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THE DIGITAL NIST: CHALLENGES AND OPPORTUNITIES IN THE DIGITAL TRANSFORMATION OF NIST'S CALIBRATION SERVICES

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Abstract – Early in 2022 NIST embarked on a pilot project to produce digital calibration reports and certificates of analysis for reference materials. The goal of the project was to produce a few examples of each for the purpose of assessing the scope and challenges of digital transformation for these measurement services. This presentation is focused on the digital calibration reports. Our aims for this portion of the pilot project are to generate a digital calibration report from calibration data, customer metadata, and other data and metadata as needed; to generate a human readable report from the digital calibration report; and to hold a workshop to gather stakeholder feedback. The digital calibration certificate (DCC), which developed as an outgrowth of the SmartCom 17IND02 project, is used as a starting point. However, challenges for NIST include the wealth of information presently contained in NIST reports, reports with complex data, and the secure nature of NIST calibration reports (NIST calibration reports, data, and metadata are not public). Other practical challenges include the wide variety of calibration services offered by NIST, as well as the needs of internal and external stakeholders. This publication reports on the progress of the NIST effort and discusses some of the challenges and potential solutions to producing digital calibration reports.

Keywords: digital transformation, DCC, digital calibration, digital SI

1. INTRODUCTION

The digital transformation of metrology is a worldwide movement. For national metrology institutes (NMIs), supporting digital technologies is now an urgent task. NMIs want to support Industry 4.0 and Internet of Things (IoT) concepts, digital twins, and many other digital technologies. Although the activities of NMIs vary, the majority provide measurement services that allow their stakeholders to obtain documented traceability to the SI. Therefore, the digital delivery of measurement service data is a key and fundamental digital technology that NMIs seek to support. To that end "A universal and flexible structure for digital calibration certificates (DCC)" was developed under the auspices of the EMPIR project SmartCom 17IND02 [1]. Practically speaking, the DCC uses an XML schema that serves as a template for producing digital calibration certificates. The DCC continues to be supported and is presently on version 3.1.0, and many NMIs are now adapting the DCC for use in their own institutions.

NIST has recognized expertise in many digital technologies, including IoT, cybersecurity, artificial intelligence (AI), etc., but has not yet endeavoured to deliver measurement service data in a digital format. In 2022, NIST embarked on a pilot project to product examples of digital calibration reports and certificates of analysis for NIST Standard Reference Materials® (SRMs). The main objective of the pilot project is to assess the resources and effort NIST will require to deliver fully digital measurement service data. Similar to the digital transformation efforts of other NMIs, NIST is using the DCC as a starting point. The efforts required to digitalize calibration reports and certificates of analysis are separate but related. For the SRM effort one of the main challenges is that the DCC has been structured for calibrations, not reference materials. Although many of the elements are similar, many are also different, particularly in the context of metadata. For calibrations, the DCC is readily adaptable for NIST purposes, but bigger challenges lie in incorporating NIST metadata, integrating the production of digital calibration report in present systems, and producing human-readable reports from the DCC. Here, we focus on the calibration side of the pilot project, and we note that at the time of writing this paper the pilot project is rapidly developing.

2. NIST CALIBRATION SERVICES

NIST offers over 450 calibration services in the following categories: biomedical, dimensional, electromagnetic, environmental, ionizing radiation, mechanical, optical radiation, thermodynamic, and time and frequency. The large number and breadth of calibration services is a long-term challenge for the digital delivery of calibration data because the data and report formats vary greatly among the various services. NIST calibration services are generally designed to deliver measurement results with the lowest measurement uncertainty available. NIST establishes metrological traceability of the calibration results and associated uncertainties and provides these measurement results to customers in the form of reports, typically as a PDF. It is the general policy of NIST that measurement results are traceable directly through NIST to the SI, i.e., not to another NMI or laboratory.

The quality management system for NIST calibrations is, to the extent allowed by statute and regulation, in conformity with the International Organization for Standardization (ISO) and the International Electrotechnical Commission (IEC) standard 17025. Because the DCC was designed to conform to the ISO/IEC 17025, most of the elements NIST requires in its calibration reports can be found in the DCC. However, it is important to note that NIST provides calibration reports rather than calibration certificates. These reports provide calibration data, but do not verify the performance accuracy of an instrument or artifact within a specific interval.

3. CHALLENGES

3.1. Digital reports

In the pilot project, NIST is using an internally developed platform, the Configurable Data Curation System (CDCS) [2], to transform calibration metadata and results into digital calibration reports based on the DCC schema. The CDCS is a NIST developed system that provides a means for capturing, sharing, and transforming unstructured data into a structured format based on XML. In the present application, it also serves as a repository for the schema and generated reports, which includes the calibration metadata and results.

A considerable effort of this pilot is developing methods required for populating the digital calibration report template, generated from the DCC XML schema, which resides in the CDCS.

Orders for NIST calibrations are placed by customers through an E-commerce platform. Much of the metadata needed for calibration reports, such as customer information and identification of calibration item(s), resides in an existing database within the system used to manage the accounts and interactions of NIST's customers. An application programming interface (API) is used to extract appropriate metadata for the digital calibration report. Although developing this type of code may be straight forward, challenges remain in gathering the proper metadata because, unfortunately, the metadata pulled from the customer input is sometimes incomplete and prone to error. Some types of metadata, such as the customer names and addresses, are likely to be correctly entered by the customer. However, other metadata, such as equipment identifications, are often incomplete, missing, or incorrectly entered. Therefore, the metadata pulled from the customer database must be checked, corrected, and validated before using to populate the digital calibration report. Additionally, most of the calibration services maintain separate databases that contain relevant metadata, such as the correct identification of equipment. Applications will be created to gather validated metadata from all the sources and populate the digital calibration report.

