Micro-physics simulations in the Virtual Observatory

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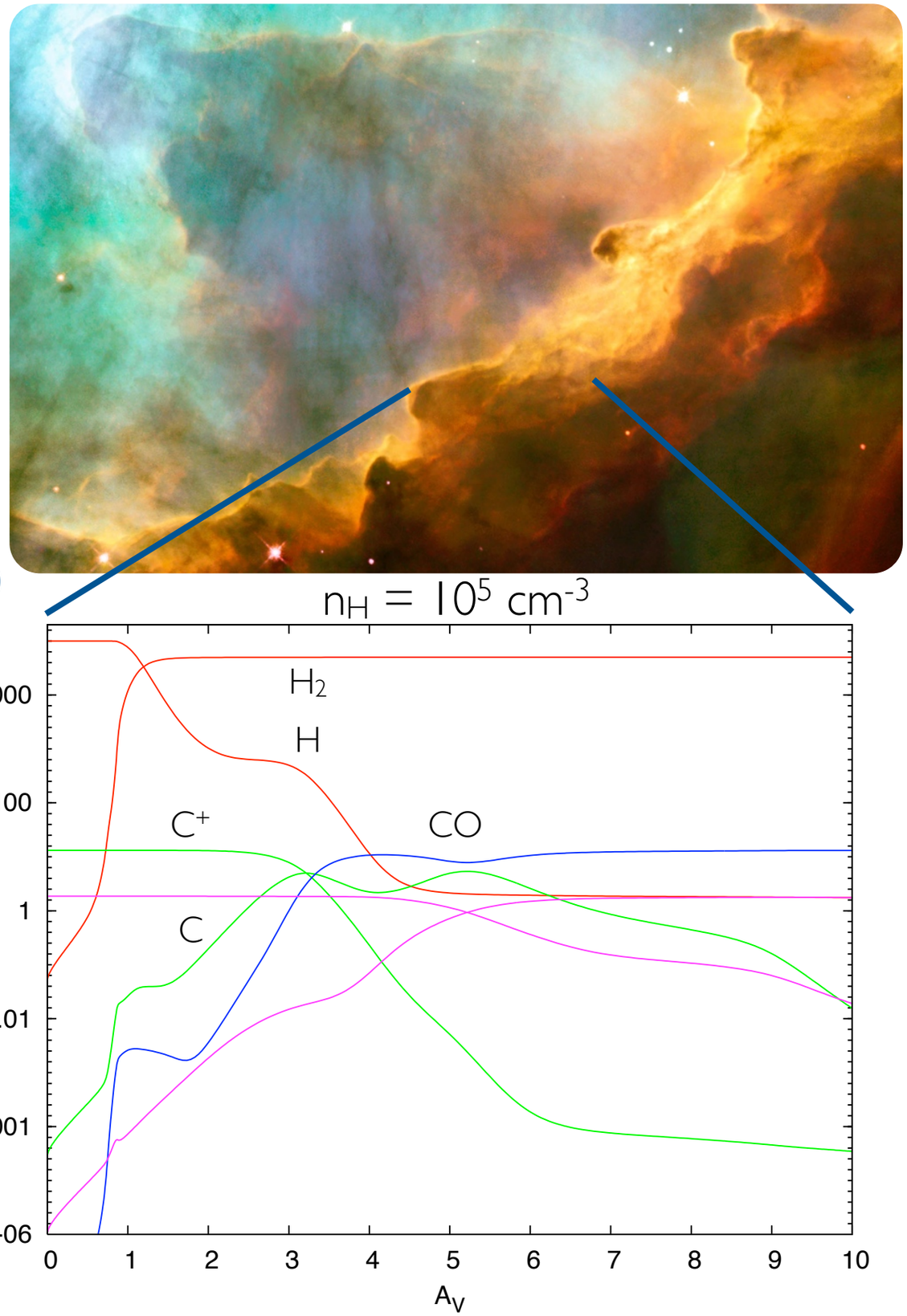
Microphysics codes (Ex: Photoionized regions, Photodissociation Regions, Chocs)

Case:
codes computing the microscopic structure of astrophysical objects

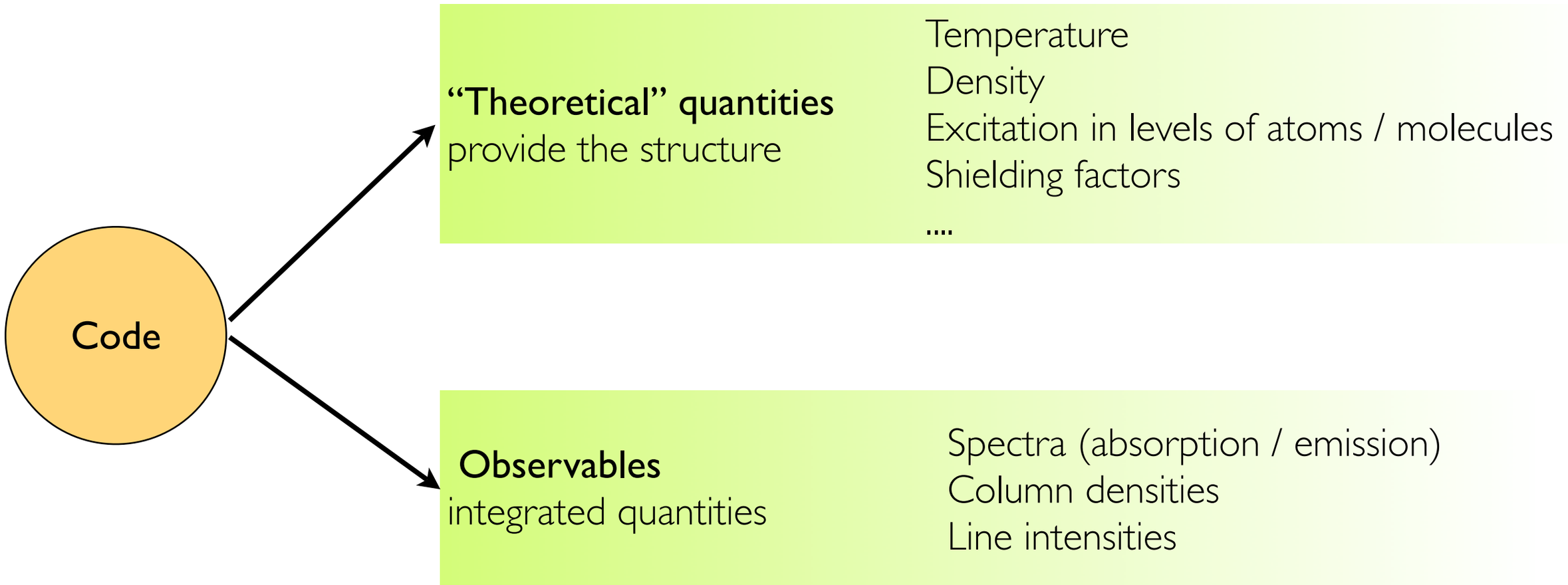
- chemical abundances
- ionization degree of species
- level excitation
- line intensities
- spectra ...

