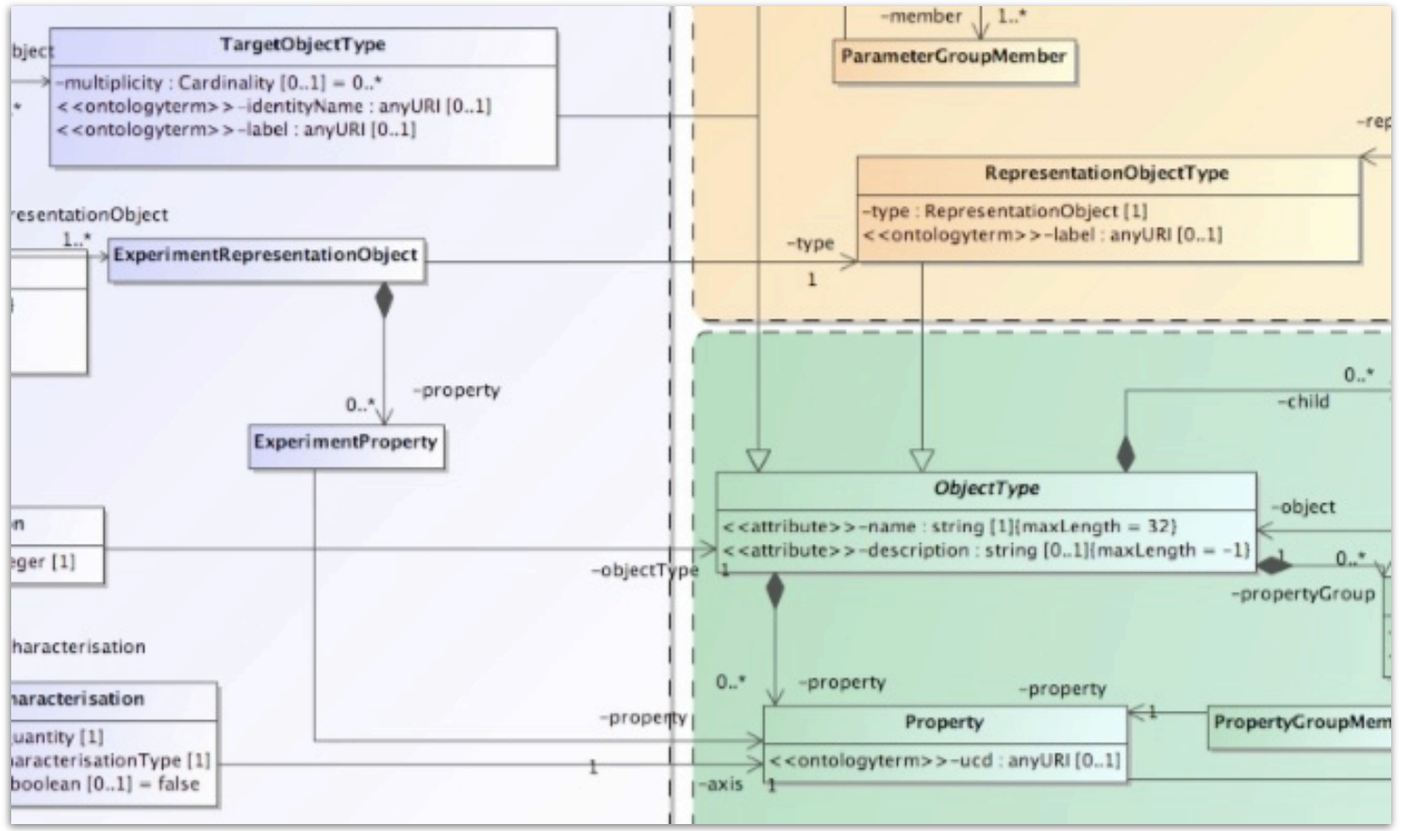
TargetObject

not implemented yet

TargetObject = Interstellar Cloud

Has for properties :
- column densities
- line intensities

-> Allow description of observables



- This is by this way the DM provides informations to solve inverse problem.
- But difficult to use in practice.