Even more challenging is the variety of formats and storage methods for calibration results that exist across the NIST calibration services. As mentioned above, many calibration services maintain databases with relevant metadata for each order as well as associated calibration data and the calibration history for that artifact at NIST. Unfortunately, there is no uniformity in the data types stored within the various databases or the format of the database itself. Initially, the pilot study is focusing on several services that are currently in the process of automating data collection and, therefore, can be easily adapted now to produce data in the suitable format for the digital calibration report template. However, going forward, a method for manually importing data will be necessary for maximum flexibility, as updating the data automation programs of NIST's many calibration services will be a lengthy process.

As mentioned in the previous section, NIST produces calibration reports, not certificates. No adjustment is ever made to the instruments or artifacts calibrated by NIST. In addition, NIST is self-traceable. NIST assures the traceability to the SI, or to other specified standards, of measurement results that NIST itself provides, either directly or through an official NIST program or collaboration. Care must be taken to ensure that the measurement results given in a NIST digital calibration report are not confused with results given in a certificate issued by another institution or organization. One way to uniquely specify elements within an XML document is by using XML attributes. In the pilot program, we have begun defining a list of attributes describing NIST measurement results, and these will be used to uniquely describe the measurement results.

Another challenge is the digital representation of SI units. Presently, NIST is not committed to a specific method, but favors flexibility in SI representation. Therefore, NIST supports the addition of an element to the DCC that specifies the system of representation being used in the digital report. For example, some stakeholders, such as the biomedical community, may prefer that units be expressed using the Unified Code of Units of Measure (UCUM) [3]; whereas stakeholders from the aerospace community may prefer units of measure as defined by the ontology for Quantities, Units, Dimensions, and Types (QUDT) [4]. One could also imagine creating an API that stakeholders could use to export their digital calibration report with their preferred system of representation.

Finally, an important aspect of producing digital calibration reports is confidentiality and security. Calibrations at NIST are produced under the authority of Cooperative Research and Development Agreements (CRADAs) and are not public. Only the customer that ordered the NIST calibration service has access to the calibration report. This is unlike a certificate of analysis for reference materials. In most cases, reference material data pertains to a group or batch of materials and the data are publicly available. The confidentiality of NIST calibration reports will place some constraints on how the digital reports are stored and delivered. Considerations include the security of the repository, security of the data in the repository from alteration once the report is finalized, and security of the method of report delivery to ensure that only the customer has access to it and data is not altered during delivery.

3.2. Human-readable reports

While the digital transformation of calibration reports is critical to the future of metrology, human-readable calibration reports will continue to be relevant for the near term. These human-readable versions of digital calibration reports must be formatted such that stakeholders can easily extract the information they need for their purposes, whether it is manually updating calibration coefficients in their instruments, serving as a resource or reference for the customer, or serving as evidence for accreditors.

Some of the components that currently exist in NIST calibration reports are intended primarily for the human

reader and should continue to be included in calibration reports.

Over the years, many NIST calibration reports have evolved from simple reports of measurement results to comprehensive reports that include results and detailed descriptions of calibration methods, uncertainty analyses, and other considerations. The intention behind these lengthier reports is to educate stakeholders about the calibration measurements and highlight issues that are relevant to the transfer of the scale from NIST to the stakeholder.

Additionally, NIST calibration reports often include figures, photos, and plots of results. The figures and photos are intended to illustrate or document measurement schemes, instrument layouts, and the condition or mounting of calibration artifacts, while plots of results provide an easy way for the human reader to digest tabulated measurement results and uncertainties.

Some NIST calibration reports may also include the calibration history of the artifact. This practice serves to provide context for the calibration and identify trends in the stability of the artifact.

It is not necessary that all these extra components be machine-readable, yet they should be incorporated within the digital calibration report in some way so that they can be produced in the human-readable version. Figures, photos, and plots, for instance, could be included as images within the digital calibration report using, for example, the Base64 method for encoding. Descriptions could be included explicitly or as links to separate documents, web resources, or publications. In some cases, these extra components may be generic, applicable to all calibrations for a particular service. A method of version control will be necessary to account for possible revisions to these components over time. It is also possible that there are extra components that pertain to a specific calibration request. For this case, the components need to be linked to its corresponding calibration report and the confidentiality of those components will need to be secured.

4. FUTURE DIRECTIONS

NIST will be hosting a workshop on 28 and 29 September 2022 for stakeholders of its calibrations and reference materials. The workshop will introduce stakeholders to the results of the pilot study, specifically beta versions of digital calibration reports and certificates of analysis and their corresponding human-readable versions and seek stakeholder feedback on these beta versions. The workshop will also be an opportunity for NIST to learn how stakeholders are responding to and implementing the digital transformation metrology.

Potential participants for the workshop were identified through a survey that was sent to customers of NIST measurement services through email blasts and posted on the NIST website. The survey gauged stakeholder interest in participating in the workshop and topics for digital transformation, such as digital calibration reports and certificates of analysis, digital traceability and security, and middleware for digital reports and certificates of analysis.

The first day of the workshop is planned to be a series of presentations followed by a question-and-answer period. Presentations will cover the following topics: introductions to the Digital NIST pilot study, including progress on the development of digital calibration reports and digital certificates of analysis; international and industry perspectives on the digital transformation of metrology; and end user concerns. These presentations are intended to introduce topics related to the digital transformation of metrology and provide context.

The second day of the workshop is planned to be a series of breakout sessions intended to answer questions and gather information from stakeholders. Topics for these sessions include digital calibration reports and digital certificates of analysis; applications for digital data; digital traceability and security; harmonization of international standards; and interoperability of units.

Following the conclusion of the workshop, NIST will develop a strategy on the full digital transformation of its measurement services.

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