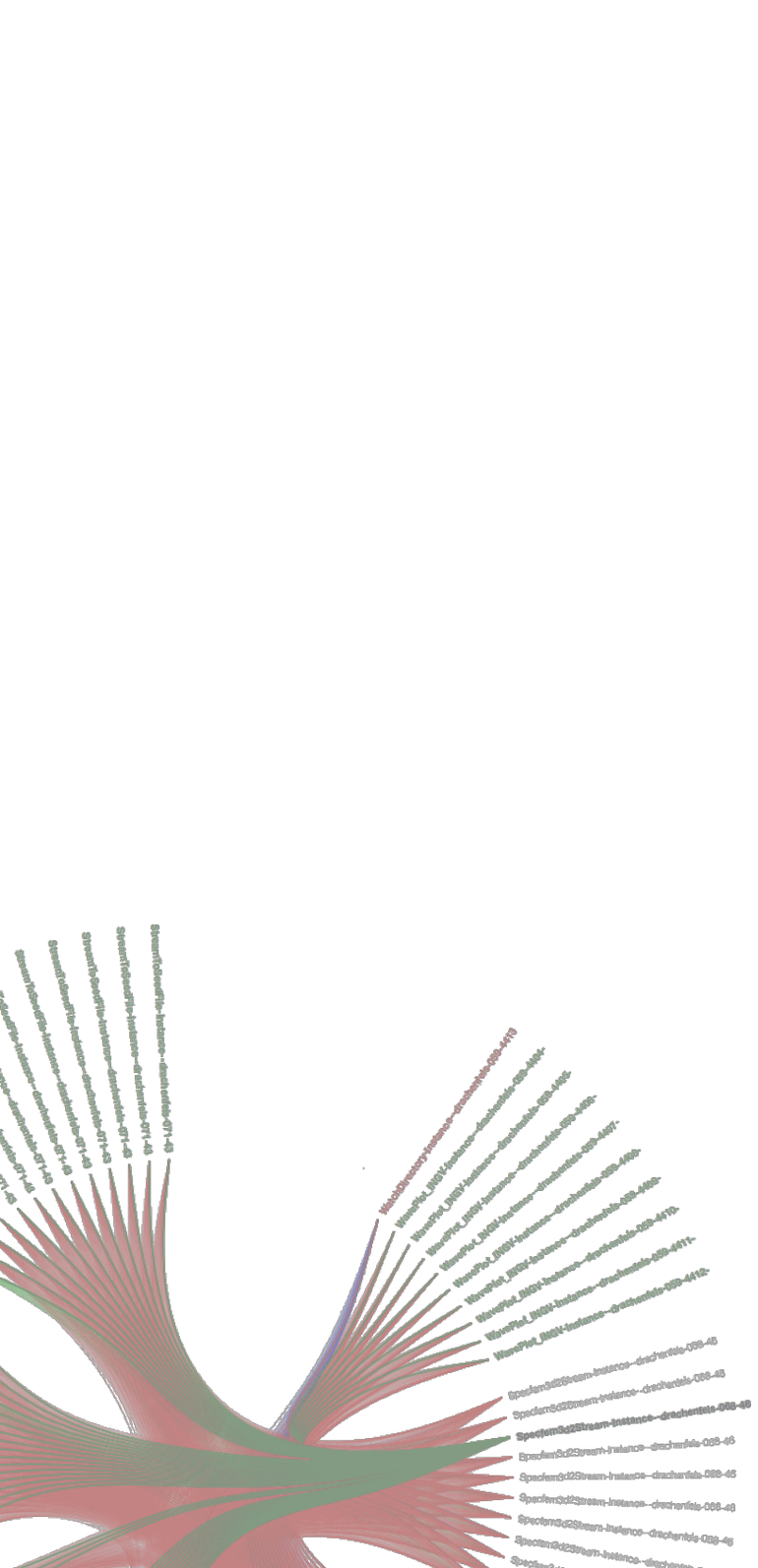
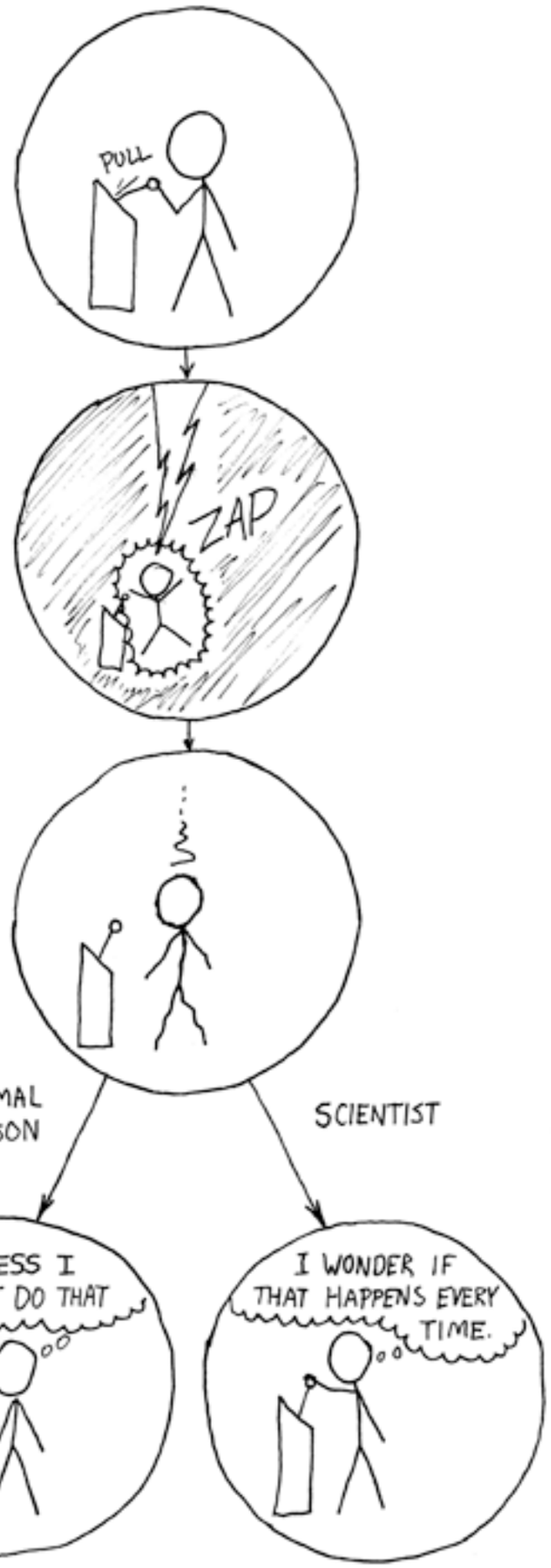
Reproducible Science



