l'Observatoire de Paris | LUTH

Laboratoire de l'Univers et de ses Théories

The Meudon PDR code in the VO

Franck Le Petit

Objectifs

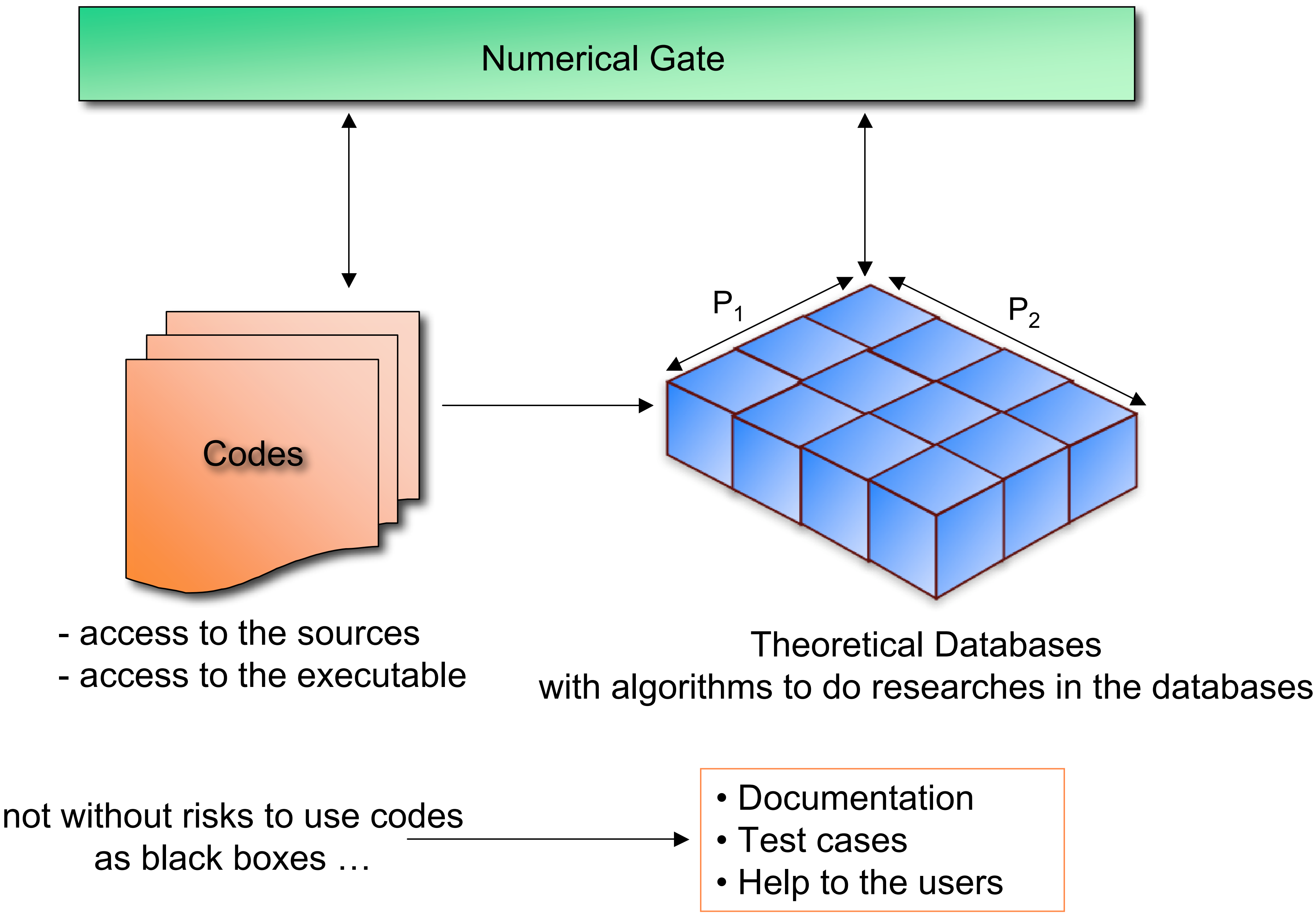
1 - Access to the codes developed at the Observatory of Paris

2 - Databases of theoretical results

3 - Codes and databases in the VO context

Purposes :

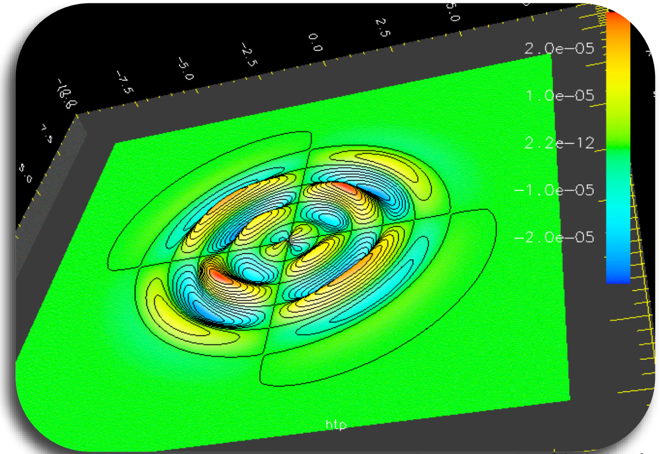
- **To make profitable the contributions asked by codes developements**
- **To facilitate the interpretation of observations**
- **To work more efficiently**


Numerical Gate
Codes
P1
P2
- access to the sources
- access to the executable
Theoretical Databases
with algorithms to do researches in the databases
not without risks to use codes
as black boxes …
• Documentation
• Test cases
• Help to the users

