Data Provenance: Use Cases for the ESO archive, and Interactions with the Virtual Observatory

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Abstract. In the Virtual Observatory era, where we intend to expose scientists (or software agents on their behalf) to a stream of observations from all existing facilities, the ability to access and to further interpret the origin, relationships, and processing steps on archived astronomical assets (their Provenance) is a requirement for proper observation selection, and quality assessment. In this article we present the different use cases Data Provenance is needed for, the challenges inherent to building such a system for the ESO archive, and their link with ongoing work in the International Virtual Observatory Alliance (IVOA).

1. The Provenance of Astrophysical Data

The ever increasing datasets archived and dealt with by astrophysical institutions and researchers are moving astrophysics into one of the fastest growing, and more public, e-Science disciplines.

Within e-Science, Data Provenance is the tracking of the origin of any piece of information that has been recorded, with knowledge of all processing steps undergone. In the astronomical realm, we need to track data Provenance in order to answer questions like what was done to the photons captured by this archived entity, and what entities were responsible for it? We need to be able to answer those questions because for typical astronomical workflows across large datasets Provenance must be recorded, and later used throughout the workflow, in order to get physically meaningful and accurate results. Fig. 1 illustrates the role of Data Provenance in astronomical workflows.

In particular, relevant questions for Data Provenance are which were the files used to create a particular data product (Associations), and which are the data products created from it? (Inverse Association). Additionally, we need to know are we using the same source data (photons) for any two given data products? (Photon Accountancy), as the use of the same photons in different data products which are later combined can produce unreliable science. Finally, we need to be able to track parameters related to the models for emission, absorption and detection used by the reduction software, as these encode implicit knowledge that needs to be made explicit in order to allow the reproduction of measurements and processes by other scientists.
Figure 1. Data reduction software are convert properties measured with the telescope detectors into files ($F_n$), and later into physical parameters and data products ($P_m$). Knowledge and models of telescope, detectors settings, astronomical source, and absorbing media is needed for the reduction.

2. Data Provenance Systems’ Requirements: High-Level Use Cases

The use cases for a Data Provenance system within the ESO archive (see Fig. 2) have been classified in three kinds of services:

- **Data Discovery services** which query on the Provenance records to find scientific data fulfilling different criteria. These data discovery encompasses the Provenance of observing projects at all stages: Organization (observing proposals, PIs and COIs), Technical (instrument setup), Ambient, and Publications. In addition, Exposure Time Calculators (ETCs) must rely on the historical information of telescope elements, such as filters or detectors, whose properties (or actual elements) can change with time.

- **Dataset Documentation services** which allow scientists to retrieve the full record of observation origin and further processing. They are the inverse of the services above, as the dataset is already known, and the inverse association must be constructed. ETCs can be used in this family of use cases to assess data quality for a particular dataset.

- **Observation Preparation services** where both observations and projects with given data acquisition characteristics are retrieved.

3. Implementing Data Provenance at ESO

3.1. Challenges

Following the taxonomy of Data Provenance systems by Simmhan, Plale, & Gannon (2005), the main elements to be specified for Data Provenance systems are Storage, Granularity, Representation, and Dissemination.

- **Storage** deals with the actual way in which Data Provenance is made persistent. While Storage implementation is not relevant from an interoperability point of view, it provides the foundation for all Provenance services.
Insertion and retrieval speeds must be able to cope with the expected data generation and query rate.

**Granularity** is the degree of detail for which Provenance metadata is collected. It must be chosen to serve all ESO use cases, and also imposes restrictions on Storage (to be able to cope with the chosen Granularity). We can also include the selection of which particular metadata (from FITS headers to observation logs) are committed to Storage as part of the Granularity. From Fig. 2 we can see that other metadata, such as Observation logs, and ADP processing logs, must be taken into account, and provide a time dimension to the problem.

**Representation** the way Provenance is expressed when shared with requesting entities (as opposed to Storage). Hierarchical trees, series of keyword/value pairs, or even plain-text files for informational use cases. However, due to the rich nature of the objects described by Provenance—a detailed description of the light-path in ESO instruments is shown by Delgado (2009)—, a hierarchical structure is preferred. Representation directly affects interoperability, so the generalization of a Provenance representation as an IVOA Data Model would be desirable.

**Dissemination** the way Provenance metadata is to be available for shared datasets. Decisions in this respect include creating Provenance services to satisfy the use cases outlined in Section 2.

The challenges, then, lie in successfully managing the huge datasets involved, do so maintaining system responsiveness, and standardize the way to retrieve and disseminate Provenance metadata.

### 3.2. Jump-Starts

In order to find the best solution for some of the issues outlined above, we can count on several already started initiatives.
There are active discussions on the Provenance of astrophysical datasets within the IVOA Working Group for Data Modelling (DM WG). A Representation, in the form of a complete IVOA Observation data model, has already been proposed by Santander-Vela (2009), and is currently under study.

In addition, ESO maintains a complete FITS keyword/metadata database (Vuong et al. 2008), which will be one of the basis for establishing Storage and Granularity of the future ESO Provenance services. Currently, that facility stores more than five thousand million keyword-value pairs, for more than ten million raw file entries, and already includes metadata versioning support (a requirement for Provenance audit trails and historical dataset documentation), while at the same time providing excellent query speed. There is also an ongoing project for using that same database to ingest keywords for highly processed datasets.

4. Conclusions

By identifying the elements needed for a successful data Provenance management system, and the selection of already in place systems, the ESO archive will be able to provide even more advanced scientific-oriented data products and services, while at the same time benefiting from existing IVOA standards for the Virtual Observatory, and helping in their development, leading by example.

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