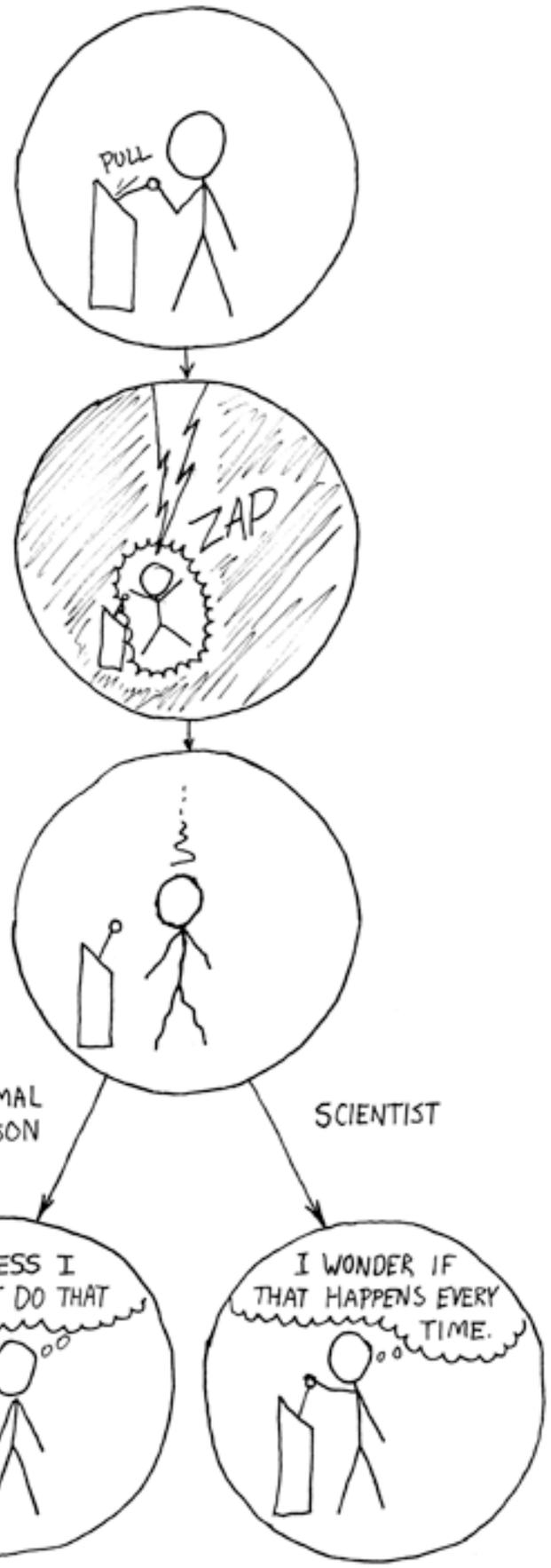


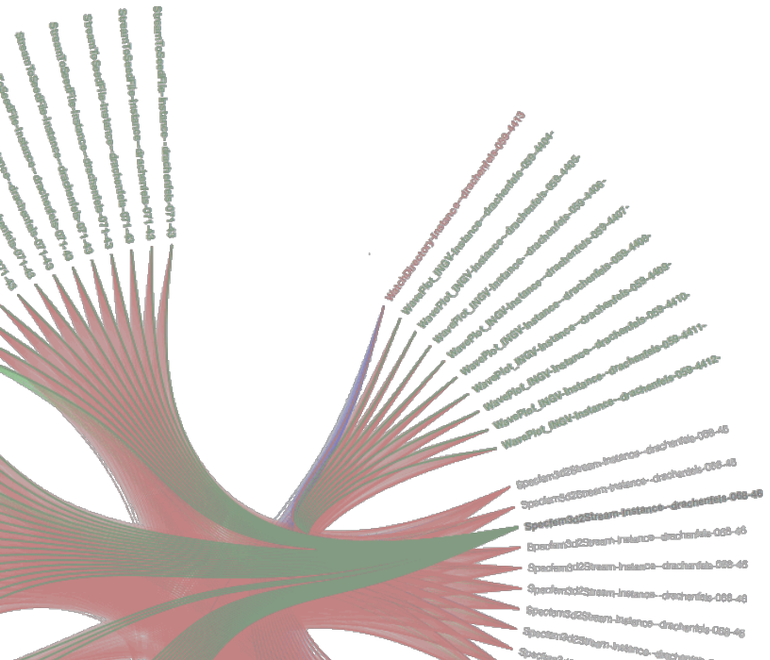
Reproducible Science

What does this suggest?