- many other quantities



Microphysics codes (Ex: Photoionized regions, Photodissociation Regions)

Two categories of outputs

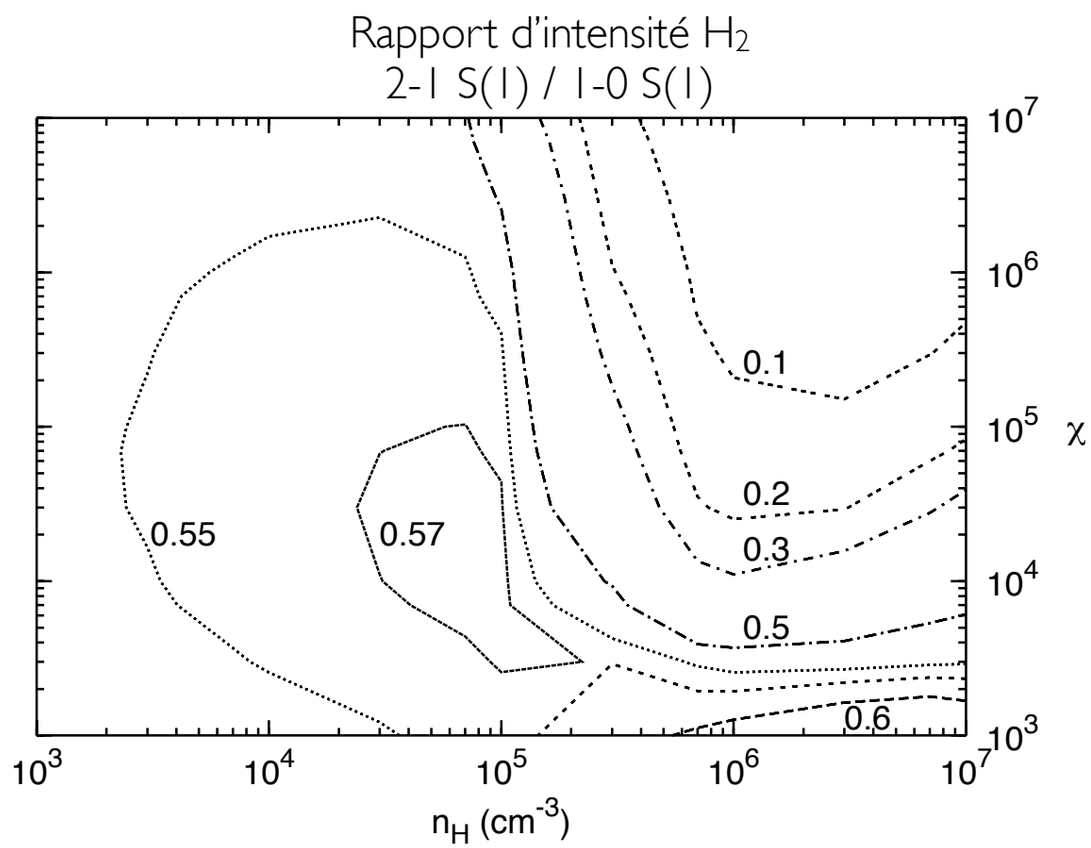


Why to publish such simulations in the Virtual Observatory

InterOperability with what ?

Observers point of view

- Interpret observations - **Inverse problem**
  - Gets observables: spectra, line intensities, column densities, emission maps, **...**
  - Want to get observables for a large set of input parameters (inverse problem)
  Deduce the best parameters to fit observations
- Want **to prepare faster observations**
  - Estimation of observables (Ex: line intensities)

