Provenance update

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FAIR principles for data sharing

https://www.go-fair.org/fair-principles

FINDABLE

Unique identifiers and metadata are used to allow data to be located quickly and efficiently

ACCESSIBLE

Data is open, free and universally available for research discovery efforts

INTER-OPERABLE

A common programming language is used to allow use in a broad range of applications

REUSABLE

All data is clearly described and outlines associated data-use standards

FAIR principles for data sharing

https://www.go-fair.org/fair-principles

Findable

F1. (Meta)data are assigned a globally unique and persistent **identifier**
F2. Data are described with rich metadata
F3. Metadata clearly and explicitly include the **identifier** of the data they describe
F4. (Meta)data are **registered** or **indexed** in a searchable resource

Interoperable

I1. (Meta)data use a formal, accessible, shared, and broadly applicable **language** for knowledge representation.
I2. (Meta)data use **vocabularies** that follow FAIR principles
I3. (Meta)data include **qualified** references to other (meta)data

Accessible

A1. (Meta)data are retrievable by their **identifier** using a **standardised** communications **protocol**
A1.1. The **protocol** is open, free, and universally implementable
A1.2. The **protocol** allows for an authentication and authorisation procedure, where necessary
A2. Metadata are accessible, even when the data are no longer available

Reusable (+ Reproducible?)

R1. (Meta)data are richly described with a plurality of **accurate** and **relevant** attributes
R1.1. (Meta)data are released with a **clear** and accessible data usage **license**
R1.2. (Meta)data are associated with detailed **provenance**
R1.3. (Meta)data meet domain-relevant community **standards**

International Virtual Observatory Alliance

IVOA Documents

http://www.ivoa.net/documents/ProvenanceDM/

IVOA Provenance Data Model
Version 1.0

IVOA Recommendation 11 April 2020

Interest/Working Group:
http://www.ivoa.net/twiki/bin/view/IVOA/IvoaDataModel
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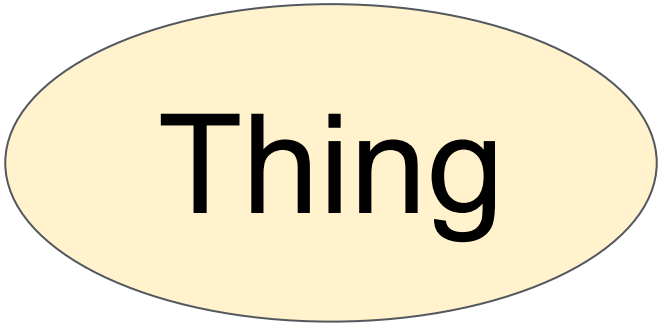
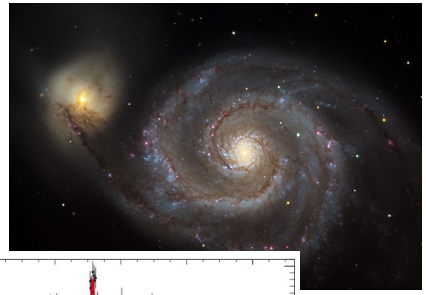
Editor(s):
Mathieu Servillat

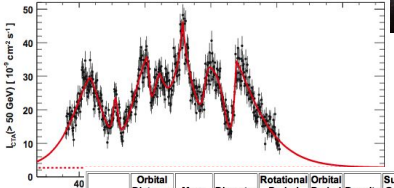


Provenance of a thing?

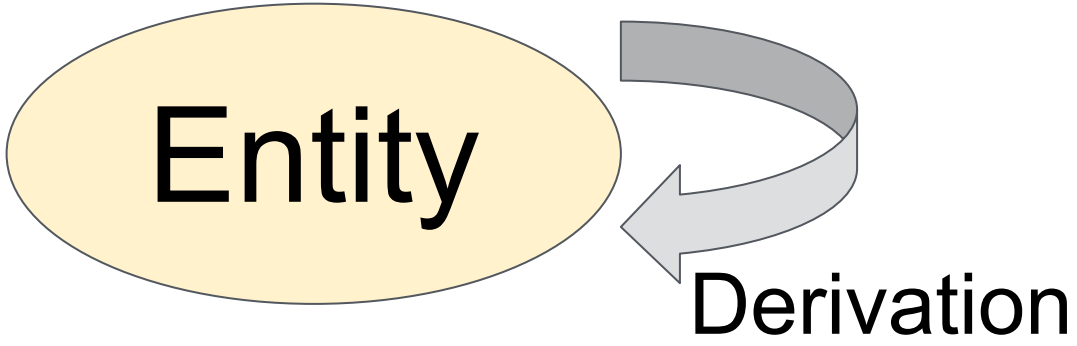
history, trace, chain of custody, location, ownership...

provenance = origin (where does it come from?) and **path** (what has been done?) gives confidence on the quality/reliability/trustworthiness of an entity (e.g. a data product).