Scientists aren't normal..

Reproducibility is masochism..





Reproducible Science

What does this suggest?

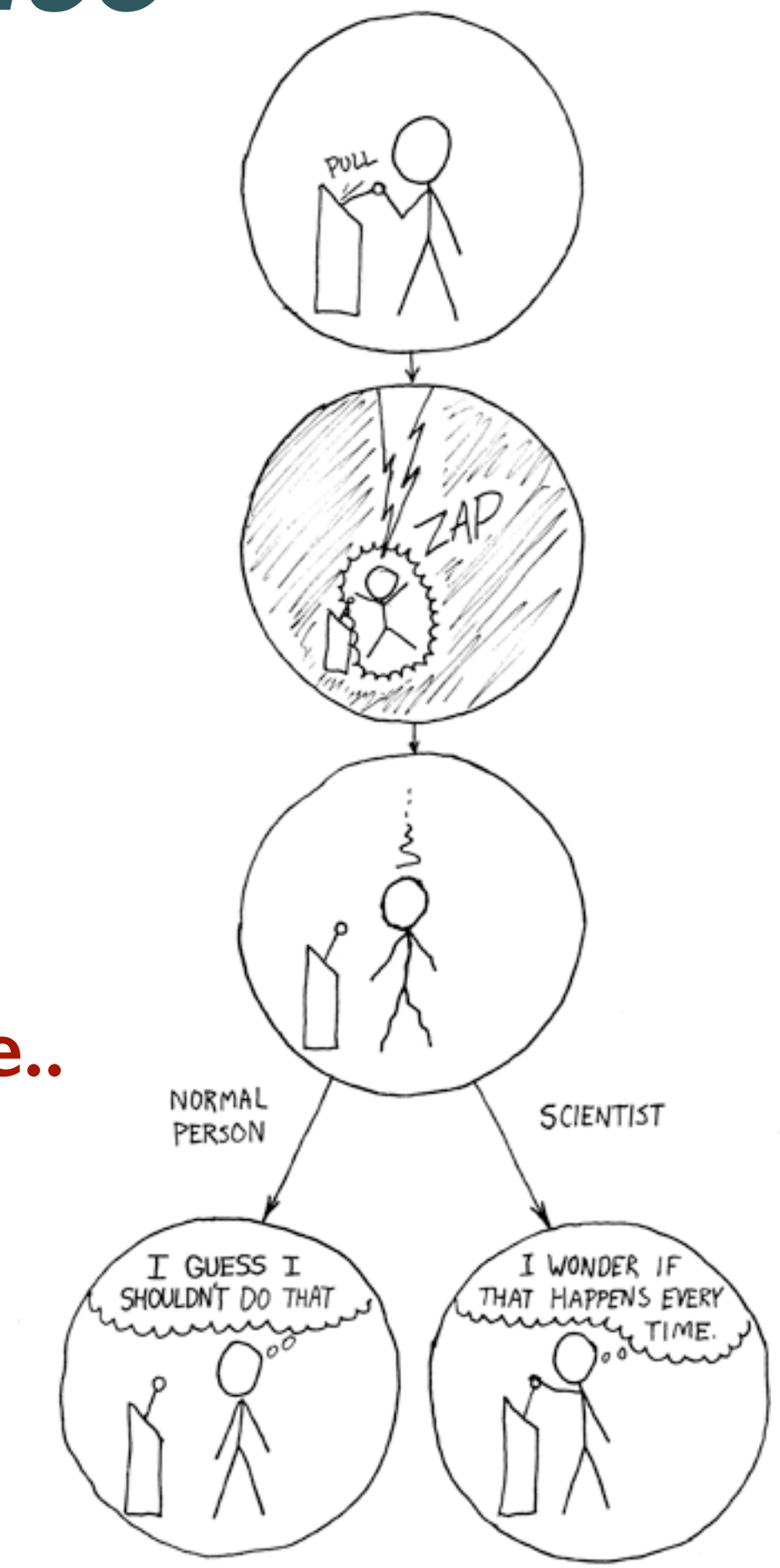
Scientists aren't normal..

Reproducibility is masochism..

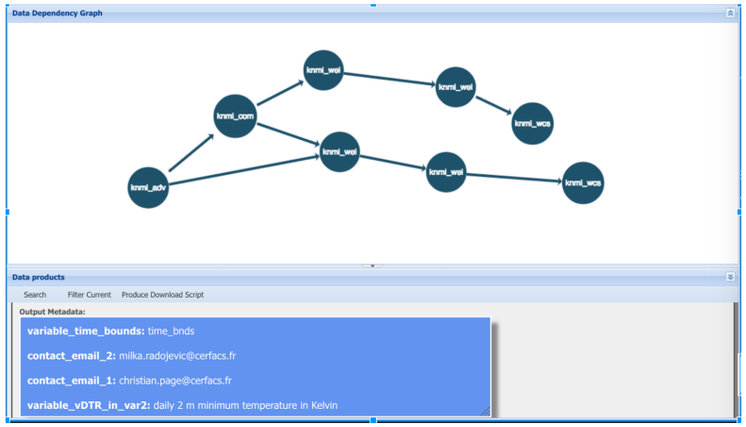
Reproducibility is fundamental but difficult to achieve.

