Revealing the Detailed History of Script Outputs with Hybrid Provenance Queries

Yang Cao[1], Duc Vu[2], Qiwen Wang[1], Qian Zhang[1], Priyaa Ramesh[3],Timothy McPhillips[1], Paolo Missier[3], Bertram Ludäscher[1]

[1]University of Illinois, Urbana-Champaign, [2]Department of Electrical and Computer Engineering, Univeristy of Illinois at Chicago, [3]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 (upstream **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.

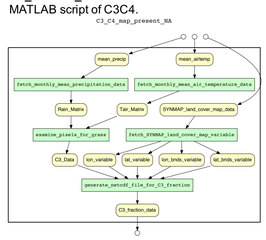

Fig 1.1 (a) YesWorkflow model of a MATLAB script of C3C4

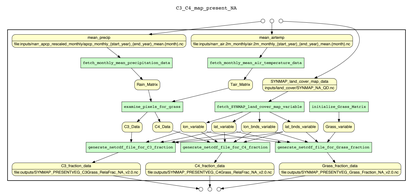

Fig 1.3 (a) Q2-Pro only shows upstream inputs of the **C3_fraction_data**; (2) Q4-pro only shows downstream outputs of **mean_airtemp**.

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.

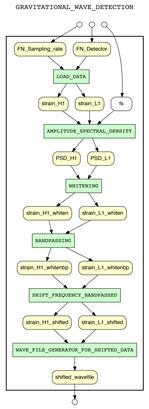

Fig 2.1 (a) YesWorkflow model of a Python script of LIGO

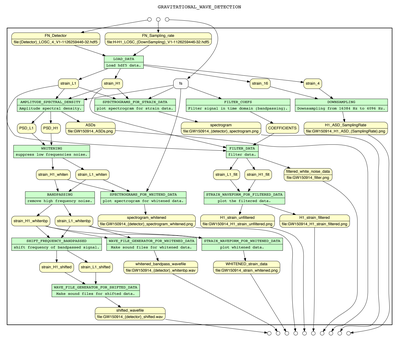

Fig 2.3 (a) Q2-Pro only shows upstream inputs of the **shifted_wavefile**; (2) Q4-pro only shows downstream outputs of **fs**.

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,'H1_strain_unfiltered').
q4_pro(fs,whitened_bandpass_wavefile).
q4_pro(fs,'H1_strain_unfiltered').
q4_pro(fs,spectrogram_whitened).

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

- **(1) YW recon (2) YW recon facts**

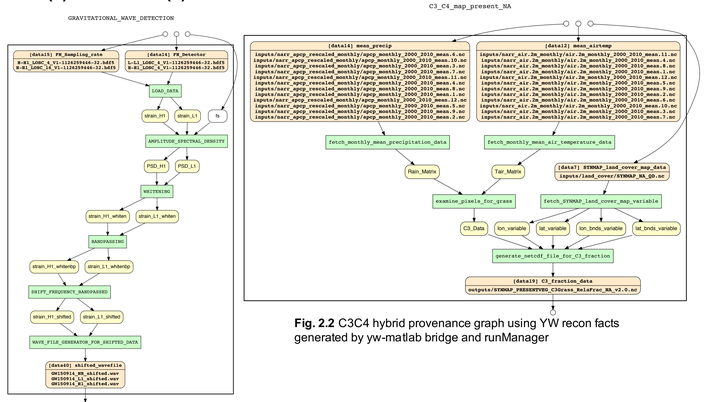

Fig. 2.1 LIGO hybrid provenance graph using yw-recon

Fig. 2.2 C3C4 hybrid provenance graph using YW recon facts generated by yw-matlab bridge and runManager

```
>> mgr.view('runNumber', 2, 'sections', {'details', 'used','generated'});
[USED]: 25 Items used by this run
'SYNMAP_NA_QD.nc'                    '52 MB'   '15-Oct-2015 17:46:03'
'air.2m_monthly_2000_2010_mean.1.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.2.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.3.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.4.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.5.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.6.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.7.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.8.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.9.nc' '1 MB'    '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.10.nc' '1 MB'   '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.11.nc' '1 MB'   '15-Oct-2015 17:46:04'
'air.2m_monthly_2000_2010_mean.12.nc' '1 MB'   '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.1.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.2.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.3.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.4.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.5.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.6.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.7.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.8.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.9.nc'   '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.10.nc'  '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.11.nc'  '1 MB'    '15-Oct-2015 17:46:04'
'apcp_monthly_2000_2010_mean.12.nc'  '1 MB'    '15-Oct-2015 17:46:04'
[GENERATED]: 7 Items generated by this run
'SYNMAP_PRESENTVEG_C3Grass_RelaFrac_NA_v2.0.nc '1 MB'  '09-Sep-2016 17:10:25'
'SYNMAP_PRESENTVEG_C4Grass_RelaFrac_NA_v2.0.nc' '1 MB'  '09-Sep-2016 17:10:25'
'SYNMAP_PRESENTVEG_Grass_Fraction_NA_v2.0.nc'   '1 MB'  '09-Sep-2016 17:10:25'
```

Fig. 2.3 C3C4 RunManager Screenshot

Demo Queries

- Q2 (**prospective query**): List the script inputs that are upsteram 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.

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

- Y Cao, D Vu, Q Wang, Q Zhang, P Ramesh, T McPhillips, P Missier, B Ludäscher (2016). DataONE AHM Provenance Demonstration: https://github.com/idaks/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-Vicenttín, 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.

School of Information Sciences, The iSchool at Illinois · Newcastle University · NCSA · ILLINOIS, University of Illinois at Urbana-Champaign · NSF · NCEAS