Priority to some « big » codes

Codes

- **Lorene**



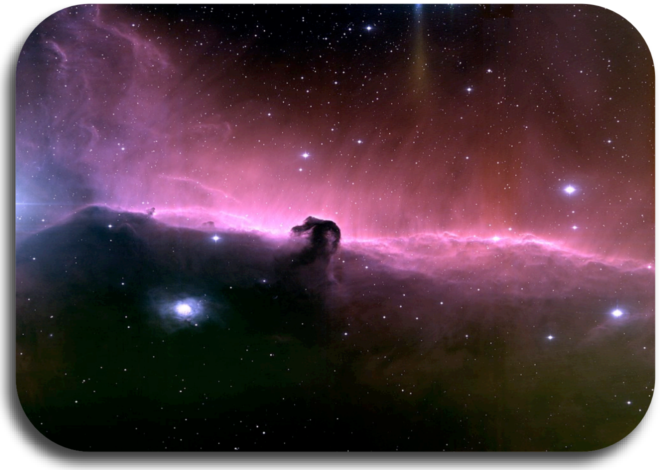
Bonazzola et al. (2004)

Relativistic team (LUTH)

- Libraries to solve partial differentials equations
  Multi-domain spectral methods

  Applications : - Compact objects
  - Relativistic jets (Zakaria Meliani)

- **The Meudon PDR code**



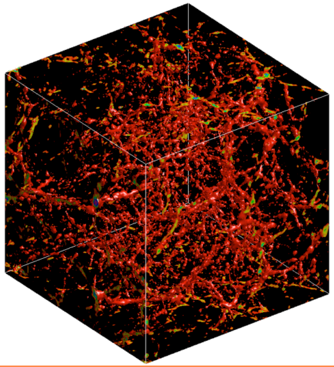
MIS team (LUTH)

Applications :
- Interpretation of observations in molecular regions
  Examples : FUSE, ISO, HST(STIS)
  Herschel, ALMA, …

Ongoing projects

- **Codes de cosmologie**

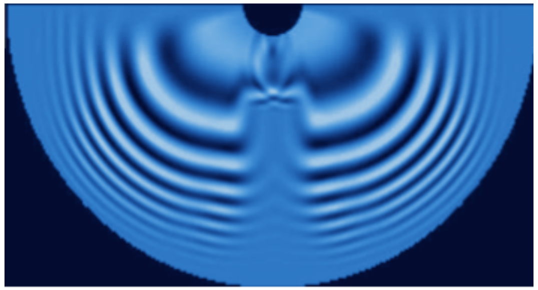
Jean-Michel Alimi, André Füzfa & collaborators



Applications : Formation of structures / galaxies
- N-body
- Hydrodynamic
- non-equilibrium chemistry

- **code MHD**

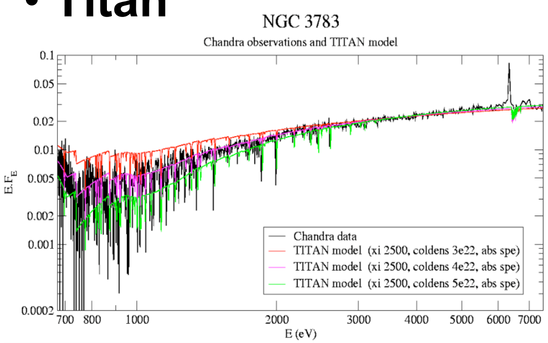
Roland Grappin, Filippo Pantellini (LESIA)



Resolution of MHD equations 1D/2D/3D
Particularities : open bounds

Applications : - stellar atmospheres, corona, winds
- stellar formation

- **Titan**



Anabela Gonçalves, Loïc Chevallier, René Goosman

Radiative transfer in optical thick medium
Applications : Interpretation of X observations
(Chandra, XMM, *XEUS*, …)

Developement of theoretical databases

1 - **Dense cores database** (P. Hennebelle - LERMA)

MHD models of the structure of dense cores : density, magnetic field, …

- Interpretation / preparation of ALMA observations ALMA (and others) of dense cores and pre-stellar regions
- Link with codes solving micro-physics / radiative transfer codes

2 - **Titan database** (Anabela Gonçalves, Loïc Chevallier)

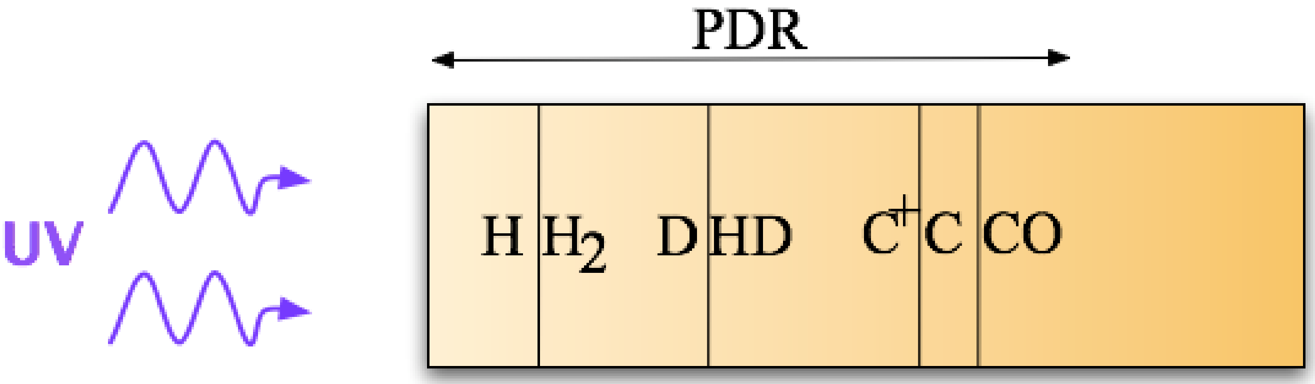
- Interpretation of X-ray observations from Chandra,XMM-Newton, Suzaku
- Preparation of future X-ray missions (Con-X, XEUS, Simbol-X)

3 - **PDR database** (MIS team - LUTH)

