

Access to simulation codes with Astrogrid & Astro-Runtime

Franck Le Petit
Jonathan Normand
Fabrice Roy
Damien Guillaume

<http://vo.obspm.fr/simulation>

Usecase and Objectives

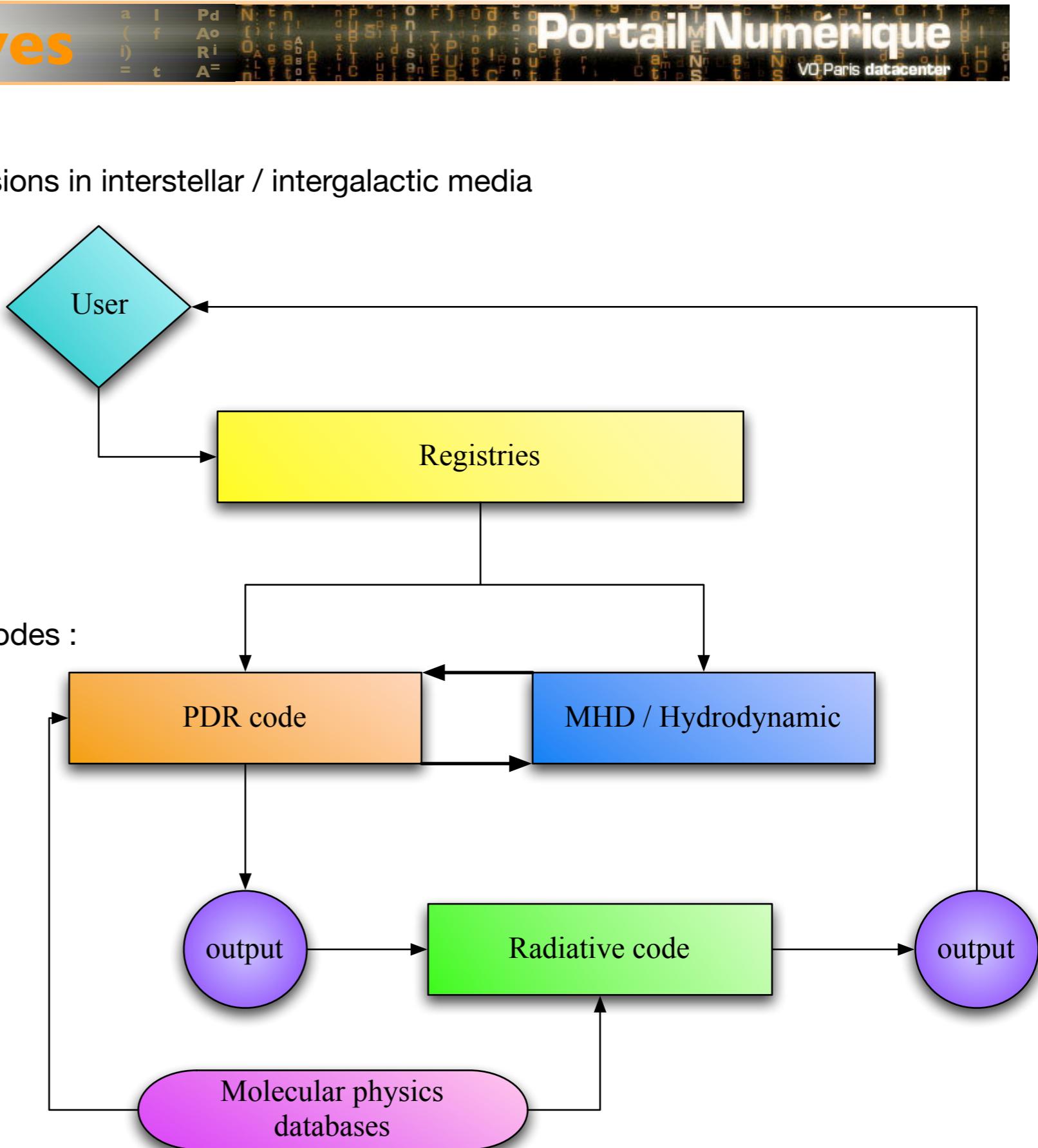
A user wants to interpretate absorptions / emissions in interstellar / intergalactic media



He needs access to simulation / modelisation codes :

- Photo-dominated regions code (Ex: PDR)
Photo-ionized regions code (Ex : CLOUDY)
- Hydrodynamical / MHD code
solves dynamics : a collapse, a shock
- Eventually radiative transfer codes

First step : To be able to run simulation codes



Objectives :

- Find codes in the VO
- Give access to simulation codes
- Give access to computing facilities
- Should be useable by non-specialists
 - documentation
 - friendly interface
- Codes in the VO should allow all possibilities than in non-VO mode
- Association of codes should be easy : Workflows

Registration in Astrogrid

- Installation of Astrogrid at the Observatory of Paris
- Registration of the Meudon PDR code as a CEA service
- Description of parameters (xml file) : generates a generic interface

```
<CmdLineParameterDefn fileRef="true" type="binary" name="chimie">
    <agpd:UI_Name>Chemistry file</agpd:UI_Name>
    <agpd:UI_Description>Name of the chemistry file to use. If no chemistry file ... </agpd:UI_Description>
</CmdLineParameterDefn>
```

```
<CmdLineParameterDefn fileRef="false" type="text" name="srcpp">
    <agpd:UI_Name>External radiation source (type spectral)</agpd:UI_Name>
    <agpd:UI_Description>Add to the UV field the radiation field of a star ... </agpd:UI_Description>
    <agpd:DefaultValue>B 1</agpd:DefaultValue>
    <agpd:OptionList>
        <agpd:OptionVal>0 3</agpd:OptionVal>
        <agpd:OptionVal>0 5</agpd:OptionVal>
        <agpd:OptionVal>0 8</agpd:OptionVal>
        <agpd:OptionVal>B 0</agpd:OptionVal>
        <agpd:OptionVal>B 1</agpd:OptionVal>
```

```
<ExecutionPath>/www/astrogrid-data/commandline-cec/apps/lancement_pdr.tcsh</ExecutionPath>
<LongName>Meudon PDR code</LongName>
<Description>The Meudon PDR code is a tool .... </Description>
<ReferenceURL>http://aristote.obspm.fr/MIS</ReferenceURL>
```

Access to codes in the VO

Portail Numérique

VO Paris datacenter

AstroGrid Workbench

Data Discovery Data Analysis System Services Helper Applications Advanced

Task Launcher Astro Grid Astro Grid Workflow Builder Myspace

Task Launcher – Meudon PDR code

Created by VO Paris

Select an Application:

Find: PDR

S... Title

- Sloan Digital Sky Survey DR3– CutOut Colour
- Sloan Digital Sky Survey DR4 – Images
- Sloan Digital Sky Survey DR4– CutOut Colour
- Sloan Digital Sky Survey DR1 –Filter I
- Meudon PDR code

Details

Meudon PDR code

Meudon PDR code, ivo://obspm.fr/pdr
Type: Long-running Task

Further information - <http://aristote.obspm.fr/MIS>
Type - Other
Subject - ???

