On the use of Abstract Workflows to Capture Scientific Process Provenance

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Overview

- Ontologies and Abstract Workflow to document scientific processes
- The Proof Markup Language (PML) to encode data provenance
- Capturing provenance about scientific processes
- Other efforts
- Conclusions

Documenting Scientific Processes with Ontologies and Abstract Workflows

- Purpose
  - Identify appropriate vocabulary for a scientific community
  - Model a scientist's understanding of a process
  - Identify the parts of a process that are of interest to scientists
- Benefits
  - Share scientist's understanding of a process with others
  - Guide the development of systems that implement scientist's understanding of a process
  - Enhance existing systems to provide functionality aligned to scientist's understanding of a process

Documenting Scientific Processes with Ontologies and Abstract Workflows

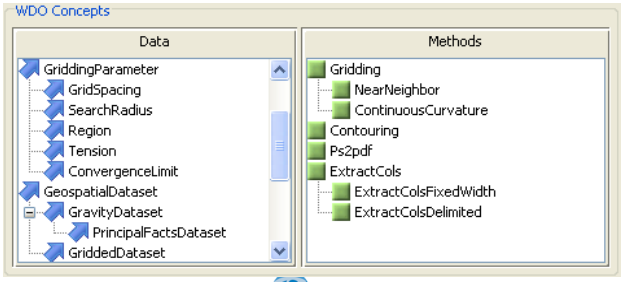
- Phase1: Capture the vocabulary of the process in a Workflow-Driven Ontology (WDO)
  - WDOs have two main classes:

Method Outputs Data

- **Data**, e.g., Gridded Dataset, Elevation Map
- **Method**, e.g., Nearest-neighbor extrapolation

Data is input to Method

  - Tool support to construct WDOs
    - Encoded in OWL
    - Reuse vocabulary from other OWL ontologies
    - Generate HTML reports



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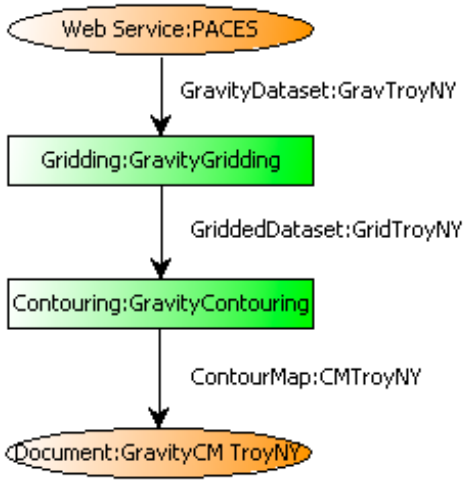
Documenting Scientific Processes with Ontologies and Abstract Workflows

- Phase2: Model the process as a Semantic Abstract Workflow (SAW)
  - Dataflow modeling
  - Graphical representation
  - Multiple levels of abstraction supported
  - Tool support to create SAWs
    - Encoded in OWL
    - Generate HTML reports
    - Generate provenance-capturing modules



Documenting Scientific Processes with Ontologies and Abstract Workflows

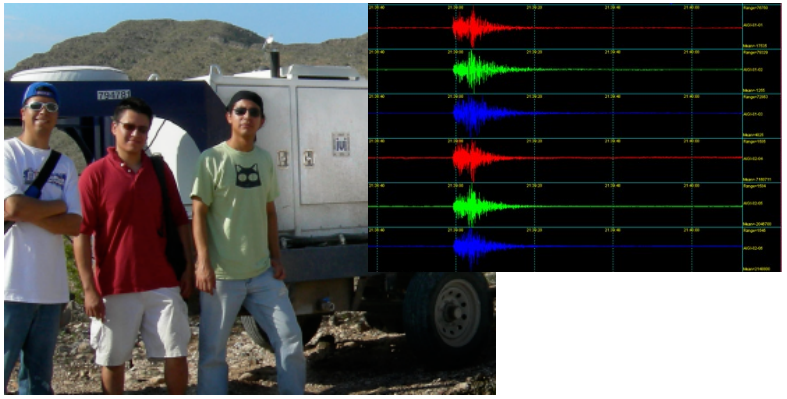
- WDOs and SAWs are intended to be authored by Scientists
  - Scientist-centered level of abstraction
  - Dataflow modeling intended to facilitate process modeling

