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Provenance information in metrological traceability: application and modeling

Ryan White[1], Julia Neumann[2], Jean-Laurent Hippolyte[3], Blair Hall[4], Thiago Menegotto[5]

[1] National Research Council Canada, Metrology Research Centre 1200 Montreal Road Bldg. M-36 Canada, ryan.white@nrc-cnrc.gc.ca, ORCID: 0000-0003-3589-5900
[2] Physikalisch-Technische Bundesanstalt, Abbestraße 2-12 Berlin Germany
[3] National Physical Laboratory, Hampton Rd, Teddington TW11 0LW UK
[4] Measurement Standards Laboratory of New Zealand, Lower Hutt, New Zealand
[5] Instituto Nacional de Metrologia, Qualidade e Tecnologia, Av. Berlim, 627, Porto Alegre, Brasil

Abstract **– This paper proposes to use provenance information to describe processes in metrology. The PROV data model is used as an example to showcase a conceptual analysis about how to improve quality, reliability, and overall interoperability within cross-domain applications that are based on metrological timeline data. The conceptual analysis will be used as a foundation for further contributions to the topic of improving metrological traceability with provenance data models.**

I. INTRODUCTION

In information technology, provenance describes the history of a piece of data, including its origin and modifications over time [1]. It is fundamental to establishing the quality and reliability of data, especially as data interoperability becomes essential for cross-domain applications. In metrology, provenance metadata documenting measurement assurance and calibration activities could underpin metrological traceability claims, enabling machine-actionable assessments of measurement data quality. This paper proposes a provenance-based approach to describing measurement assurance processes in metrology, aligning with the FAIR principles (Findable, Accessible, Interoperable, and Reusable) that are driving global digital transformation in measurement science [2].

We demonstrate the application of the W3C PROV data model to capture key events and entities in metrological processes, such as calibration and validation of measurement standards across different stages within a traceability chain [3]. Integrating provenance into the ecosystem of metrology digital documents, including Digital Calibration Certificates (DCCs), ensures compliance with specific traceability requirements and establishes a robust, machine- actionable framework for a digital quality infrastructure [4]. Provenance-enabled systems not only enhance cross-disciplinary data usability but also provide a scalable foundation for metrological traceability and digitalization in industry, where reliable measurement assurance data are critical to maintaining global standards and supporting innovation.

II. BACKGROUND AND RELEVANCE OF PROVENANCE IN METROLOGICAL TRACEABILITY

Metrological traceability ensures the comparability of measurement results across different times, locations, and measuring instruments, thus providing a foundation for reliable decision making when dealing with information about physical quantities. Establishing traceability requires the coordination of metrological processes through a sequence of intermediate stages—called a traceability chain—ensuring that information is available where needed. The staged nature of a traceability chain enables stage-specific information to accumulate at each step, while intermediate results are passed along the chain. As a result, downstream process participants typically lack access to details about activities carried out upstream. To ensure the reliability and integrity of staged activities in practice, metrological traceability stipulates that each stage must conform to international standards for the competence of testing and calibration laboratories, such as ISO/IEC 17025:2017 [5]. Conformance to such standards involves regular independent assessments of a laboratory's capabilities, which, when deemed satisfactory, lead to accreditation. Such quality assurance requires meticulous documentation management. Maintaining a coherent system of traceable measurements requires sustainable, verifiable processes to assess quality and reliability.

Ehrlich and Rasberry noted that, at the turn of the 20th century, NIST defined traceability as follows [6, 7]:

"The property of the result of a measurement or the value of a standard whereby it can be related to stated references, usually national or international standards, through an unbroken chain of comparisons all having stated uncertainties. It is noted that traceability only exists when scientifically rigorous evidence is collected on a continuing basis showing that the measurement is producing documented results for which the total

measurement uncertainty is quantified."[1]

Recognizing the importance of the second sentence, which distinguishes metrological traceability as a scientific principle, Ehrlich and Rasberry introduced the concept of metrological timelines—explicit sequences of key measurement events—to strengthen the collection of evidence of traceability [7].

Timelines are used to gather data about the systems contributing to a traceable measurement. Results from independent measuring systems are compared with those obtained from systems within the traceability chain. This comparison helps assess whether the systems in the chain are under metrological control, a crucial requirement for ensuring that the accuracy of results is objectively justifiable.