Abundances of molecular species, excitation state, temperature profiles for a wide range of parameters of interstellar clouds

- Interpretation of observations of PDRs (ISO, VLT, Herschel, Spitzer, ALMA)
- diffuse clouds (FUSE, HST, CFHT, …)

The Meudon PDR code



Stationnary model solving:

- Radiative transfer: absorption in the lines of H, H_2, CO, HD, …
  absorption in the continuum

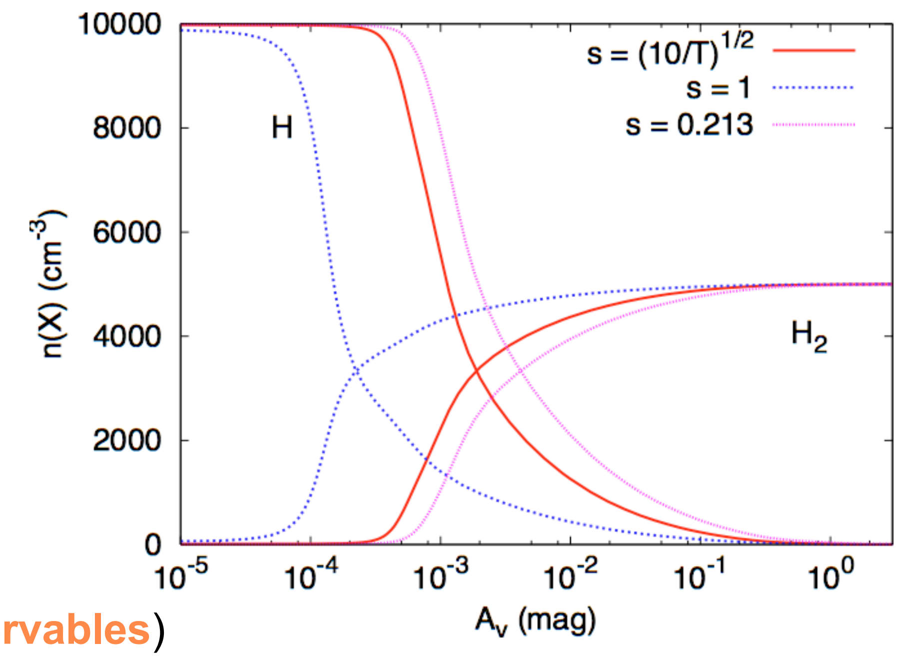
- Chemistry: more than 100 chemical species
  network of more than 1000 chemical reactions
  photoionization

- Statistical equilibrium of the populations in the levels of H_2, HD, CO, HCO^+, CS, …
  takes into account: radiative and collisional excitation / de-excitations
  photodissociation

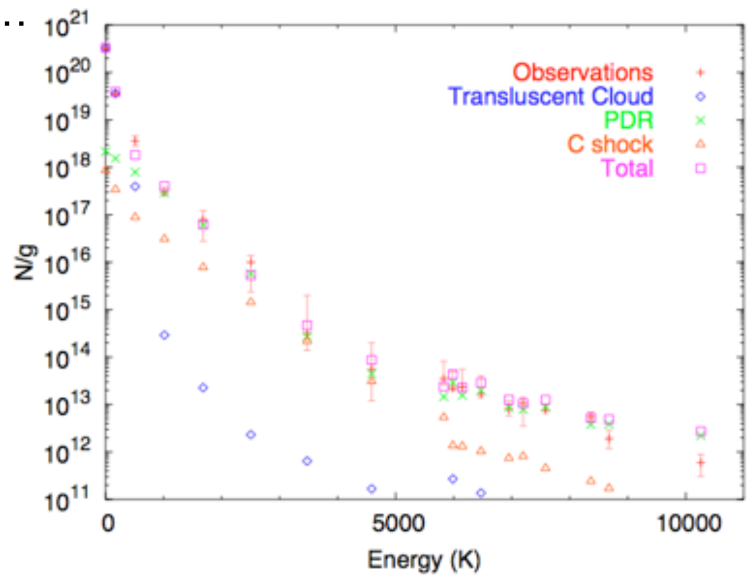
- Thermal balance: heating by photoelectric effect, chemistry, cosmic rays …
  cooling in the lines of atoms and molecules

Outputs :

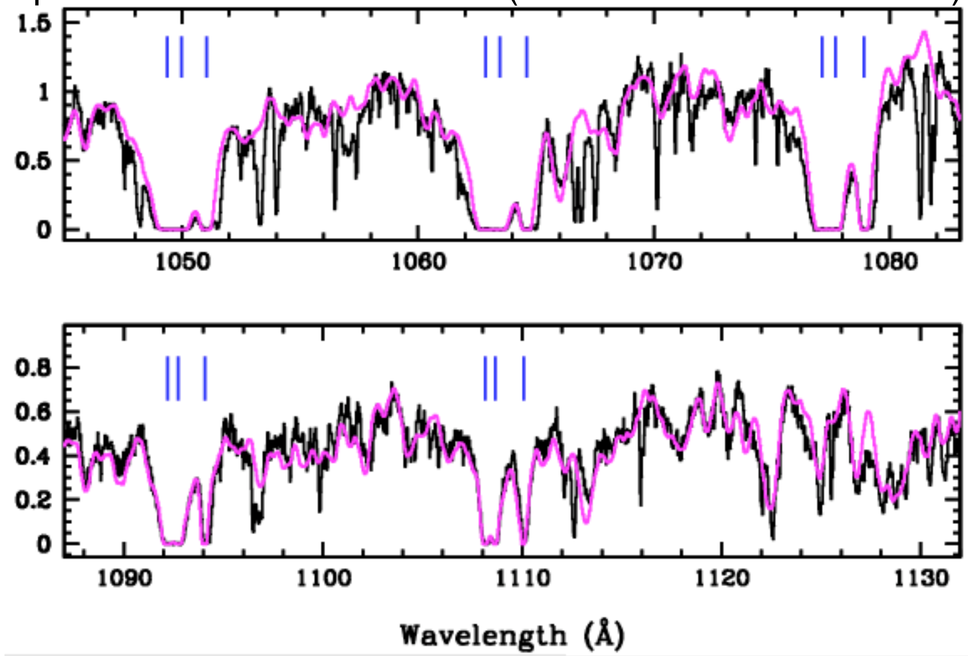
local quantities (at each point of the cloud) :
- abundance and excitation of species
- temperature of gas and dust
- heating rates for each heating mechanism
- cooling rates for each mechanism
- density of energy
- rates of chemical reactions
-…



integrated quantities on the line of sight (Observables)
- column densities
- intensities in lines
- absorption of the radiation field
- …



