Semantics & Theory

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InterOp - Urbana - 2012

Reminder

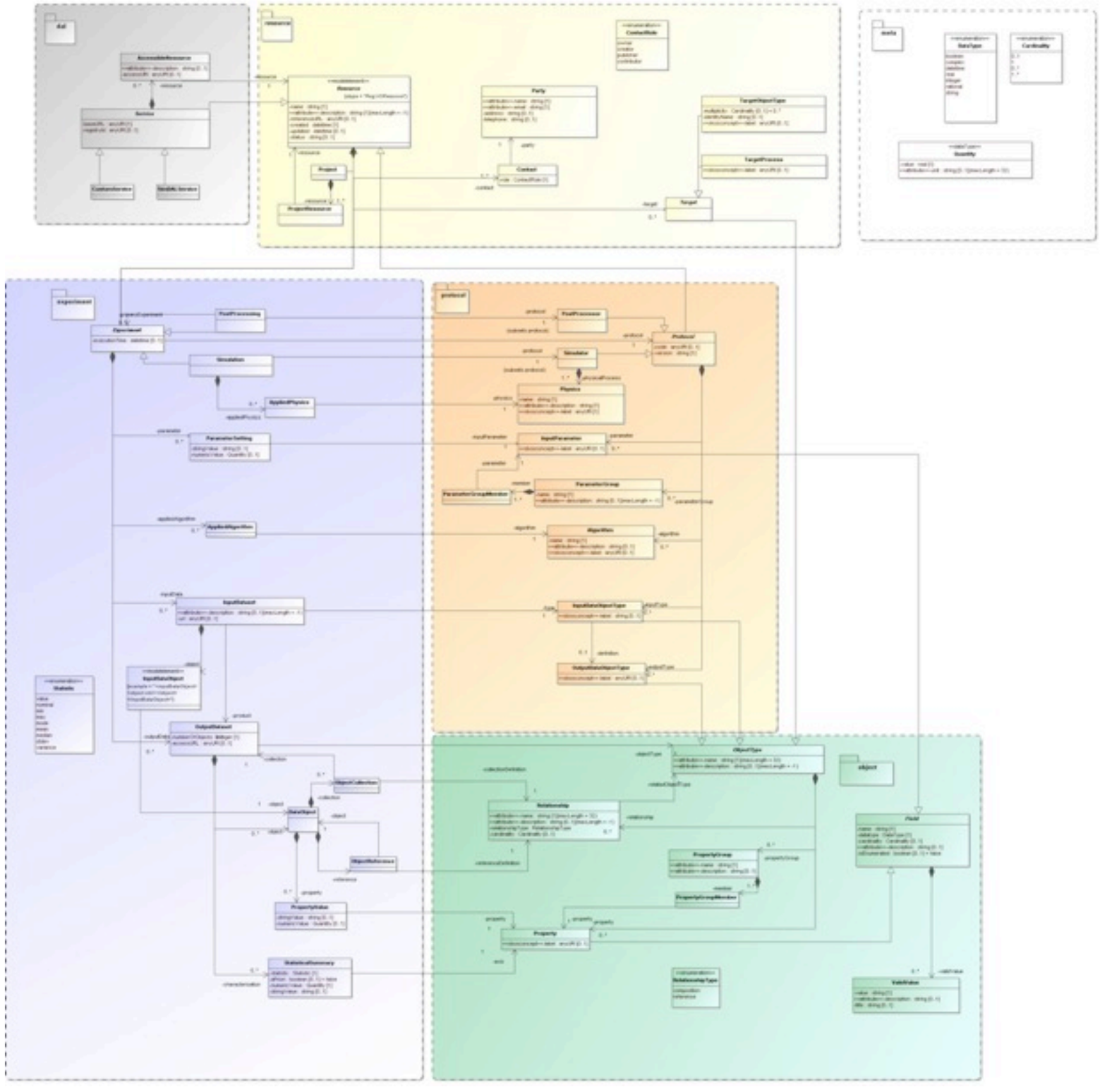
Simulation Data Model uses SKOS concepts to define quantities described by the DM

Classes :

- Physical quantities
- Physical processes
- Astronomical objects
- Algorithms
- Representation Object Type
- ...

