

Revealing the Detailed History of Script Outputs with Hybrid Provenance Queries

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Motivation

- Data- and Workflow-Provenance are crucial for **transparency** and **reproducibility** in computational and data-driven science.
- Scientific workflow systems provide both **prospective provenance** (the workflow graph) and **retrospective provenance** (runtime observables).

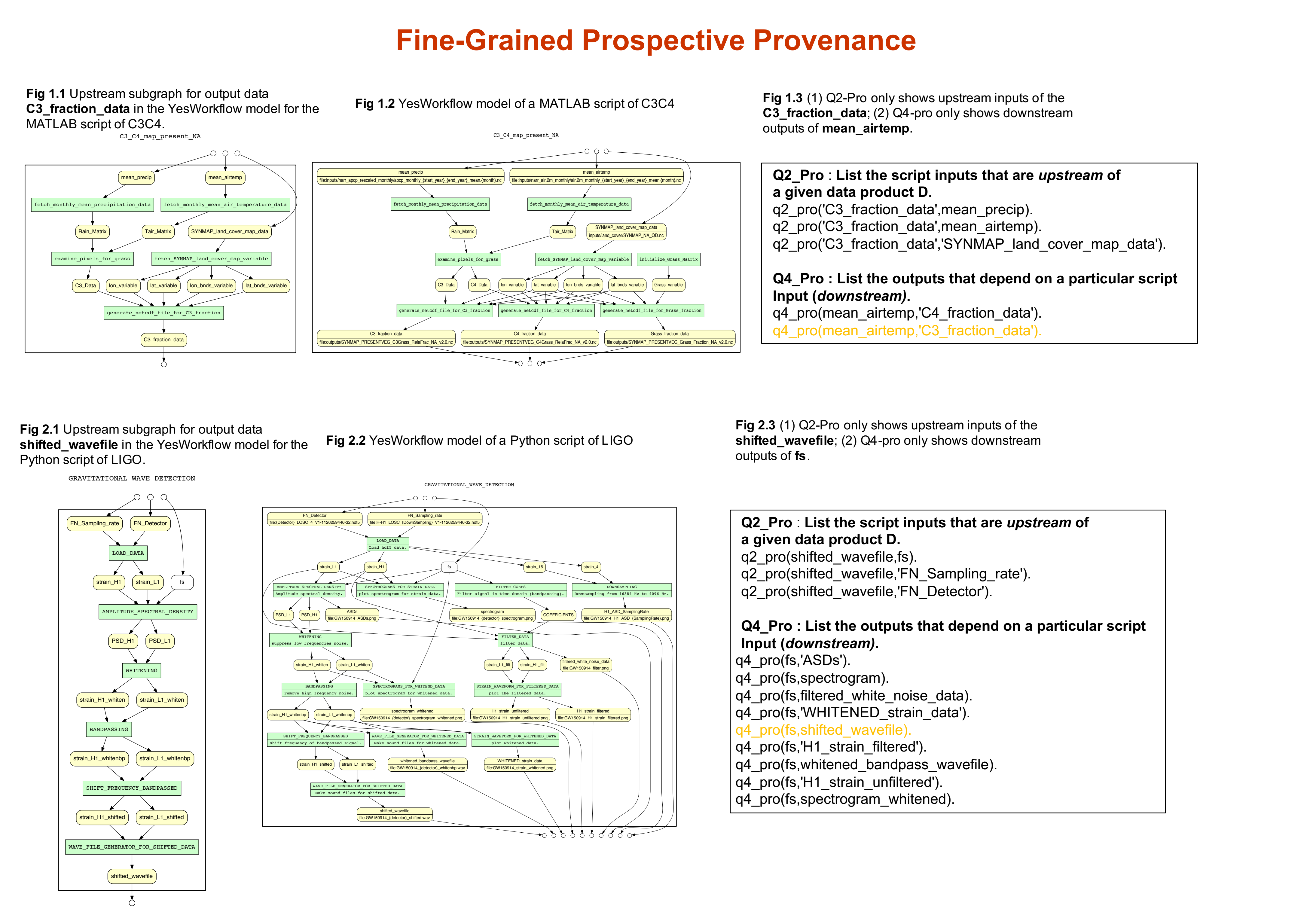
Challenges

- Most computational analyses and workflows are conducted using **scripts** (Python, R, MATLAB, bash, ...) rather than workflow systems.
- **Retrospective Provenance Observables** at different levels only yield **isolated fragments** of the overall data lineage and processing history.
- **Prospective Provenance** could be used to link and contextualize fragments into a meaningful and comprehensible workflow, but **scripts alone do not reveal the underlying workflow graph**.
- Provenance (like other metadata) appears to be useful “*for others*”.

Approach

Simple **YesWorkflow (YW)** annotations allow users to **reveal workflow** (prospective provenance graph) **implicit in scripts**.

- **Prospective provenance queries to expose and test data dependencies** at the workflow level.
- **Hybrid provenance queries that situate runtime observables** (retrospective provenance) in the overall workflow, yielding meaningful knowledge artifacts.
- Easily **share comprehensible workflow graphs and customizable provenance reports for script runs**, along with data, code in scientific studies (“*provenance for self*”).