Interfaces

- simple

Inputs - chimie, ifafm, Avmax, densh, radm, radp, srapp, d_sour, fmrc, ieqth, tgaz, ifisob, presse, vturb, itrfer, jfgkh2, l0h2, ichh2, los_ext, rrr, cdunit, alb, gg, gratio, rhogr, alpgr, rgmin, rgmax, iforh2, istic

Outputs - dernier_binaire.bin, avant_dernier_binaire.bin, modele

Parameter Details

Name	Type	Description
Scaling factor of the radiation field (right side)	double	UV field scaling factor on the right side of the cloud (back of the cloud). To get a semi-infinite cloud choose 0 and do not introduce a star on the right side of the cloud.
R = Av / E(B-V)	double	Ratio between visual extinction and reddening. This value is linked to the choice of the ligne of sight. Typical value for the Galaxy is 3.1
Isobaric Model	boolean	If checked, pressure will be kept constant at the value in the next field (density and temperature will vary accordingly)
Minimum grain radius	double	Minimal radius of dust grains in cm ; Typical value: 3.0E-7 cm
...	...	Control the distribution of energy during H2 formation on dust :

Task Launcher – Meudon PDR code

Created by VO Paris

Inputs

Name	Value	Ref	Rep	Del
Chemistry file	ivo://uk.ac.le.star/FranckLePetit#Drco...	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Number of global iterations	10	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Av integration limit	1.00E+00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Initial density (cm-3)	1.00E+03	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Scaling factor of the radiation f...	1.00E+00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Scaling factor of the radiation f...	1.00E+00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
External radiation source (typ...	B 1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Distance of the source (pc)	0.00E+00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Ionization rate by cosmic rays	5.00E+00	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Thermal equilibrium	true	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Initial temperature (in Kelvin)	1.00E+02	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

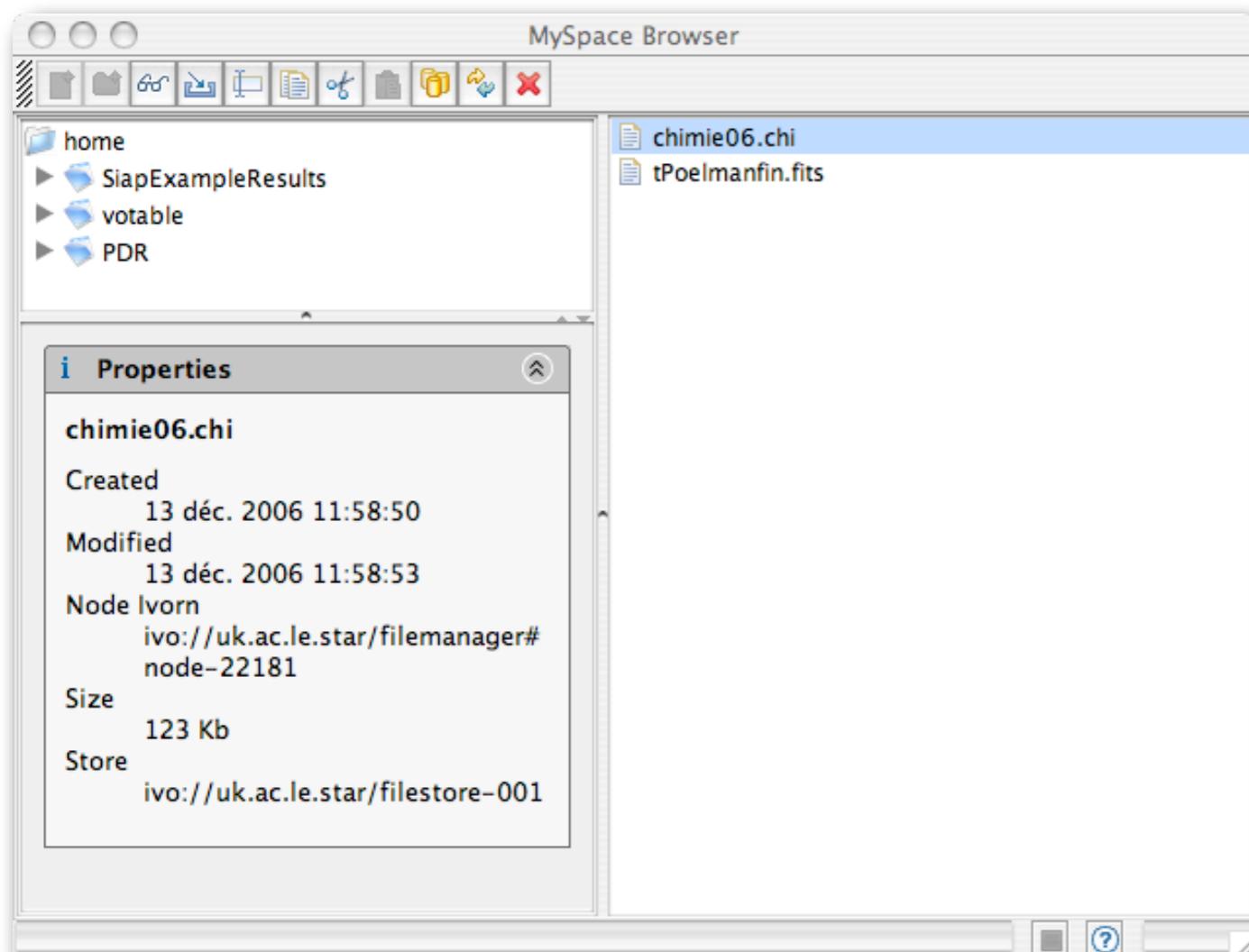
Outputs:

Name	Value	Ref	Rep	Del
dernier_binaire.bin		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
avant_dernier_binaire.bin		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Results file	dcl_3	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

