



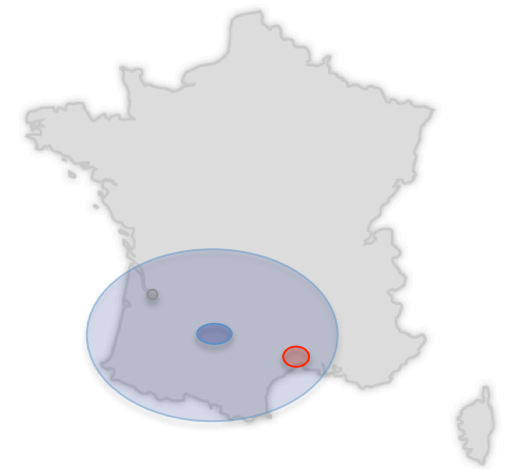
Pollux and Provenance

Scientists :

Ana Palacios, Agnès Lèbre

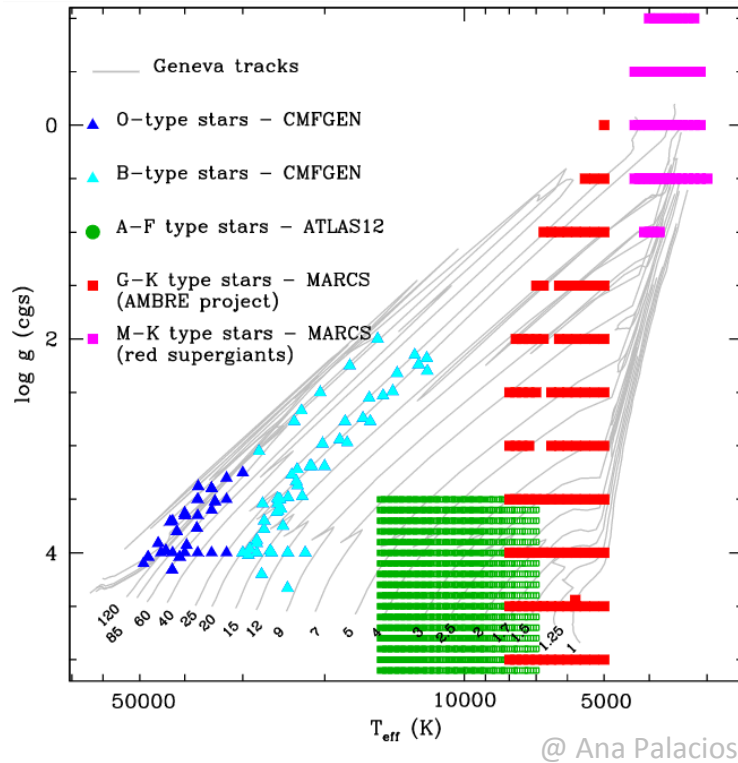
Software engineer :

Michèle Sanguillon





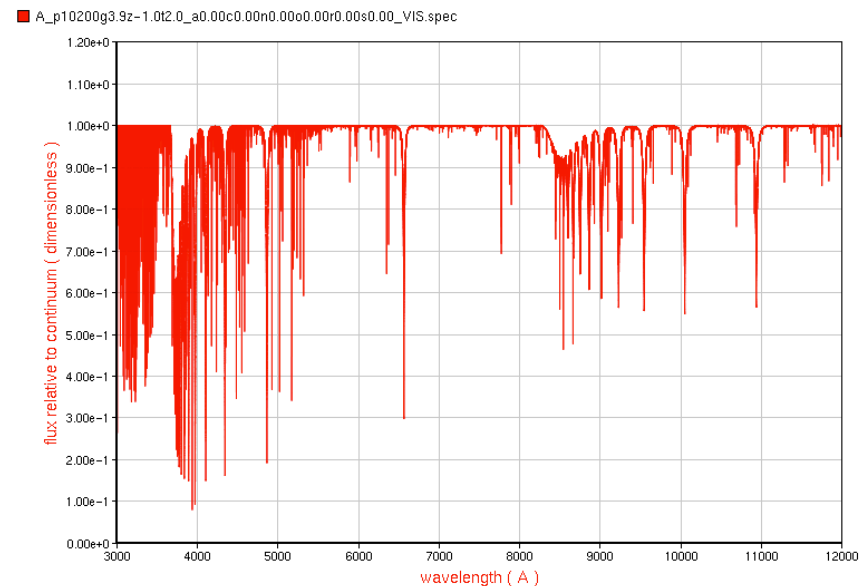
Pollux Database



Data include the absolute flux and the flux normalized to the continuum.