Spectre FUSE vers HD76534 (C. Martin-Zaïdi et al. 2006)

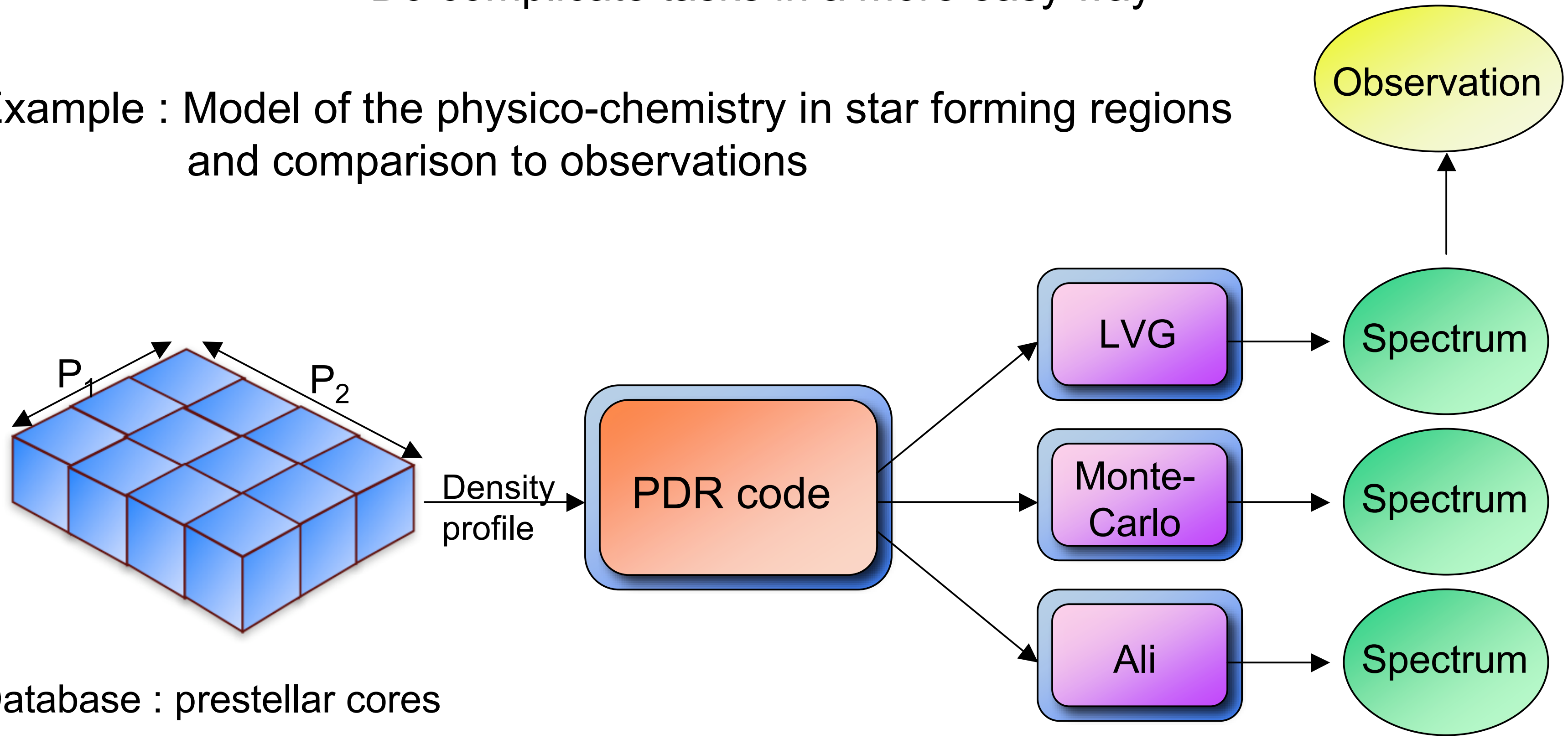


Virtual Observatories

Standardization inputs/outputs → Interoperability

Do complicate tasks in a more easy way

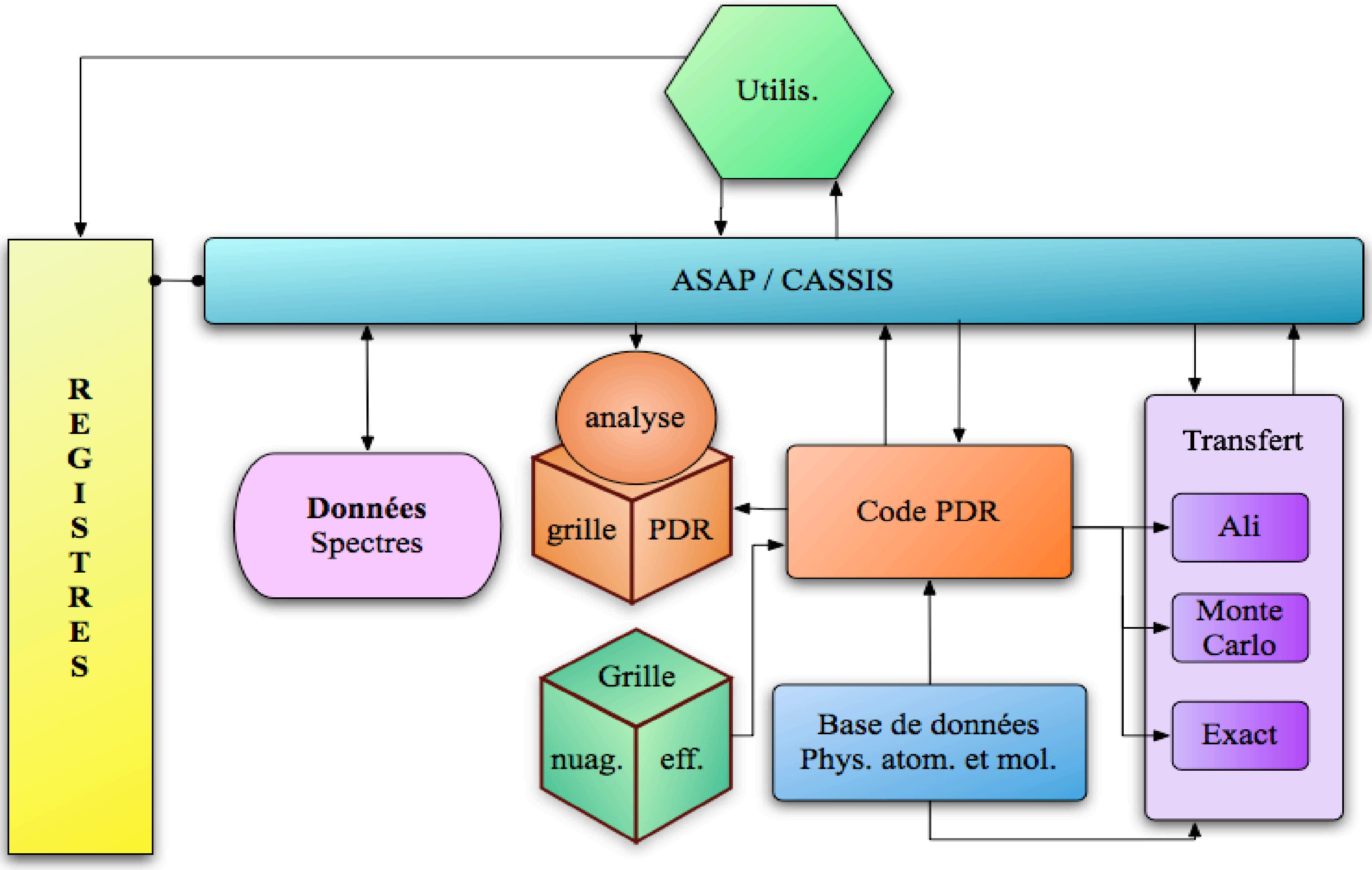
Example : Model of the physico-chemistry in star forming regions and comparison to observations



Database : prestellar cores

Usecase

Next generation of instruments : huge amount of data
⇘ need efficient tools to analyse and interpret the observations



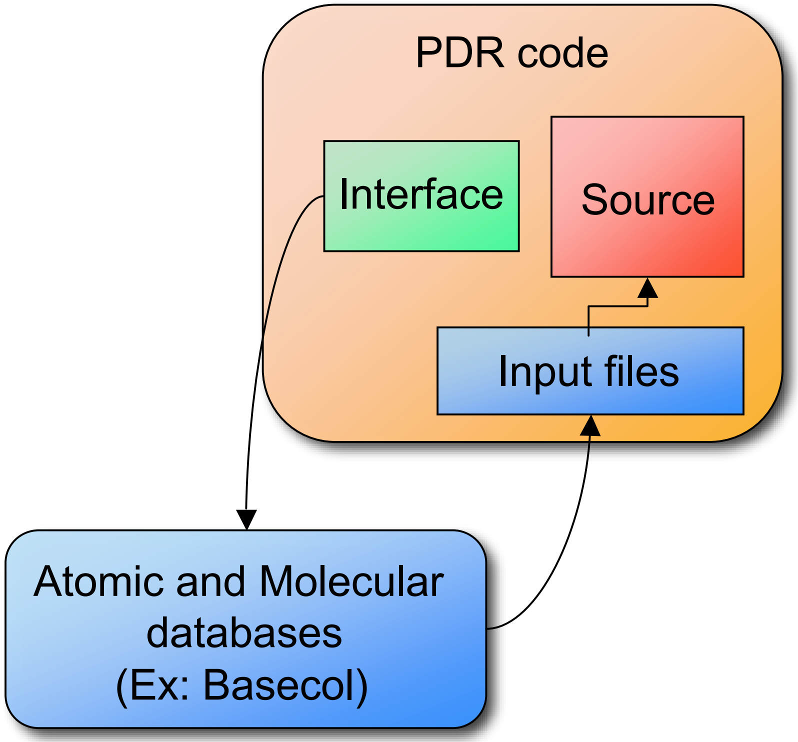
Step 1 : Use of the VO :

Link : PDR code / databases (1)

Data used by PDR codes :

- Atomic and molecular properties :
    - Energy levels
    - Einstein coefficients

- Reactions between elements
    - collision rates
    - chemical reaction
        - gas phase reactions
        - surface reactions
        - photo-process cross sections



Data stored in :
• files
• directly inside the code
↳ modification of the code

→

• re-writing of the code to use only datafiles
• script looking for data in databases
• automatic implementation of new data

Link PDR code / databases (2)