Not always convenient/possible..

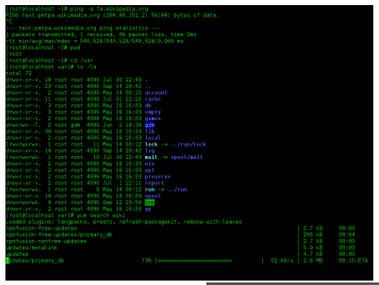
We need more than just rerun

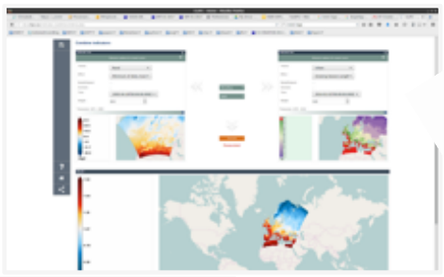


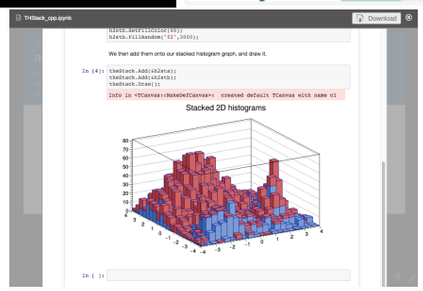
Reproducibility Cycle(s)



Validate







Procedures / Tools / Development

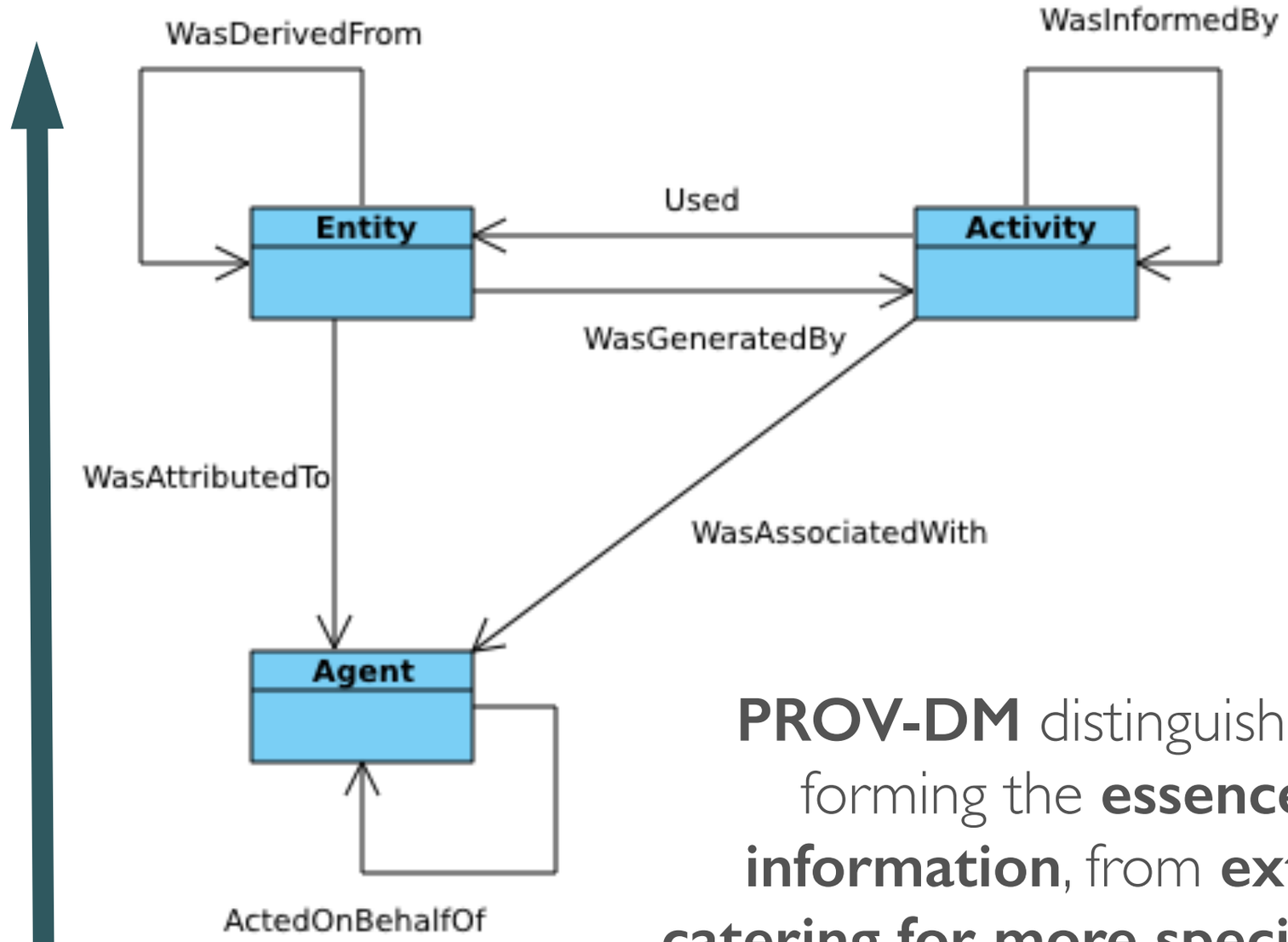
Analyse / Discover

Report / Outreach / Preserve

Repeat / Verify

Provenance Model

Data-Lineage → ***Knowledge***



W3C PROV

PROV-DM distinguishes **core structures**, forming the **essence of provenance information**, from **extended structures catering for more specific** uses of provenance.