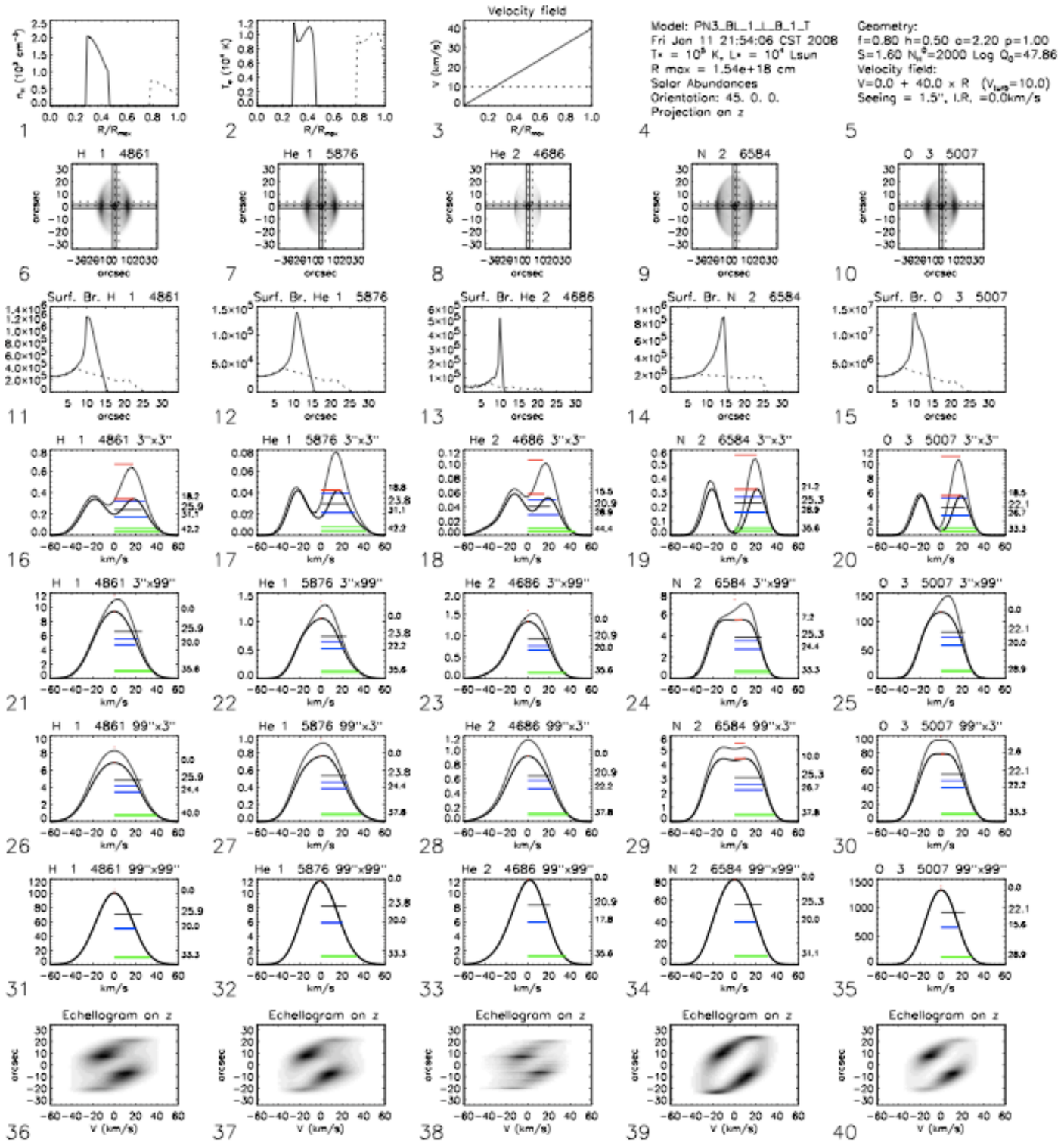


Most of the time queries will be done
on observables (outputs of the simulations)

Example: Which category of nebula produce an O+
column density above a value

Need to publish data
- should be published in the V.O. for easy recovery
- Data as spectra may be interoperable with VO-plotting Tools

Microphysics codes (Ex: Photoionized regions, Photodominated regions)