Goals :

- use SKOS to describe simulations
- use SKOS to discover simulations



Reminder

Several vocabularies have been developped

- http://votheory.obspm.fr

- provide access to URIs of SKOS concepts
  - Browse by PrefLabel or AltLabel
  - No search by narrower / broader yet

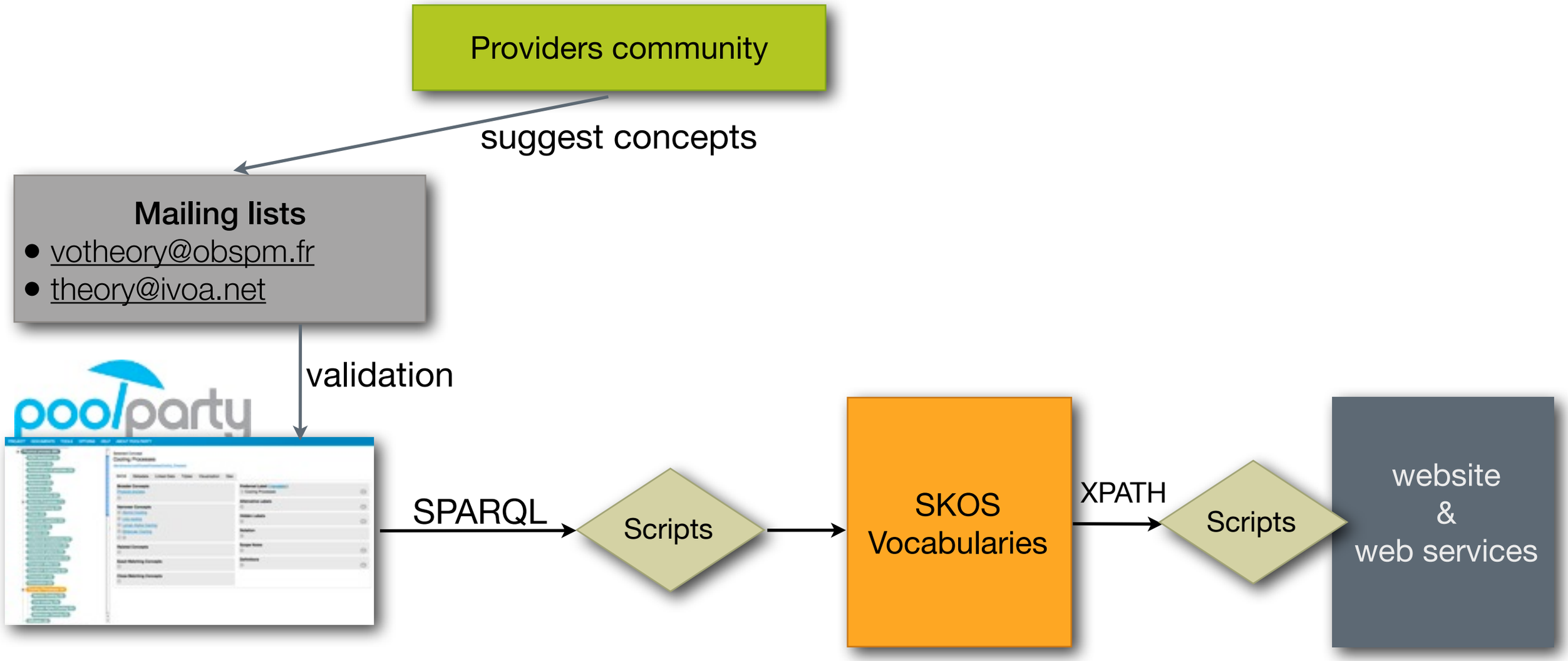
- provide webservices to check the existence of SKOS concepts

From last InterOp
- Add a lot of concepts in algorithms, Physical Processes, Physical Quantities
- Ex : Stellar physics, Asterosismology