Enactment ← ***Machinery & Data***

Provenance Challenges

*"**Automated** system should provide support for a **consistent and effective acquisition** of provenance metadata." [A. Misra] [I. Foster.]*

Expert users are part of the process - configuration and contextualisation:

"How much domain metadata should be contained?"

Scale of the provenance records:

"What level of granularity is needed to describe provenance of complex objects?
"Manage the scale of the provenance records to be recorded and processed"

Multiple levels of understanding:

"Provenance at different levels of abstraction, extract high-level summaries of provenance from detailed records."

Roles in Computational Research

research-developers (data-scientists):

Empirical implementation and evaluation of new methods and advanced tool

Direct observations at **different scales** and across **execution environments (PaaS)**.

end-users (domain-scientists):

Use tools via **virtual environments**

Confidence and trust in the tool requires **feedback** and **contextual information** (**SaaS**). **Share - Reuse**

data-architects:

The **improved understanding** of the execution's details lead to **better systems**.

data-curators and administrators:

Long-term preservation of scientific results **and exploitation of tools**.

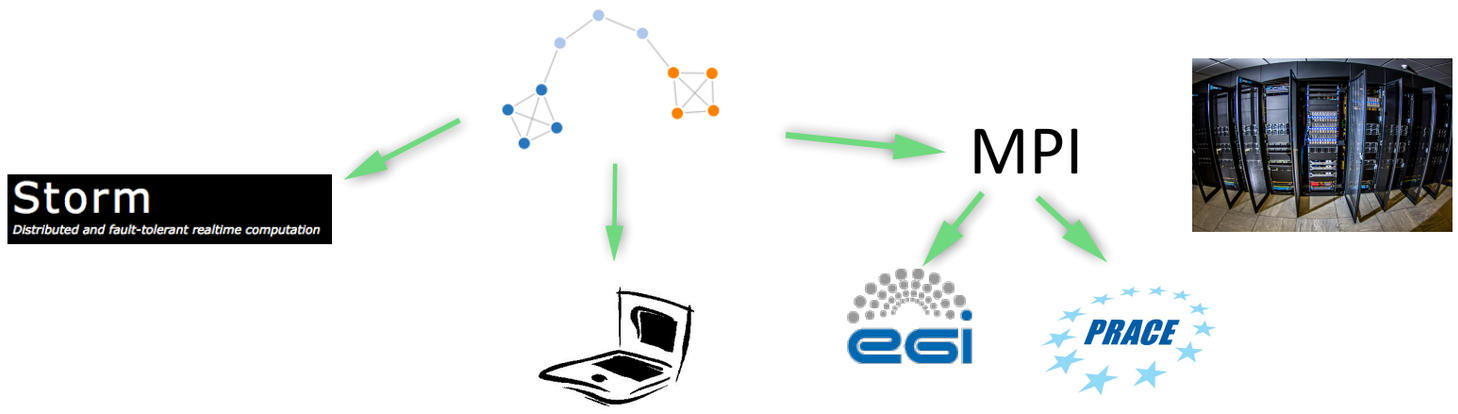
S-PROV

Provenance and Reproducibility in S-PROV:

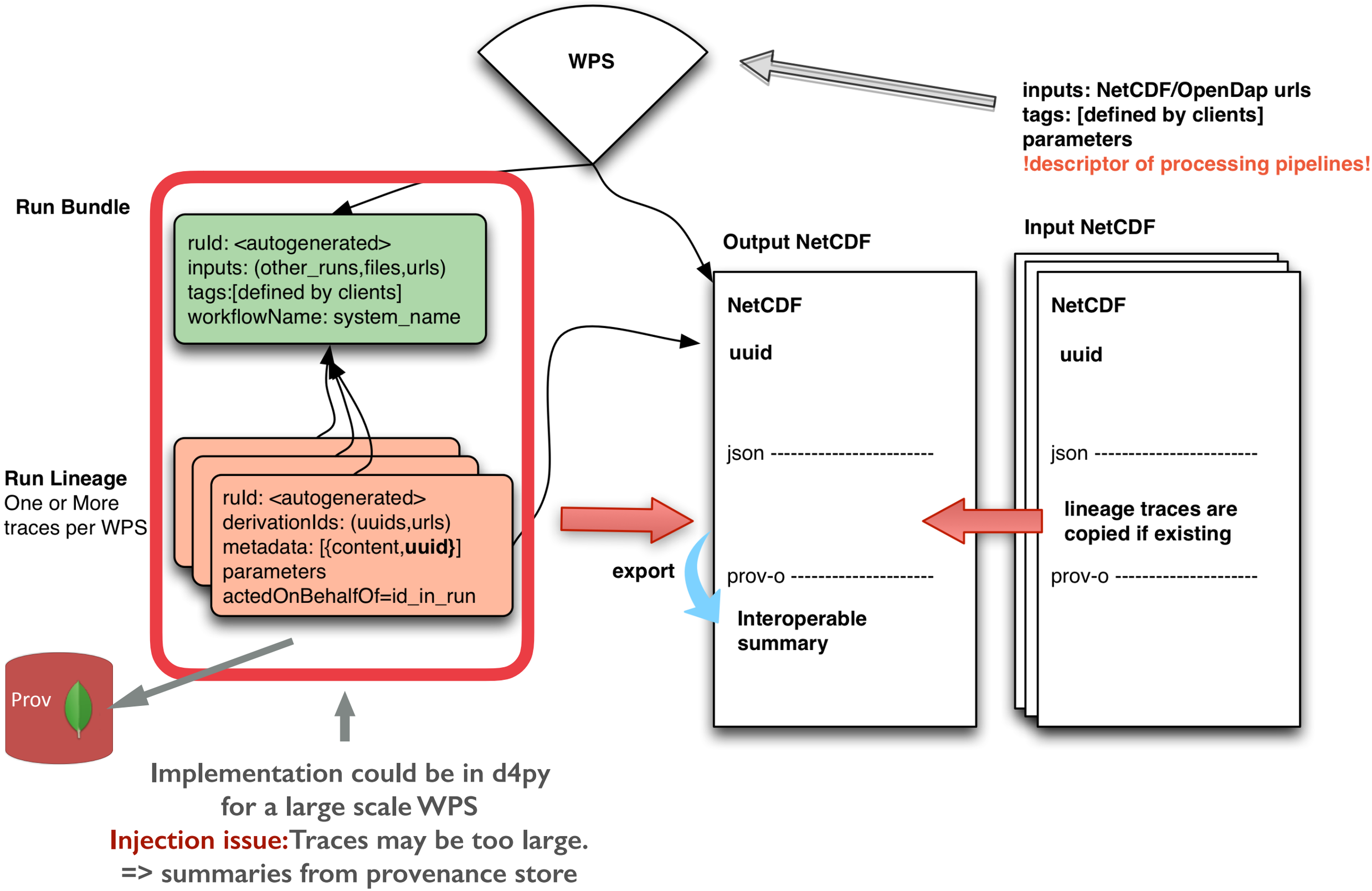
- Represents the **relationships** occurring between the players of a **data-intensive** computation in a **scientific domain**.
- Captures information at **multiple level of detail** within an **holistic data-model** (W3C PROV)
- Allows for **contextual switch** among **expertise** and **understandings**
- **Active Provenance** Use Cases: Monitor, validate, steer, compare, repeat, document.

Target System

- Systems where the data-intensive applications are specified with a **high-level language or API** (eg. ToolBox, dispel4py)
- Users define **abstract, machine-agnostic, workflows**.



Enabling S-PROV in WPS and NetCDF Injection



Implementation could be in d4py
for a large scale WPS

Injection issue: Traces may be too large.
=> summaries from provenance store

Enabling S-PROV in WPS and NetCDF Injection

Sensible issues:

Generation of *UUID*:

-The *WPS* framework should automatically produce and assign UUID

-UUID are used also into the lineage trace to match the output data with its provenance

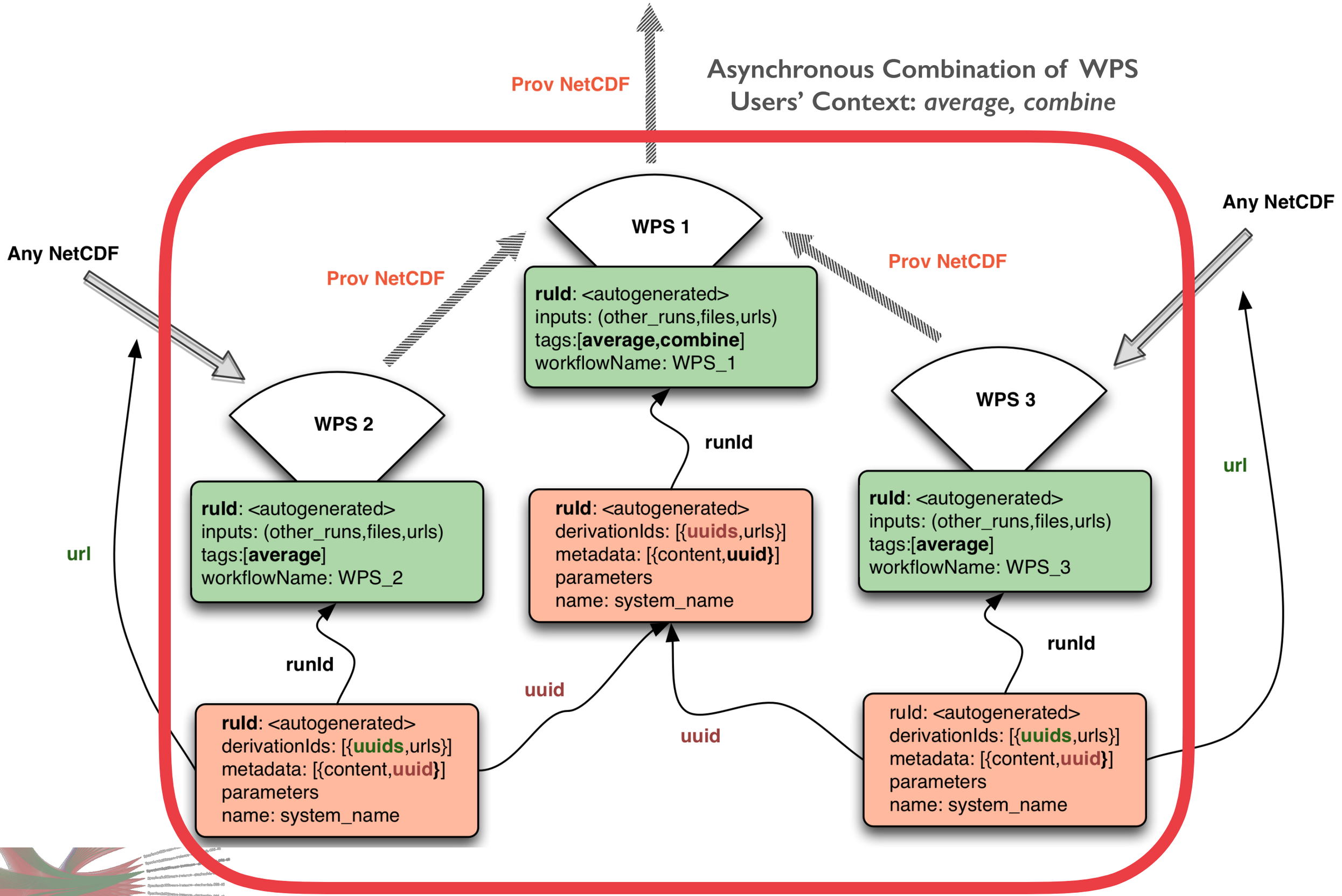
Derivation ID *UUID* (Chaining of WPS and associated outputs):