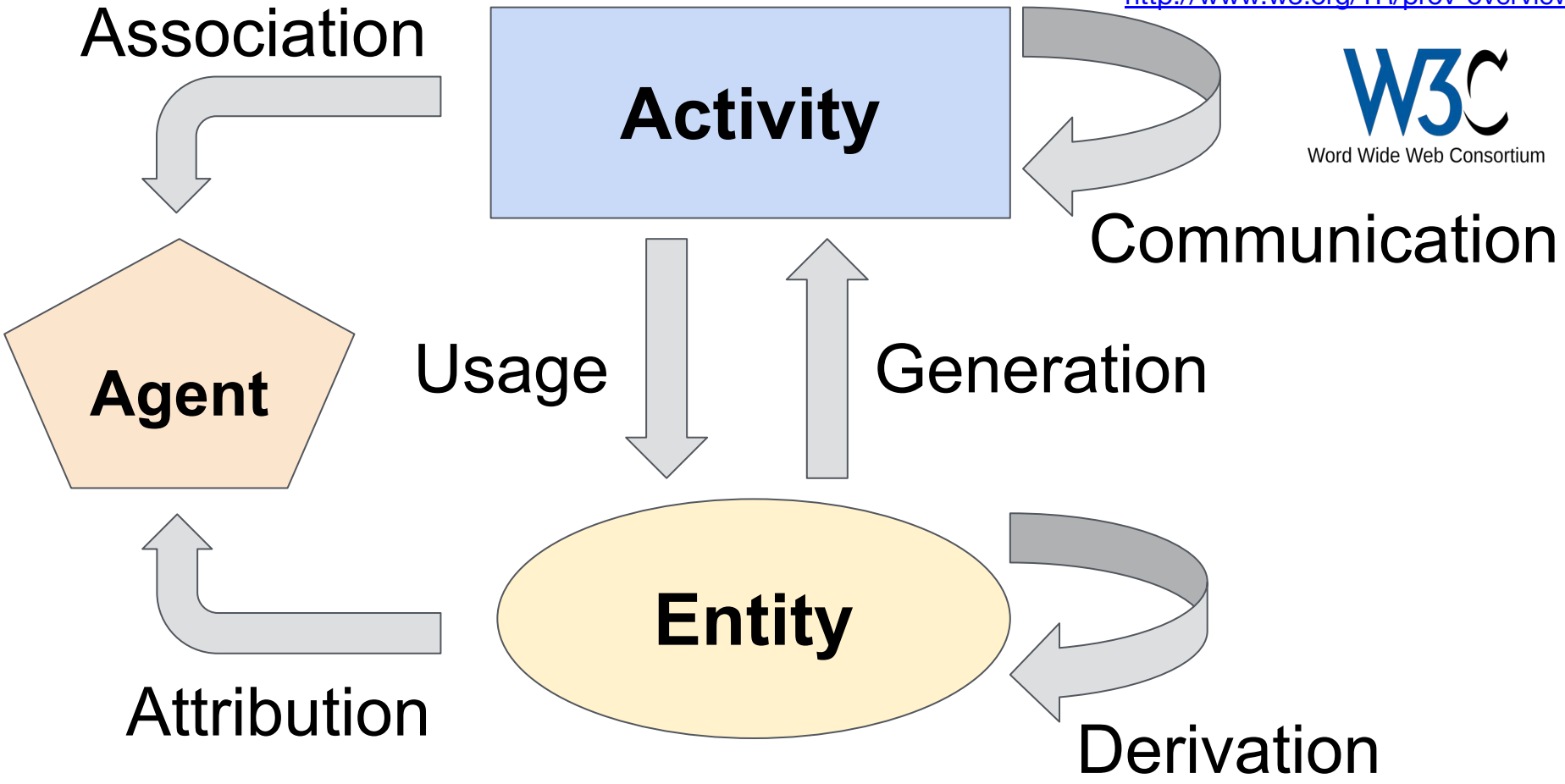




	Orbital Distance (AU)	Mass (earths)	Diameter (earths)	Rotational Period (days)	Orbital Period (years)	Density (earths)	Surface Gravity (earths)	Moons
Sol	0.0	330,000	109.2	25.4	...	1.42	28	...
Mercury	0.4	0.06	0.38	59	0.24	0.98	0.38	0
Venus	0.7	0.81	0.95	243	0.62	0.95	0.90	0
Earth	1.0	1.00	1.00	1.00	1.0	1.00	1.00	1
Mars	1.5	0.11	0.53	1.03	1.9	0.71	0.38	2
(Ceres*)	2.8	0.00015	0.07	0.38	4.6	0.38	0.03	0
Jupiter	5.2	317.8	11.2	0.42	11.9	0.24	2.34	63
Saturn	9.5	95.2	9.4	0.44	29.4	0.12	1.16	60
Uranus	19.2	14.5	4.0	0.72	83.7	0.23	1.15	27
Neptune	30.1	17.2	3.9	0.67	163.7	0.30	1.19	13
(Pluto*)	39.4	0.002	0.18	6.40	248.0	0.37	0.04	3
(Eris*)	67.7	0.002?	0.18	~8	557	?	?	1