Vocabularies development and access

Development of vocabularies is done thanks to Poolparty

- http://poolparty.biz
- Free commercial licence



Use Poolparty

- to enter concepts
- to define relationships

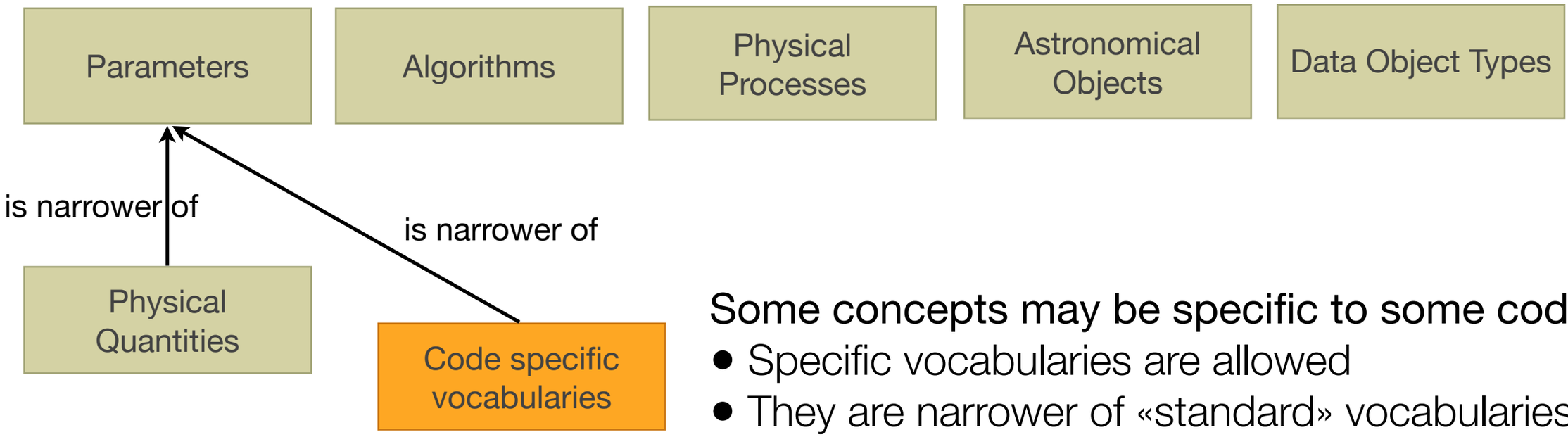
Scripts

- Get SKOS vocabularies
- Correct URIs for IVOA
- Relationships between vocabularies

Vocabularies organization

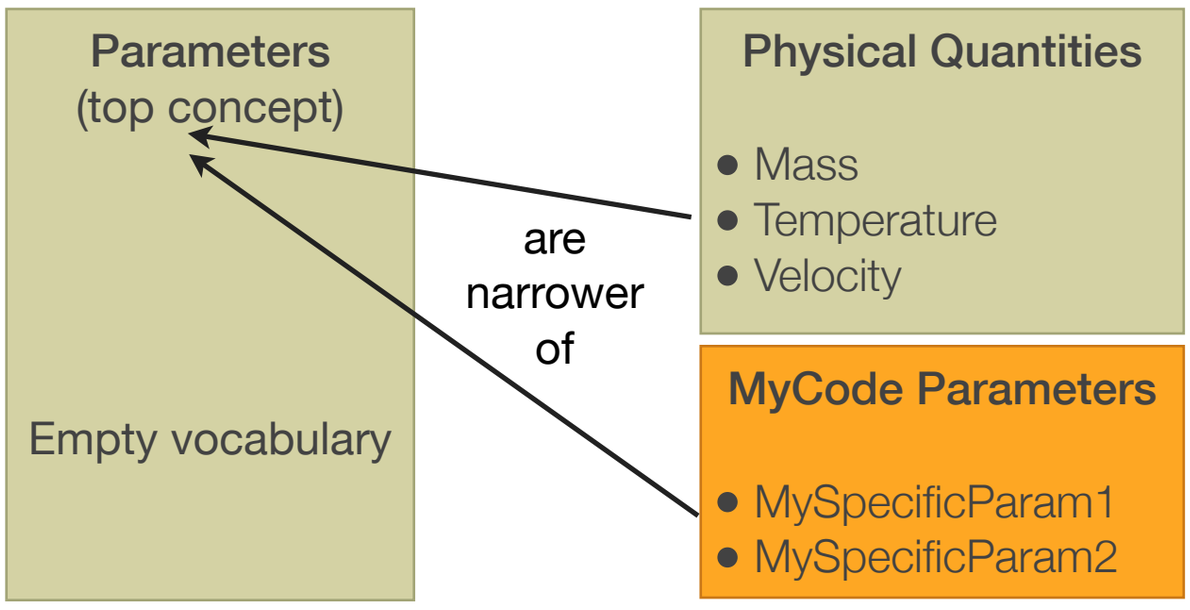
Content of some vocabularies is related to other vocabularies

- Example : Input Parameters of codes are often Physical Quantities
  => Physical Quantities become narrower of Input Parameters



Some concepts may be specific to some codes

- Specific vocabularies are allowed
- They are narrower of «standard» vocabularies



Requirement :

- Register vocabularies in registries

How to do it ?
How to define it ?