- **IF input files have *prov*** attributes we re-use the uuid ad *DatasetDerivationID*
- **ELSE** we may directly use the links (URLS) to the file.
- Links are used anyway in the Run Bundle to describe the WPS inputs

Tagging (Chaining of WPS and associated outputs)

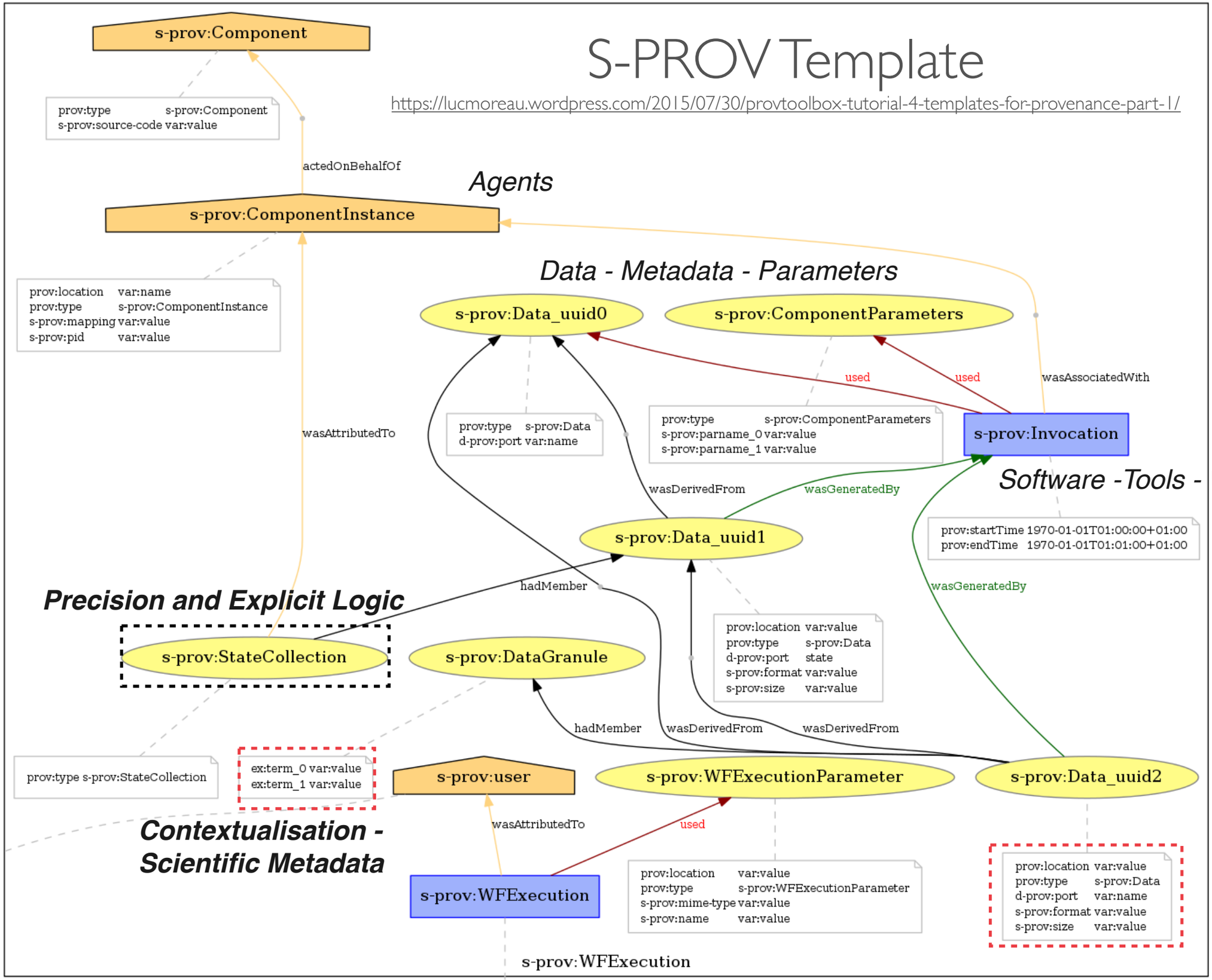
- **The WPS should** allow for a *tags* parameter
- **This will allow to link Run Bundles** together, describing workflows according to the users' contexts.