Difficulty: description of atoms, molecules, lines, quantum levels

Try to use SimDB for PDR simulations

Some other difficulties

No way to describe **stationnary simulations**:

SimDB done for cosmology and assumes implicitly that simulations are time dependant
BUT: can describe stationnary simulations, there is just one snapshot

How to do the difference between an experiment with only 1 snapshot
- corresponding to 1 time step for a time dependant code
- corresponding to a stationnary solution
-

No way to describe the **number of dimensions or the geometry**:

Example : How to discover through SimDB
- PDR simulations with plan parallel geometry
- PDR simulations with spherical geometry

No way to describe **relationships between properties and axis**

Use of SimDB

Two ways to discover simulations

1 - Query on input parameters to find simulations
Example : search for all simulations with proton density of 10^4 cm^{-3}

2 - Query on characterisations
Example : search all PDR simulations with CO column density above 10^{14} cm^{-3}
(inverse problem)

Use of SimDB

Both present difficulties

1 - Difficulty for queries on parameters:

- The number of parameter is a challenge to browse simulations
- The experiments in a PDR SimDB will vary often

Example on the Meudon PDR code
Only a few of the 60 parameters can vary in the DB

If the user has to choose values for all parameters there is a high probability that there is no answer corresponding to his query.
=> need dynamical browser

The informations to build directly such a browser are not in SimDB DM.
=> requires many queries

Use of SimDB

1 - choose protocol
2 - choose parameters

Query the model parameters :

Back to : **Index** - **Previous Page**

To query the PDR models, please select a protocol :

refresh | cancel

Pdr1.2_chimie08-test | select

Protocol : Pdr1.2_chimie08-test
First test protocol

Please select a least one criteria on parameters :

ID	Parameter	Possible values	Value
282	nH_init	100.0, 500.0, 1000.0, 10000.0	
328	radp_ini	1.0, 5.0	
323	radm_ini	1.0, 5.0, 10.0	
317	Av_max	1.0	