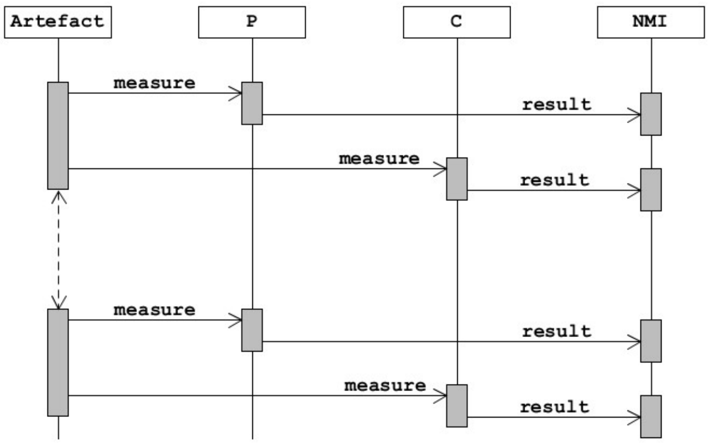

Fig. 1 A UML sequence diagram for the metrological timeline discussed here. Time progresses from top to bottom with horizontal lines used to represent events. The artifact is measured using systems P and C on two occasions (a substantial time apart). The NMI collects the results for quality assurances purposes.

The scenario considered in this paper is a simple timeline described by Ehrlich and Rasberry [6]. It involves a primary measurement standard, *P*, maintained by a national metrology institute (NMI) and an ensemble of control standards that perform at a level commensurate with *P* but are not considered primary standards. For simplicity, we will refer to a single control standard, *C*. The NMI also has an artifact that can be characterized using the systems *P* and *C*.

The timeline we are interested in describes a sequence of measurements of this artifact, using both *C* and *P*. Fig. 1 shows a UML sequence diagram of the scenario considered. The artifact is measured on two occasions using both systems P and C. The measurement results are retained by the NMI and used to check that P is operating at a satisfactory level, providing evidence of traceability claims on an ongoing basis.

III. APPLYING PROVENANCE IN METROLOGICAL TRACEABILITY

Generally speaking, provenance is a set of structured metadata that provides information about an object of interest, the origin of the object, the processes applied to the target object over time, including sources from which data have been derived and characterization or justification of the creation and transformation processes [8]. Fig. 2 shows the core information of the W3C PROV family of specifications:

- Agents, that perform processes on or own the objects of interest in the provenance description, whether they are software, hardware or human.
- Entities, the virtual or physical objects of interest in the provenance description.
- Activities, digital or physical manipulations applied to the objects of interest.
- Relationships that link agents, entities and activities, such as association of an agent with an activity or derivation of an entity from another entity.

[1] The International Vocabulary of Metrology defines metrological traceability as a property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty. [14, §2.41]

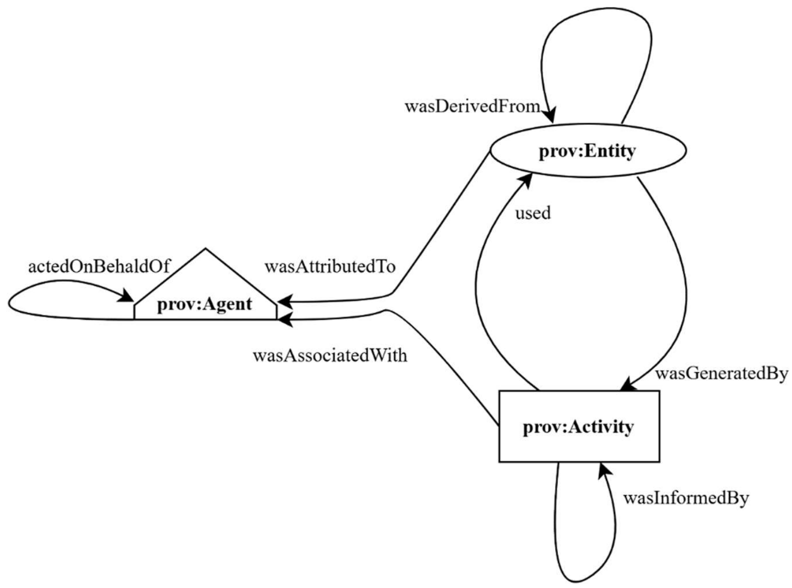

Fig. 2. Figure based on the starting point classes of W3C PROV-O ontology [13].

Provenance metadata take the form of a "graph describing the relationships among all the elements (sources, processing steps, contextual information and dependencies) that contributed to the existence of a piece of data [9]." Since provenance metadata offers a formal way to track data transformations and ownership, it is essential to support semantic procedures to assess the quality, verify authenticity, and evaluate the trustworthiness of data [10]. As a specification of provenance, the W3C PROV semantic model must accommodate different uses of provenance given that different perspectives on provenance may be applicable, resulting in different information that can be captured in metadata records [11].