Theory Workshop - Garching
C. Morisset

- need to define precisely lines, species, quantum levels

- a problem related to Line DM

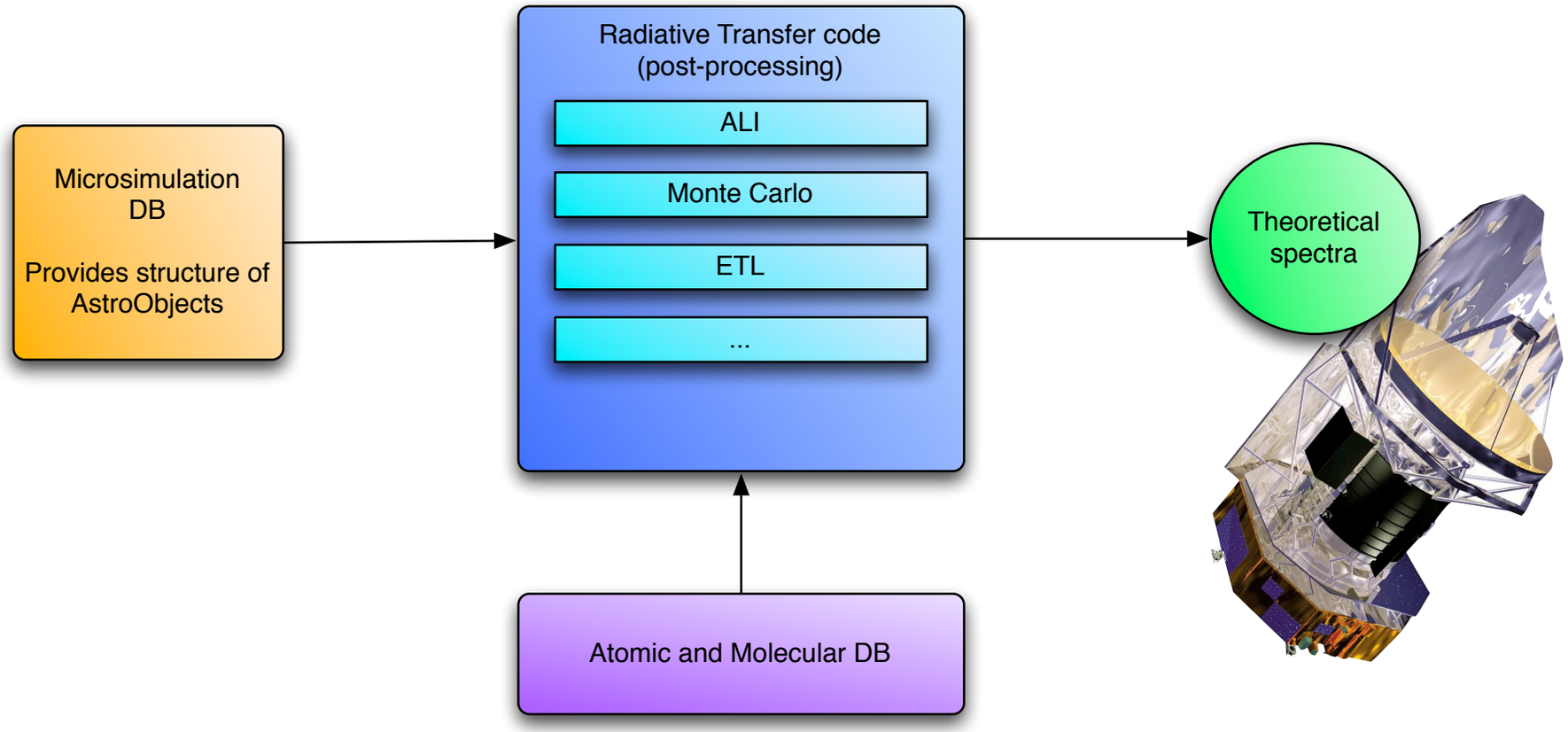
Why to publish such simulations in the Virtual Observatory

InterOperability with what ?

Theorists point of view

- postprocessing
- Towards interoperability between codes

1 - Find a model in a D.B.
2 - Extract profiles (Temperature, some abundances)
3 - Send them to a radiative transfer code
4 - Computes line intensities / spectra



Caracteristic of these simulations:

- 1D or more
- stationnary or time dependant

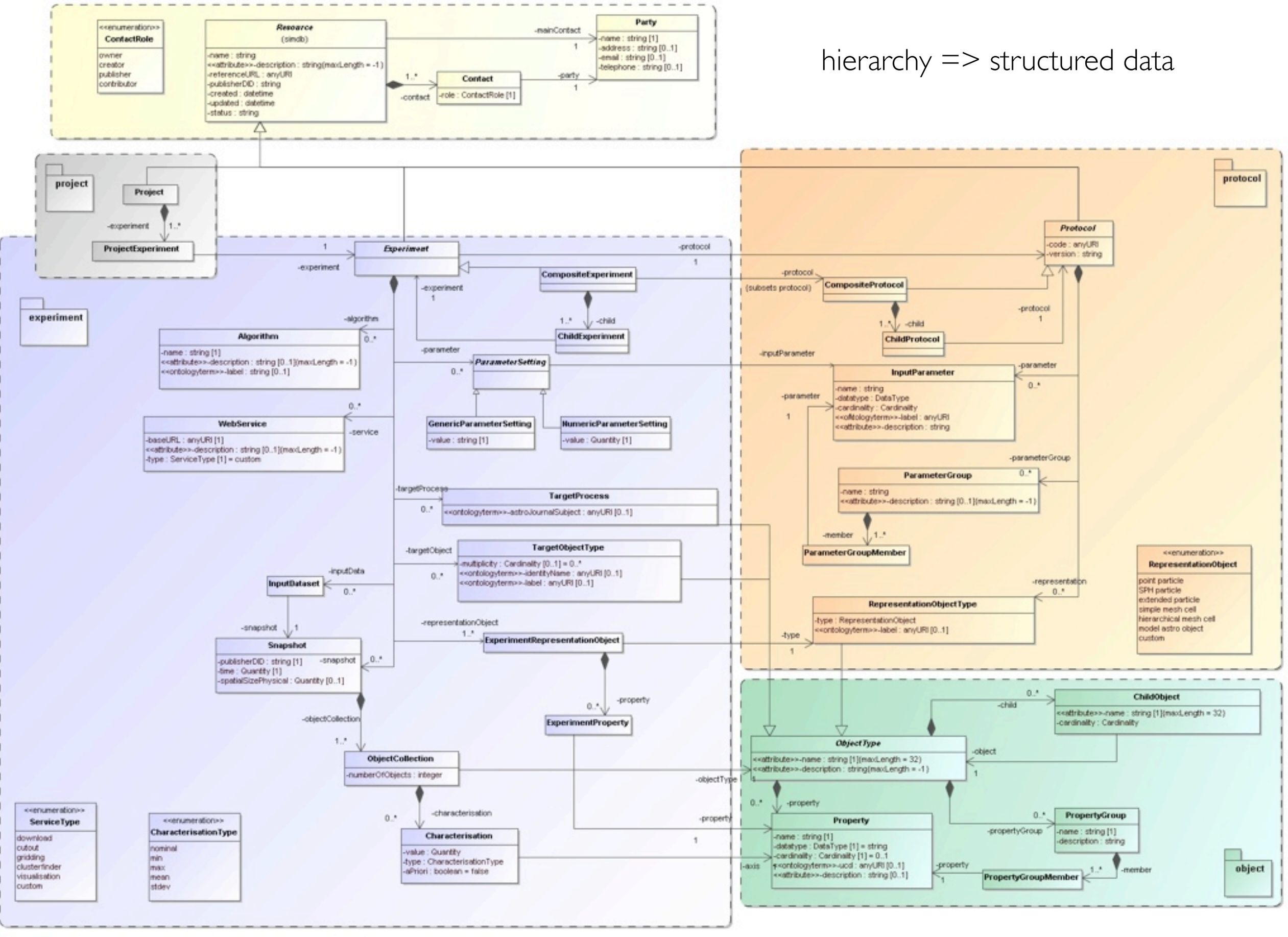
- A large number of input parameters
  - Property of gas
    - Ex: density profile, metallicities, incident radiation field, ...
  - Property of grains
  - Parameters controling algorithms

