Towards A Practical Provenance Framework for Scientific Data on HPC Systems

Runzhou Han
Iowa State University

Suren Byna
Lawrence Berkeley National Laboratory

Mai Zheng
Iowa State University

1 Motivation

Data-driven scientific discovery has been well acknowledged as a new fourth paradigm of scientific innovation [17]. The shift toward the data-driven paradigm imposes new challenges in data reproducibility, explainability, trustworthiness, etc [7], all of which demand innovative solutions for modeling and capturing provenance, i.e., the lineage of data life cycle.

While the importance of provenance has been well recognized across communities (e.g., databases [1] [10] [12] [6] [19], operating systems [9, 8], eScience [5] [13] [2] [16] [15]), we find that there are three major gaps between the available solutions and the real needs of domain scientists.

First, in terms of provenance modeling, we find that existing standards (e.g., W3C PROV [18]) are too vague to describe the specific needs of scientific data and scientists precisely. Scientists often seek a variety of information from scientific workflows on high performance computing (HPC) systems, including the origins of data products, the configurations used for deriving results, the usage patterns of datasets, and so on, which cannot be described effectively using any existing provenance models. Such ambiguity fundamentally limits the usability of existing provenance products for scientific data.

Second, in terms of provenance systems, existing products are largely incompatible with the scientific workflows or HPC systems. For example, it is common for HPC workflows to use HDF5 library [4] or a combination of HDF5 and POSIX system calls [11] to perform I/O operations and access data in different granularity (e.g., file, dataset, attribute). However, to the best of our knowledge, none of existing products can handle HDF5-related I/O operations effectively or efficiently. Moreover, existing systems lack the flexibility to handle high-level semantic information that is much needed by domain scientist (e.g., high-level metrics of a workflow).

Last but not the least, existing solutions often require manual efforts to identify relevant source code locations for instrumentation [14, 15], which is inconvenient for domain scientists and impractical for large-scale scientific workflows.

2 Our Approach

To address the challenge, we first analyze three representative scientific workflows in collaboration with domain scientists. In doing so, we identify the unique characteristics of the workflows (e.g., I/O interfaces, data formats) as well as the specific needs for provenance (e.g., lineage at file, dataset, or attribute granularity).

Based on the first-hand investigation, we propose a practical provenance framework for scientific data on HPC systems. Our key observation is that I/O operations are critically important in affecting the state of data that form the lineage. So we derive an I/O-centric provenance model, which enriches the W3C PROV standard [18] with a variety of concrete sub-classes to describe both the data and the associated I/O operations and execution environments precisely with extensibility.

Moreover, based on the unique provenance model, we are building a practical prototype which includes three major components: (1) Provenance Tracking for capturing diverse I/O operations; (2) Provenance Storage for persisting the captured provenance information as standard RDF triples [3] ; (3) User Engine for querying and visualizing provenance. The prototype can provide end-to-end provenance support with little manual effort, which is essential for addressing the provenance problem in complex HPC environments.

Our preliminary evaluation on a state-of-the-art HPC system with realistic scientific workflows show that the provenance framework incurs reasonable tracking and storage overhead for the use cases evaluated. More importantly, through the query and visualization support, the prototype can address the data provenance needs of the end users effectively.

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