Provenance concepts and uptake within IVOA

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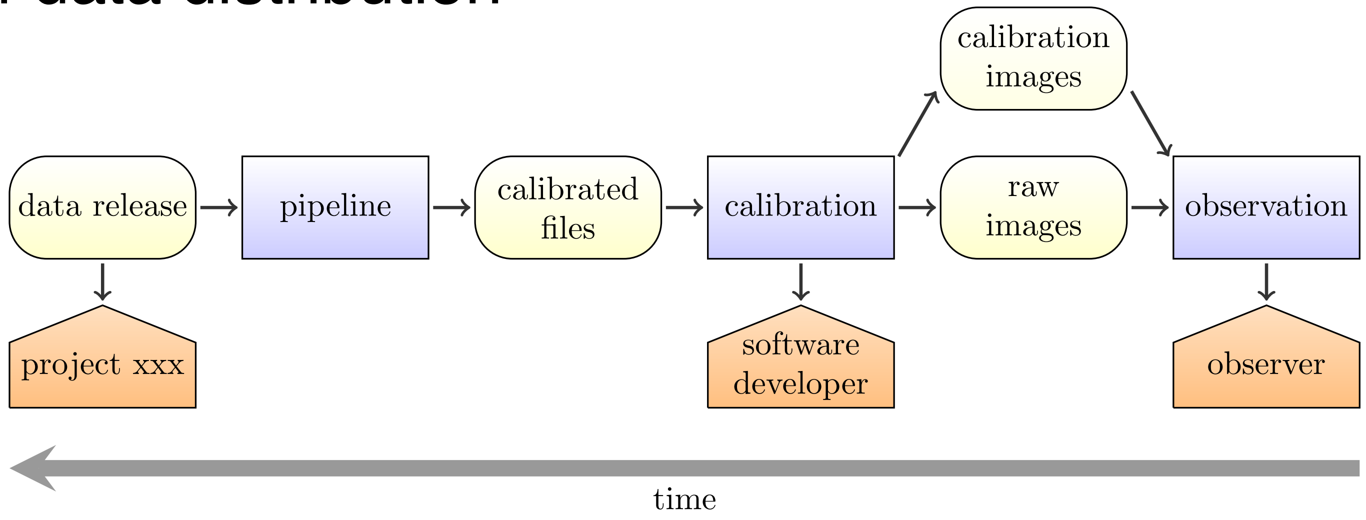
ESCAPE
VO Virtual Observatory

IVOA

Provenance definition

- Provenance is a structured representation of the information necessary to capture, store, and analyse the history of data production. It supports trust and efficiency for the management of data archives in a re-usable and machine readable format.
- A notion that came with the automation of data production pipelines data and the large expansion of data distribution



- Crucial in science, and especially when data are widely distributed and re-used

□ Provenance goals

- Managing Provenance info allows for:

A: Tracking the production history

Find out which steps were taken to produce a dataset and list the methods/tools/software that was involved.

B: Attribution and contact information

Find the people involved in the production of a dataset, that need to be cited or can be asked for more information.

C: Locating error sources

Find the location of possible error sources in the generation of a dataset.

D: Quality assessment

Judge the quality of an observation, production step or dataset.

E: Searching in structured provenance metadata

This would allow one to also do a “forward search”, i.e. locate derived datasets or outputs.

Provenance history (1)