- A very large number of outputs
  - Structure of the astrophysical object
    - Profiles of density, temperature, pressure, ...
    - Profiles of abundances of chemical species with level populations
    - Line intensities
    - Column densities
    - Spectra

SimDB like

Can we use SimDB ?

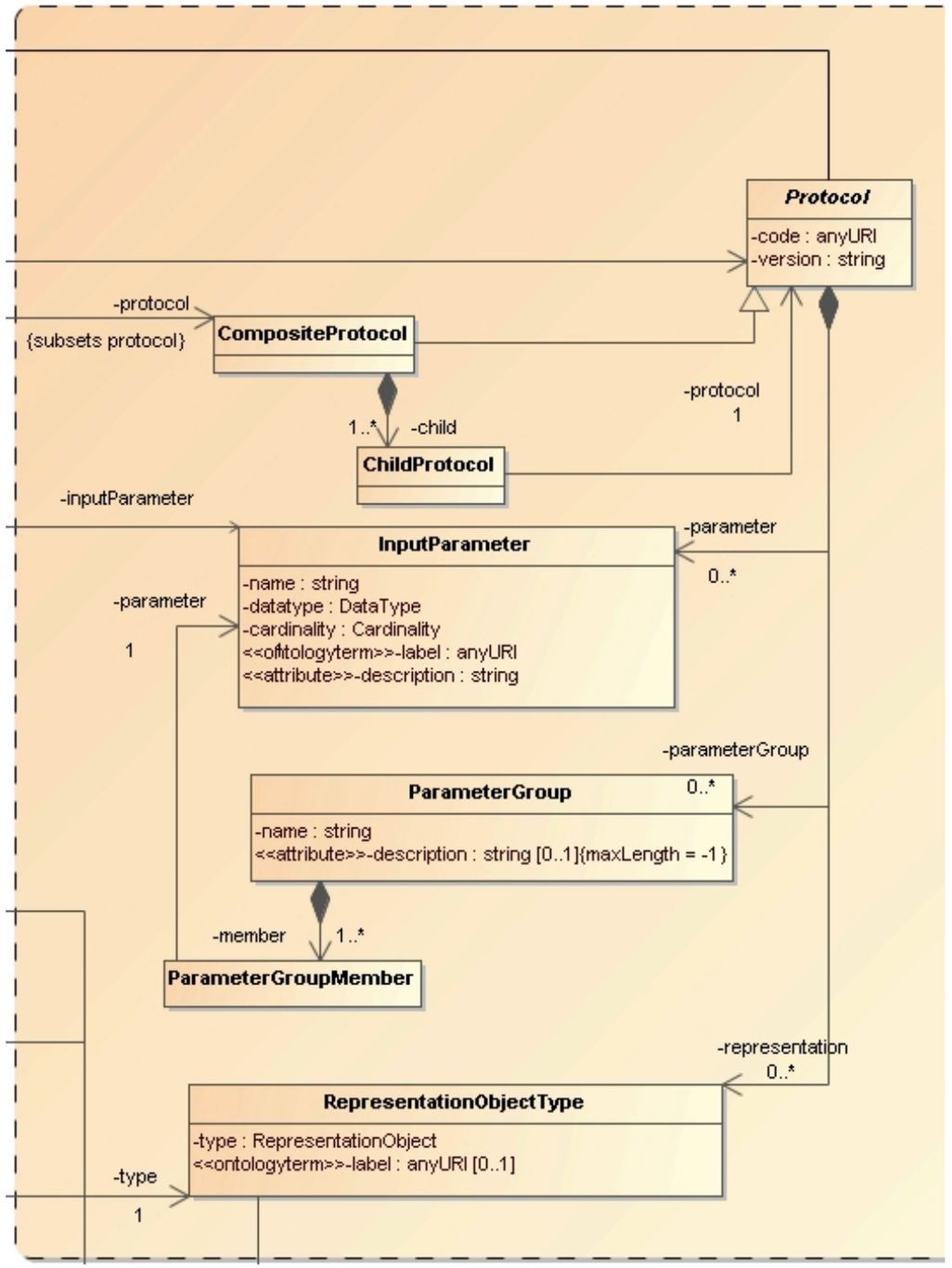
hierarchy => structured data



Parameters

A large number of parameters

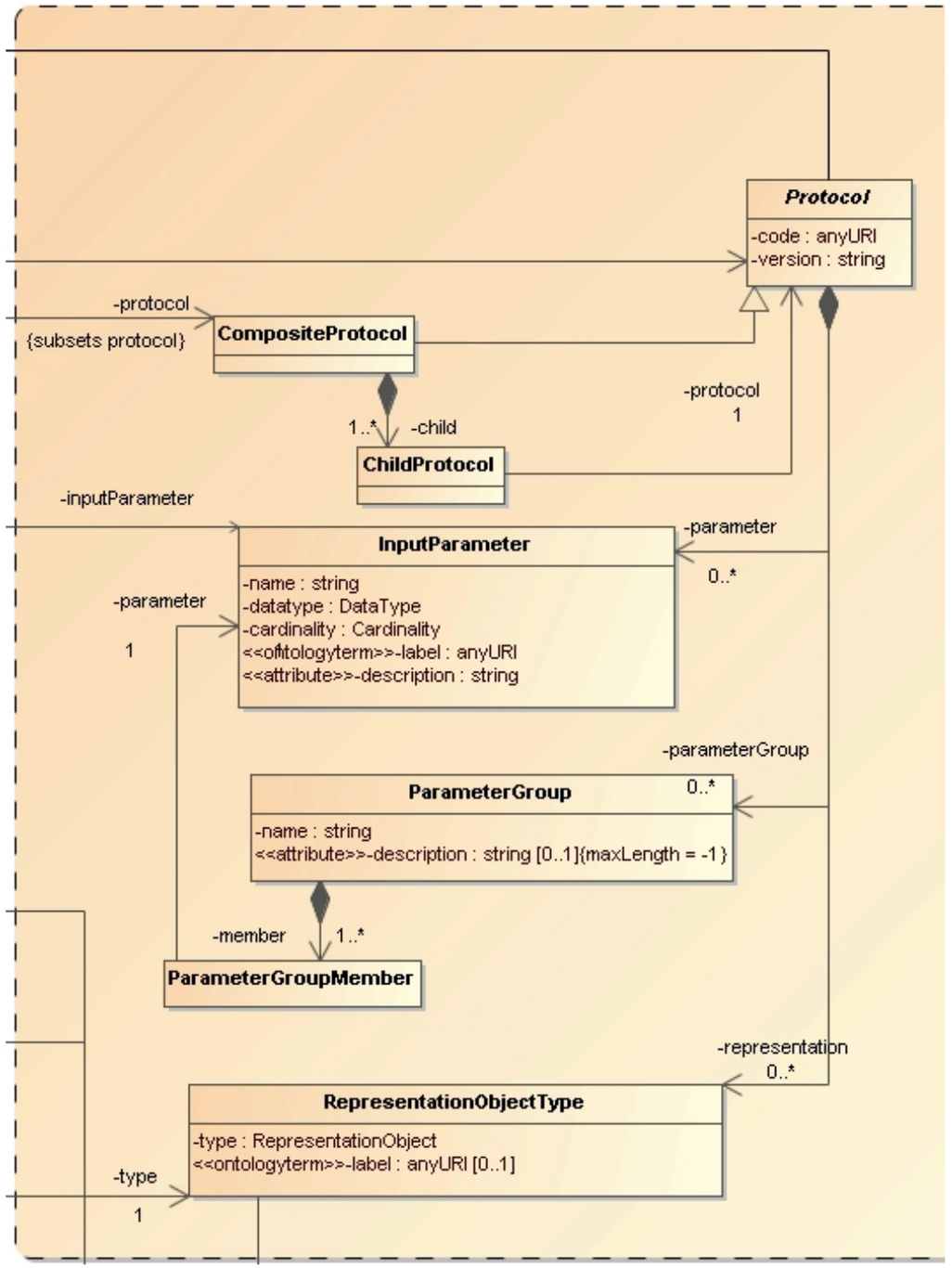
- gas properties
  - density
  - incident radiation field
  - composition
  - ...
- grains properties
  - composition
  - size
  - ...
- algorithm properties



Parameters

```
<parameters>
  <name>FD_NHINIT : Initial proton density</name>
  <description></description>
</parameters>
<parameters>
  <name>FD_RADM_INI</name>
  <label>Initial ISRF scaling factor (observer side) </label>
  <description>Scaling factor to Draine radiation field</description>
</parameters>
<parameters>
  <name>FD_RADP_INI</name>
  <label>Initial ISRF scaling factor (backside) </label>
  <description>Scaling factor to Draine radiation field</description>
</parameters>
```

```
<parameterGroup>
  <name>gas parameters</name>
  <description>Parameters controling gas properties</description>
  <member>
    <parameter>#FD_NHINIT</parameter>
  </member>
  <member>
    <parameter>#FD_RADM_INI</parameter>
  </member>
  <member>
    <parameter>#FD_RADP_INI</parameter>
  </member>
</parameterGroup>
```