- *Agent-centered provenance* describes the people and organizations involved in generating or manipulating the object of interest.
- *Object-centered provenance* traces the origins of the different elements of an object of interest to other entities.
- *Process-centered provenance* captures the actions and steps taken to generate the object of interest.

In measurement assurance, provenance could track the generation of, and updates to, a chart monitoring the stability of a measurement standard across its metrological timeline. Measurement assurance data provenance would include critical details of calibration activities, control standards, and associated measurement uncertainties. This metadata effectively describes a metrological timeline at a stage in a traceability chain, ensuring all relevant measurement and quality assurance activities are accurately represented, universally interpreted and machine-actionable.

IV. METROLOGICAL TIMELINE – PROV-O USE CASE

The concept of the metrological timeline is a compelling use case for provenance metadata. The use case details the provenance of internal measurement assurance data, supporting traceability to a primary standard. The provenance metadata links documented measurement results to a relevant quality assurance event from an object-centered perspective, documenting the origins of measurement assurance data to a reference. The provenance metadata is generated using the PROV ontology (PROV-O) specification of the PROV data model, and the model is illustrated graphically following the PROV graph layout convention [12, 13]. The intention of the provenance layout is to show the essence a set of provenance descriptions for this particular timeline scenario.

The object-centered provenance of measurement assurance data for an event in a metrological timeline, illustrated in Fig. 3, originates from the first stage of a traceability chain, measuring a quantity X. The primary measurement standard, P, is used (`prov:used`) in a primary calibration activity (`prov:Activity`) to measure the value X of a physical artifact (`prov:Entity`), part of an NMI's internal measurement assurance. This activity generates (`prov:generated`) a measurement result, X_P, linking the measured property of the artifact with the primary standard. A control standard, C (`prov:Entity`), is used in a control calibration activity (`prov:Activity`) to measure the value X of the physical artifact to serve as an independent check on the stability of P over time. This activity generates a second measurement result X_C. Together, X_P and X_C contribute measurement assurance data that can be displayed on a chart, the entity of interest (`prov:Entity`) in this provenance record, which is derived from both the measurement results (`prov:wasDerivedFrom`).

One example for Fig. 3 could be the traceability chain for silicon trap detectors used in radiometry. The primary calibration of trap detectors (measurement artifact) is done by using a cryogenic radiometer (primary standard). One possible approach for measurement assurance is to use a set of control standards that are of the same type as the measurement artifact, i.e., silicon trap detectors. The control standards are used to check the stability of the cryogenic radiometer scale, under specific conditions, when this is used to calibrate another silicon trap detector. The provenance layout provides guidance for implementing provenance descriptions for silicon trap detectors in radiometry.

The use case demonstrates a laboratory's internal application of provenance metadata to document metrological timelines. However, the value of documenting metrological timelines is to communicate quality assurance information at any point in the traceability chain as supporting evidence of traceability claims. The timeline scenarios that introduce the comparison of standards along a traceability chain need to be modeled and validated with specific examples. The resulting provenance layouts would introduce an entity representing calibration certificates. The layouts that incorporate calibration certificates would illustrate sets of provenance descriptions that relate downstream calibrations to upstream measurement assurance activities.