Example, *average and combine*

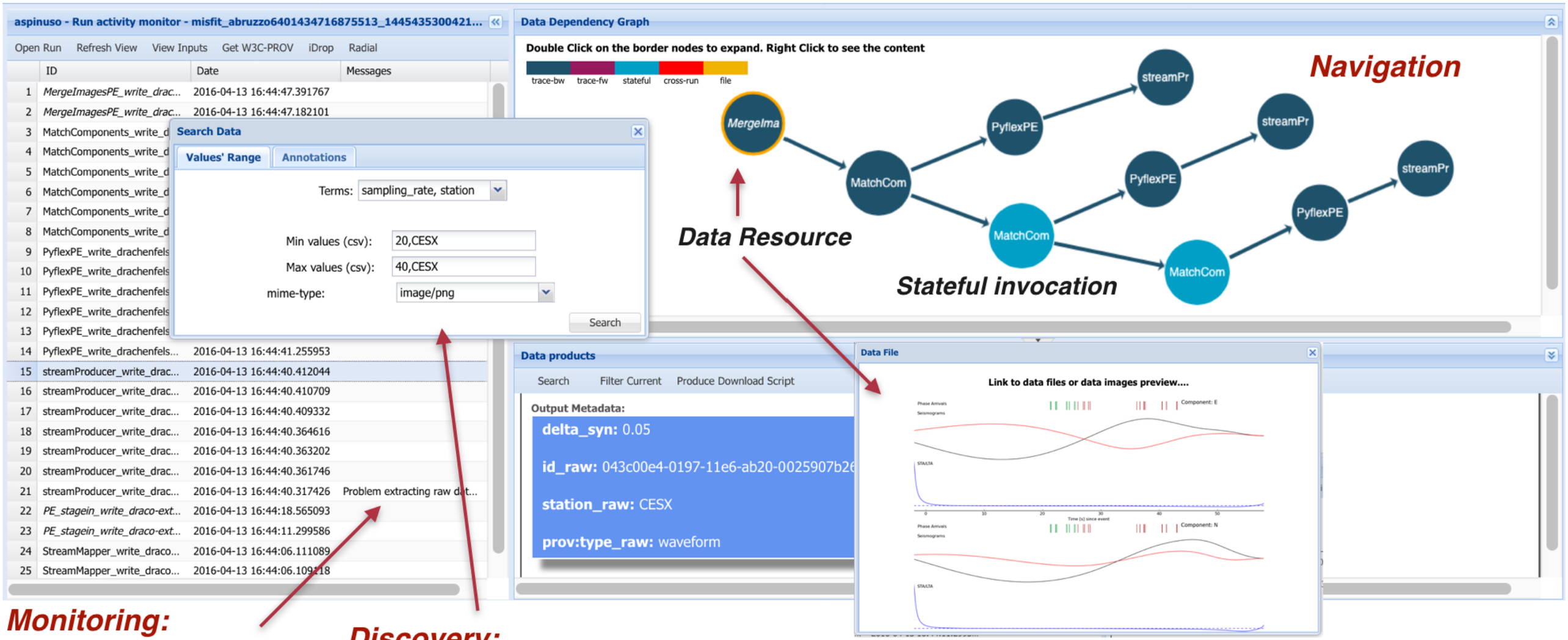


S-PROV Template

https://lucmoreau.wordpress.com/2015/07/30/provtoolbox-tutorial-4-templates-for-provenance-part-1/



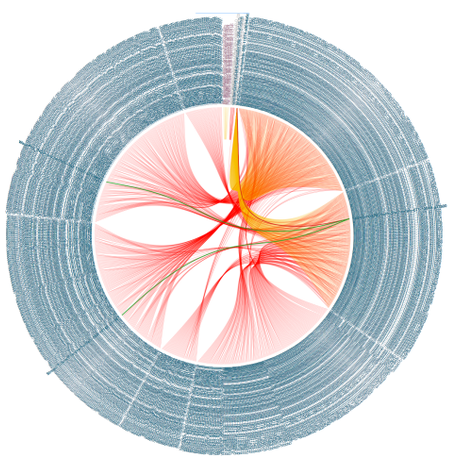
Tools: S-ProvFlow - Reproducibility as a Service

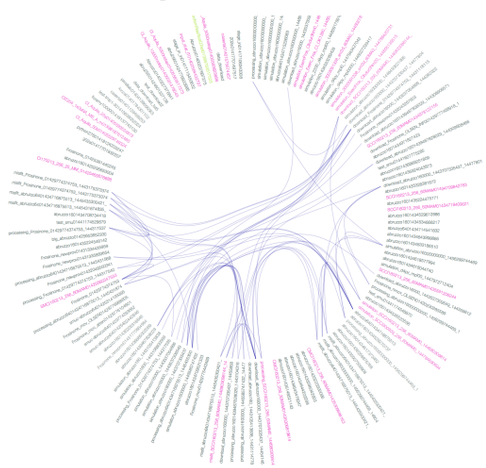


Monitoring:
System and user Messages

Discovery:
Search on contextual metadata (within and across runs)

Preview and Download





Visual analytics techniques on provenance

Perspectives on:

- data-intensive processes
- users and applications interactions
- data-reuse
- exploitation of resources..