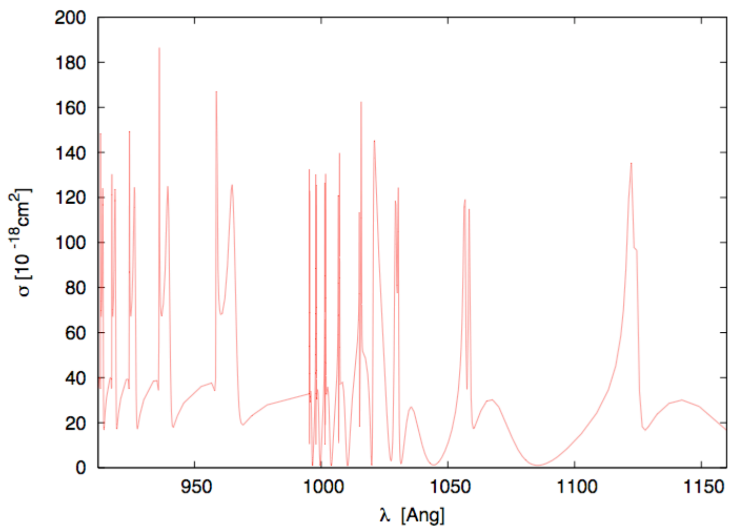
- **Photo-processes:** X + hν ⟶ Y + Z

Up to now : $P = P_0 \exp(-\beta A_V)$

↳ replaced by direct integration of cross sections

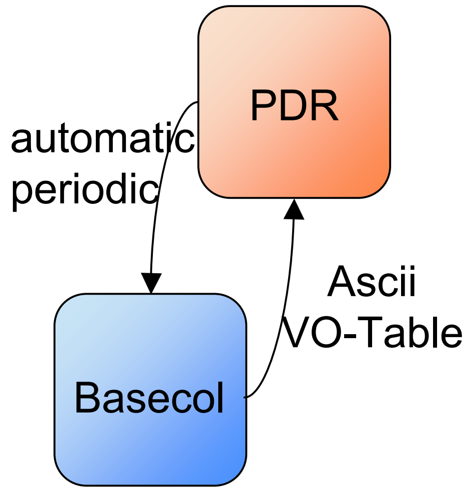
$$P = \frac{1}{h}\int_{\lambda_0}^{\lambda_{cut}} \sigma(\lambda)\, I(\lambda)\, d\lambda$$

Problem : no databases of this kind in VO-format



- **Collision rates :** used to solve statistical equilibrium equation
  - excitation of species
  - cooling ⟶ thermal balance

Basecol (Obs. Paris / M.-L. Dubernet) ⟶ VO-standards



Very simple developement of the code
(Auto-developement of the code)

Step 2 : PDR code in the VO (1)

PDR codes as other codes are used in 2 steps :

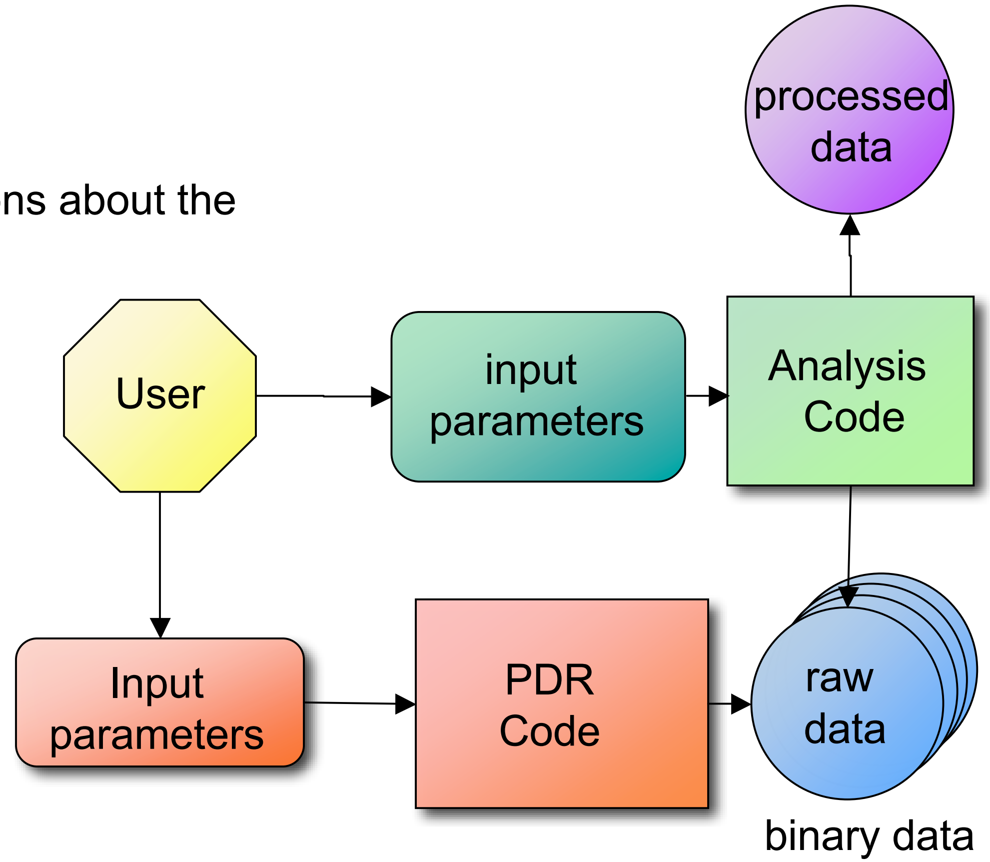
1 - PDR code

- Give entrance parameters
- run the code

=> production of a binary file
contains all the informations about the
structure of the cloud

2 - Analysis code

- Reads the binary file
- Give entrance parameters
- (optional: computation)
- Give results in a human readable format

