

# 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 (Kepler, Taverna, ...) 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**, e.g., from DataONE RunManagers (file-level), ReproZip (OS-level), or noWorkflow (Python code-level) 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 **rarely actionable or immediately useful** for those who are expected to provide it (provenance is “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 (**prospective query**): Render prospective upstream subgraph of the YW model of the script for a given output data product D.
- Q5 (**hybrid query**): Render retrospective graph with with concrete filename for a given output data product D.

### Fine-Grained Prospective Provenance

**Fig 1.2** (a) Upstream subgraph for output data **C3\_fraction\_data** in the YesWorkflow model for the MATLAB script of C3C4.

**Fig 1.1** (a) YesWorkflow model of a MATLAB script of C3C4

**Fig 1.3** (a) Q2-Pro only shows upstream inputs of the **C3\_fraction\_data**; (2) Q4-pro only shows downstream outputs of **mean\_airtemp**.

**Q2\_Pro** : List the script inputs that are *upstream* of a given data product D.  
q2\_pro('C3\_fraction\_data',mean\_precip).  
q2\_pro('C3\_fraction\_data',mean\_airtemp).  
q2\_pro('C3\_fraction\_data',SYNMAP\_land\_cover\_map\_data).

**Q4\_Pro** : List the outputs that depend on a particular script Input (*downstream*).  
q4\_pro(mean\_airtemp,'C4\_fraction\_data').  
q4\_pro(mean\_airtemp,'C3\_fraction\_data').

**Fig 2.2** (a) Upstream subgraph for output data **shifted\_wavefile** in the YesWorkflow model for the Python script of LIGO.

**Fig 2.1** (a) YesWorkflow model of a Python script of LIGO

**Fig 2.3** (a) Q2-Pro only shows upstream inputs of the **shifted\_wavefile**; (2) Q4-pro only shows downstream outputs of **fs**.

**Q2\_Pro** : List the script inputs that are *upstream* of a given data product D.  
q2\_pro(shifted\_wavefile,fs).  
q2\_pro(shifted\_wavefile,FN\_Sampling\_rate').  
q2\_pro(shifted\_wavefile,FN\_Detector').

**Q4\_Pro** : List the outputs that depend on a particular script Input (*downstream*).  
q4\_pro(fs,ASDs').  
q4\_pro(fs,spectrogram).  
q4\_pro(fs,filtered\_white\_noise\_data').  
q4\_pro(fs,'WHITENED\_strain\_data').  
q4\_pro(fs,shifted\_wavefile).  
q4\_pro(fs,H1\_strain\_filtered').  
q4\_pro(fs,whitened\_bandpass\_wavefile).  
q4\_pro(fs,H1\_strain\_unfiltered').  
q4\_pro(fs,spectrogram\_whitened').

**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 (optional) workflow modeling constructs (e.g., simple control-flow to complement dataflow); 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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