



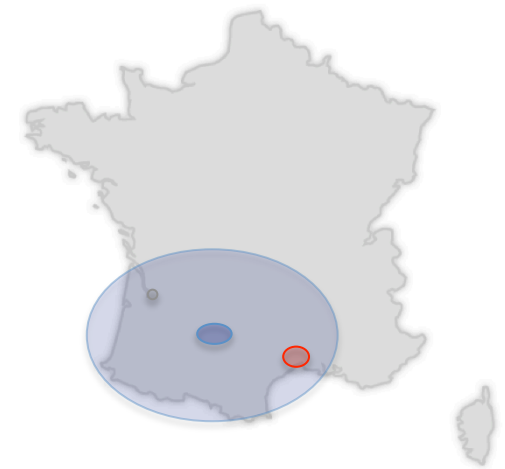
Pollux and Provenance

Scientists :

Ana Palacios, Agnès Lèbre

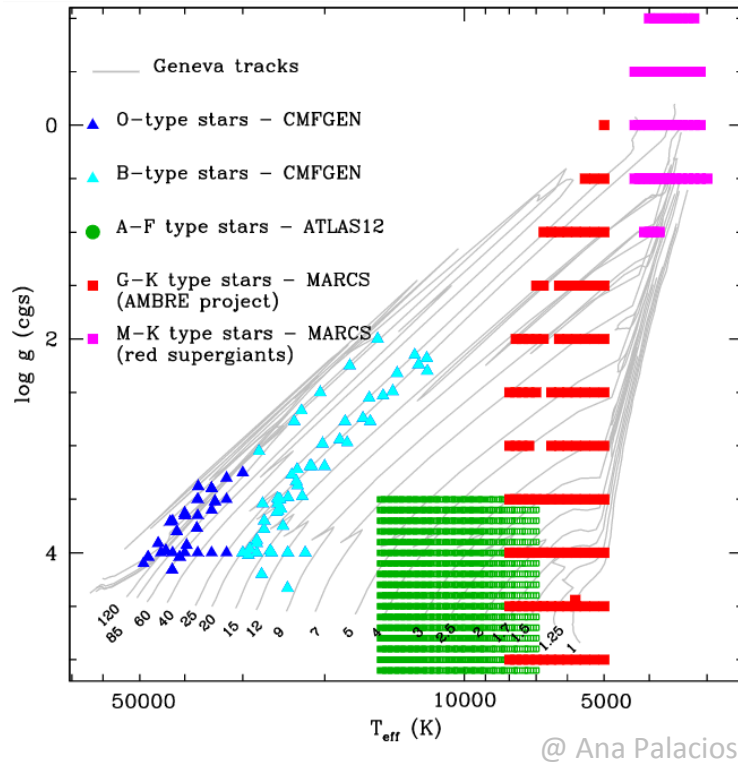
Software engineer :