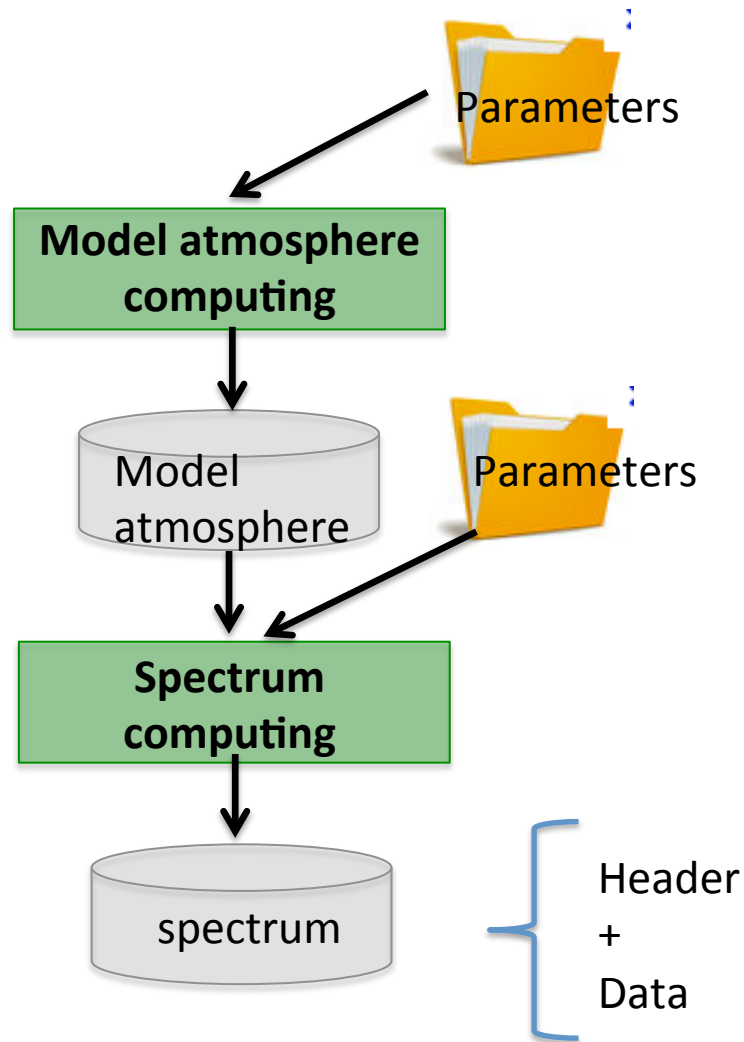
Database of very high resolution ($R \geq 150\,000$) synthetic spectra in the optical domain (3000 Å to 12000 Å).

Spectra exist for many spectral types (O to M and Wolf-Rayet stars.)





Pollux data and workflow



Only the spectra are available on the VO



Pollux accessibility



- via Web for Internet users:
 - Spectra in flat, fits, xml, votable formats (header + data)
- via SSA protocol for VO users:
 - Spectra in fits format (header + data)



Pollux accessibility via Web



The interface shows a sidebar with a tree view of data sources (SSHR, MARCS, CMFGEN, CMFGEN-WR, ATLAS, MARCS & CMFGEN & ATLAS) and filter options (parallel, spherical, parallel & spherical). The main panel has several input fields for physical parameters:

Parameter	lowest	lowequal	high	highest
effective temperature (K)	3000	7250	7250	49091
gravity log10 (cgs)	-1.00000			5.00000
mass (solar mass)	1.00000			84.91000
luminosity (log10 of solar luminosity)	1.18800			6.07000
microturbulent velocity (km/s)	1.00000			10.00000
metallicity ([Fe/H])	-5.00000			1.00000