http://www.w3.org/TR/prov-overview/



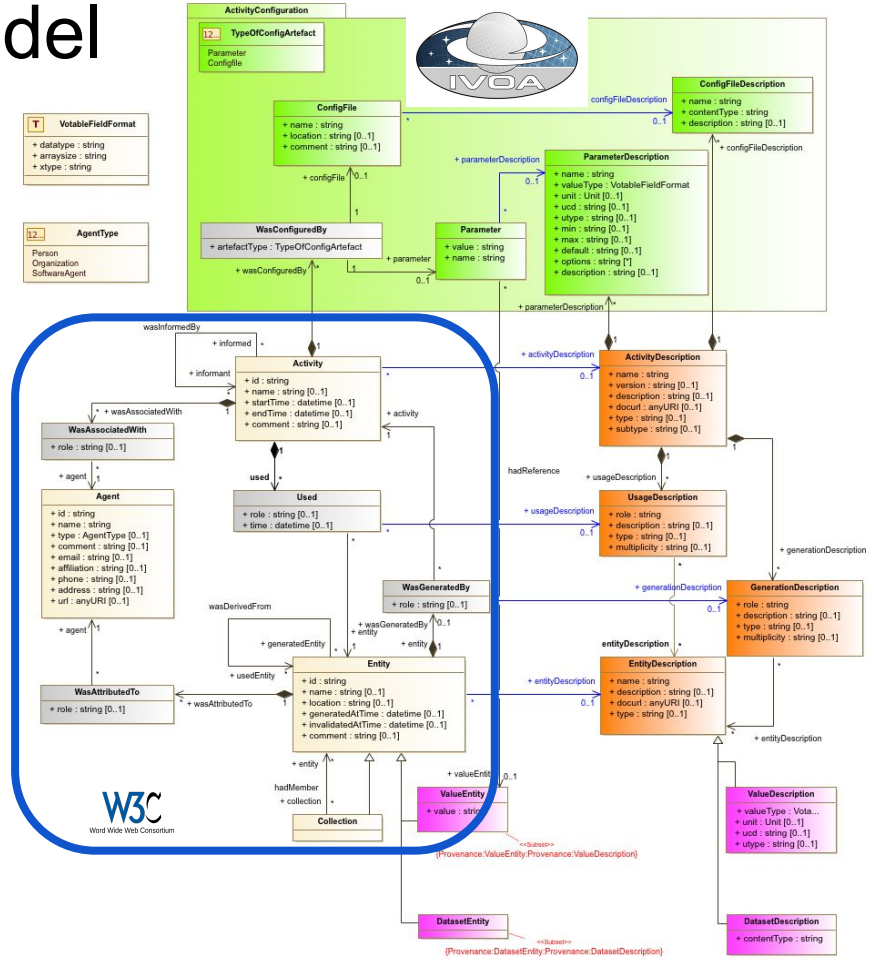
Word Wide Web Consortium

IVOA Provenance Data Model

http://www.ivoa.net/documents/ProvenanceDM/

Recommendation in April 2020

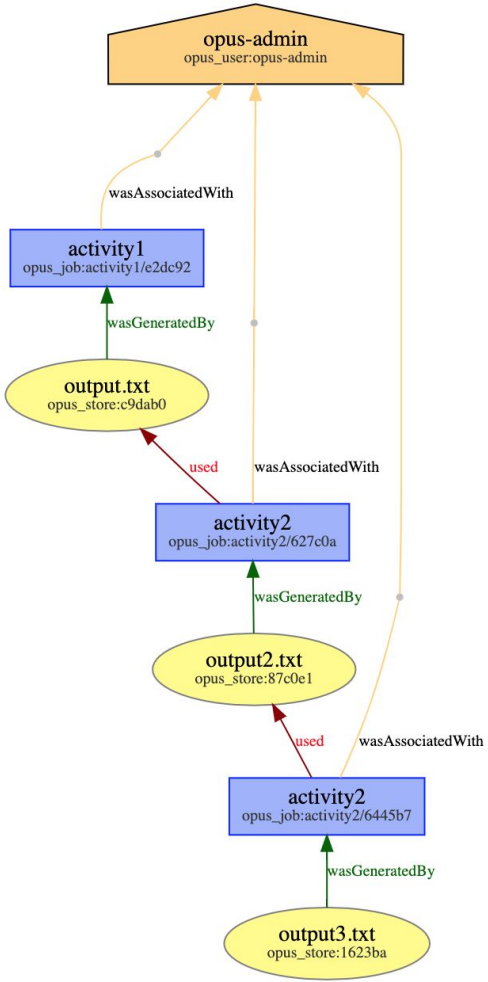
- Adds “**Description**” classes
- Adds “**Configuration**” classes
- Plugged in with
  - **VO** data models and concepts
    (UCD, VOUnit, VOTable…)
  - **VO** access protocols
    (ProvTAP, ProvSAP)
- Serializations
  - W3C PROV (XML, JSON, SVG…)
  - **VO** specific (VOTable)



Why recording structured provenance?

- **Make data FAIR** (Findable, Accessible, Interoperable, Reusable)
  - https://www.go-fair.org/fair-principles/
  - "**rich**" metadata, following standard data model, protocols and formats
  - "**detailed provenance**"
- **Quality** / **Reliability** / **Trustworthiness** of the products
- **Reproducibility requirement** in projects
  - Be able to rerun each activity (maybe testing and improving each step)
  - Not necessary to keep every intermediate file that is easily reproducible (possible gain on disk space and costs)
- **Debugging**
  - Not necessary to restart from scratch: locate in the provenance tree the faulty parts or the products to be discarded

→ We often realize too late that there are missing elements or links in the provenance. The capture of the provenance should be as detailed as possible and as naive as possible (simply record what happens).



Provenance graph

Provenance is :