Michèle Sanguillon





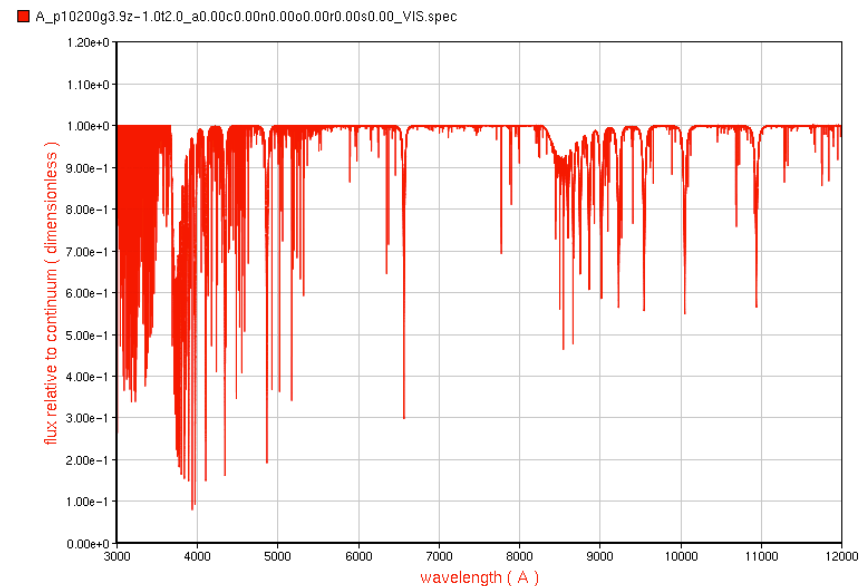
Pollux Database



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

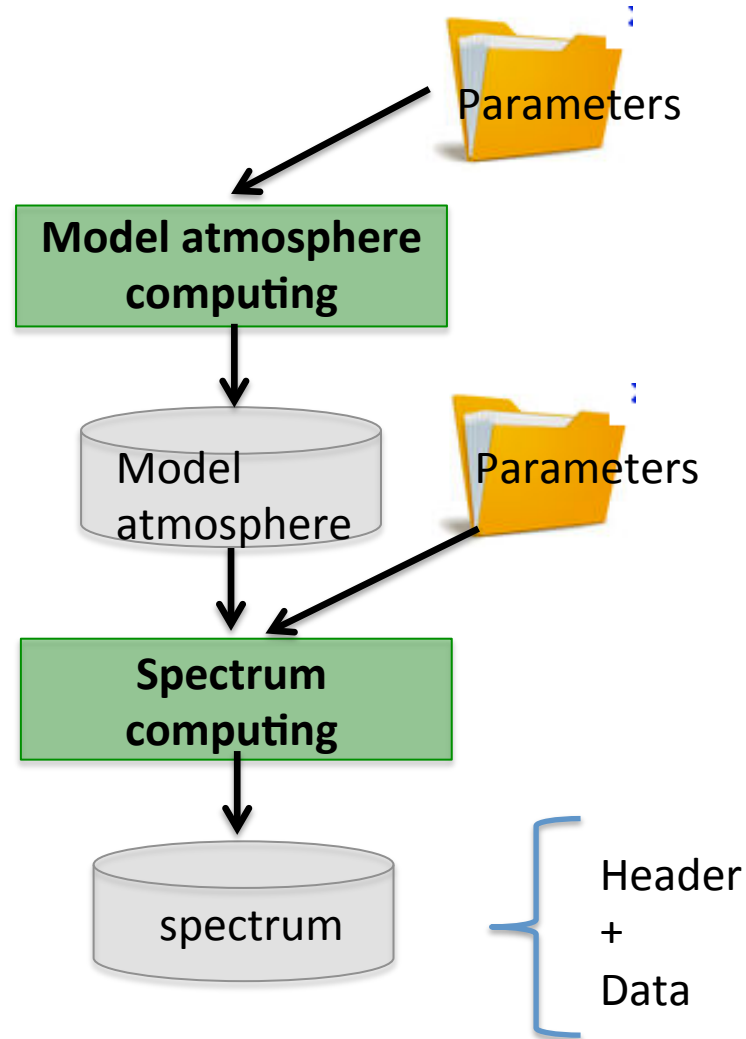
Spectra exist for many spectral types (O to M and Wolf-Rayet stars.)

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





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 OV users:
 - Spectra in fits format (header + data)



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' section has 'POLLUX Database' checked. The 'Request' section shows various parameters like Object name, RA, DEC, SIZE, BAND, TIME, and FORMAT. A blue circle highlights the 'Optional Parameters' table, which lists parameters like logg_max, logg_min, MAXREC, meta_max, meta_min, model, pertinence, teff_max, teff_min, vturb_max, and vturb_min. The 'Results' section displays a table with columns for Index, teff, logg, mass, lum, vturb, meta, pert, title, SpectralAxis, FluxAxis, UNITS, SpectralSI, FluxSI, DataLength, Format, Location, and Exte.