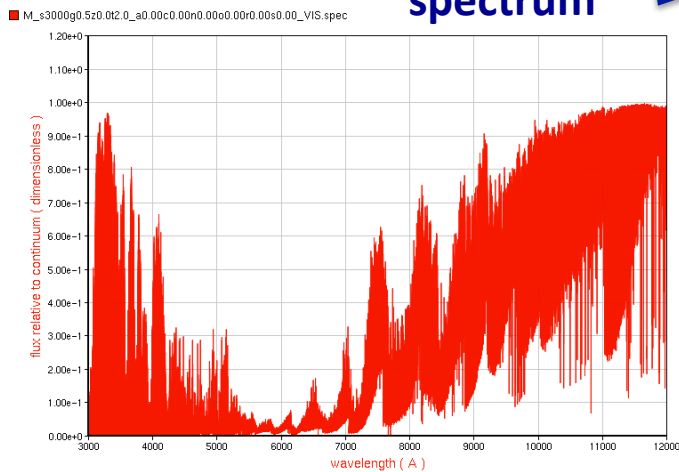
Below these are sections for 'Specific Abundances (optional)' and 'Cart Status'. The 'Cart Status' section indicates 'No spectra to be downloaded'. To the right, a data table shows columns for selection criteria and physical parameters. The table header is: '0 spectra to be downloaded - 97 available(s)'. A blue arrow points from the table to the 'Header' section.

Display spectrum

Header

Download

Provenance information



Spectrum: M_s3000g0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0

```

code1                = marcs35                code for atmosphere model
version1              = 2006.1                version of code for model
type                  = s                      type of model atmosphere
filename               = 3000g0.5m15z0.00t2.0.mod model atmosphere file
author_mod            = plez                  model atmosphere creator

Teff                  = 3000                  effective temperature (K)
logg                  = 0.5                  log10(gravity) (cgs)
mass                  = 15.0                 mass (solar mass)
lum                   = 3.977                log of luminosity (solar)
turbvel               = 2.00                 microturbulent velocity (km/s)

conv_alpha            = 1.5                  convection parameter (conv)
conv_ny               = 8.0                  convection parameter (conv)
conv_y                = 0.076               convection parameter (conv)
conv_beta             = 0.5                  convection parameter (conv)
macroturbvel         = 0.0                  macroturbulence parameter
macrobeta             = 0.0                  macroturbulence parameter

Mdot                  = irrelevant            log10(mass loss) (solar mass)
Vinfy                 = irrelevant            terminal velocity (km/s)
beta                  = irrelevant            velocity law parameter
finfy                 = irrelevant            1st clumping law parameter
vcl                   = irrelevant            2nd clumping law parameter

metallic_mod          = 0.000                metallicity ([Fe/H])
alpha_mod             = 0.000                [alpha/Fe]
r_process_mod         = 0.000                [r elements/Fe]
s_process_mod         = 0.000                [s elements/Fe]

```



Pollux accessibility via a VO tool



CASSIS A free interactive spectrum analyser

Selection depending on a very few provenance criteria

The screenshot shows the CASSIS web interface. The 'Registry & Services selection' panel on the left has 'POLLUX Database' checked. The 'Request' panel on the right shows various parameters like Object name, RA, DEC, SIZE, BAND, TIME, and FORMAT. A blue circle highlights the 'Optional Parameters' table in the Request panel.

Use	Name	Value
<input type="checkbox"/>	logg_max	
<input type="checkbox"/>	logg_min	
<input type="checkbox"/>	MAXREC	
<input type="checkbox"/>	meta_max	
<input type="checkbox"/>	meta_min	
<input type="checkbox"/>	model	
<input type="checkbox"/>	pertinence	
<input type="checkbox"/>	teff_max	
<input type="checkbox"/>	teff_min	
<input type="checkbox"/>	vturb_max	
<input type="checkbox"/>	vturb_min	