Documenting Scientific Processes with Ontologies and Abstract Workflows

- Some efforts where WDOs and SAWs are being used

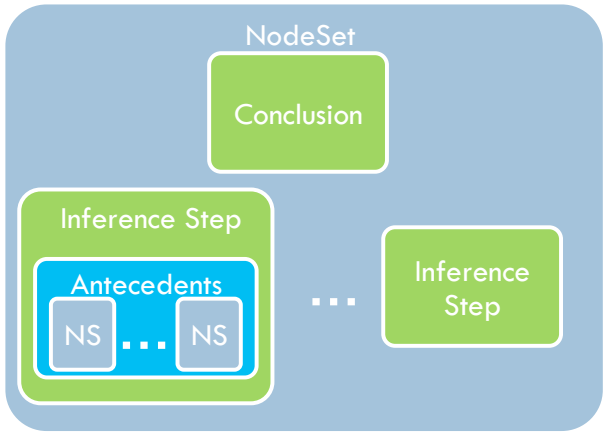
Environmental data collection at
- La Jornada Experimental Range
- The arctic region (Barrow, Alaska)

Seismic refraction experiments at Potrillo mountains



Encoding Provenance with PML

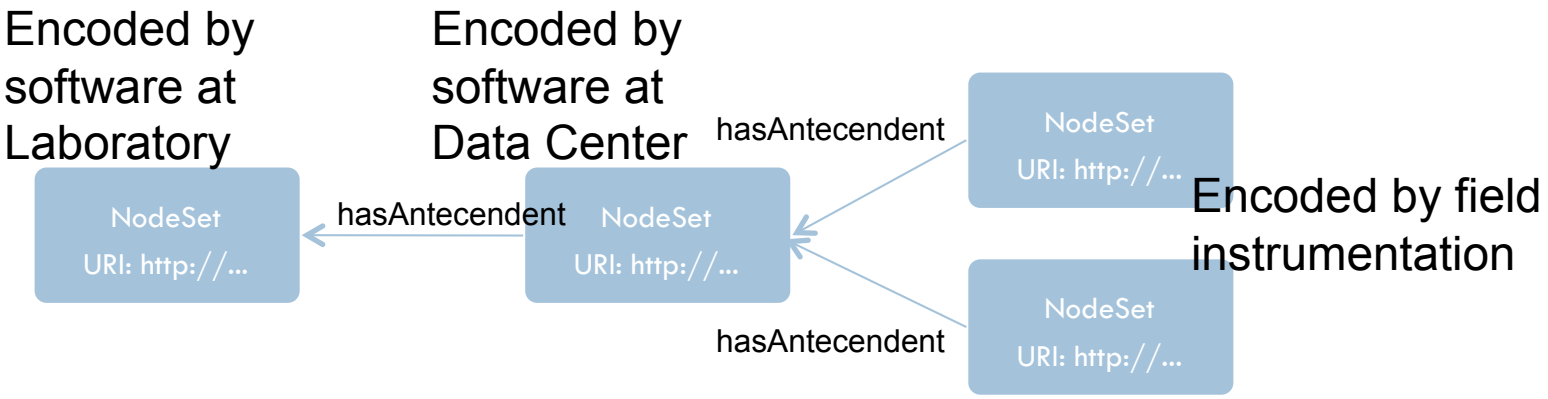
- Proof Markup Language (PML)
  - Derived from the theorem proving community
  - Divided into three parts:
    - PML-Provenance
    - PML-Justification
    - PML-Trust



With respect to provenance

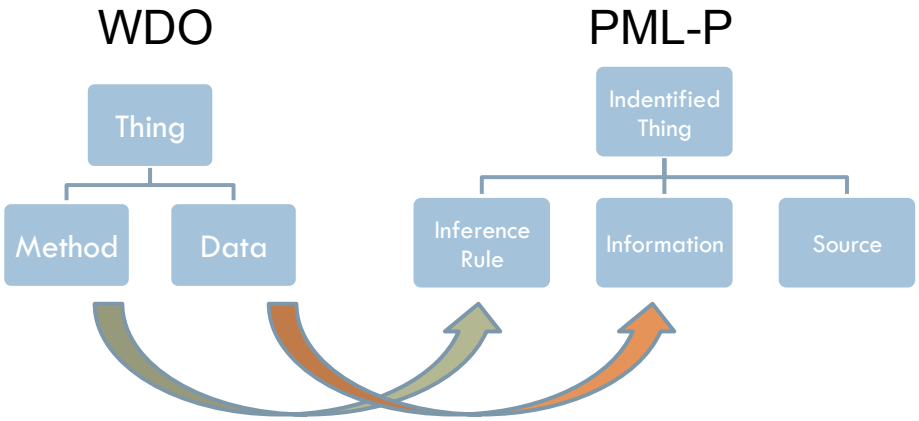
Encoding Provenance with PML

- Distributed provenance
  - NodeSets generated by distributed components
  - NodeSets linked through Web conventions