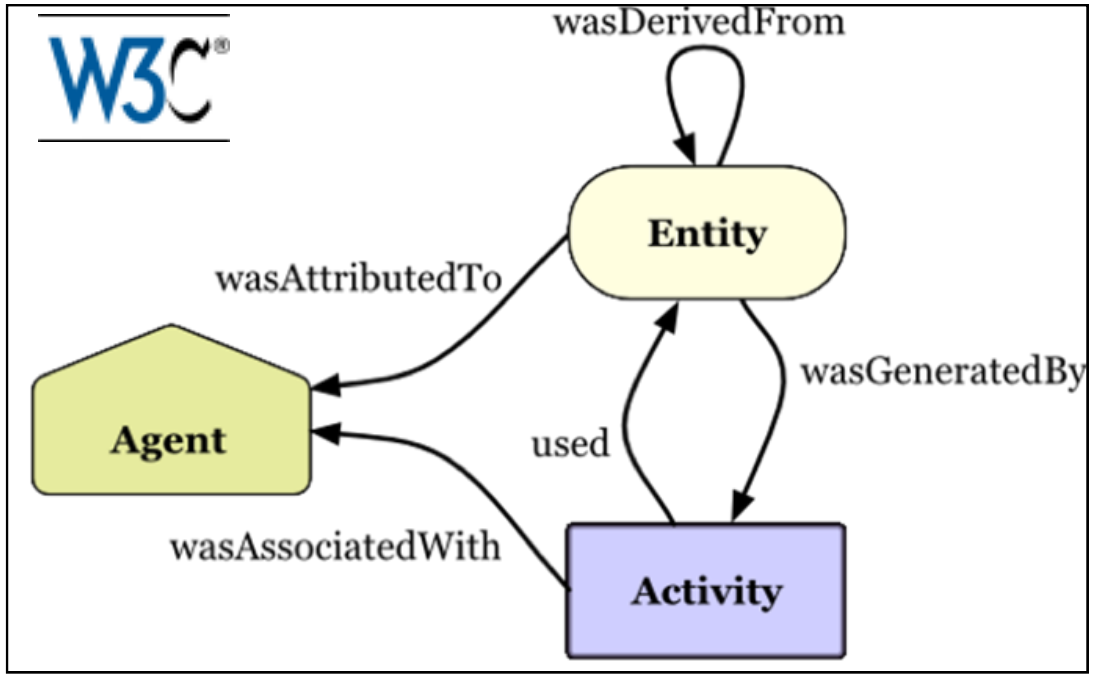
- a concern in various domains and science communities
  - document processing —> design and maintain workflows
  - genetics, molecular biology —> reproduce experiments
  - today for all observing science in general
- considered at beginning of IVOA data modeling group
  - for the Observation Data model 2005, J. Mc Dowell
  - for a reflexion on observing configurations, instruments, across various projects 2010, F. Bonnarel and coll.
  - see the history summary on the wiki page
    - https://wiki.ivoa.net/twiki/bin/view/IVOA/ProvenanceDataModelLegacy

□ Provenance history (2)

- developed and experienced in computer science research
  - 'Provenance Week' events since 1990, **IPAW conference**
  - modeled by the **W3C** consortium : a very general approach **PROV-DM** recommendation (2013)

    https://www.w3.org/TR/prov-overview/
- in parallel, description of Workflows have been developed with distributed computing
  - XML description, adhoc scripting languages, etc.
  - workflow management applications (Common Execution Architecture, Astrogrid)
- http://www.ivoa.net/documents/Notes/AstrogridWorkflow/AstrogridWorkflow-20060227.pdf
  - workflow management systems, e.g Taverna, grid management systems, etc.
- benefits from the development of **Metadata formats** : XML, JSON, …

W3C Provenance Pattern



- In our context

Entity

- data products (files), ancillary data (calibration, instrumental response, etc.), processing parameter files

Activity

- data acquisition, mosaicing, regridding, fusion, calibration, transformation

Agent

- Telescope astronomer, pipeline operator, principal investigator, data engineer, etc.
- W3C relations can make explicit:
  - Processing steps
  - Chain of dependencies
  - Responsibilities