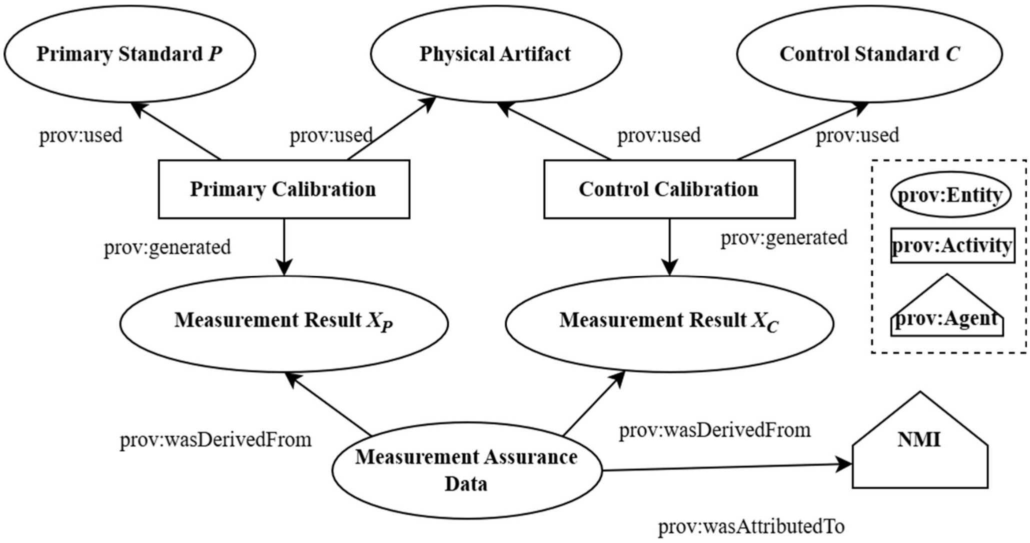

Fig. 3. PROV-O data model example applied to a metrological timeline describing the provenance of measurement assurance data. The subscripts P and C denote primary and control standards, which are used to measure the property X of a physical artifact.

V. DISCUSSION: PROVENANCE AND TRACEABILITY

The value of provenance metadata depends on the ability to distinguish the concept of provenance from metrological traceability, and model provenance metadata to adequately capture details of sequences of key measurement events to support metrological traceability.

Provenance captures the historical context and record of processes that influence a piece of data or thing, including what happened, why it happened (e.g., triggering entities), and the conditions under which changes occurred. Processes can include information about the creation, update, transcription, abstraction, validation and transferring ownership of data [1].

Traceability is the ability to verify and validate each step in a chain of custody through documented evidence, establishing accountability and reliability. Metrological traceability is a property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to measurement uncertainty [14]. The stated measurement uncertainties should be backed by rigorous scientific evidence collected over time.

Measurement assurance data provenance documents its origin from a reference and its evolution over time to support traceability claims. While accreditation to ISO 17025 provides assurance to clients of calibration providers, provenance metadata can accompany calibration certificates, providing detailed records of measurement assurance data over time at any stage in the traceability chain. The ability to exchange and interoperate provenance metadata, to accompany digital calibration certificates, can facilitate visualization of measurement relationships, measurement assurance data and sequences of measurement events Along a traceability chain, provenance metadata linked to references provides access to quality assurance details both downstream and upstream in the chain. The capabilities that provenance metadata provides can increase trust and reliability of digital measurement data, and support metrological traceability as a scientific principle

PROV-O classes provide structured data to support evidence of traceability claims collected by quality assurance systems [12]. Mapping components and events to PROV-O classes enables the capture of metrological timelines. Additionally, the core classes of PROV-O serve as flexible containers for detailed, metrology-specific metadata, which further enhances the provenance record. For example, measurement results can be described with digital representation of quantity and units and attributed to a measurand [15, 16]. Measurands can be fully specified within a controlled taxonomy and quantity and units uniquely identified from authoritative metadata repositories to enhance interoperability.

Process-centered provenance metadata may provide information of the specific steps or actions taken at each calibration activity. The details of the calibration method and specific software used and their provenance (e.g. the documented changes to those methods and software) can be documented with extended components of PROV-O, such as `prov:Plan` (a subclass of `prov:Entity`). The provenance of the software used may give details of changes over time with the accounting of measurement errors and quantification of measurement uncertainties.

Agent-centered provenance documents the roles and responsibilities within the NMI's organizational structure, assigning specific activities to roles such as metrologists, technicians, and quality managers. Provenance metadata attributes changes in calibration methods, procedures and software to measurement experts, technicians or quality managers.

This paper advocates for the implementation of object-centered provenance to support the scientific principle of metrological traceability. Provenance metadata documents the relationship between the metrological entities — measurement results, measurement standards and calibration certificates. Provenance metadata also documents the historical context of measurement assurance of a standard which can be provided, along with the calibration certificate derived from the measurement result, at any point in a traceability chain.

VI. CONCLUSION

The W3C standard for provenance, the PROV data model provides a domain-agnostic reference model for describing certain aspects of metrological processes. This paper demonstrates that metrological timelines can be adequately represented to capture the details of activities and events that continuously monitor the stability of measurement standards and contribute to the generation of measurement assurance data. As a specification, provenance provides a digital-ready and interoperable foundation to support various metrological and quality processes that need to represent, exchange and integrate information generated from different systems and different perspectives. Interoperability remains a challenge without standardization of measurement concepts, their representation and relationships with provenance concepts. PROV-O can be used as reference model to develop metrology-specific provenance ontology.

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