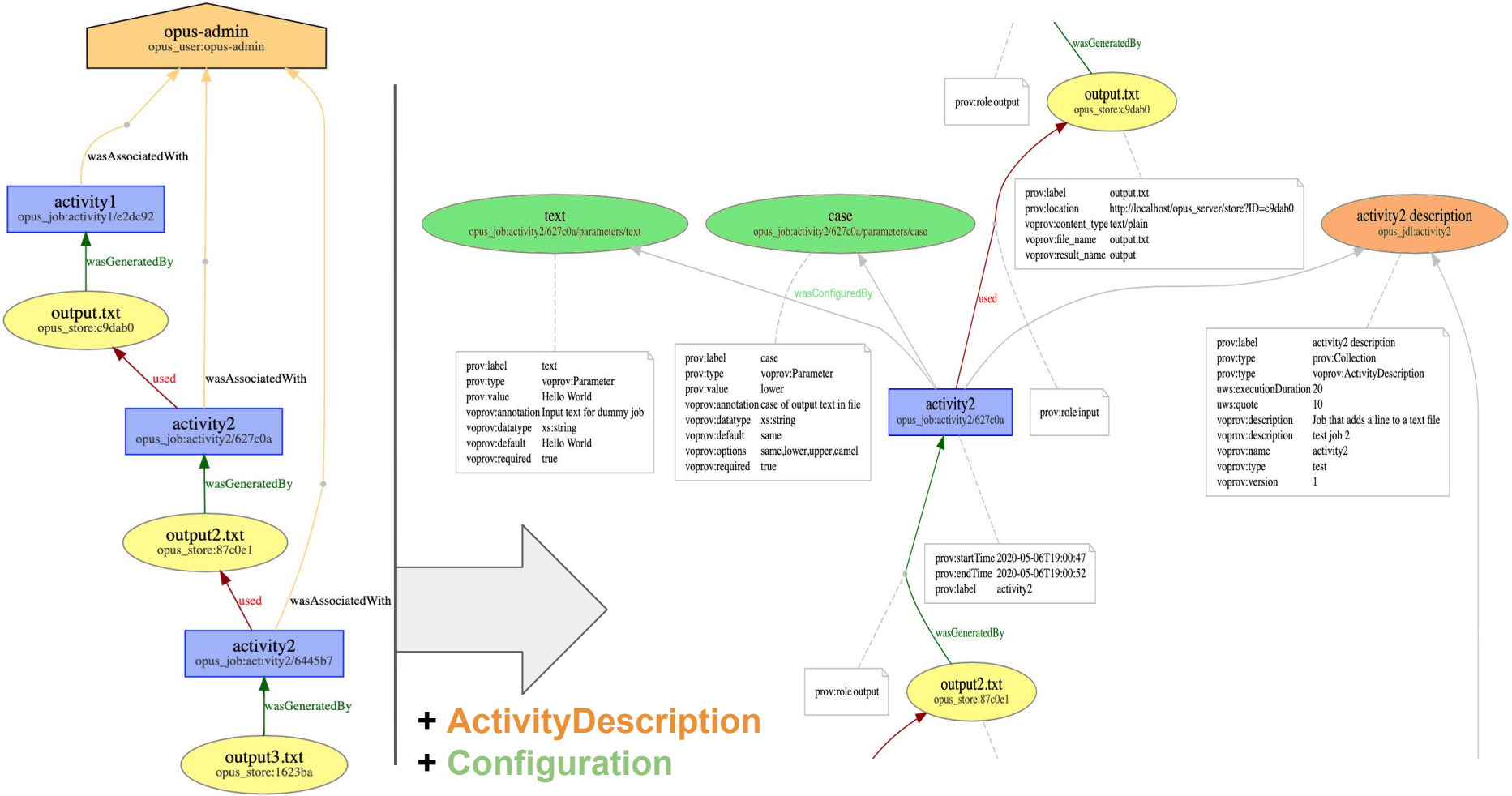
- a **chain** of activities and entities (used and generated)
- that occured in the **past**

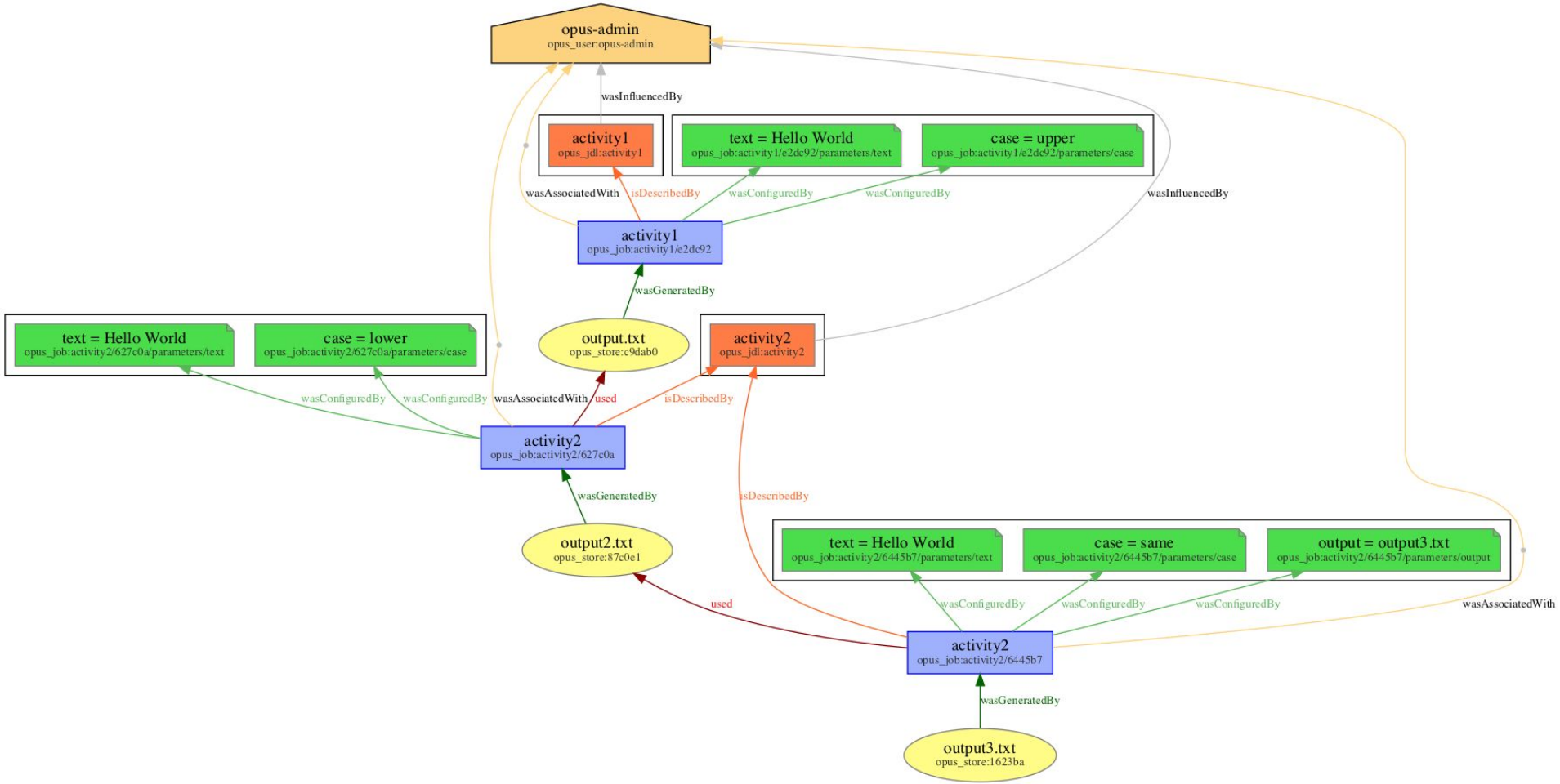
Using the **core data model**, some goals are achieved:

- **Unique identifiers**
- **Traceability**
- **Contact and Acknowledgement**

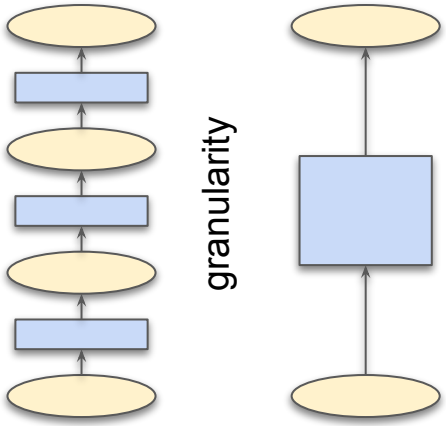
By using the **full IVOA data model**, more questions are answered:

- What **happened** during each **activity**?
- How was the **activity tuned** to be executed properly?
- What **kind of content** is in the **entities**?


opus-admin
opus_user:opus-admin
wasAssociatedWith
activity1
opus_job:activity1/e2dc92
wasGeneratedBy
output.txt
opus_store:c9dab0
used
wasAssociatedWith
activity2
opus_job:activity2/627c0a
wasGeneratedBy
output2.txt
opus_store:87c0e1
used
wasAssociatedWith
activity2
opus_job:activity2/6445b7
wasGeneratedBy
output3.txt
opus_store:1623ba
+ ActivityDescription
+ Configuration
wasGeneratedBy
prov:role output
output.txt
opus_store:c9dab0
prov:label output.txt
prov:location http://localhost/opus_server/store?ID=c9dab0
voprov:content_type text/plain
voprov:file_name output.txt
voprov:result_name output
text
opus_job:activity2/627c0a/parameters/text
case
opus_job:activity2/627c0a/parameters/case
activity2 description
opus_jdl:activity2
wasConfiguredBy
used
prov:label text
prov:type voprov:Parameter
prov:value Hello World
voprov:annotation Input text for dummy job
voprov:datatype xs:string
voprov:default Hello World
voprov:required true
prov:label case
prov:type voprov:Parameter
prov:value lower
voprov:annotation case of output text in file
voprov:datatype xs:string
voprov:default same
voprov:options same,lower,upper,camel
voprov:required true
activity2
opus_job:activity2/627c0a
prov:role input
prov:label activity2 description
prov:type prov:Collection
prov:type voprov:ActivityDescription
uws:executionDuration 20
uws:quote 10
voprov:description Job that adds a line to a text file
voprov:description test job 2
voprov:name activity2
voprov:type test
voprov:version 1
prov:startTime 2020-05-06T19:00:47
prov:endTime 2020-05-06T19:00:52
prov:label activity2
wasGeneratedBy
prov:role output
output2.txt
opus_store:87c0e1


opus-admin
opus_user:opus-admin
wasInfluencedBy
activity1
opus_jdl:activity1
text = Hello World
opus_job:activity1/e2dc92/parameters/text
case = upper
opus_job:activity1/e2dc92/parameters/case
wasAssociatedWith
isDescribedBy
wasConfiguredBy
wasConfiguredBy
wasInfluencedBy
activity1
opus_job:activity1/e2dc92
wasGeneratedBy
text = Hello World
opus_job:activity2/627c0a/parameters/text
case = lower
opus_job:activity2/627c0a/parameters/case
output.txt
opus_store:c9dab0
activity2
opus_jdl:activity2
wasConfiguredBy
wasConfiguredBy
wasAssociatedWith
used
isDescribedBy
activity2
opus_job:activity2/627c0a
wasGeneratedBy
isDescribedBy
output2.txt
opus_store:87c0e1
text = Hello World
opus_job:activity2/6445b7/parameters/text
case = same
opus_job:activity2/6445b7/parameters/case
output = output3.txt
opus_job:activity2/6445b7/parameters/output
used
wasConfiguredBy
wasConfiguredBy
wasConfiguredBy
wasAssociatedWith
activity2
opus_job:activity2/6445b7
wasGeneratedBy
output3.txt
opus_store:1623ba

Applying the model

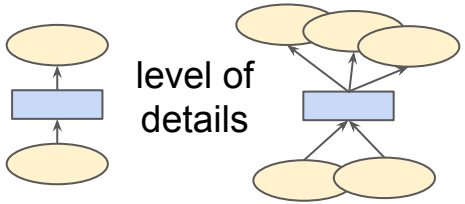


Different contexts in use cases

- Two flavours:
  - **on-top** (data products/collection already exist)
  - **inside** (save provenance information during the processing)
- **Identifiers:** unique and without meaning (if possible)
- **Granularity** (what steps? what objects?)
- **Level of details** (descriptions? configuration?)