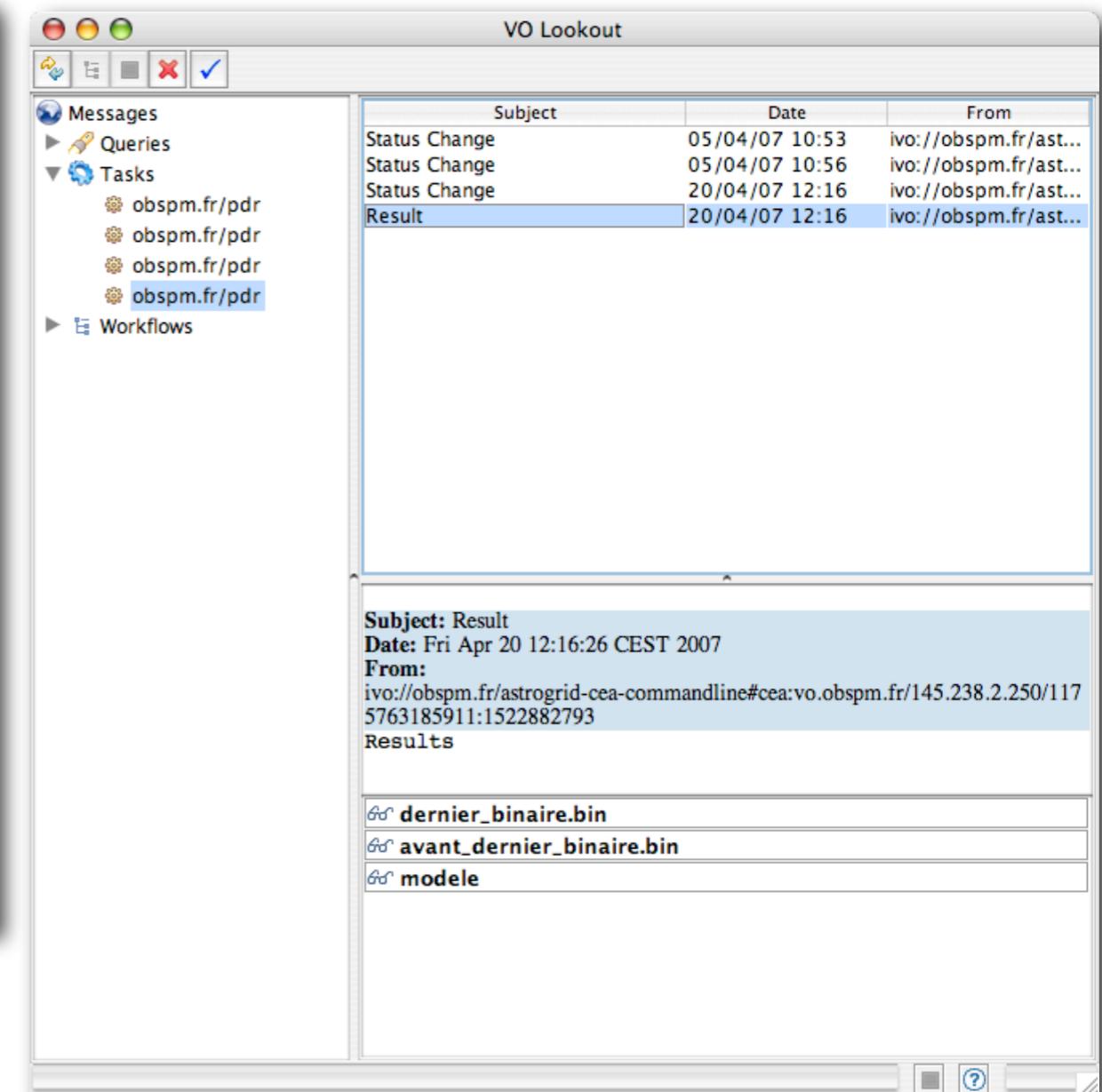
Access to codes in the VO

Portail Numérique

VO-Paris datacenter



MySpace

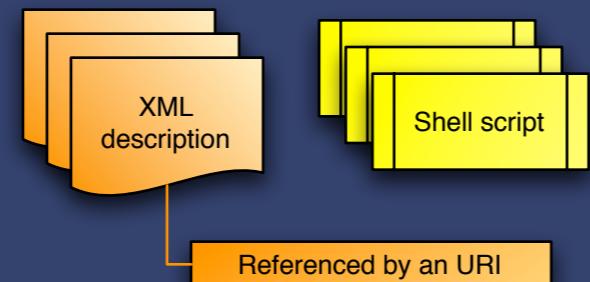


Lookout

Astrogrid
(England)

VO-Paris
Portal

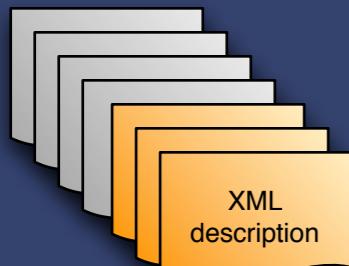
VO-Paris
Computing center



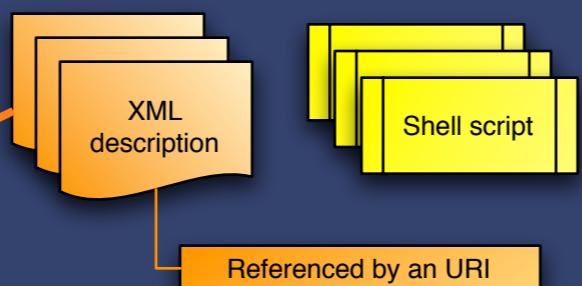
On VO-Paris portal (where Astrogrid is installed)

- XML description of services
- Shell scripts corresponding to services

Astrogrid
(England)