- RDF / SKOS
- ontologies

Atoms and Molecules

Question at the Napoli InterOp :

- How to describe quantities related to atoms and molecules ?

Examples :

- Service provides simulations about abundance of H_2O
- Service provides line intensities of CO

Solutions :

- Ontologies : more powerful but more complex
- SKOS : more direct

Proposition for URIs for atoms and molecules :

- Isotopologs, isomers, ... : C_2OH_6 could be : CH_3-CH_2-OH or CH_3-O-CH_3

- need unicity in URIs : use INCHI keys in the URIs

- Example : CO

http://purl.org/astronomy/vocab/ChemicalSpecies/UGFAIRIUMAVXCW-UHFFFAOYSA-N

CO

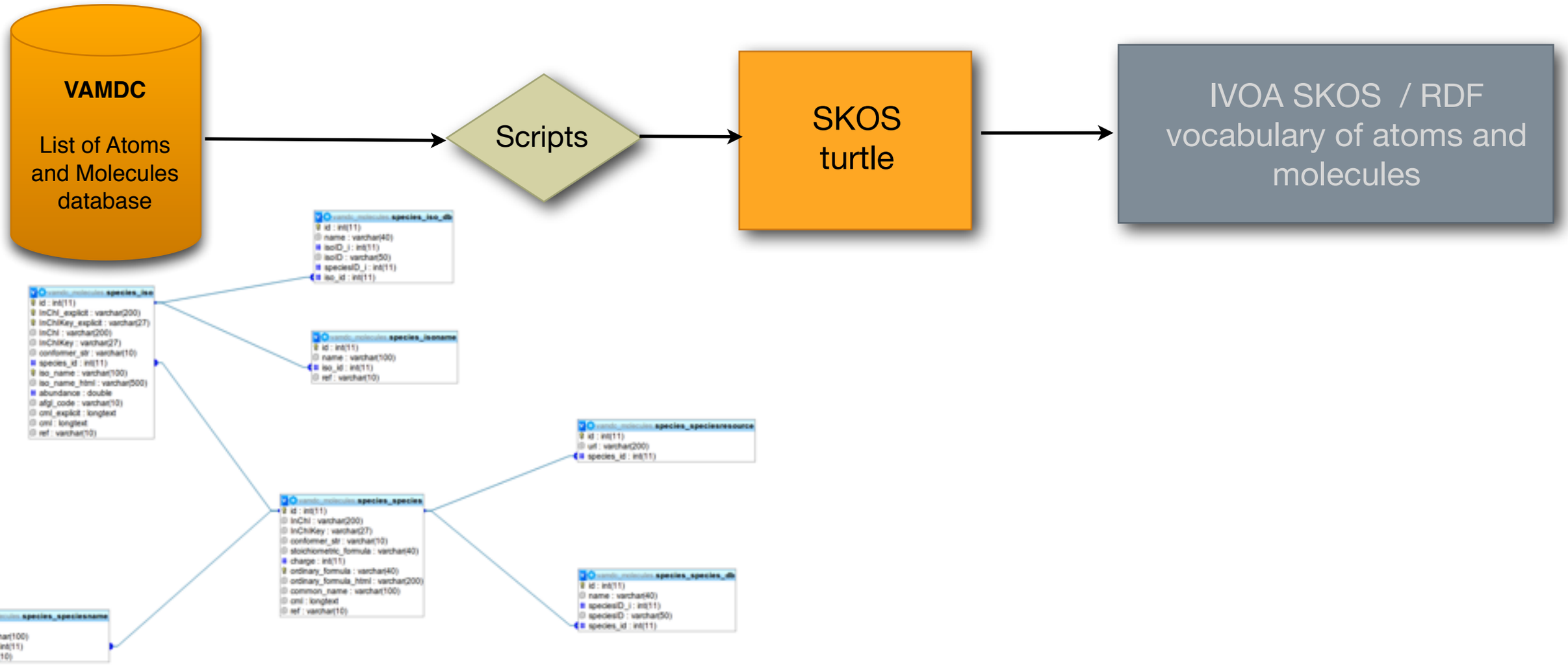
Atoms and Molecules

VAMDC develops and maintains a data base of chemical species

- use INCHI key to identify species
- INCHI used as ID for interoperability of VAMDC services