Different steps in provenance management

- How to **capture** the provenance information
- How to **store** this information
- How to **access** it
- How to **visualize** a provenance graph



Some terminology

See ADASS XXX proceedings : https://arxiv.org/abs/2101.08691

- **full provenance**: graph/tree/chain of activities and entities up to the raw data. This information is not hosted by the entities themselves (stored on an external server? as separate files?)
- **minimum/last-step provenance**: attached to an entity, list of keywords that gives some context and info on **last activity** (general process/workflow, software versions, contacts...).
  Note: it would be interesting to include used entities, so that a full provenance may be reconstructed from each minimum provenance. However, such information on what was used may not be kept, or may not be complete.
- **end-user/specific "provenance"**: attached to an entity, list of keywords or data that provides **key information to use/analyse** the entity (e.g. for CTA: event class, event type, telescope configuration, sky conditions, reco method...)
  Note: may be extracted from full provenance (some parameters or entities generated at a given step), but it is considered as data here. Reversely, this specific "provenance" information may be a source of information to be mapped in the standard in order to fill the full provenance graph with more details.

See ADASS XXX proceedings : https://arxiv.org/abs/2101.08691

1. Defining the content of a **minimum provenance (last-step provenance)**
   - List of keywords related to the last activity and context
2. **Serializing** provenance
   - Both **human** and **machine** readable
   - Explore W3C formats, and YAML / VOTABLE / VOEvent formats
3. Provenance and **workflows**
4. From provenance "**on-top**" to provenance "**inside**"
   - How to map specific provenance information into the IVOA model?
   - How to introduce provenance **capture** inside a pipeline?
5. Provenance **storage**
6. Provenance **exploration** and **visualization**
   - Access protocols (ProvTAP, ProvSAP)
   - `voprov` Python package, or other tools