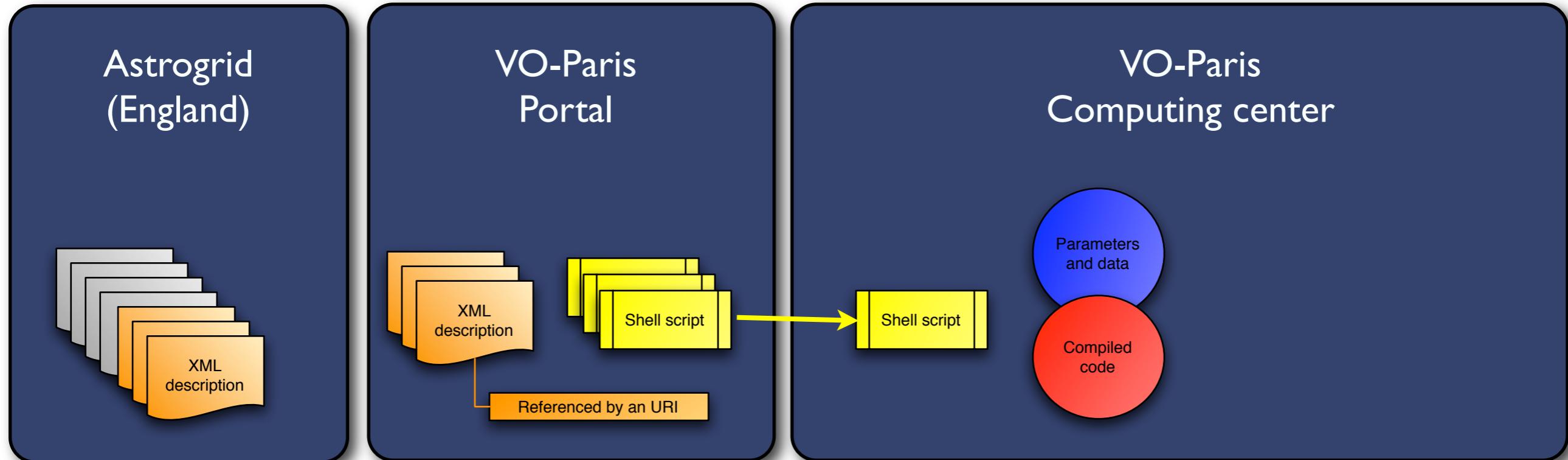


VO-Paris
Portal



VO-Paris
Computing center

- Services are harvested by Astrogrid
- Identified by an URI



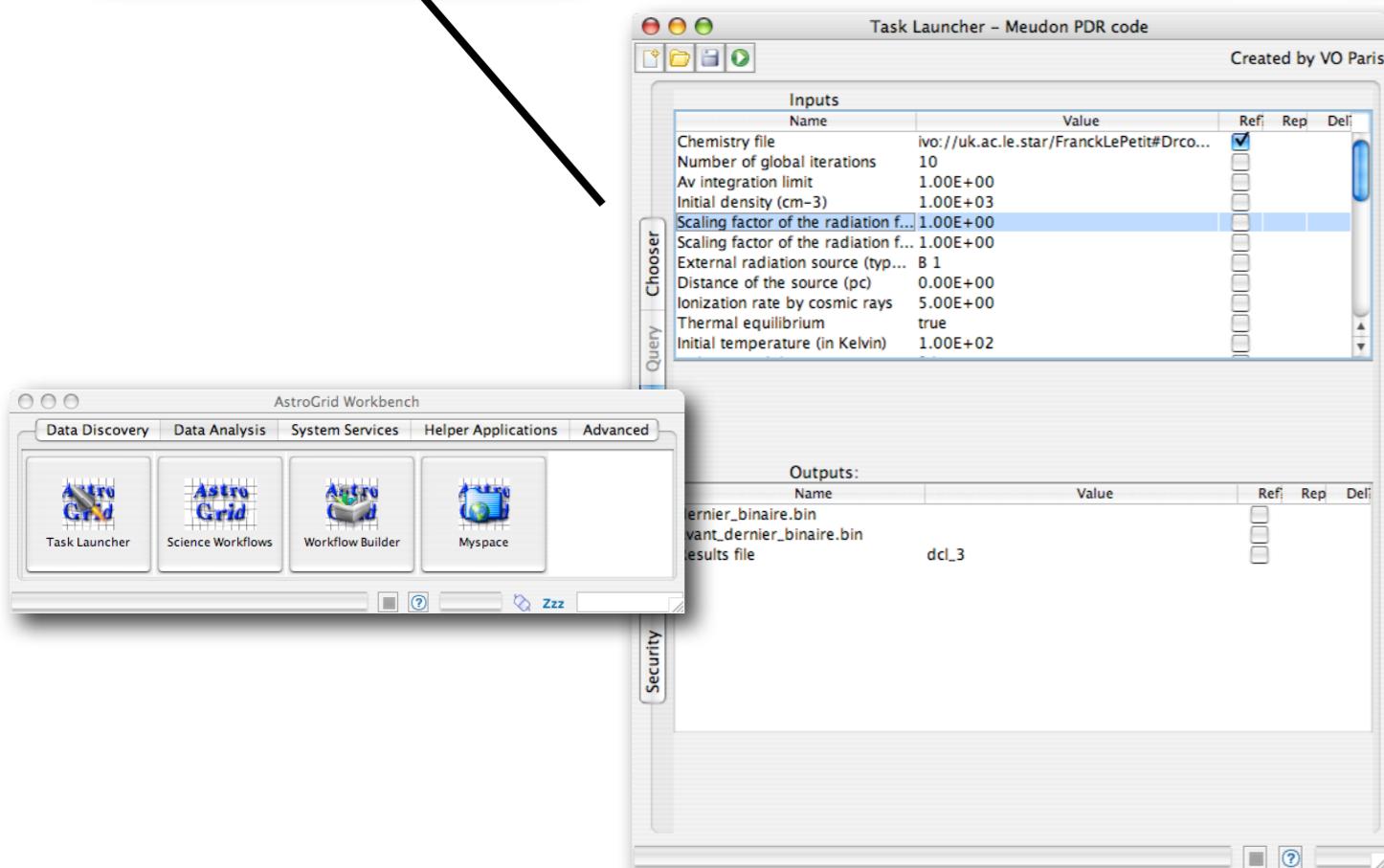
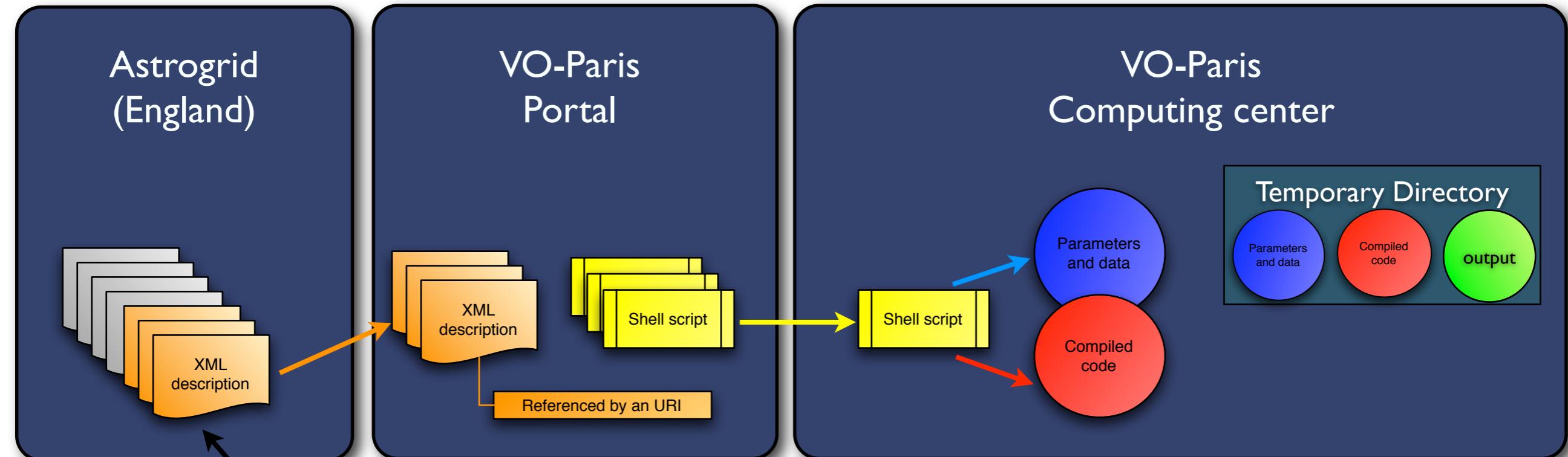
Computing center

- Shell script to command the execution
- Compiled code

Access to codes in the VO

Portail Numérique

VO-Paris datacenter

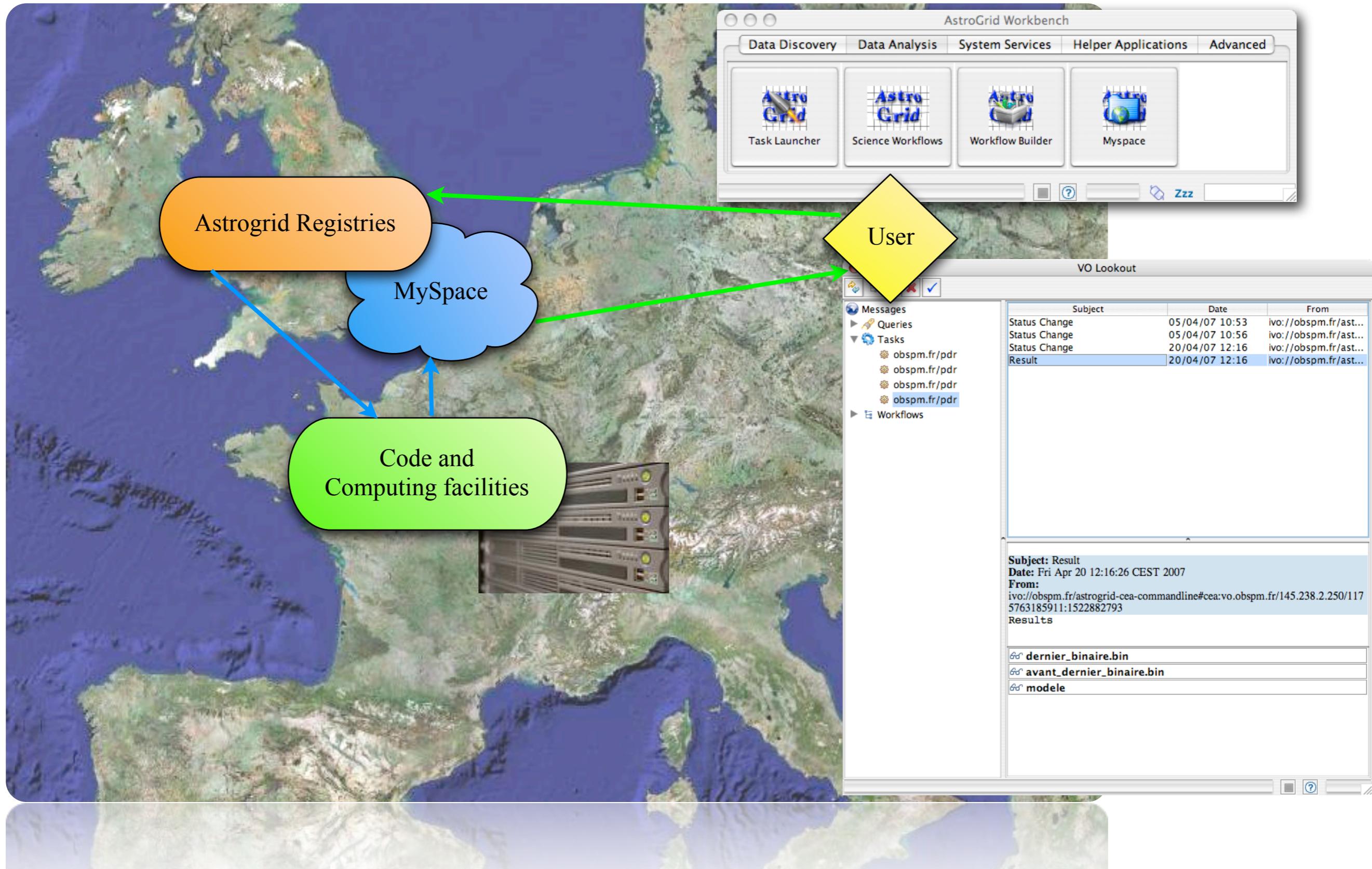


- Parameters are transmitted as command lines parameters
- Shell script on Computing center transforms them in the input file waited by the code
- multi-user : copy of the executable + parameters and data