Index	teff	logg	mass	lum	vturb	meta	pert	title	SpectralAxis	FluxAxis	UNITS	SpectralSI	FluxSI	DataLength	Format	Location	Exte
1	3000	0.5	15.0	3.977	2.0	0.0	1	FLUX_M_s3000g0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	flux	A erg/cm^2 /s/A	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
2	3000	0.5	15.0	3.977	2.0	0.0	1	NORMFLUX_M_s3000g0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	normalized flux	A dimensionless	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
3	3100	-0.5	15.0	5.034	2.0	0.0	1	FLUX_M_s3100g-0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	flux	A erg/cm^2 /s/A	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
4	3100	-0.5	15.0	5.034	2.0	0.0	1	NORMFLUX_M_s3100g-0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	normalized flux	A dimensionless	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
5	3100	0.0	15.0	4.534	2.0	0.0	1	FLUX_M_s3100g0.0z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	flux	A erg/cm^2 /s/A	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
6	3100	0.0	15.0	4.534	2.0	0.0	1	NORMFLUX_M_s3100g0.0z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	normalized flux	A dimensionless	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
7	3100	0.5	15.0	4.034	2.0	0.0	1	FLUX_M_s3100g0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	flux	A erg/cm^2 /s/A	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
8	3100	0.5	15.0	4.034	2.0	0.0	1	NORMFLUX_M_s3100g0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	normalized flux	A dimensionless	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
9	10200	3.9			2.0	-1.0	1	FLUX_A_p10200g3.9z-1.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	flux	A erg/cm^2 /s/A	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
10	10200	3.9			2.0	-1.0	1	NORMFLUX_A_p10200g3.9z-1.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	normalized flux	A dimensionless	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
11	3200	-0.5	15.0	5.089	2.0	0.0	1	FLUX_M_s3200g-0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	flux	A erg/cm^2 /s/A	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
12	3200	-0.5	15.0	5.089	2.0	0.0	1	NORMFLUX_M_s3200g-0.5z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	normalized flux	A dimensionless	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7
13	3200	-1.0	15.0	5.589	2.0	0.0	1	FLUX_M_s3200g-1.0z0.0t2.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.FITS	wavelength	flux	A erg/cm^2 /s/A	1E-10 L	1E+7 ML-1T-3	450001	application/fits	7.5-7	9E-7

Currently no possibility to see the header or the provenance information because DATALINK is not yet implemented in spectra visualization tools .



Our motivations for Provenance



- **1) A Data Model** to **describe** our data (spectra and provenance) => use of **utypes** for every piece of information:
 - Spectrum DM 1.1 / Spectral DM 2.0:
 - **adequate for spectra**
 - **but ours have 3 columns (wavelength, flux, normalized flux)**
 - **with a ObsConfig part**
 - **provenance information not included**
 - SimDM:
 - **adequate for simulations**
 - **complex**
 - **doesn't describe the spectrum**
 - Future spectral DM (with 2 flux columns)
+ (ProvDM or SimDM):
 - **could describe our spectra and the way they were produced**



Our motivations for Provenance



2) A way to **display** all our provenance information in VO spectra tools, **easy readable** and **normalized**

Flat header (Web users)

```

header_name_SSHR = 'M_p7250g5.0z1.00t1.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.txt'
short_name_SSHR = 'M_p7250g5.0z1.00t1.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec'
Key_SSHR        = 'M_p7250g5.0z1.00t1.0_a0.00c0.00n0.00o0.00r0.00s0.00_convai.5convny0.076convb0.5mt'

code1           = 'marcs'           / code for atmosphere model
version1       = '2008.5'          / version of code for model atmosphere
type           = 'p'              / type of model atmosphere (Spherical/Parallel)
filename       = 'p7250_g+5.0_m0.0_t01_st_z+1.00_o+0.00_c+0.00_n+0.00_o+0.00_r+0.00_s+0.00.mod' / model atm
author_mod     = 'Marcs-team'      / model atmosphere creator name

Teff           = '7250'           / effective temperature (K) - model atmosphere data
logg           = '5.0'            / log10(gravity) (cgs) - model atmosphere data
mass           = 'irrelevant'     / mass (solar mass) - model atmosphere data
lum           = 'irrelevant'     / luminosity (solar luminosity) - model atmosphere data
turbvel       = '1.00'           / microturbulent velocity (km/s) - model atmosphere data

conv_alpha    = '1.5'            / convection parameter (conva) - model atmosphere data
conv_ny       = '8.0'            / convection parameter (convny) - model atmosphere data
conv_y        = '0.076'          / convection parameter (convy) - model atmosphere data
conv_beta     = '0.5'            / convection parameter (convb) - model atmosphere data
macrotrubvel = '0.0'            / macro turbulence parameter (mt) - model atmosphere data
macrobeta     = '0.0'            / macro turbulence parameter (mb) - model atmosphere data

Mdot           = 'irrelevant'    / log10(mass loss) (solar mass/year) - model atmosphere data
Vinfity       = 'irrelevant'     / terminal velocity (km/s) - model atmosphere data
beta          = 'irrelevant'     / velocity law parameter - model atmosphere data
finfity       = 'irrelevant'     / 1st clumping law parameter - model atmosphere data
vcl           = 'irrelevant'     / 2nd clumping law parameter (km/s) - model atmosphere data

metallic_mod  = '1.00'           / metallicity ([Fe/H])
alpha_mod     = '0.000'          / [alpha/Fe]
r_process_mod = '0.000'          / [r elements/Fe]
s_process_mod = '0.000'          / [s elements/Fe]