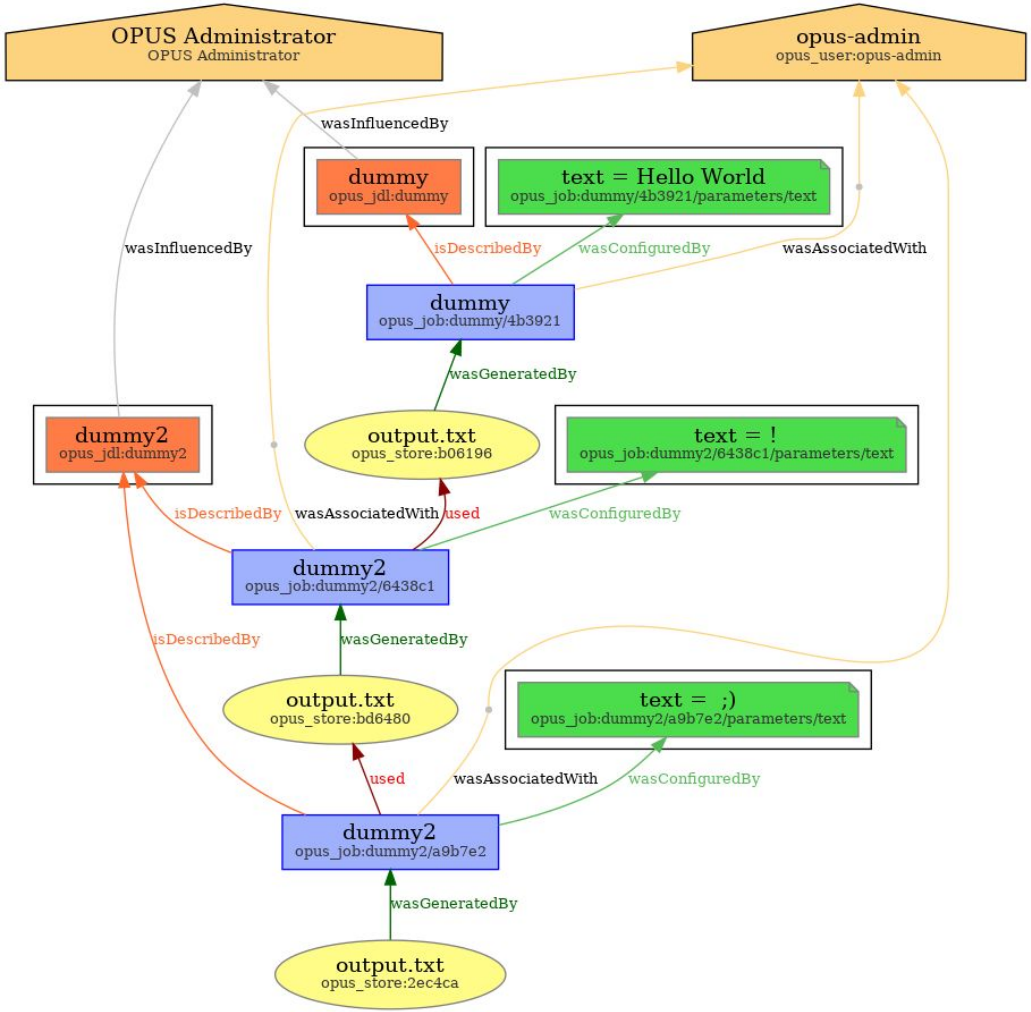
`voprov` Python package

- `prov` is a Python package that implements W3C PROV
  - https://github.com/trungdong/prov
- `voprov` extends `prov` to implement the IVOA Provenance DM
  - https://github.com/sanguillon/voprov
  - *Development Lead*: Jean-François Sornay, Michèle Sanguillon
  - *Contributors*: Mathieu Servillat, Mireille Louys, François Bonnarel, Catherine Boisson
- Main features
  - Description and Configuration classes and relations
  - Coloured graph to visualize IVOA objects
  - Conversion to a W3C graph

ProvSAP: Simple Access Protocol

- Simple HTTP endpoint
- Query string with arguments:
  - **ID** = a9b7e2 (activity or entity)
  - **DEPTH** = ALL / 1..
  - **DIRECTION** = FORWARD / BACKWARD
  - **RESPONSEFORMAT** = PROV-SVG / PROV-JSON / PROV-XML
  - **MODEL** = IVOA / W3C
  - **AGENTS** = 0 / 1
  - **CONFIGURATION** = 0 / 1
  - **DESCRIPTIONS**= 0 / 1 / 2
  - **ATTRIBUTES** = 0 / 1
- https://voparis-uws-test.obspm.fr/provsap?**ID**=a9b7e2&**DESCRIPTIONS**=1&**CONFIGURATION**=1&**ATTRIBUTES**=0&**DEPTH**=ALL&**MODEL**=IVOA

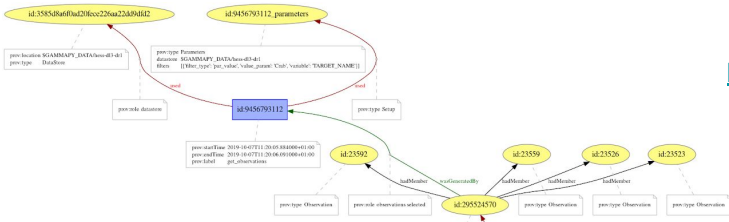
See ADASS XXX proceedings on OPUS : https://arxiv.org/abs/2101.08683


OPUS Administrator
OPUS Administrator
opus-admin
opus_user:opus-admin
wasInfluencedBy
dummy
opus_jdl:dummy
text = Hello World
opus_job:dummy/4b3921/parameters/text
wasInfluencedBy
isDescribedBy
wasConfiguredBy
wasAssociatedWith
dummy
opus_job:dummy/4b3921
wasGeneratedBy
dummy2
opus_jdl:dummy2
output.txt
opus_store:b06196
text = !
opus_job:dummy2/6438c1/parameters/text
isDescribedBy
wasAssociatedWith
used
wasConfiguredBy
dummy2
opus_job:dummy2/6438c1
isDescribedBy
wasGeneratedBy
output.txt
opus_store:bd6480
text = ;)
opus_job:dummy2/a9b7e2/parameters/text
used
wasAssociatedWith
wasConfiguredBy
dummy2
opus_job:dummy2/a9b7e2
wasGeneratedBy
output.txt
opus_store:2ec4ca

`logprov` Python package

- `logprov`: https://github.com/mservillat/logprov
- Capture provenance transparently
  - For Python tools (in particular data analysis on a laptop)
  - Make provenance info compatible between different software (ctapipe, gammapy, …)
  - Minimum effort from the developers, reuse existing tools
- Development drivers
  - Use **logging** system
    - known by developers, already integrated (base Python package)
    - log **dictionaries** to structure the information
  - **Non-intrusive** addition of code
    - use **decorators** for classes and methods
  - Fill with useful information
    - **descriptions** in a `definition.yaml` file
    - log parameters, arguments...

Provenance in `gammapy`



https://openprovenance.org/store/documents/1191.svg

1/ definition.yaml file for description/template
(already **integrated** to the code by the developers)

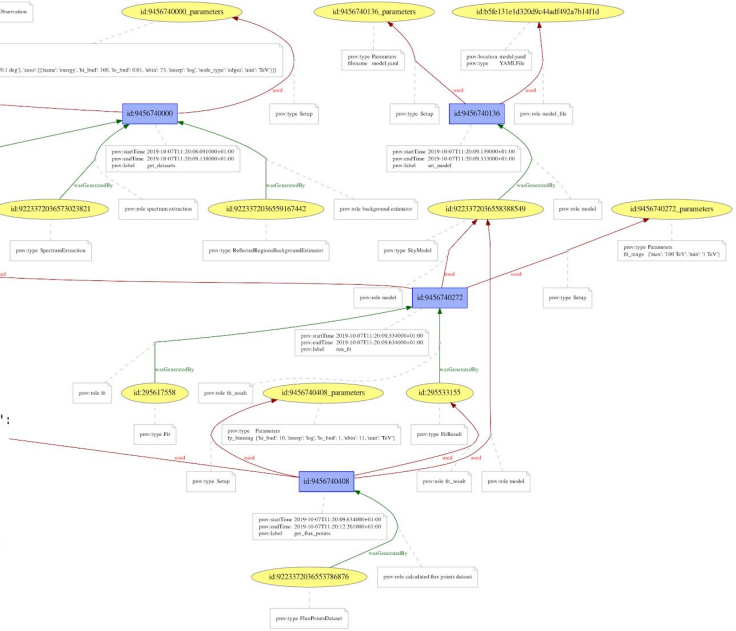
```
activities:

    get_observations:
        description:
            "Fetch observations from the data store according
            to criteria defined in the configuration"
        parameters:
            - name: datastore
              description: "DataStore path as string"
              value: settings.observations.datastore
            - name: filters
              description: "Filter criteria to select observations"
              value: settings.observations.filters
        usage:
            - role: datastore
              description: "DataStore object file"
              entityType: DataStore
              location: settings.observations.datastore
        generation:
            - role: observations selected
              description: "Observations selected"
              entityType: Observations
              value: observations
              has_members:
                  entityType: Observation
                  list: observations.list
                  id: obs_id
                  namespace: ""

    get_datasets:
        description: "Produce reduced datasets"
        parameters:
```