Access to codes in the VO

Portail Numérique

VO Paris datacenter

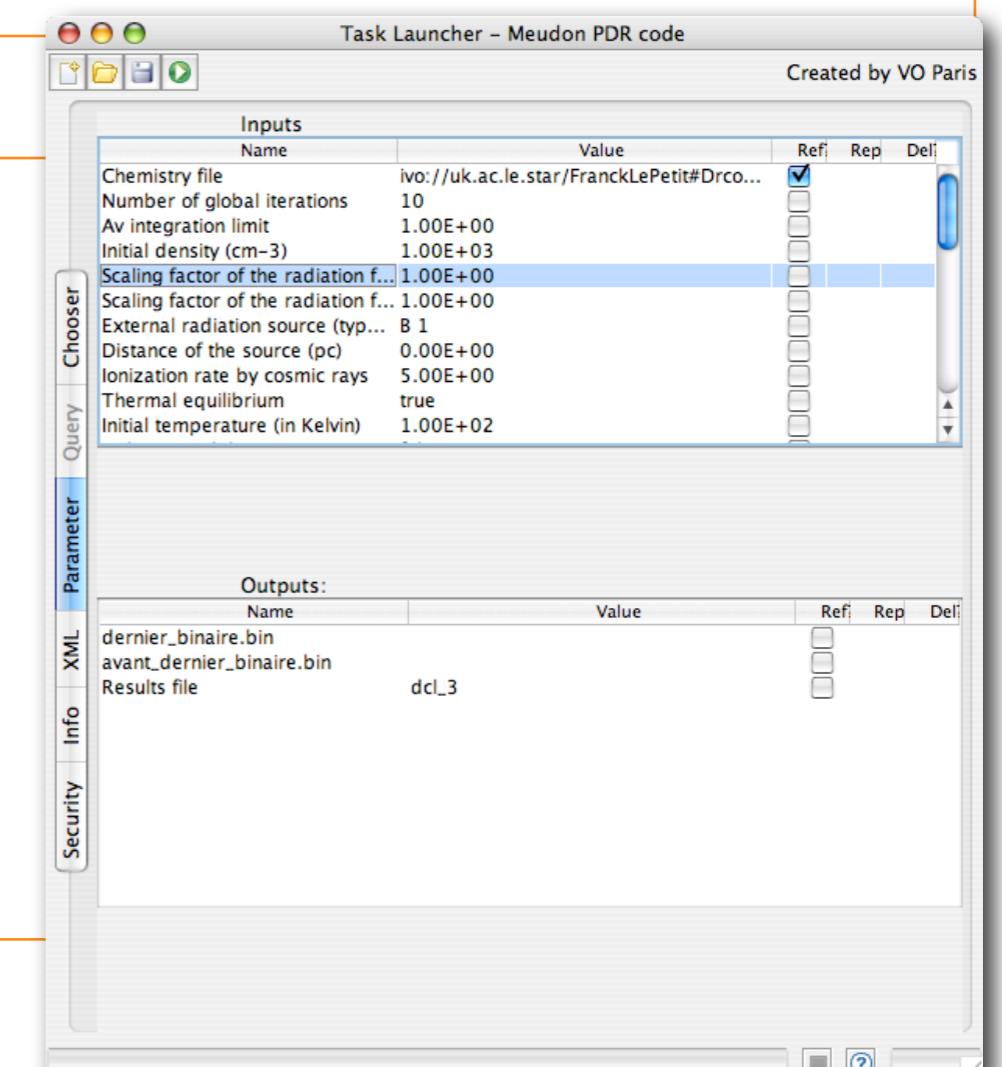


Advantages :

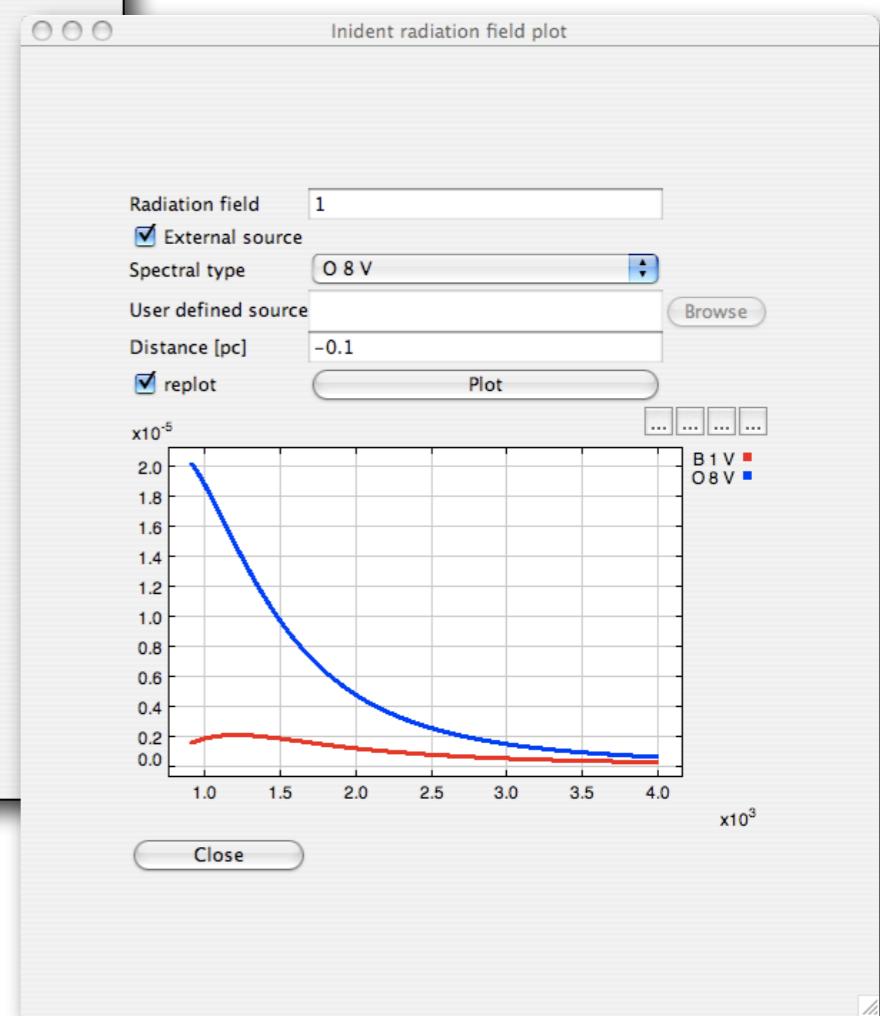
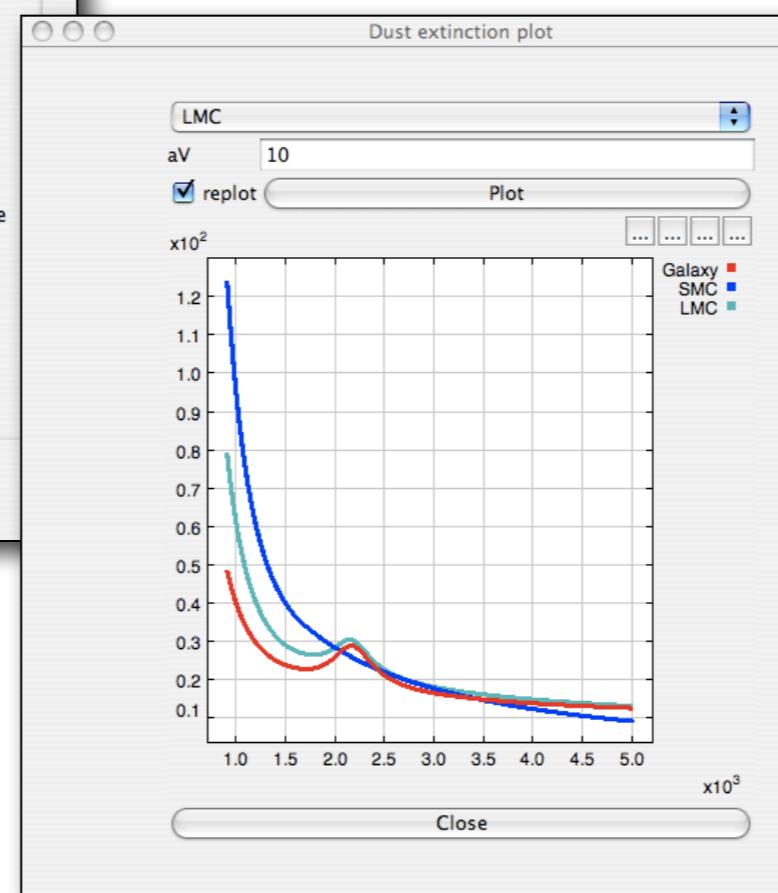
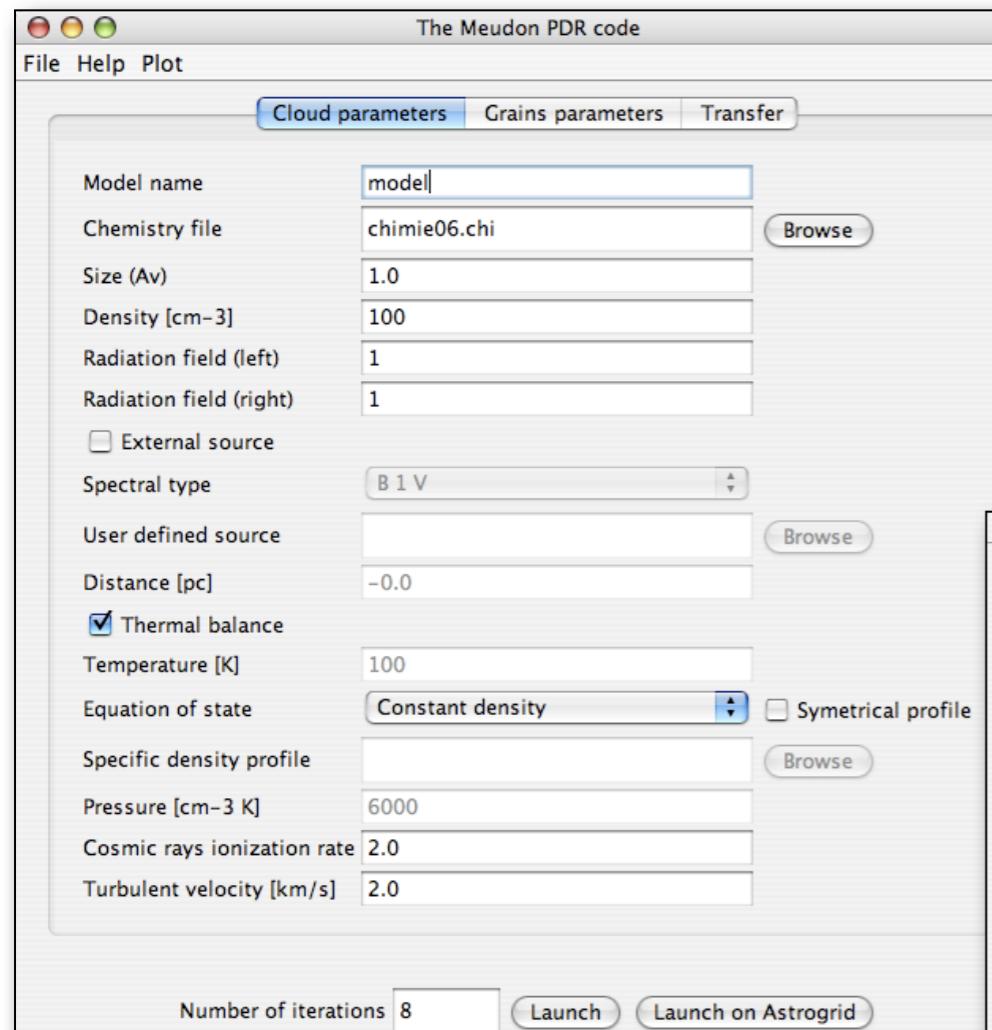
- Easy to use
- Produces automatically a generic interface
- Description of parameters, default values
- Use “Identification” from Astrogrid
- Can run codes on computing centers
- Access to MySpace (disk storage accessible from anywhere)