VAMDC Virtual Atomic and Molecular Data Centre

http://vamdc.eu



Atoms and Molecules

Example of a molecule on votheory.obspm.fr

H2O

Pref Label

URI :

http://purl.org/astronomy/vocab/ChemicalSpecies/XLYOFNOQVPJJNP-UHFFFAOYSA-N

URI

Alternative labels :

- Dihydrogen monoxide (en)
- Dihydrogen oxide (en)
- Distilled water (en)
- H2(16O) (en)
- Tritiotope (en)
- Water (en)
- Water vapor (en)

Alt Label

Narrower terms :

- XLYOFNOQVPJJNP-DQGQKLTASA-N
- XLYOFNOQVPJJNP-DYCDLGHISA-N
- XLYOFNOQVPJJNP-NJFSPNSNSA-N
- XLYOFNOQVPJJNP-OUBTZVSYSA-N
- XLYOFNOQVPJJNP-XKYOGGAFSA-N

isotopologs for example

Narrower (in development)

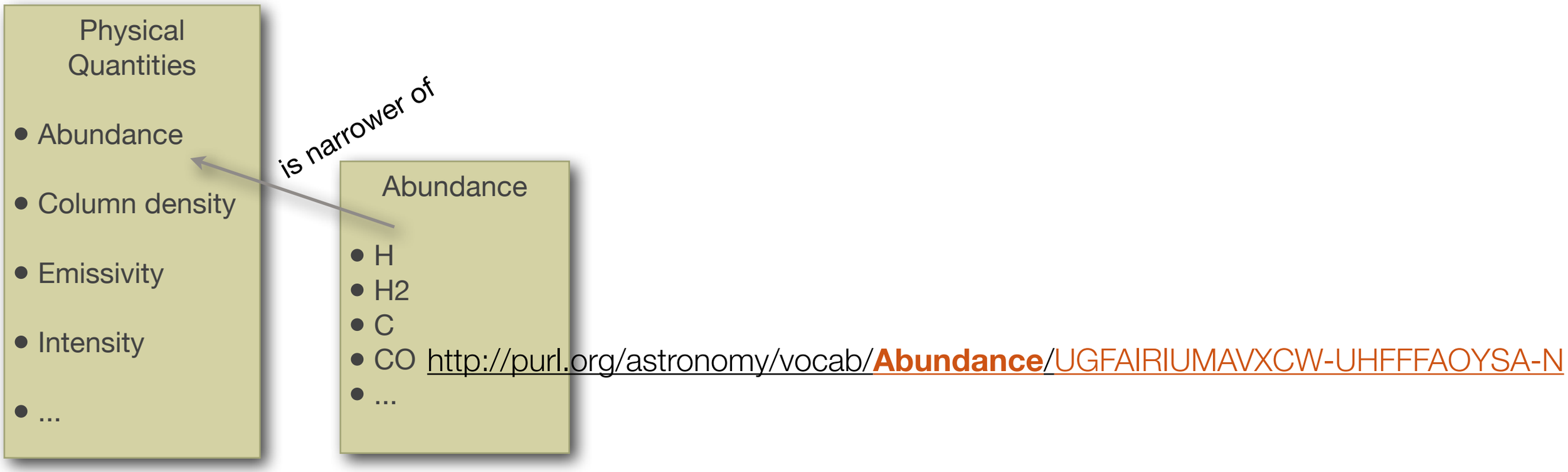
Atoms and Molecules

How to build a SKOS URI for the concept : «Abundance of CO» ?

- Solution 1 : **Abundance Of INCHI key**

  http://purl.org/astronomy/vocab/PhysicalQuantities/**AbundanceOf**UGFAIRIUMAVXCW-UHFFFAOYSA-N

- Solution 2 : **Specific narrower vocabularies**



Next steps and questions to the Semantics W.G.

- Question 1: How to specify SKOS concepts in VO-Tables ?
  - Attribute UCD but nothing for semantics
  - Plan extension from SKOS to ontologies ?

- Question 2: How to register vocabularies in IVOA registries ?

- Question 3: How to query in IVOA registries using SKOS concepts ?