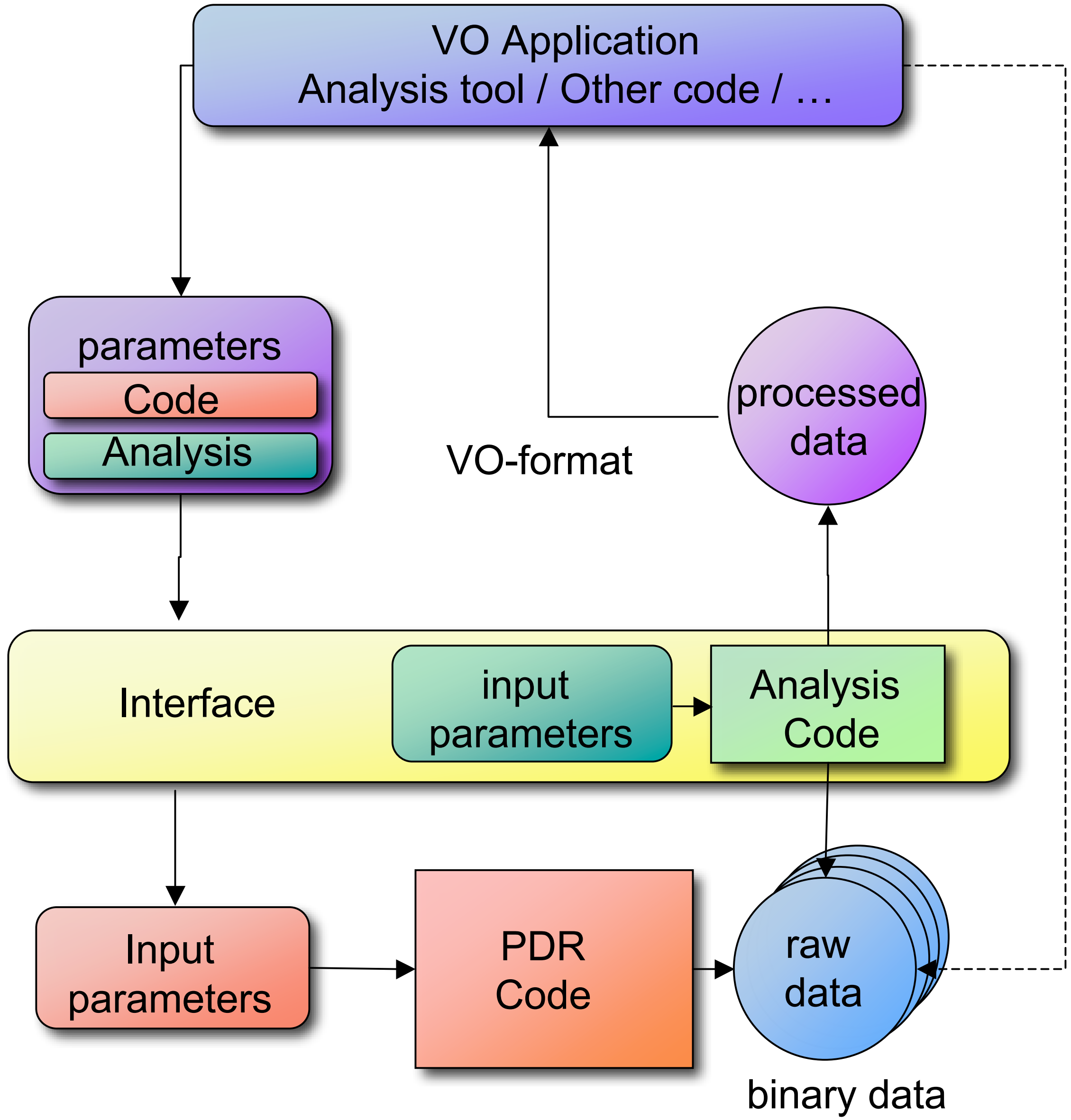


Step 2 : PDR code in the VO (2)

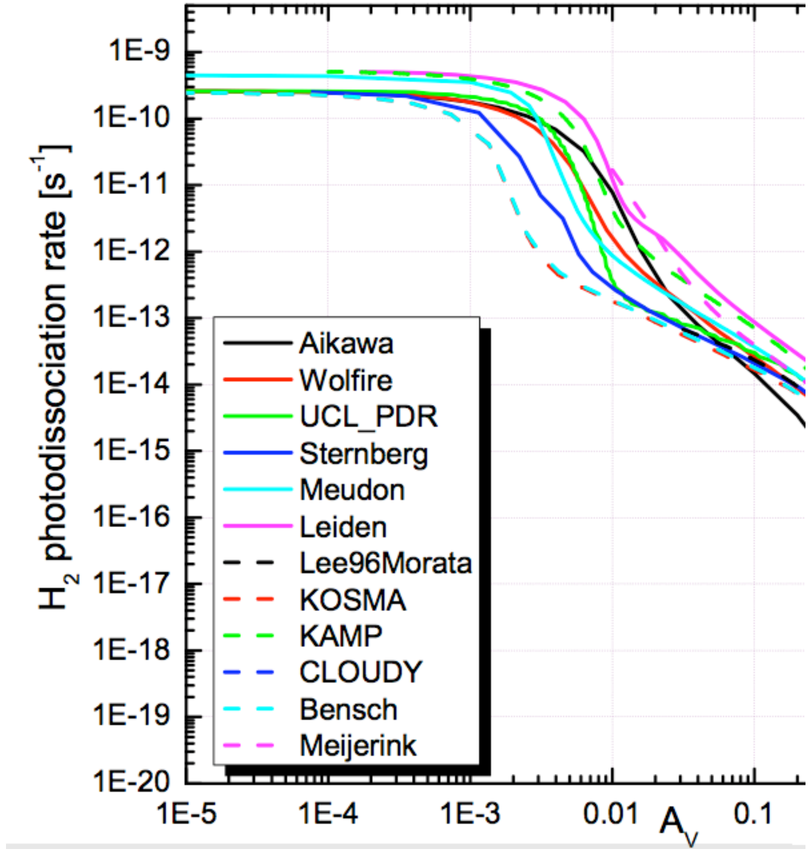
- Only VO-Tables are required
- Except if raw data have to be accessible

Needs in term of VO-definition:

- **definition of all quantities transmitted (UCDs)**
- **definition of the result (metadata)**



Definition of UCDs for simulations



- **Physical quantities**
  - Example : Temperature
    Density
    ….