Drawbacks :

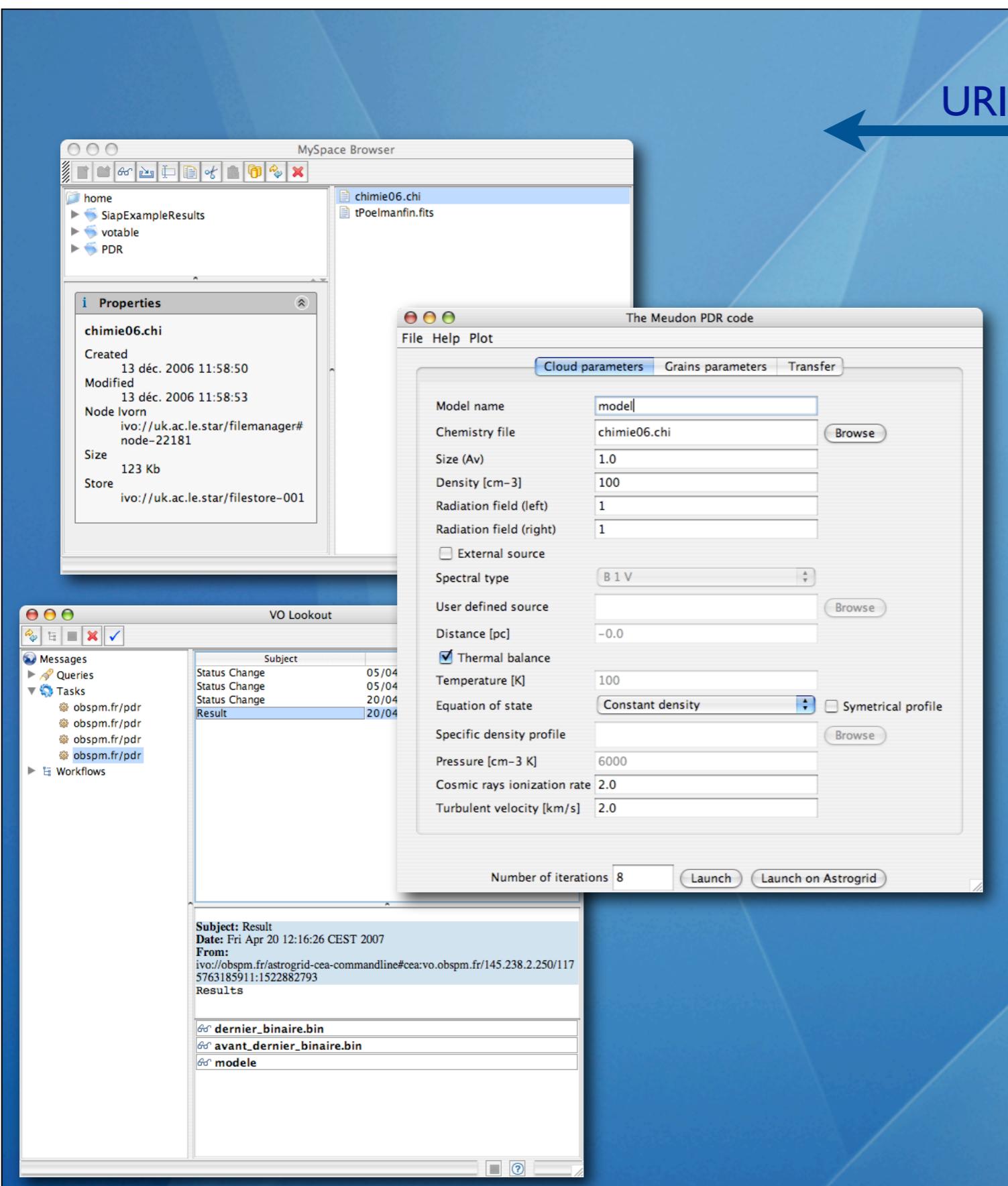
- Generic interface
- Not adapted to non specialists
- Not linked to the code
 - Developpement of the code more complex
 - No verification of parameters
 - No link between parameters
- Not possible to visualize parameters (curves)



