

# Revealing the Detailed History of Script Outputs with Hybrid Provenance Queries

Yang Cao<sup>1</sup>, Duc Vu<sup>2</sup>, Qiwen Wang<sup>1</sup>, Qian Zhang<sup>1</sup>, Priyaa Ramesh<sup>3</sup>, Timothy McPhillips<sup>1</sup>, Paolo Missier<sup>3</sup>, Bertram Ludäscher<sup>1</sup>

<sup>1</sup>University of Illinois, Urbana-Champaign, <sup>2</sup>Department of Electrical and Computer Engineering, Univeristy of Illinois at Chicago, <sup>3</sup>School of Computing Science, Newcastle University, UK



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/Q3 (**prospective query**): Render prospective upstream/downstream subgraph of the YW model of the script for a given output data product D.
- Q2/Q4 (**prospective query**): *List the script inputs that are upstream/downstream of a given data product D*
- Q5 (**hybrid query**): Render retrospective graph with concrete filename for a given output data product D.

Fine-Grained Prospective Provenance

Fig 1.1 Q1: The prospective upstream subgraph of the YW model for output data **Grass\_fraction\_data**.

Fig 1.2 The complete YesWorkflow-generated (prospective) workflow graph (with @URI annotation) for a MATLAB script of C3C4 example - **C3\_C4\_map\_present\_NA with comments.m**

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

Fig 2.1 Q1: The prospective upstream subgraph of the YW model for output data **shifted\_wavfile**.

Fig 2.2 The complete YesWorkflow-generated (prospective) workflow graph (with @URI annotation) for a Python script of LIGO example - **GW150914 tutorial\_uri.py**

Fig 2.3 (a) Q2-Pro only shows upstream inputs of the 'shifted\_wavfile'; (b) Q4-Pro only shows downstream outputs of 'fs'.

Run Reconstruction

- YW recon**
- YW recon facts**

Coarse and Fine-Grained Observations of Runs

- Matlab Run Manager -> list of files input or output
- YesWorkflow -> list of files matching @URI annotations
- noWorkflow -> values assigned to variables

Hybrid Queries for Fine-Grained Retrospective Provenance

Fig. 3 Q5: LIGO hybrid provenance graph using yw-recon

Fig. 2.2 C3C4 hybrid provenance graph for 'C3\_fraction\_mapping' using YW recon facts generated by yw-matlab bridge and runManager together.

Fig. 2.3 C3C4 hybrid provenance graph for 'Grass\_fraction\_data' using YW recon facts generated by yw-matlab bridge and runManager together.

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 to facilitate querying log files for hybrid provenance at data level.
- 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

- Y Cao, D Vu, Q Wang, Q Zhang, P Ramesh, T McPhillips, P Missier, B Ludäscher (2016). DataONE AHM Provenance Demonstration: <https://github.com/idsk/dataone-ahm-2016-poster>
- YesWorkflow Project and Tools, <https://github.com/yesworkflow-org>
- T. McPhillips, T. Song, et al.(2015). YesWorkflow: A User-Oriented, Language-Independent Tool for Recovering Workflow Information from Scripts. Intl. Journal of Digital Curation 10, 298-313.
- T. McPhillips, S. Bowers, K. Belhajjame, B. Ludäscher (2015). Retrospective Provenance Without a Runtime Provenance Recorder. Workshop on the Theory and Practice of Provenance (TaPP).
- Cao, Y., Jones, C., Cuevas-Vicentín, V., Jones, M.B., Ludäscher, B., McPhillips, T., Missier, et al., 2016, June. DataONE: A Data Federation with Provenance Support. Intl. Provenance and Annotation Workshop (IPAW). Springer.
- Pimentel, J.F., Dey, S., McPhillips, T., Belhajjame, K., Koop, D., Murta, L., Braganholo, V. and Ludäscher, B., 2016, June. Yin & Yang: demonstrating complementary provenance from noWorkflow & YesWorkflow. Intl. Provenance and Annotation Workshop (IPAW). Springer.

Acknowledgments. Supported by NSF awards ACI-1430508 and NSF ABI-1262458.

School of Information Sciences  
The iSchool at Illinois