```

Easy to read and to understand
 Keywords and format not normalized
 No UCD, no utypes

Fits header (OV users)

```

<PARAM arraysize="60" datatype="char" name="short_name_SSHR" value="M_p7250g5.0z1.00t1.0_a0.00c0.00n0.00o0.00r0.00s0.00_VIS.spec.txt">
<PARAM arraysize="106" datatype="char" name="Key_SSHR" value="M_p7250g5.0z1.00t1.0_a0.00c0.00n0.00o0.00r0.00s0.00_convai.5convny0.076convb0.5mt">
<DESCRIPTION>code for atmosphere model</DESCRIPTION>
</PARAM>
<PARAM datatype="float" name="version1" ucd="meta.code;meta.version" value="2008.5">
<DESCRIPTION>version of code for model atmosphere</DESCRIPTION>
</PARAM>
<PARAM arraysize="1" datatype="char" name="type" ucd="meta.code.class" value="p">
<DESCRIPTION>type of model atmosphere (Spherical/Parallel)</DESCRIPTION>
</PARAM>
<PARAM arraysize="76" datatype="char" name="filename" ucd="meta.id;meta.file" value="p7250_g+5.0_m0.0_t01_st_z+1.00_o+0.00_c+0.00_n+0.00_o+0.00_r+0.00_s+0.00.mod">
<DESCRIPTION>model atmosphere filename</DESCRIPTION>
</PARAM>
<PARAM arraysize="10" datatype="char" name="author_mod" ucd="meta.bib.author" value="Marcs-team">
<DESCRIPTION>model atmosphere creator name</DESCRIPTION>
</PARAM>
<PARAM datatype="int" name="Teff" ucd="phys.temperature.effective" unit="K" value="7250">
<DESCRIPTION>effective temperature (K) - model atmosphere data</DESCRIPTION>
</PARAM>
<PARAM datatype="float" name="logg" ucd="phys.gravity;arith.zp" unit="log(cm/s2)" value="5.0">
<DESCRIPTION>log10(gravity) (cgs) - model atmosphere data</DESCRIPTION>
</PARAM>
<PARAM arraysize="10" datatype="char" name="mass" ucd="phys.mass" unit="M_sun" value="irrelevant">
<DESCRIPTION>mass (solar mass) - model atmosphere data</DESCRIPTION>
</PARAM>
<PARAM arraysize="10" datatype="char" name="lum" ucd="phys.luminosity" unit="L_sun" value="irrelevant">
<DESCRIPTION>luminosity (solar luminosity) - model atmosphere data</DESCRIPTION>
</PARAM>

```

Not very easy to read and to understand
 VOTable (normalized)
 UCD, no utypes



Our motivations for Provenance



3) **Select** spectra **on provenance criteria** as...

- **Use case 1:**

Show me a list of synthetic spectra satisfying :

- domain of wavelength = visible
- domain of effective temperature = [4000, 5000]

- **Use case 2:**

Show me a list of synthetic spectra satisfying :