□ Requirements listed for IVOA

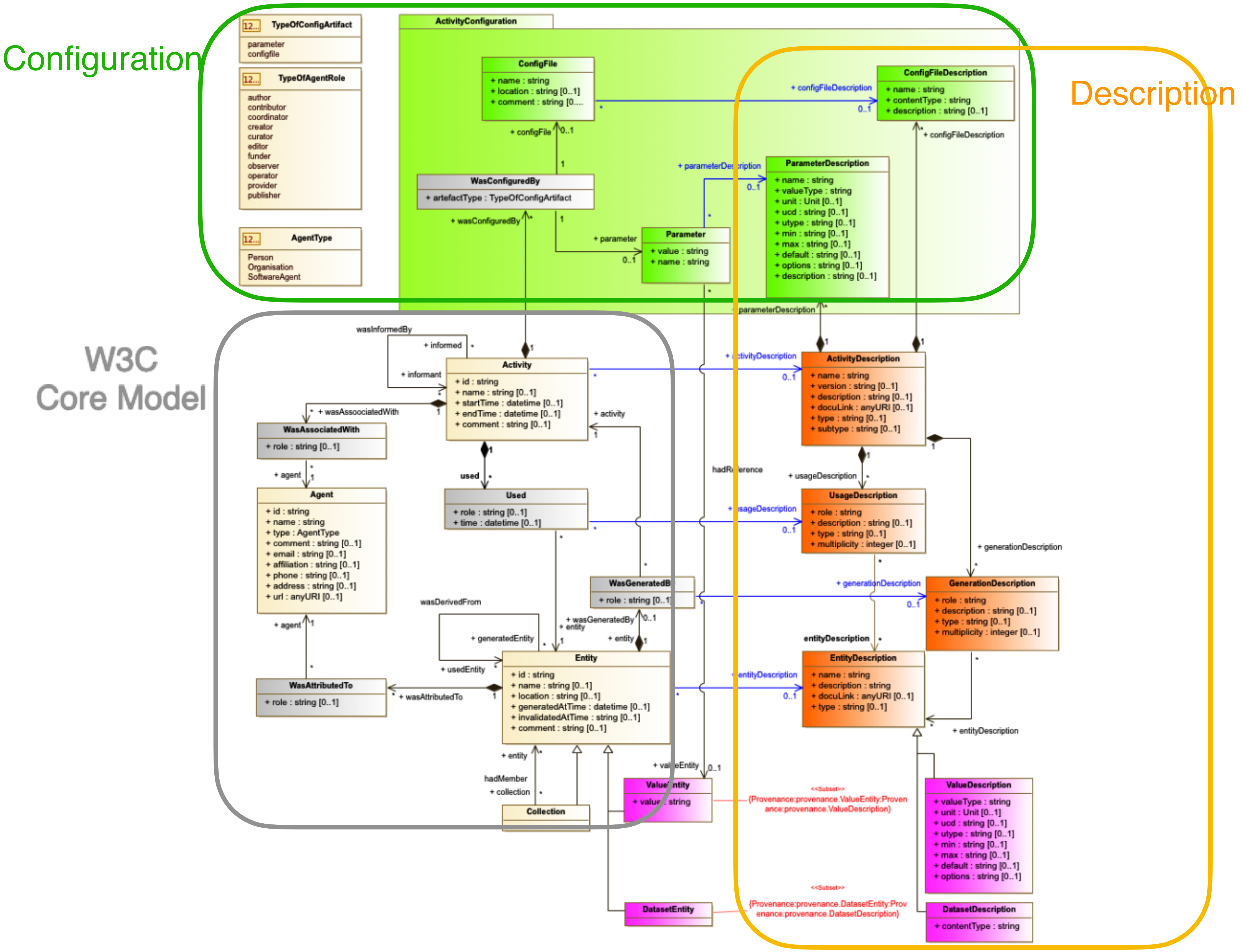
1. Provenance information must be stored in a **standard model**, with **standard serialization formats**.
2. Provenance information must be **machine readable**.
3. Provenance data model classes and attributes should be **linked to IVOA semantics, data models and formats** (DatasetDM, ObsCoreDM, SimDM, VOTable, UCDs, …).
4. Provenance information should be **serializable into the W3C provenance standard formats** (PROV-N, PROV-XML, PROV-JSON) with minimum information loss.
5. Provenance metadata must contain information to find immediate **progenitor(s)** (if existing) for a given entity, i.e. a dataset.
6. An entity must be linked to **the activity that generated it** (if the activity is recorded).
7. Activities must be linked to **input entities** (if applicable).
8. Activities may point to **output entities**.
9. Provenance information should make it possible to derive the **chronological** sequence of activities.
10. Entities, Activities and Agents must be **uniquely identifiable** within a domain
11. Released entities should have a **main contact**.
12. It is recommended that all activities and entities have **contact information** and contain a (short) **description** or link to a description