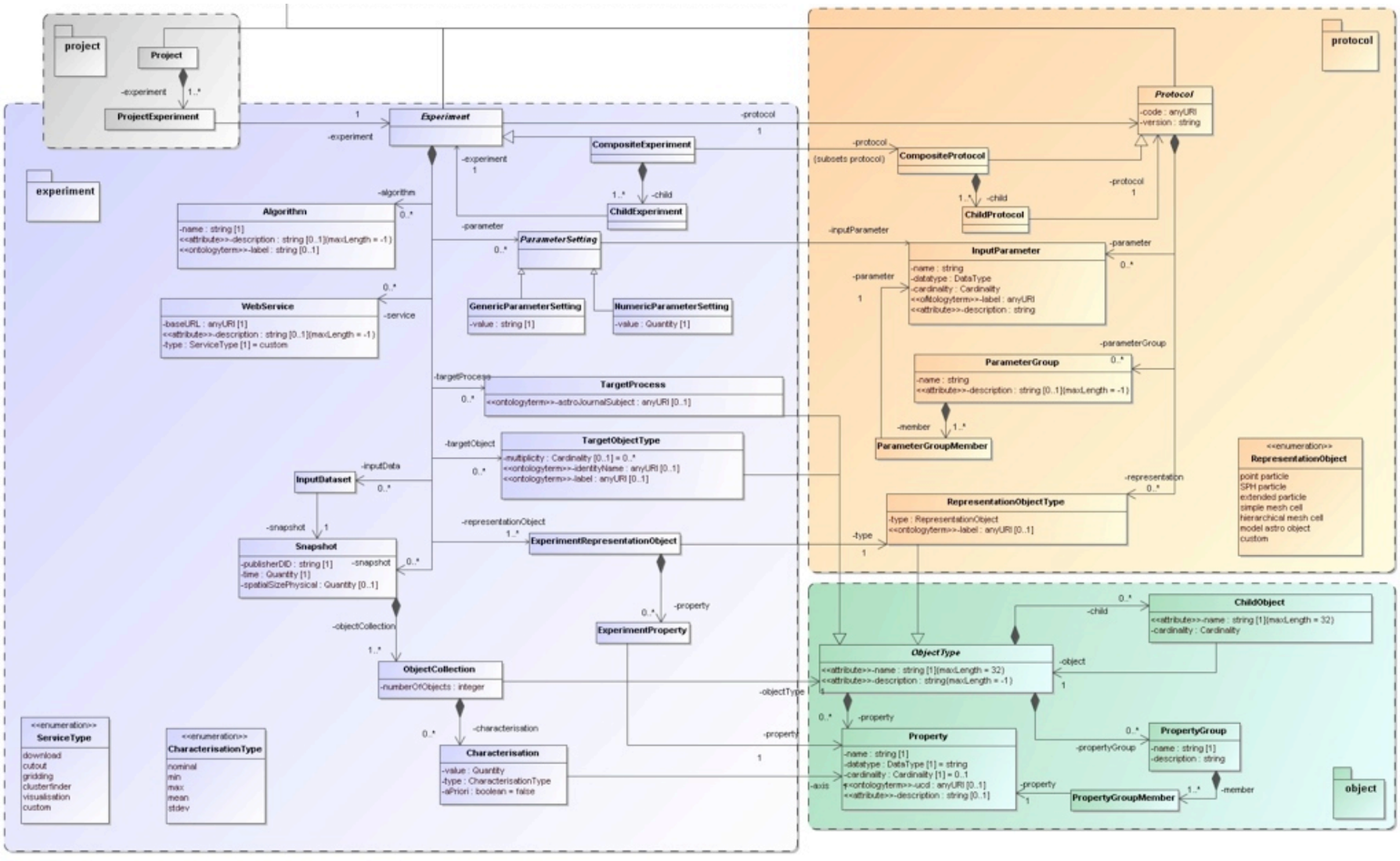
Add another table in SimDB DM to list mandatory parameters ?

Use of SimDB

2 - Difficulty for queries on Characterisation:

SimDB DM is very hierarchical

Experiment -> RepresentationObject -> Properties -> characterisation



Queries on characterisation are very difficult to build.

PDR simulations and SimDAP

SimDAP is promissing for PDR simulations

Context:
PDR simulation produces more than 10 000 outputs
BUT users are usually interested in only a few of them 20 (?)
=> cutout service can be used on it

Challenge:
How to deal with 10 000 properties in SimDAP services ?
Sending the 10 000 properties to the client to allow him to choose is a bit tough ...