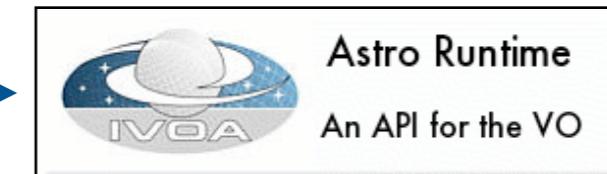
Specific interface communicating with Astrogrid : ASTRO RUNTIME



- Structuration of parameters
- Relations between parameters
- Link between code and interface
 - Code is more easy to develop
- Documentation
- Vizualisation tools



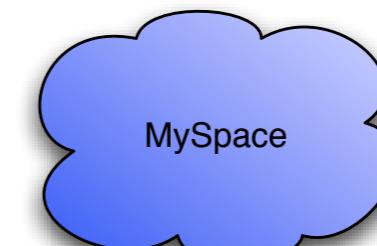
URI



get XML template

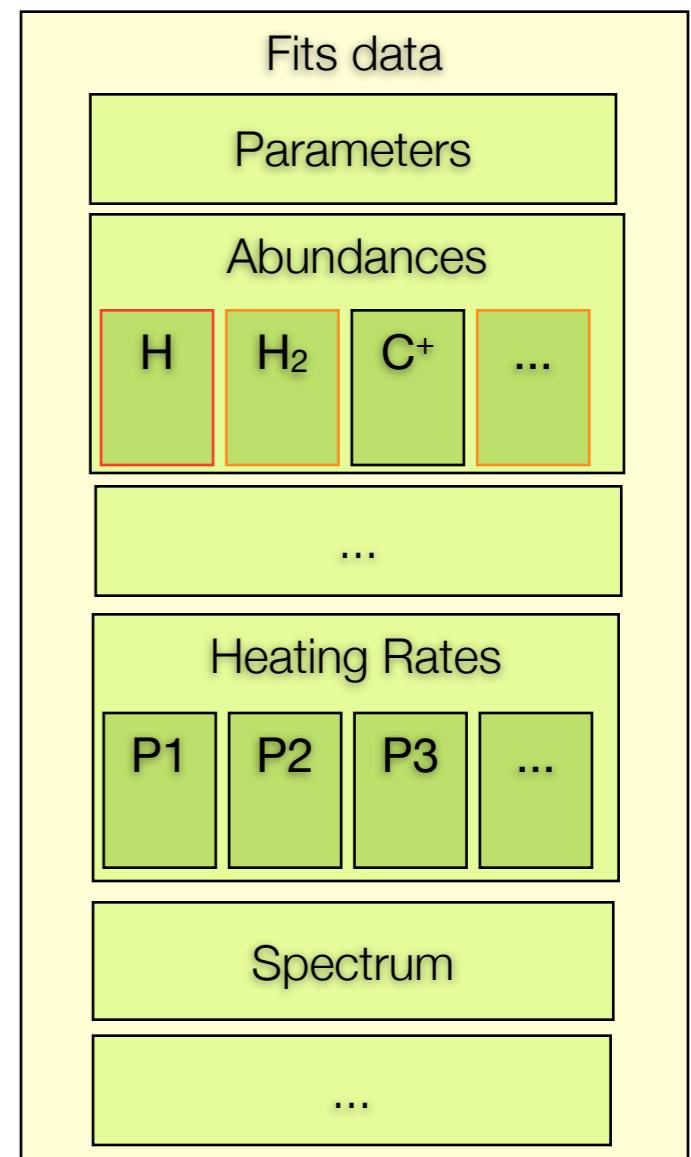
Registries

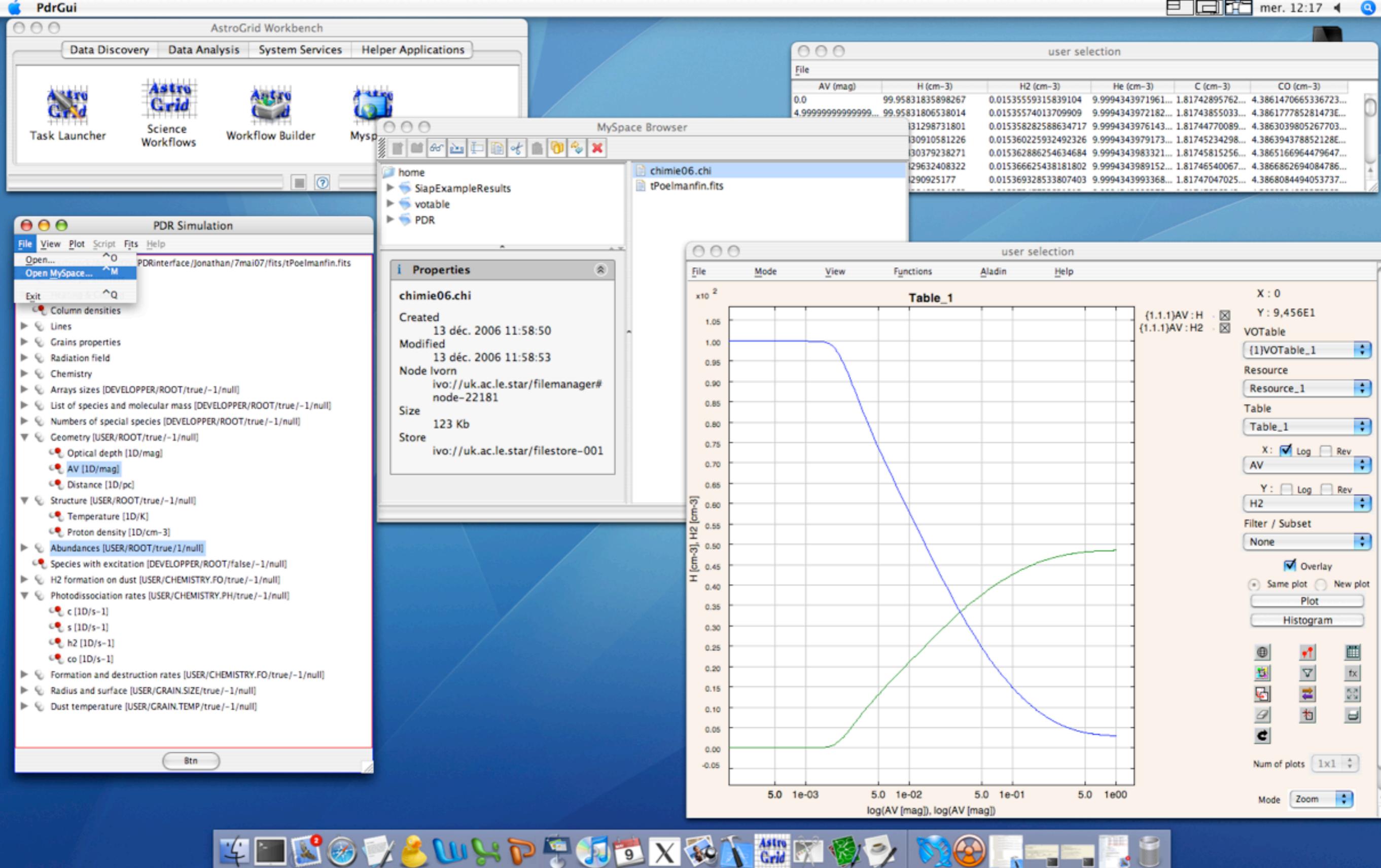
Services
identified by URI



Computing center
(VO-Paris)

- Problem of portability :
 - fits (only data at present - metadata will come later in VO-Table)
- Outputs of models / simulation codes
 - Some are observables : Spectrum, intensities, column densities
 - Some are not observables : abundances, excitation, physical processes ...
- Access to output
 - on the computer it has run
 - on MySpace (with Astro-runtime)
 - Data are not big compared to cosmological codes
 - download all results