- code for model atmosphere = MARCS
- type of model atmosphere = spherical

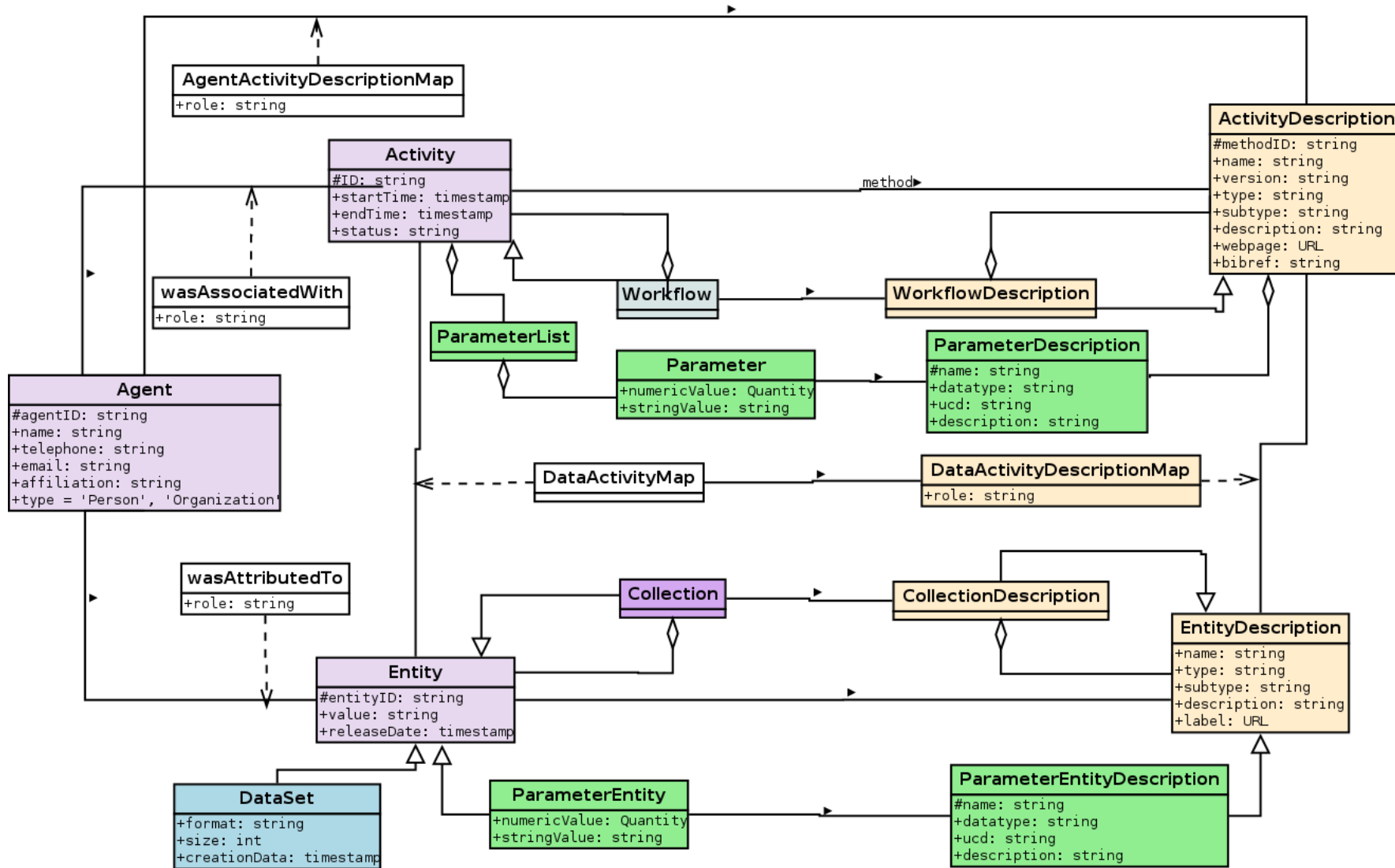
- **Use case 3:**

Show me a list of synthetic spectra satisfying :