order of
importance
depends on
projects
-> core profile
+ options
tuning

□ PROV for the astronomical domain

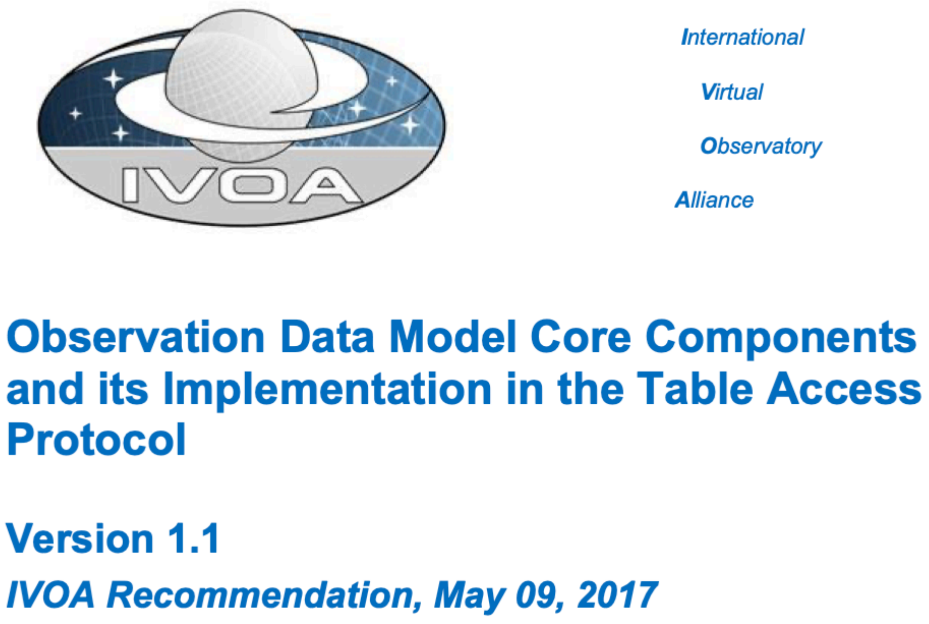
- W3C Provenance DM project is
  - good to understand concepts
  - very general —> not tuned to science data
- PROV-Store : a demo application for W3C ProvDM
  - https://openprovenance.org/store/
  - helps to build up examples
  - to practice various serialization languages: e.g. PROV-XML, PROV-N , PROV-JSON
  - does not scale easily with our datasets production chain
- Need more rules and customization to support project implementations
  - W3C PROV-Constraints REC https://www.w3.org/TR/prov-constraints/
  - Proposal in PROV-ONE (W3C Note) —> workflow and grid management
  - PROV-Template, etc. cf Luc Moreau 's team @Kings College London

IVOA provenance data model



□ IVOA landscape

- IVOA PROV-DM extends and restricts the general W3C PROV-DM
- It adds the data history
- IVOA has stable sets of metadata definitions for
  - data identification
  - data access and format
  - data curation
  - data physical properties (Characterization DM)