ObjectTypes

Simple Mesh Cells

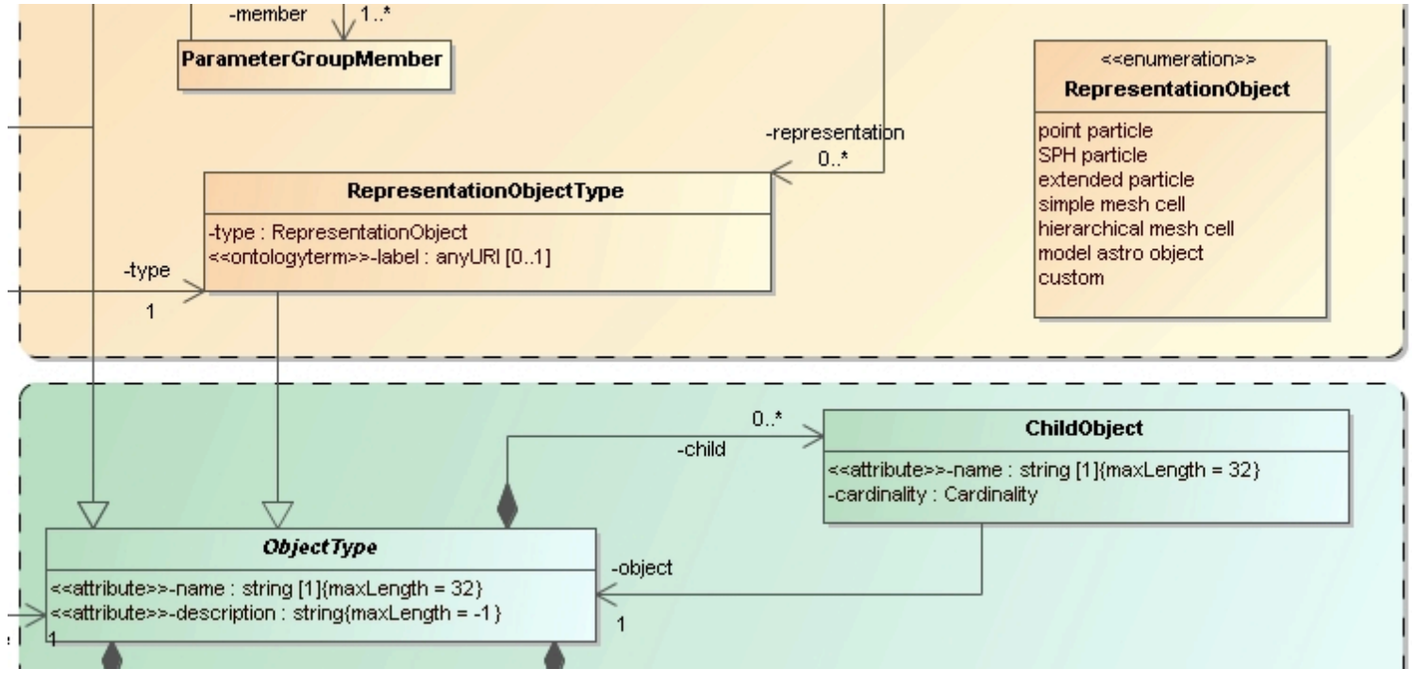
- Gas
  - H
  - H_2
    - Level 1
    - Level 2
    - Level 3
    - ...
  - C^+
    - Level 1
    - ...
  - C
  - CO
  - CH
  - ...

About 300 levels

Between 100 - 400 species

- Grains
  - Size 1
  - Size 2
  - ...

About 10 sizes



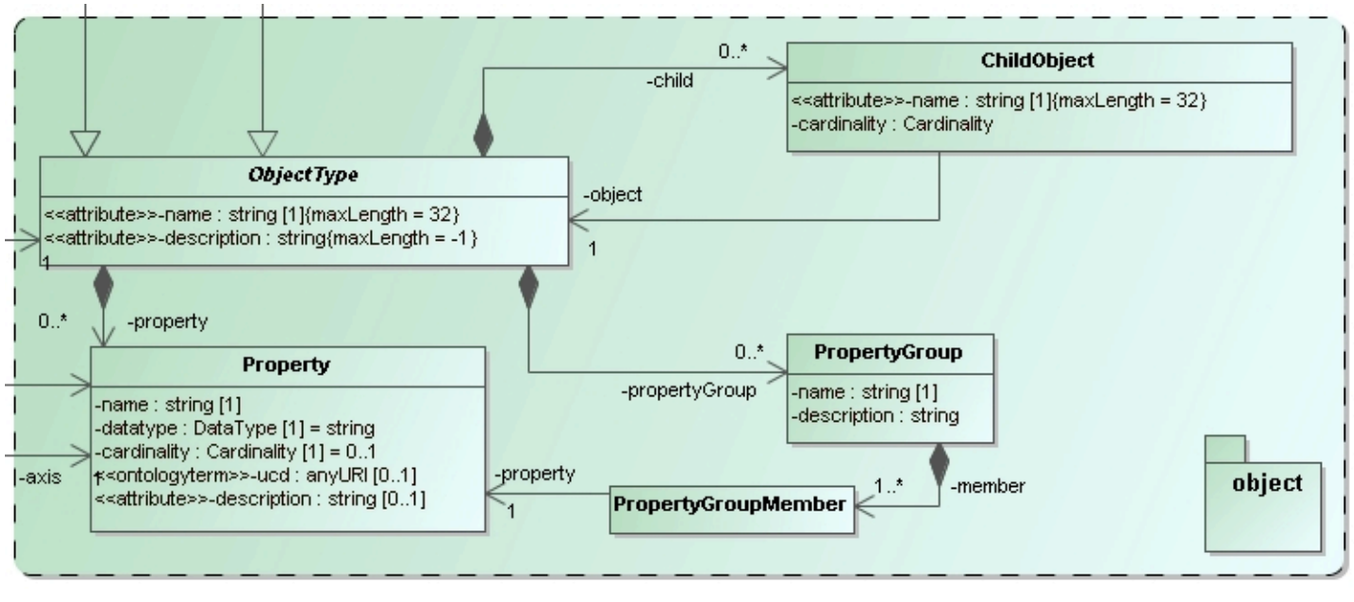

```
<representation>
   <name>gas  ID="R_GAS"</name>
   <description>Interstellar gas</description>
   <child>
     <name>H</name>
     <object>R_H</object>
   </child>
   <child>
     <name>H2</name>
     <object>R_H2</object>
   </child>
   ...
   <label></label>
   <astroJournalSubject>ISM</astroJournalSubject>
</representation>
<representation>
   <name>H ID="R_H"</name>
</representation>
<representation>
   <name>H2 ID="R_H2"</name>
   <child>
     <name>H2 Level 1</name>
     <object>R_H2_Level_1</object>
   </child>
   <child>
     <name>H2 Level 2</name>
     <object>R_H2_Level_2</object>
   </child>
```