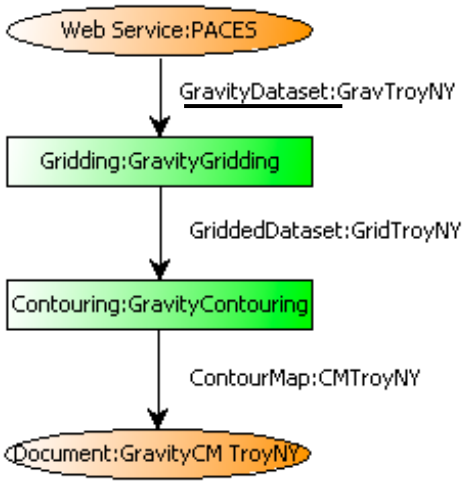
Capturing Scientific Process Provenance

- The framework:
  - Process and Provenance ontology alignment
    - WDO: Identify things that can be used to document how things **can happen** (i.e., process)
    - PML-P: Identify things that can be used to document how things **happened** (i.e., provenance)



Capturing Scientific Process Provenance

- The framework:
  - WDO reuses concepts from the PML-P ontology
  - WDO adds properties to the concepts from PML-P
  - WDO vocabulary can be used for Provenance queries!



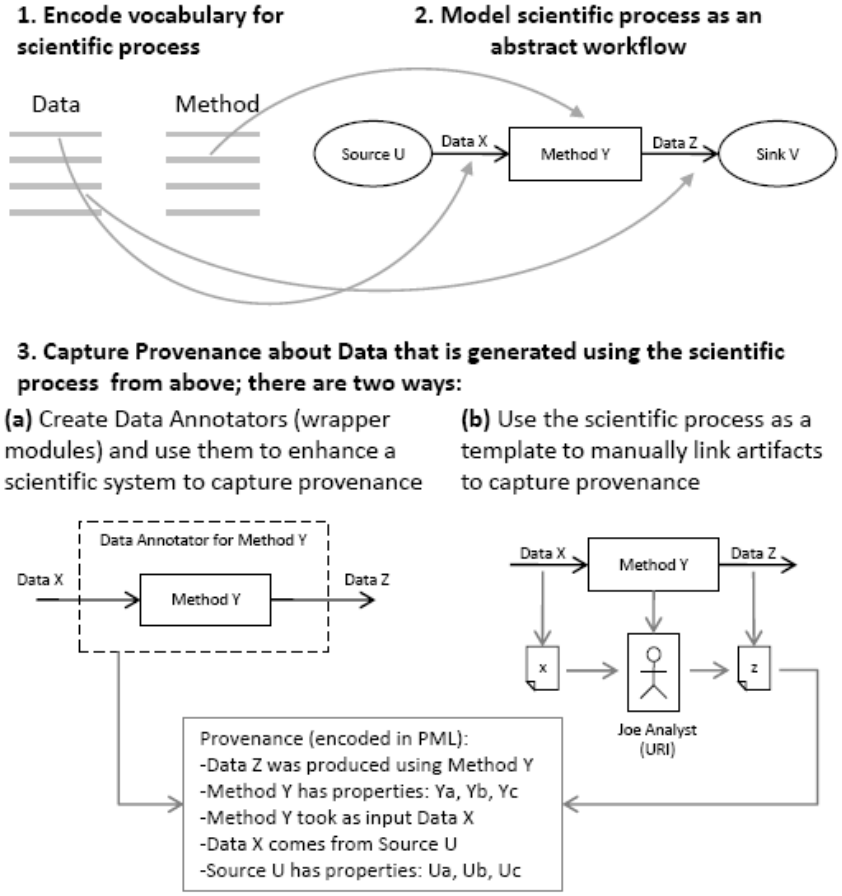
Vocabulary identified by scientist to document process