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

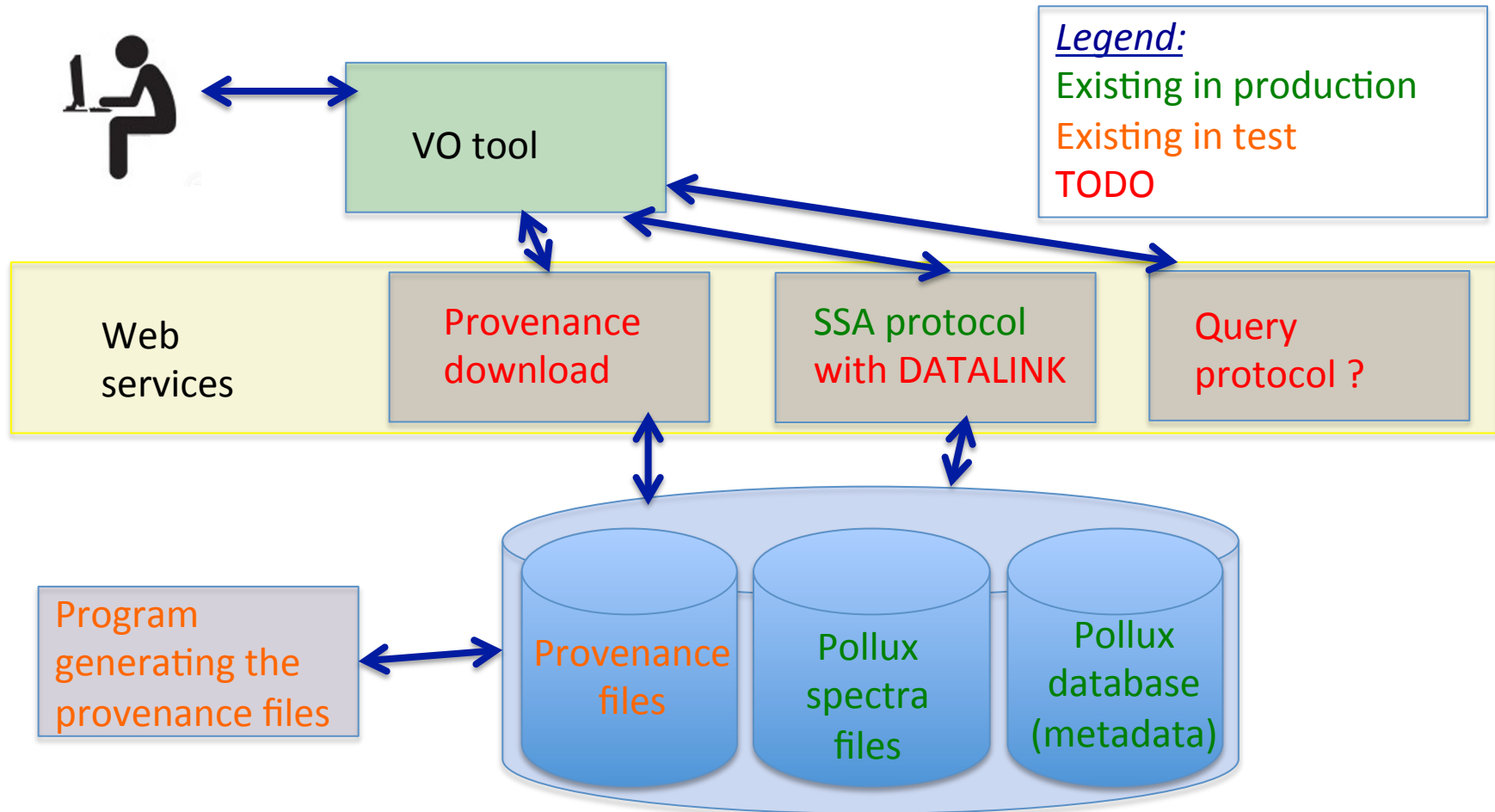
- **Use case 3:**

Show me a list of synthetic spectra satisfying :

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



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>
```

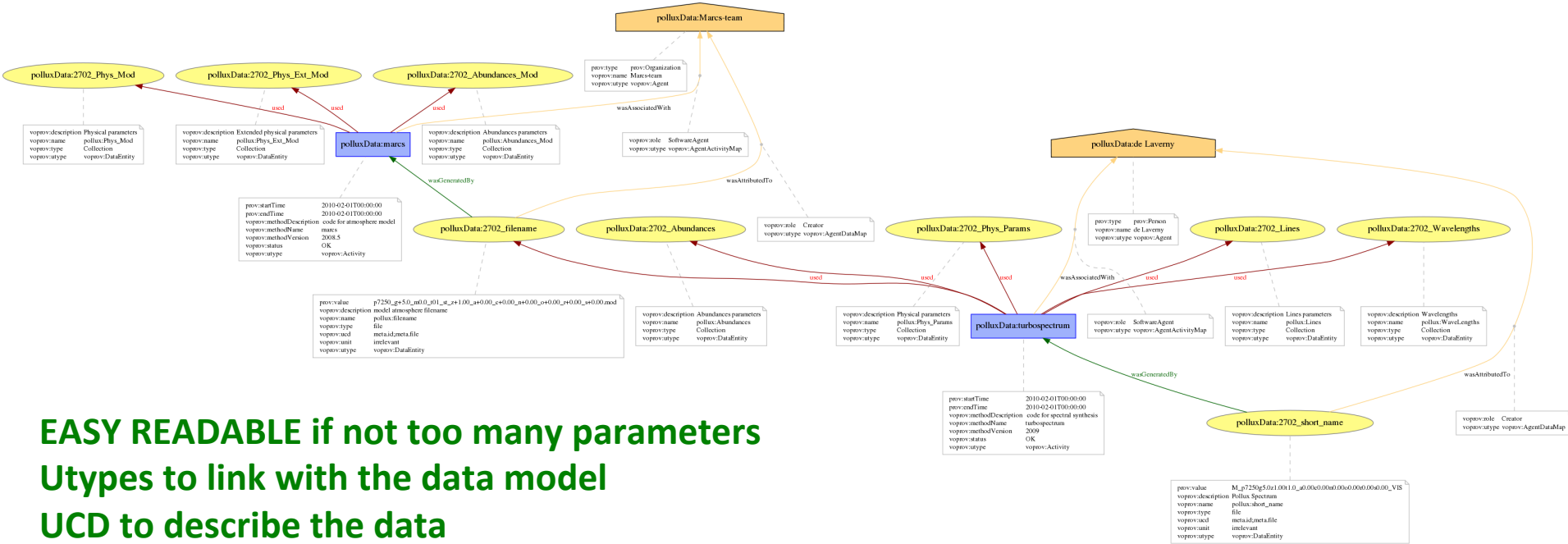
```
entity(pollux:14800g4.1z0.0a0.0C0.0.mod_2012_Teff, [voprov:description="effective  
temperature (K) - model atmosphere data", voprov:type="int", prov:value="14800",  
voprov:unit="K", voprov:ucd="phys.temperature.effective"])
```



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