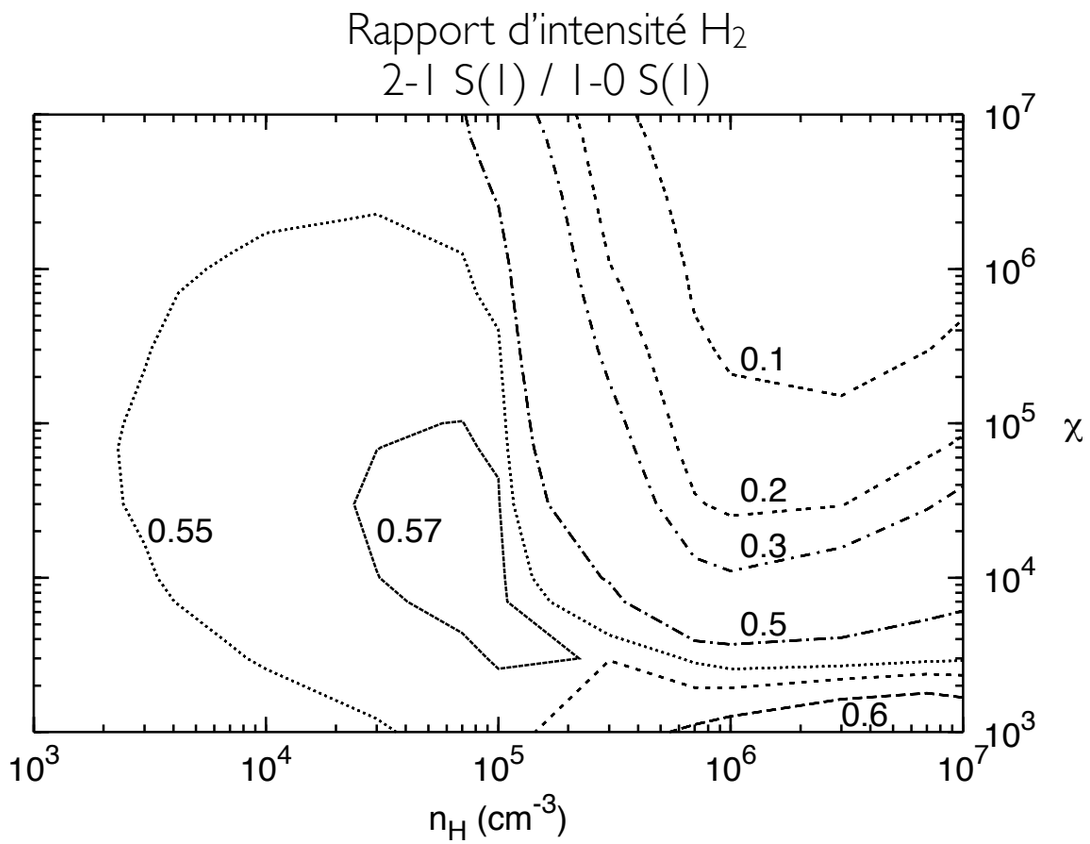
Requirement 1 : Queries to discover parameters should use PropertyGroups.

Possible solution:
Need iterative communication using PropertyGroup:
1 - client requires properties for experiments
2 - server answer PropertyGroup
    2.1 - client choose a PropertyGroup
    2.2 - server sends contain of PropertyGroup
3 - client choose property
4 - ...

PDR simulations and SimDAP

Users may wish to get properties for several simulations:

Example :
Contour maps in space parameters
build from one property extracted in more than 100 experiments