International
Virtual
Observatory
Alliance

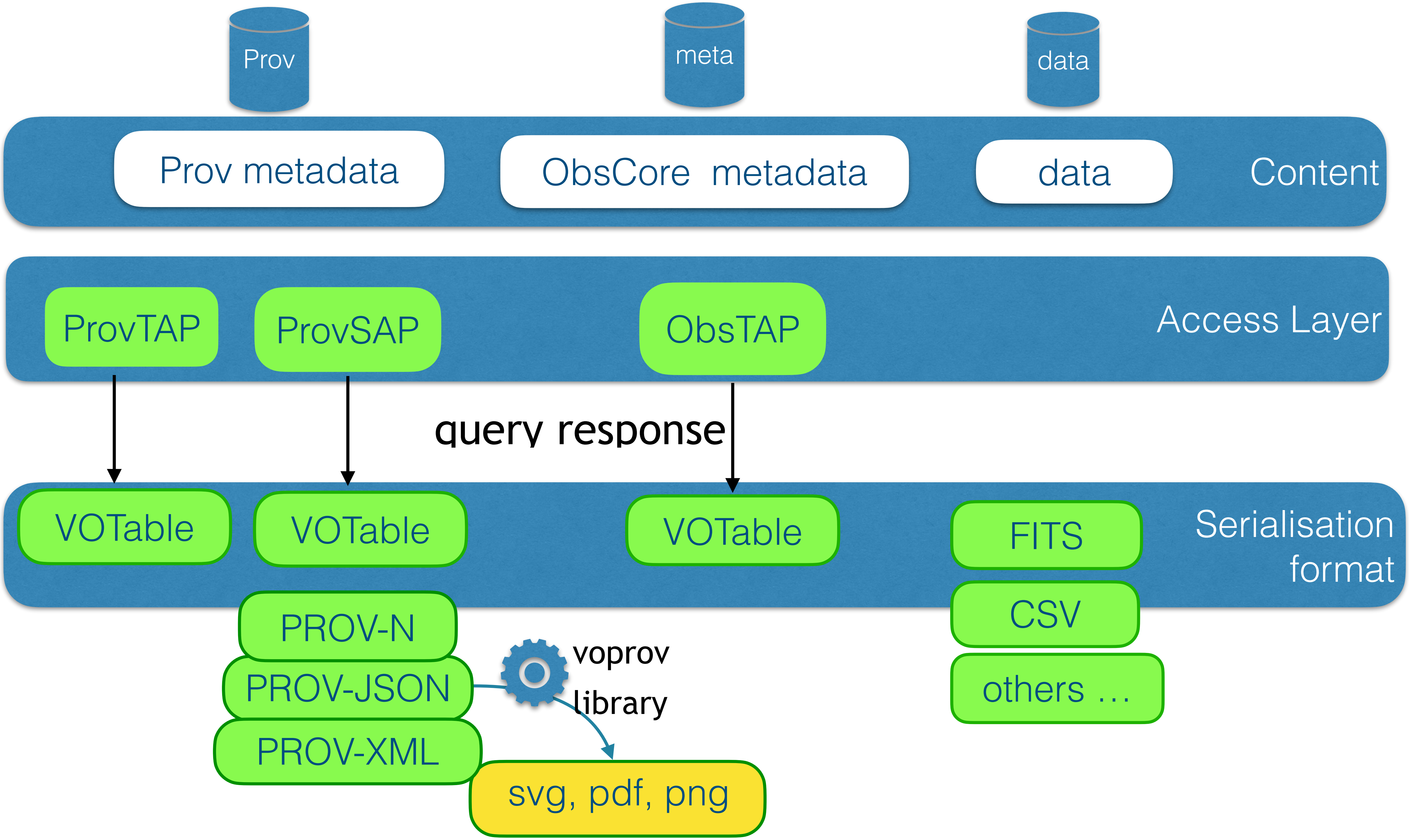
Observation Data Model Core Components and its Implementation in the Table Access Protocol