Used to query provenance:

Select NodeSets that have an antecedent of type GravityDataset

Capturing Scientific Process Provenance

- The process of capturing provenance:



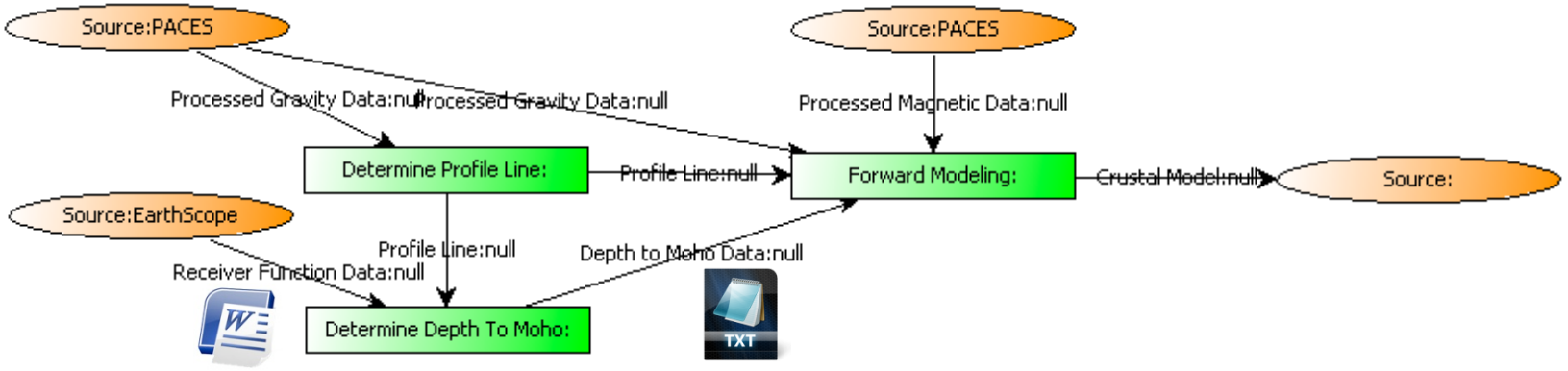
Goal: Facilitate provenance encoding in PML

Capturing Scientific Process Provenance

- Automated scientific systems
  - Use process knowledge to generate data annotator modules
    - Instrument system to call data annotators to record provenance during execution
      - E.g., C-shell scripts
    - Use data annotators after system execution to construct provenance from logs/temp files generated by the system
      - E.g., field data-gathering instruments with proprietary software and extensive logging features

Capturing Scientific Process Provenance

- Manual scientific systems
  - Tool support to encode PML using process knowledge a as template:

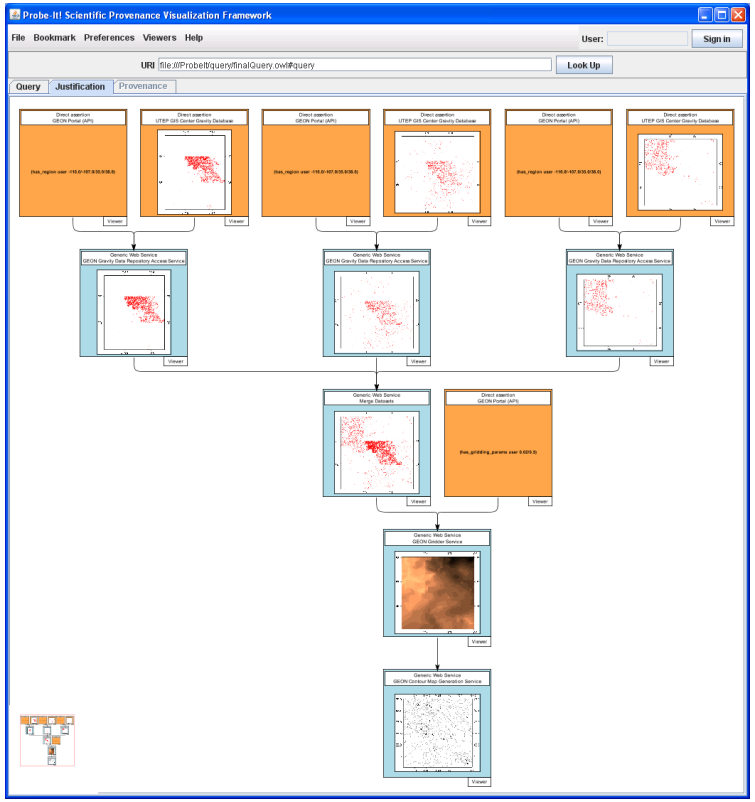


Technical Report

Manually entered parameters

Other Efforts

- Provenance Query
  - Build RDF triple stores from PML encodings
  - SPARQL queries
- Provenance Visualization
  - Probe-It!