Properties

Gas

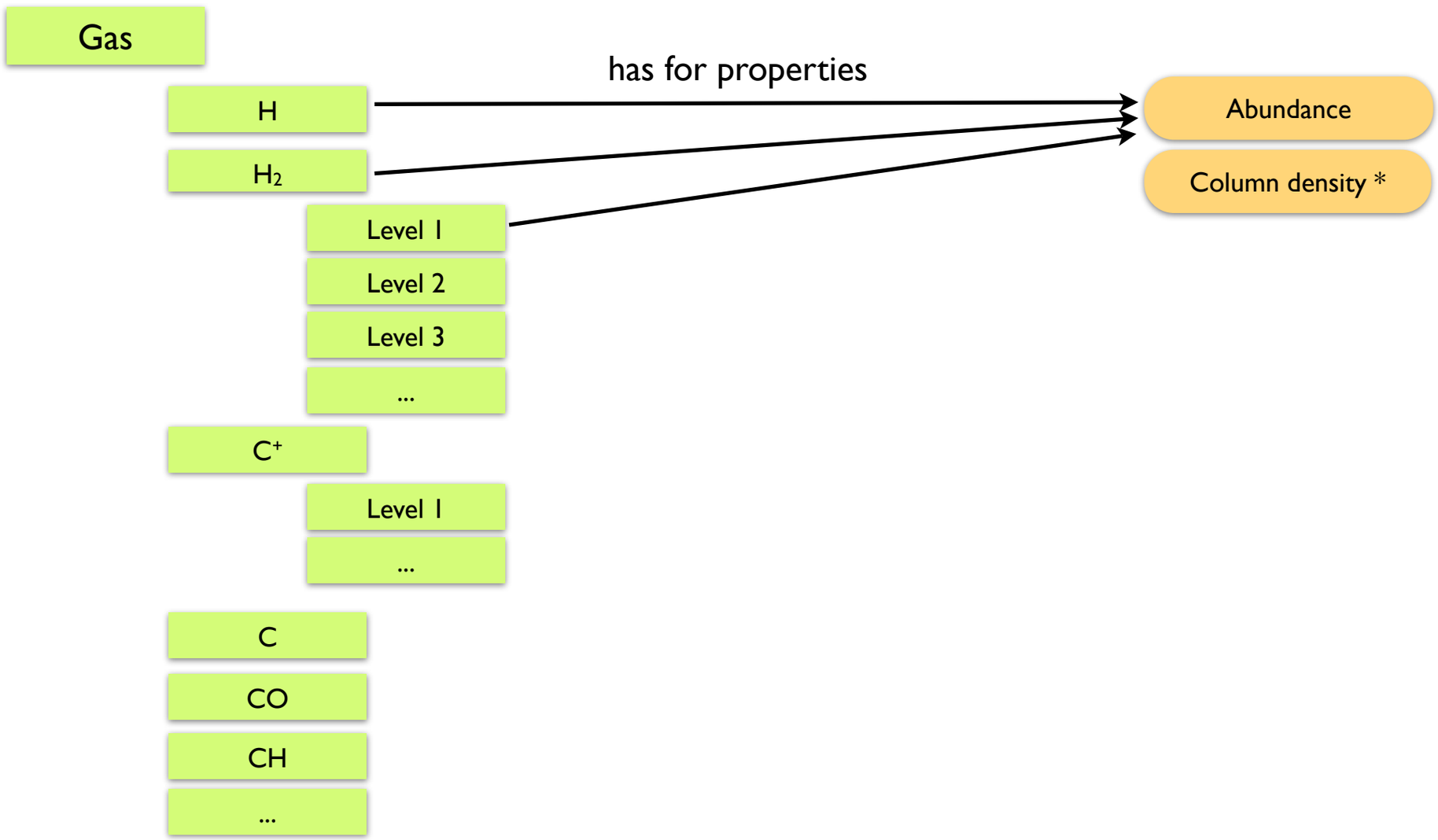
has for properties

- Temperature
- Total density
- Proton density
- Ionization degree
- Pressure
- Lines intensities
- ...
- Heating rate
  - Total
  - Photoelectric
  - Cosmic rays
  - ...
- Cooling rate
  - Total
  - C
  - CO
  - ...




```
<property>  <!-- Objects concern: Gas -->
        <name> Heating rates </name>
        <description>Profiles of heating rates in erg cm-3 s-1</description>
        <child>
            <property>
                <name>Total heating rate</name>
                <datatype>double<datatype>
                <cardinality>1..*</cardinality>
                <ucd></ucd>
                <description>Heating rate in erg cm-3 s-1</description>
            </property>
        </child>
        <child>
          <property>
                <name> Photoelectric Heating </name>
                <datatype> double </datatype>
                <cardinality>0</cardinality>
                <ucd></ucd>
                <description>Heating rate by photo-electric effect on grains in erg cm-3 s-1</description>
          </property>
        </child>
```

Properties


Gas
H
H_2
Level 1
Level 2
Level 3
...
C^+
Level 1
...
C
CO
CH
...
has for properties
Abundance
Column density *

Conclusion on SimDB for such kinds of microphysics codes

SimDB seems to permit the description of protocols and some parts of the experiment.
In particular:

- the structure of an object.
- the hierarchy in Objects / Parameters / Properties
- detail description of protocol

But difficulties:

- Definition of a snapshot
- Integrated quantities related to a snapshot
  Ex: Column densities, Line intensities

- Semantics: Atoms, Ions, Molecules, levels and lines

- These simulations produce also spectra

Conclusion on SimDB for such kinds of microphysics codes

some microphysics simulations are at the boarder of several domain