2/ entries **automatically** stored in the log file

```
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:05
  .884436_PROV_{'activity_id': 9456793112, 'activity_name': 'get_observations', 'startTime':
   '2019-10-07T11:20:05.884419'}
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:06
  .091102_PROV_{'activity_id': 9456793112, 'parameters': {'datastore':
  '$GAMMAPY_DATA/hess-dl3-dr1', 'filters': [{'filter_type': 'par_value', 'value_param':
  'Crab', 'variable': 'TARGET_NAME'}]}}
INFO:gammapy.utils.provenance.provenance:_PROV_The entity is a file with
  hash=3585d8a6f0ad20fece226aa22dd9dfd2 ($GAMMAPY_DATA/hess-dl3-dr1/obs-index.fits.gz)
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:06
  .091413_PROV_{'activity_id': 9456793112, 'used_role': 'datastore', 'used_id':
  '3585d8a6f0ad20fece226aa22dd9dfd2', 'entity_type': 'DataStore', 'entity_location':
  '$GAMMAPY_DATA/hess-dl3-dr1'}
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:06
  .091474_PROV_{'activity_id': 9456793112, 'generated_role': 'observations selected',
  'generated_id': 295524570, 'entity_type': 'Observations'}
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:06
  .091527_PROV_{'entity_id': 295524570, 'member_id': 23592, 'member_type': 'Observation'}
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:06
  .091571_PROV_{'entity_id': 295524570, 'member_id': 23523, 'member_type': 'Observation'}
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:06
  .091613_PROV_{'entity_id': 295524570, 'member_id': 23526, 'member_type': 'Observation'}
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:06
  .091653_PROV_{'entity_id': 295524570, 'member_id': 23559, 'member_type': 'Observation'}
INFO:gammapy.utils.provenance.provenance:_PROV_2019-10-07T11:20:06
  .091691_PROV_{'activity_id': 9456793112, 'endTime': '2019-10-07T11:20:06.091068'}
```



3/ export to W3C PROV
or search in provenance records

@ M. Servillat & J. E. Ruiz

Serializations

https://etherpad.in2p3.fr/p/provyaml

- **W3C PROV** standards + **`prov/voprov`**
  - XML & JSON, not easy to read by humans : lists of classes (entity, activity, agent, used, ...)
  - But visualizations possible : SVG, PNG, PDF
- **YAML** proposed solution
  - Machine readable **and** human readable
  - Structure with only 3 main groups :
    - activities : contains the links to reconstruct the chain of activities-entities
    - entities : contains information on how to find the entities and what they are
    - agents : contains contact information only (no roles)
  - **Relations** are attached to the above objects
- See example of Vizier (talk by Gilles Landais)
  - Model Mapping in VOTable with similar structure

```
agents:
    mservillat:
        name: MS
        email: m..@obspm.fr
entities:
    1234:
        name: input.txt
    5678:
        name: output.txt
        generatedAtTime: 2021-...
activities:
    9876:
        name: transform
        startTime: 2021-...
        endTime: 2021-...
        parameters:
            <name>: <value>
        used:
          - entity_id: 1234
            role: input
        generated:
          - entity_id: 5678
            role: output
        associated:
          - agent_id: mservillat
            role: operator
```

Minimum/Last-step provenance

https://etherpad.in2p3.fr/p/miniprov

- List of keywords
- Attached to an entity
- Gives info on last activity and context
- Enables full provenance reconstruction

⇒ Such a list is a restriction of the full provenance information, that is more easily stored in a header (FITS) or a flat table (same as ObsCore)

⇒ Identifiers must be “resolvable” to provide further provenance information

- entity_
  - id
  - creation_time
  - name
  - location
  - comment
  - content_type
  - description
- agent_
  - name
  - email
  - affiliation
- activity_description_
  - name
  - version
  - docurl
- activity_
  - id
  - name
  - type
  - start_time
  - stop_time
- used
  - [entity_id]
- generated
  - [entity_id]

ProvTAP and last-step provenance

François Bonnarel @ IVOA Nov 2020:
https://wiki.ivoa.net/internal/IVOA/InterOpNov2020DM/ProvTAPevolution.pdf

- Provenance information can be attached to data in various ways:
  - Embedded in the data « header » itself
  - Linked to the data record via DataLink or URL
  - Retrievable via ProvSAP via data id
- ProvTAP allows to discover « data » by constraining provenance features
  - Table Access Protocol using ADQL for queries and a TAP Schema
  - It's a « reverse » mechanism
- Last step provenance
  - `select * from last_step_provenance where entity_name = "..."`
  - Provides the Minimum/Last-step provenance for an entity in one line