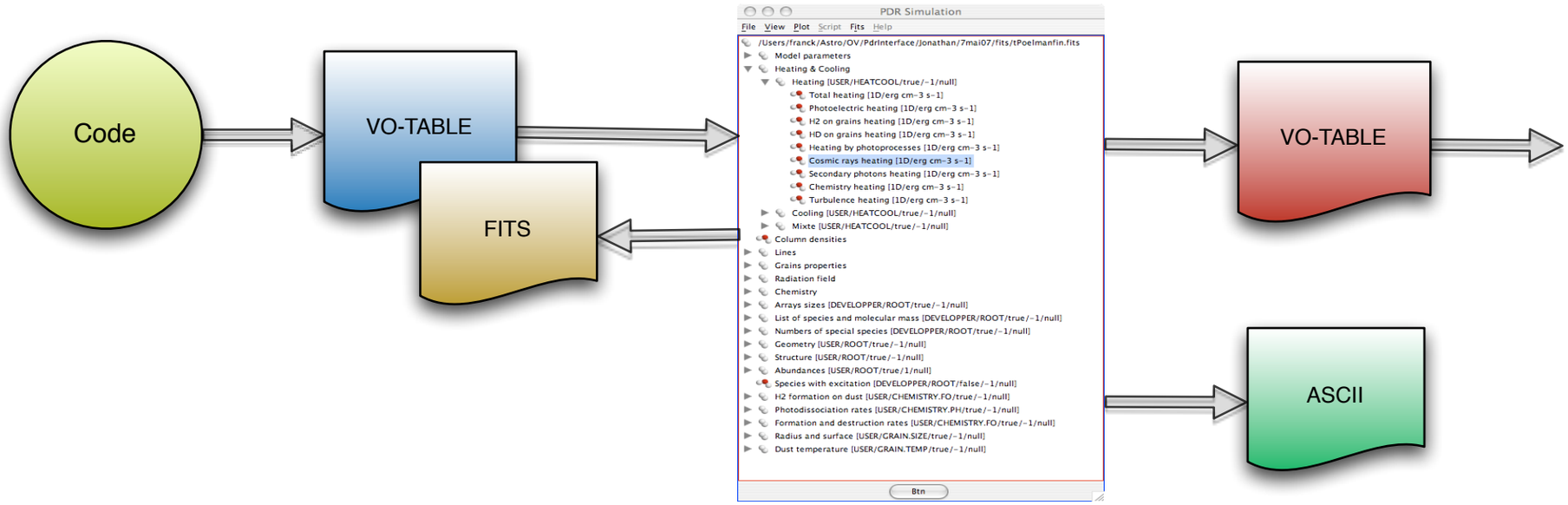


Requirement: Download results for several Experiment/Snapshots at the same time

PDR simulations and SimDAP

Data Format

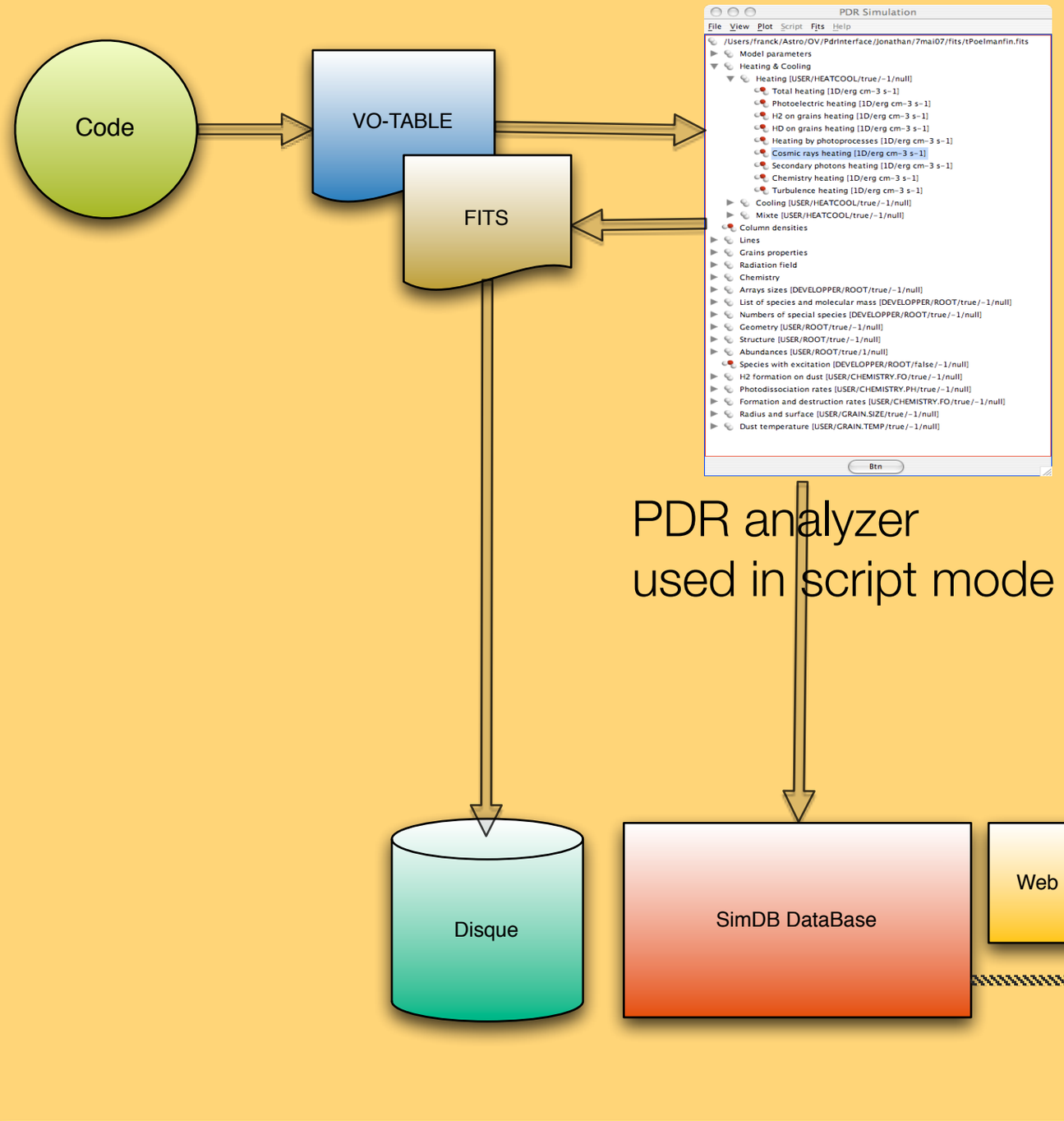
No standard for file format in PDR community
Outputs are heterogenous (quantities function of position, of wavelength, of both)
=> a tool to read data is required