Version 1.1

IVOA Recommendation, May 09, 2017

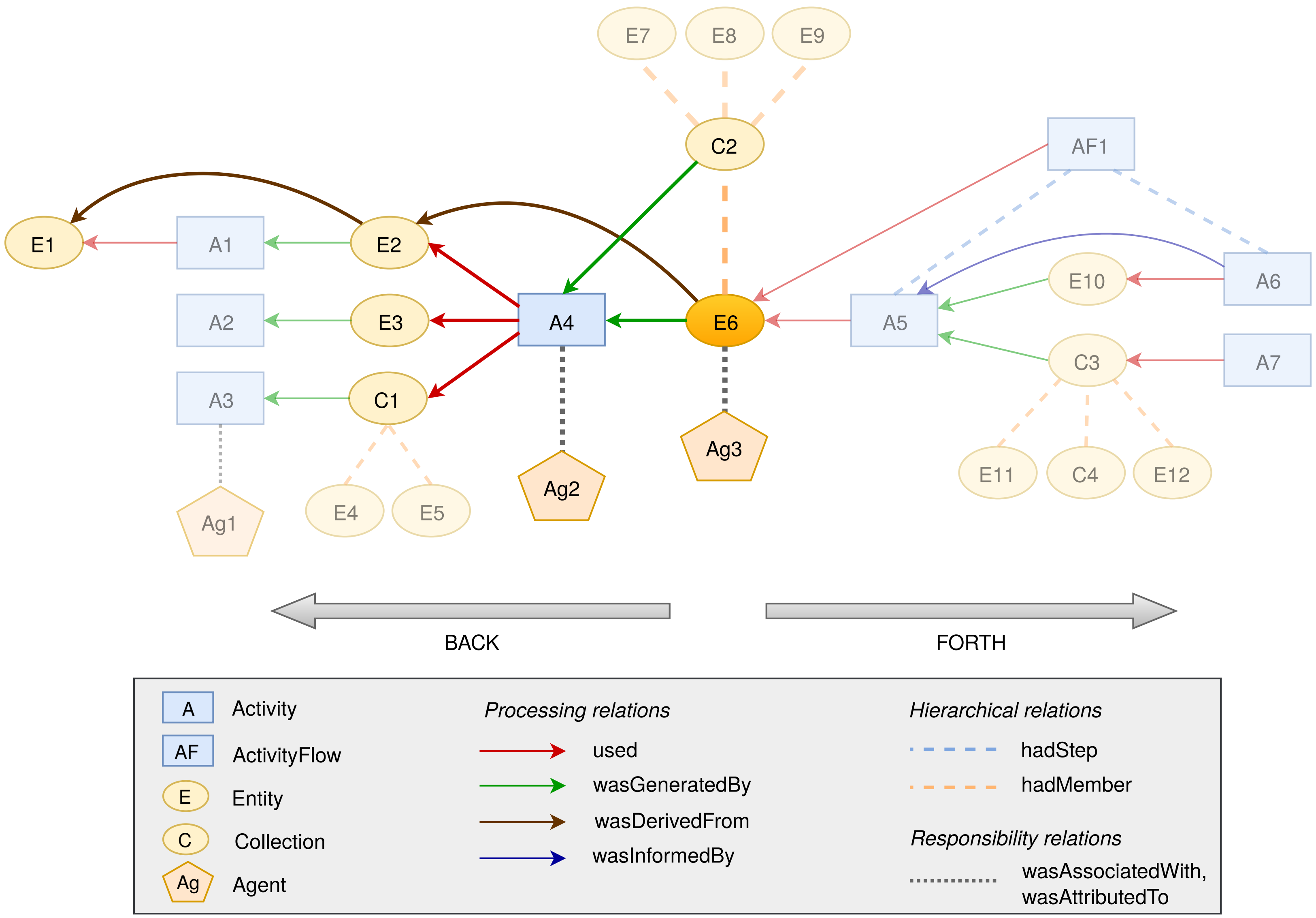
  - Various strategies to consider how to serve data, metadata, and Provenance records

VO building blocks



Implementation choices

- For each project
- Mapping for Entity
- define at which granularity to expose entities
  - datasets, collections of sub-observations, etc…)
- select the entity relations to implement
  - core: used +wasgeneratedBy
  - progenitor view : wasDerivedFrom
  - activity chaining : wasInformedby



credits : K. Riebe, AIP, Postdam

□ Implementation choices (2)

- For each project
- Mapping for Activity
- define granularity for task definition : ActivityDescription
    - existing dictionary of tasks? templates ?
    - interface to existing workflow descriptions language
        - e.g. CWL:Common Workflow Langage, Yaml
    - relations between Used—> UsageDescription, etc. or only Activity—> ActivityDescription
    - format for description : yaml, xml, cwl, scripting language, etc.

□ Conclusion

- The distribution of provenance metadata comes with a best effort strategy.
- On the data provider's side, the cost in implementing these features needs to be balanced with
  - an understandable content exportable outside the project
  - metadata clearly mapped means better queries prepared by the user or by the wrapping API (translator)
  - maintenance benefits to better monitor the archive collections (quality control, reprocessing, …)
- On the client side, an application querying several data centers will have to deal with the various level of completeness chosen by the data centers.
  - define various depth for provenance profiles : Core, Workflow description, all, etc.
  - enhance data search with provenance profile flavor selection

Thanks

Questions ?
Comments ?

□ Serialisation Formats

- Ready :
  - Gammapy Provenance embedded VOTable, PROV-N, PROV-XML
  - CTA Pipe/DIRAC text JSON
  - OPUS job submission and execution (LUTH) VOTable, JSON
  - Image database prototype in Triplestore (CDS) RDF/ttl
  - HiPS Image database (CDS) with PROV-TAP VOTable
  - Applause VOTable
  - RAVE implementation (AIP, Postdam)
    - Simple access (Prov-SAP) prototype Prov-N, PROV-JSON
  - Provenance for Pollux DB & *voprov* library (LUPM) VOTable, Prov-N, PROV-JSON
  - Under study :
  - SVOM pipeline execution tracking JSON FITS embedded