Conclusions

- Abstraction is used to comprehensively document scientific processes
- Encoding provenance in PML is not straight-forward, but tools can help
- Not all scientific processes are implemented as software systems
- This approach to document provenance may not be scalable for all systems, but it is useful for some:
  - Scientists building custom systems to gather data

Thank you!

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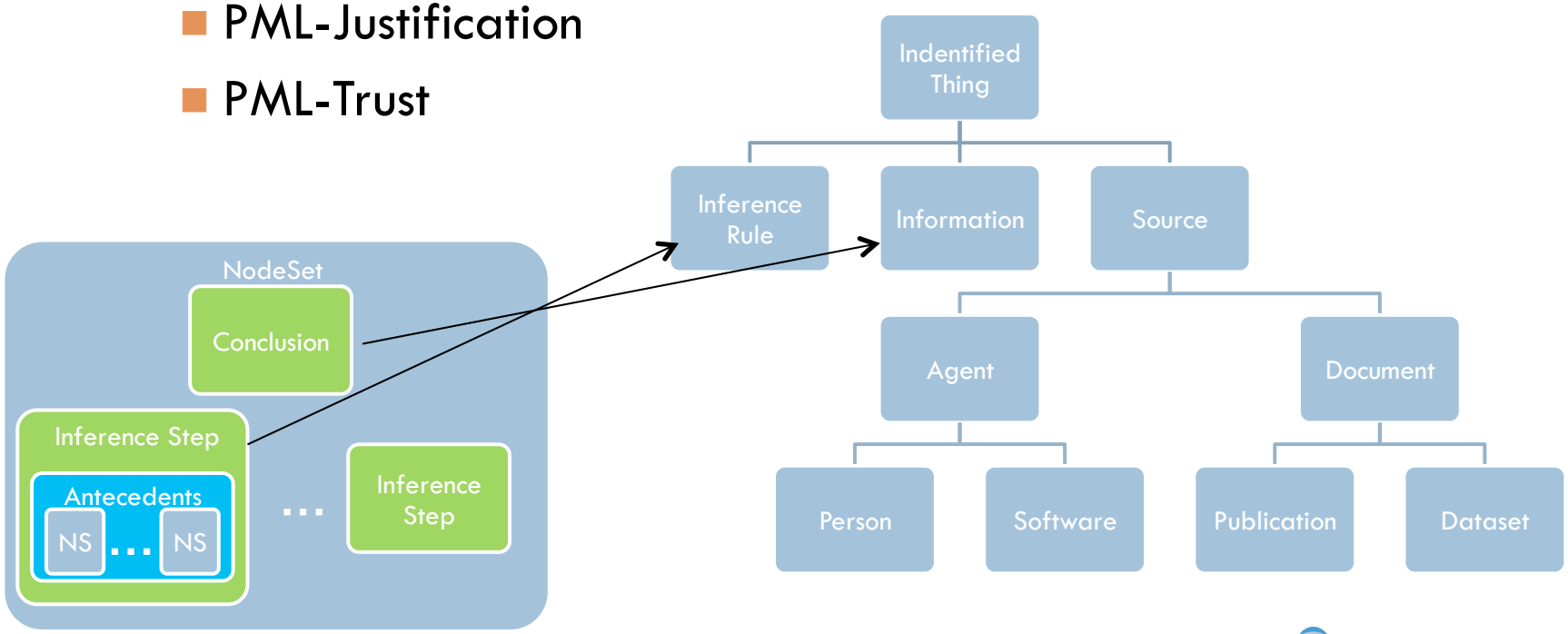
Encoding Provenance with PML

- More details about PML
  - Divided into three parts:
    - PML-Provenance
    - PML-Justification
    - PML-Trust



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