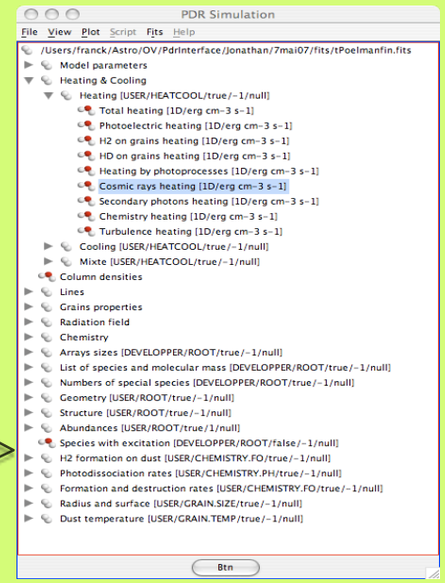

```
      <FIELD name="AB_H3CO+"   ID="DU_ABUNDANCES.FD_AB_H3COp"   datatype="double"      unit="cm-3"   ucd="phys.density"   utype="" />
      <FIELD name="AB_H2CS+"   ID="DU_ABUNDANCES.FD_AB_H2CSp"   datatype="double"      unit="cm-3"   ucd="phys.density"   utype="" />
      <FIELD name="AB_H3CS+"   ID="DU_ABUNDANCES.FD_AB_H3CSp"   datatype="double"      unit="cm-3"   ucd="phys.density"   utype="" />
      <DATA>
         <FITS extnum="0"         >
            <STREAM encoding=""   href="file///./fits/BINFITS/model.fits />
         </FITS>
      </DATA>
</TABLE>
```

PDR simulations and SimDAP

Server side



Client side



Conclusion

Partial implementation of SimDB on PDR simulations done
- SimDB can describe PDR simulations
- no reflexion on spectra yet : related to SSAP

Difficulties to implement SimDB:
- to fill RepresentationObject / Properties
- Vocabulary is missing for:
  - quantities related to Atomic and Molecular physics
  - name for chemical species
  - specific parameters

Difficulties to use SimDB
  - to query on parameters when the number is large
  - to query on characterisation for inverse problem

SimDAP
- should be usefull for PDR simulations

need to take into account:
  - Problem of large number of properties
  - Multi-download