Data Provenance Hybridization Supporting Extreme-Scale Scientific Workflow Applications

ERIC STEPHAN
Pacific Northwest National Laboratory
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Provenance Definitions

- A computable and semantically meaningful historical explanation of influential factors, process flows, and data flows.
- Provenance is information about entities, activities, and people involved in producing a piece of data or thing, which can be used to form assessments about its quality, reliability or trustworthiness [W3C PROV].
- **Disclosure** – evidence provided from the perspective of the running application.
- **Observation** – measurements collected about the computational environment while disclosure is taking place.

Provenance Graph
Tracing Data Origin
Provenance at scale

- **Minimize impact**, control granularity (coarse to fine) and retention of provenance
- **Retrieval**, how to retrieve, explore, and analyze large amounts of collected provenance
- **Scalability**, provenance collection from concurrent large-scale scientific workflows will require a scalable solution
- **Dynamic interference**, provide real-time monitoring and analysis to support runtime workflow steering
- **Context**, integrate system level data to extend provenance descriptions
- **Provenance by Design**, provenance disclosure designed for workflow domain objectives:
  - Reproducibility, Results Explanation, Performance Optimization, Anomaly Detection, Monitoring, Others…
**Provenance Environment (ProvEn) Services Overview**

**Provenance Environment (ProvEn)** is a provenance management platform consisting of loosely coupled components supporting the disclosure, storage, and access to provenance information.

**Producer API (PAPI)**
- ProvEn’s provenance disclosure library. Scientific workflow applications instrumented with PAPI can produce and disclose their provenance data.

**Provenance Cluster**
- ProvEn’s scalable approach for collecting concurrent provenance data streams from PAPI sources.

**Hybrid Store**
- ProvEn combines system level metrics (Metric Store) with the traditional disclosed provenance (Semantic Store) to create an extended provenance view.
Standards-based Provenance

- **W3C PROV** data model published in 2013 defines a core data model for provenance for building representations of the entities, people and processes involved in producing a piece of data or thing in the world.

- **Workflow Performance Provenance** (WFPP) data model is an extension to PROV that will enable the empirical study of workflow performance characteristics and variability including complex source attribution.

- **Provenance Environment** (ProvEn) data model provides concepts specific to the ProvEn provenance management software platform.

- **Domain Specific Descriptive** integration

![Diagram showing JSON-LD and data models]
Research Focus

ACME Results Explanation and Performance Tuning

Scheduler Optimization on Belle II

Belle II: A Truly International Team
599 Collaborators, 97 institutes, 23 countries

Reproducible Mass Spectrometry Workflows

Model Federation and Message Profile Tool Chains

Horizontally Scaling Hybrid Analytical Database

Cyber Reporting Machine Learning Decision Support
Provenance Message

- PAPI’s “unit of” provenance
- Each message is a fragment of the complete provenance graph
- Every message created uses the same structure (Header + Body)
- Provenance by design – messages tailored per PAPI distribution. Ad-hoc also supported
- Messages are serialized as JSON-LD for a direct interchange to Semantic Store – RDF Database
- Offline messaging capability
Lifecycle of Provenance Message

- **Provenance Message Design**
  - Involves domain expert to identify the provenance messages to support experimental design
  - Uses foundation ontology (e.g. W3C PROV, ProvEn) and domain ontology (WFPP)

- **Assembly**
  - A domain specific provenance context file is created based on the identified ontological concepts. Enumerated constants are generated for compile time checking

- **Message Creation**
  - PAPI generates provenance messages based on context file and are serialized into JSON-LD.
When collected by ProvEn provenance message fragments are integrated into a connected provenance graph to answer the questions posed earlier. The gray outline on entity ovals indicates where messages are connected to form the complete provenance graph.
Provenance Disclosure Strategies

- Collecting only relevant information that is used to answer direct questions.

Provenance API (PAPI) calls from standalone or distributed apps

ProvenanceMessage pm = createMessage(START_APPLICATION);
pm.sendMessage();

PAPI enabled Harvesting

APACHE nifi
Types of Querying

- Regular Expression searches
- Searches
  - Semantic
  - Time-series
- Tracing origin
- Detecting repeating patterns
- Semantic reasoning

Sub-graph partitioning

Tracing Data Origin

Detecting Repeating Patterns in subgraphs

Domain and foundation

multi-layer searches

December 7, 2016
Hybrid Store
What are Provenance Metrics?

- **Provenance Metrics** are discrete pieces of semantic provenance (a single triple) identified in a Provenance Message, and serialized into a time-series format for storage in a registered Metric Store.
- Occurs at time of disclosure, at a minimum alignment of data is by time

```
acme:simulation_1 wfpp:hasStartTime "1471355953002"^^xsd:dateTime
acme:simulation_1 wfpp:hasStopTime "1471355959001"^^xsd:dateTime
```

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How will your efforts help the ESGF community of users?

- As an active member of standards communities we can both represent needs and notify the ESGF of trends and solutions emerging from any synergistic technological efforts.

- **ProvEn Services**
  - As an analytical platform, ProvEn could be used as an integration point for provenance inter-comparison or runtime analytics.
  - As a repository, ProvEn could be hosted by those who lack a provenance solution.

- **PAPI Java client API**
  - Used standalone or integrated as a client to ProvEn Services.

- Working with ESGF to standardize what provenance analytics means for climate science and what disclosures are required to answer priority questions.
What is your timeline for releasing your efforts?
- We plan to deploy ProvEn in Docker in FY2017.
- We are in the process of making ProvEn Services and PAPI open source (possibly Spring 2017)
- Limited deployments could be supported as early as February.

What standards and services need to be adopted within the environment that will allow ESGF to participate in early adoption?
- Minimum is dedication of linux box
- Determining provenance requirements.

How are you funded for longevity?
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Eric.stephan@pnnl.gov