- code for spectral synthesis = turbospectrum
- version of this code = 2008.1

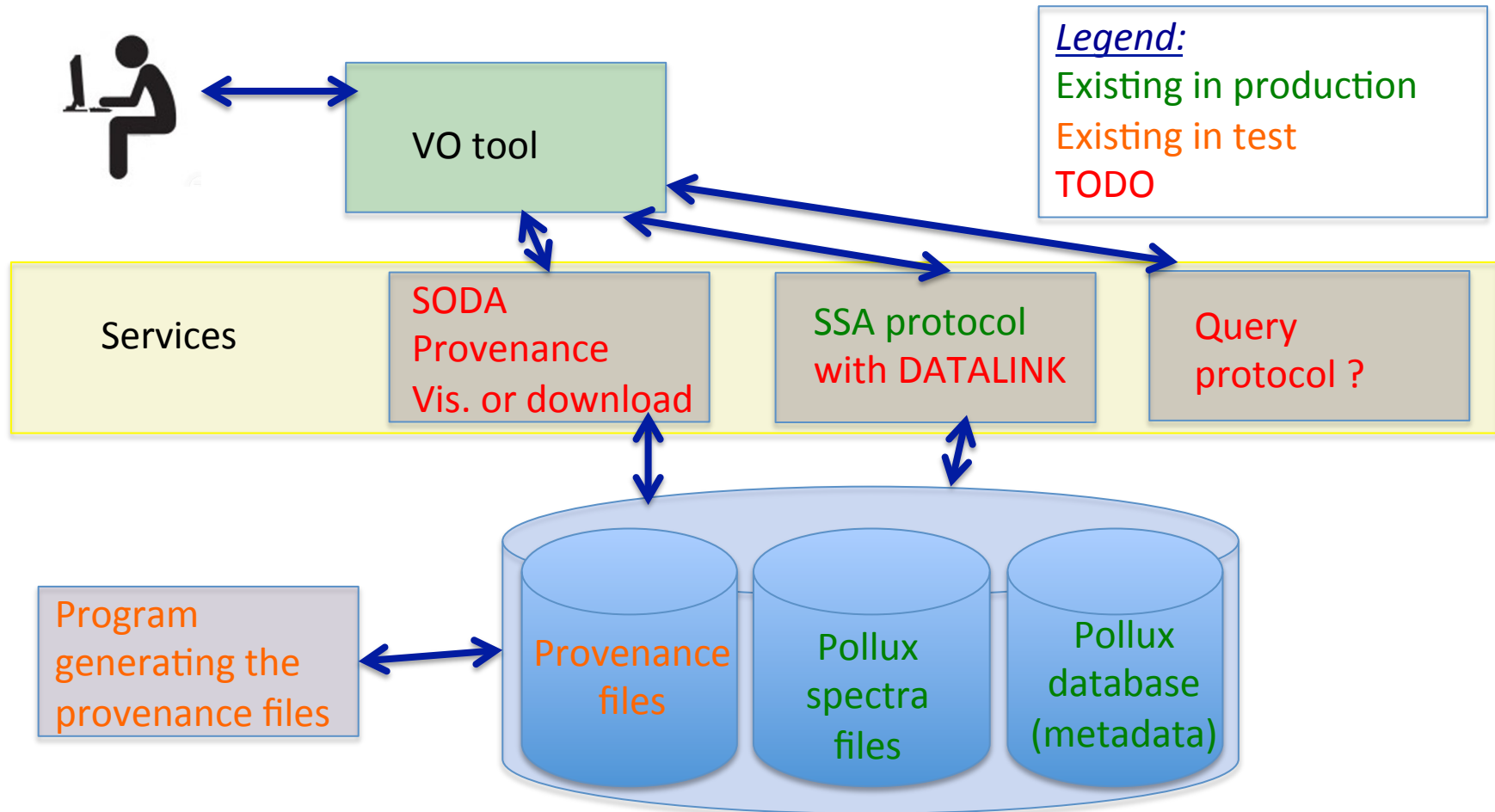


Data Model used





A beginning of implementation





Creation of provenance files



- Code : use of the prov 1.4.0 python package (developed at the University of Southampton)
 - A library for W3C Provenance Data Model
 - Can generate different formats:
 - Serialized formats: **PROVN**, **JSON**, **XML**, **VOTABLE**
 - Graphic formats: **PNG**, **SVG**, **PDF**
 - Uses namespaces:
 - prov:
<http://www.w3.org/ns/prov#>
 - voprov (TBD):
<http://www.ivoa.net/documents/dm/provdm/voprov/>
 - polluxData:
<http://dev-pollux/datalink/provenance?Id=>
- Validation: use of the **Southampton Provenance Suite**
<https://provenance.ecs.soton.ac.uk/>