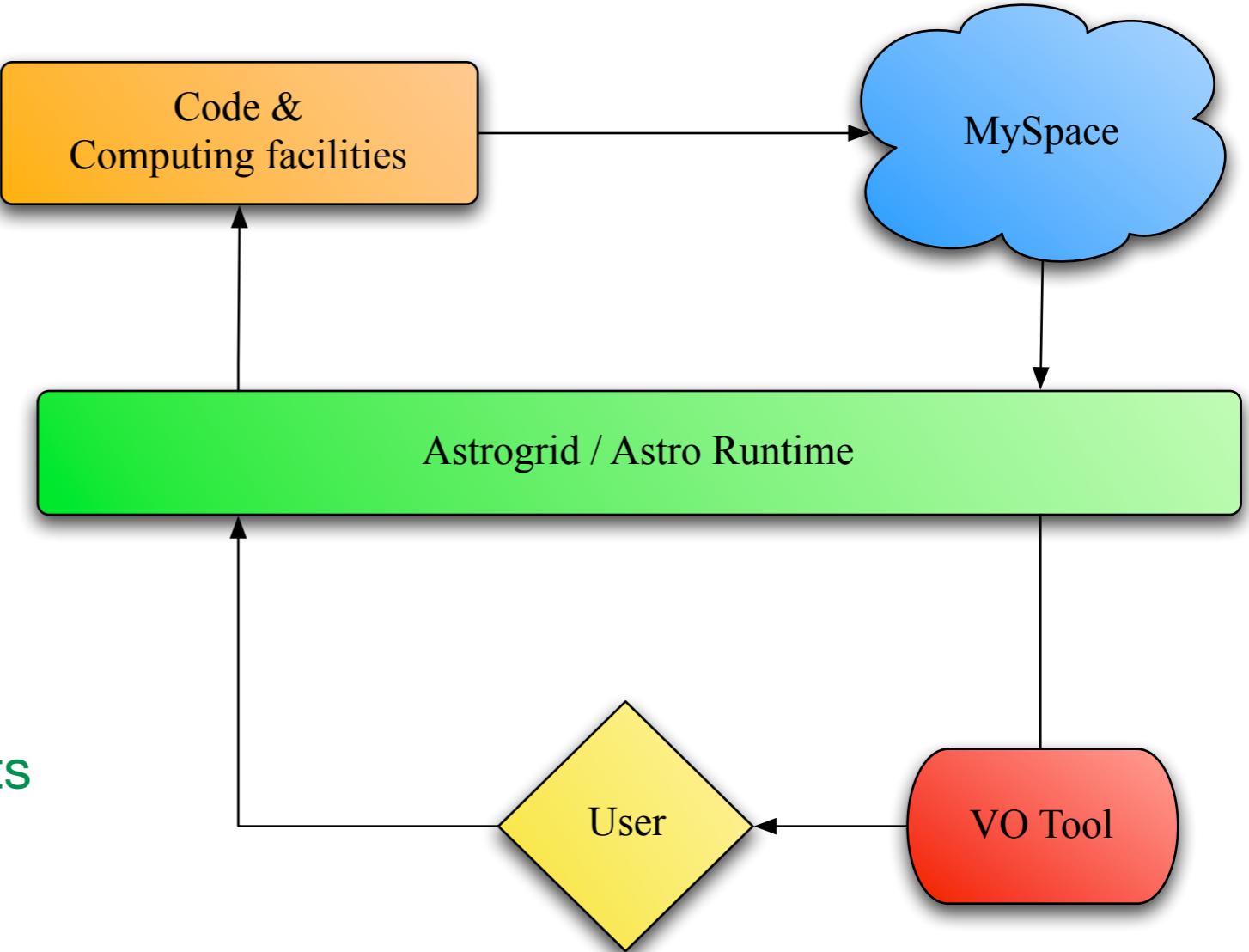
Read .fits output file (local computer or MySpace)

- Send results in VO-Plot
- ASCII file
- VO-Table

- Comparison of models
- Plastic

Objectives :

- Give access to simulation codes
- Give access to computing facilities
- Should be useable by non-specialists
 - documentation
 - friendly interface
- Codes in the VO should allow all possibilities as in non-VO mode



Next step :

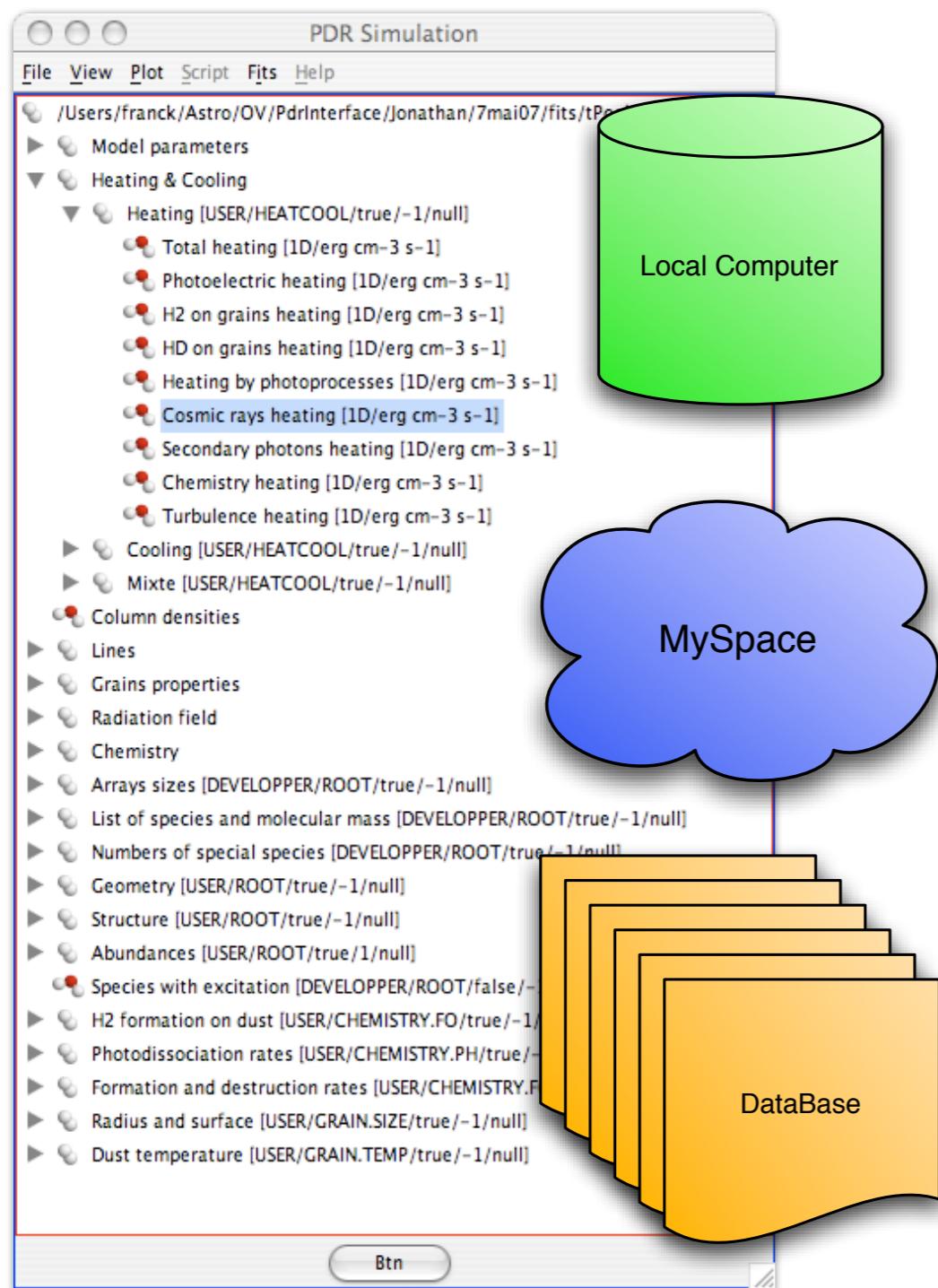
- Workflows

PDR codes / Photo-ionization codes:

1 dimension → few points

Lots of physical quantities

Hydrodynamic / N-body
3 dimensions → lots of points
few physical quantities



SNAP
get some physical
quantities for all spatial
points