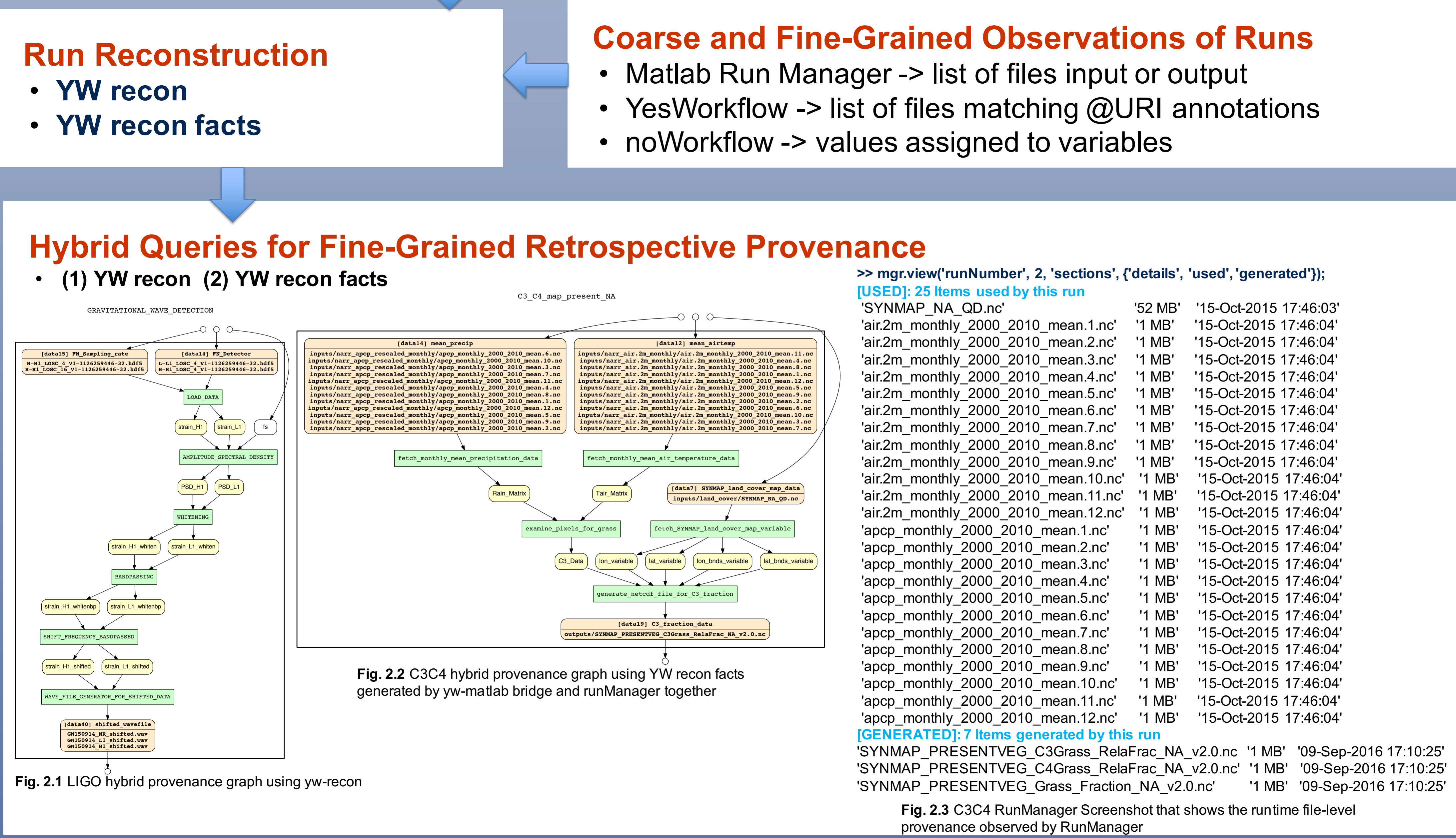


Demo Queries

- Q1 (upstream prospective query): **Render** prospective upstream subgraph of the YW model of the script for a given output data product D.
- Q2 (prospective query): **List** the script inputs that are upstream of a given data product D..
- Q3 (downstream prospective query): **Render** everything downstream of a given data product D, where D can be any one (input or intermediate) data element of the YW model of the script.
- Q4 (prospective query): **List** the script outputs that are downstream of a given data product D.
- Q5 (hybrid query): **Render** retrospective graph with with concrete filename for a given output data product D.

Conclusions and Future Work

- Provenance from script runs can be revealed graphically and made actionable (e.g., to yield customizable data lineage reports) via (1) simple YW user annotations, (2) linking runtime observables (e.g. DataONE RunManager, ReproZip, noWorkflow), and (3) sharing provenance artifacts and executable queries.
- Extend YW toolkit to support other workflow modeling constructs; to support graph pattern queries; to support project-level provenance.
- Evolve ProvONE to support project-level provenance and graph queries.



References

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