Creation of provenance files



- **Serialized formats:**

- JSON: 3906 lines
- PROVJ : 613 lines
- XML: 3800 lines
- VOTable : not yet implemented

```
"entity": {  
  "pollux:14800g4.1z0.0a0.0C0.0.mod_2012_Teff": {  
    "voprov:ucd": "phys.temperature.effective",  
    "voprov:type": "int",  
    "voprov:description": "effective temperature (K) ",  
    "voprov:unit": "K",  
    "prov:value": "14800"  
  },  
}
```

```
<prov:entity prov:id="polluxData:2702_Teff">  
  <prov:value xsi:type="xsd:string">3000</prov:value>  
  <voprov:description>effective temperature (K)</voprov:description>  
  <voprov:name>pollux:Teff</voprov:name>  
  <voprov:type>int</voprov:type>  
  <voprov:ucd>phys.temperature.effective</voprov:ucd>  
  <voprov:unit>K</voprov:unit>  
  <voprov:utype>voprov:DataEntity</voprov:utype>  
</prov:entity>
```

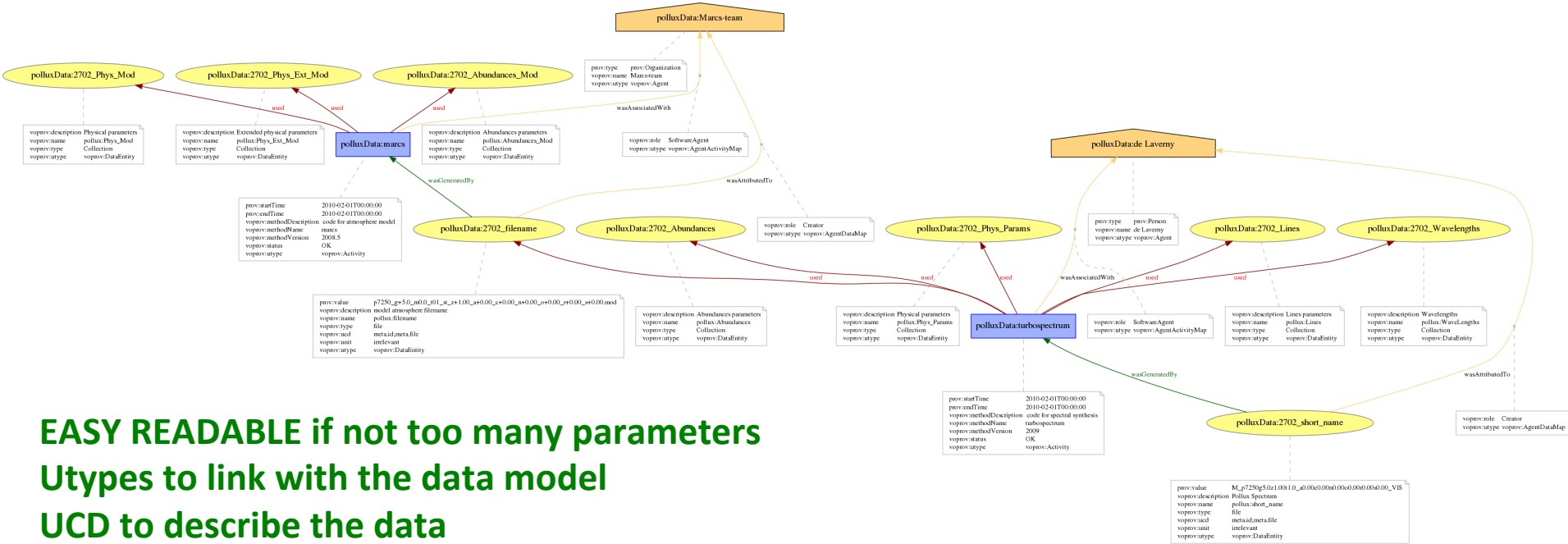
```
entity(pollux:14800g4.1z0.0a0.0C0.0.mod_2012_Teff, [voprov:description="effective  
temperature (K) - model atmosphere data", voprov:type="int", prov:value="14800",  
voprov:unit="K", voprov:ucd="phys.temperature.effective"])
```



Creation of provenance files



- **Graphic formats:**
 - SVG: you can click on each declaration
 - PNG : only a picture
 - PDF : currently a picture



EASY READABLE if not too many parameters
Utypes to link with the data model
UCD to describe the data



Conclusions



- It is just a beginning of implementation
- Interesting stuffs:
 - Existing tools: Prov python package + Southampton suite for validation
 - SVG format with the use of namespaces
- A lot of things to do:
 - Explore SimDM
 - Implement DataLink descriptors and link resources
 - Serialize the provenance in a VOTable
 - Think about how to query