  These UCDs still exist

- **Numerical quantities** : particular to simulations
  Example : number of iterations
  numerical methods

  In discussion in the VO-Theory Group

- **Other quantities** : between simulation and physical quantities

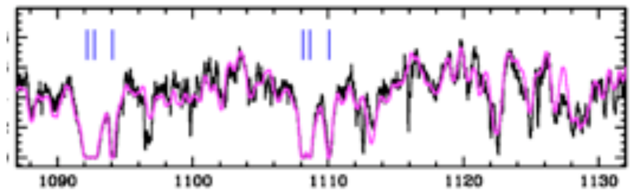
  Example : Intensity of the incident radiation field on a cloud : χ

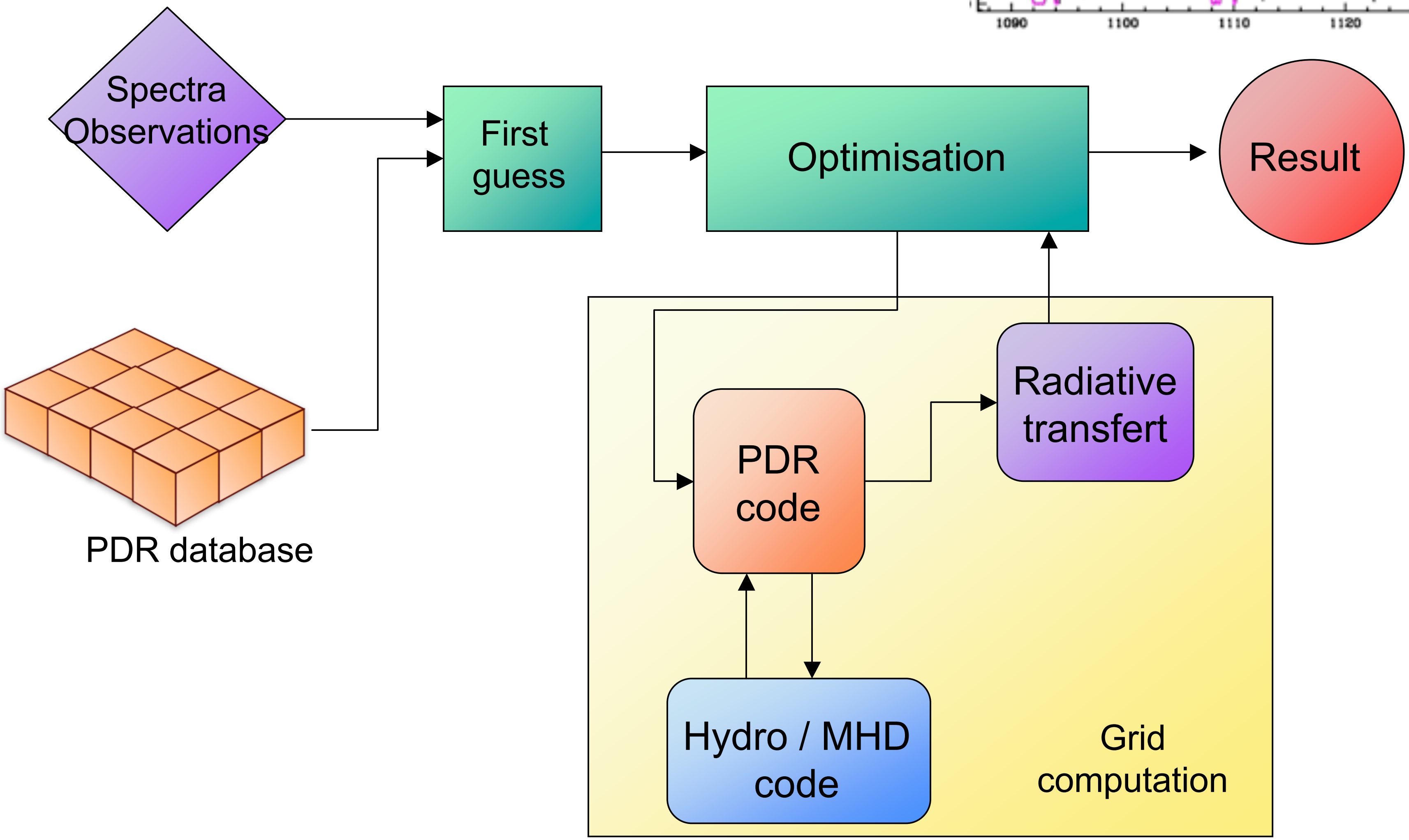
  Flux of the cosmic rays : ζ
  Example : H + cosmic ray ⟶ $H^+ + e^-$ $k = 0.46 \times \zeta$

↳ **The meaning of these quantities depends on how they are used in the codes**
Need for precise definitions of these quantities

Step 2 : PDR code in the VO (3)

Workflows / Grids





Conclusion

Codes in the VO will allow to do complicate things in a simple way
and to facilitate interpretation of observations

- Requirements :
  - **Progress in the definitions of the standards for simulation** :
    - UCD
    - Metadata

    →
    - may require to precise the meaning of some commonly used quantities
    - where to stop the description of a code ?

    - Standards for binary data produced by codes
  - Developement of tools to use simulations in workflows and grids
- But some **risks** : bad use of codes or of results of simulations
  - Documentation
  - Help to the users
  - Well thinked interfaces to minimize possible errors