IMEKO TC8, TC11 and TC24 Joint Conference
October 11-13, 2023, Madeira, Portugal

THE DIGITAL NIST: STEPS TOWARD THE DIGITAL TRANSFORMATION OF NIST'S MEASUREMENT SERVICES

R.J. Hanisch,[1] J. Fedchak,[2] C. Cooksey,[3] K. Delak,[4] S. Choquette,[5]
W.D. Camara,[6] K. Rimmer,[7] I. Dominguez Mendoza[8]

[1] Material Measurement Laboratory, NIST, USA, robert.hanisch@nist.gov
[2] Physical Measurement Laboratory, NIST, USA, james.fedchak@nist.gov
[3] Physical Measurement Laboratory, NIST, USA, catherine.cooksey@nist.gov
[4] Information Technology Laboratory, NIST, USA, katya.delak@nist.gov
[5] Material Measurement Laboratory, NIST, USA, steven.choquette@nist.gov
[6] Material Measurement Laboratory, NIST, USA, william.camara@nist.gov
[7] Material Measurement Laboratory, NIST, USA, catherine.rimmer@nist.gov
[8] Informática, CENAM, Mexico, idomingu@cenam.mx

Abstract:
Beginning in 2022, NIST began a project called *The Digital NIST* which aims to make our measurement services—calibrations, standard reference materials, standard reference data--fully digital and fully FAIR [1]. We reported on this work previously [2] but provide here an update on further progress and prospects for future developments.

Keywords: calibrations; reference materials; reference data; measurement services; digitalization

1 INTRODUCTION

NIST is in the early phases of the digital transformation of metrology within its measurement services. Two key NIST services are the calibrations, of which there are over 400 services in nine different areas, and the standard reference materials (SRMs), of which NIST has more than 1100 in its catalog. Two separate but related projects are underway in each of these services: first, to develop a tool to both produce human readable calibration reports and NIST digital calibration reports (NDCR); the second is to produce a digital reference material certificate (DRMC) for our SRMs. Challenges for the calibration projects include the wide variety of reports NIST produces; a standard template must be developed for the human readable reports, and the elements of the reports must also be mapped into a digital report. NIST will leverage the XML schema DCC presently under development by PTB for calibration reports as much as possible. For the DRMCs, the metadata descriptors for reference materials are quite different and the DCC schema will need certificate-specific extensions. Demonstrating traceability to the SI is fundamental to both SRM products and calibration services and a digital representation of this traceability could be an important feature of digital certificates. Concerns regarding privacy and business identifiable information (BII) is particularly a challenge to calibration services. We describe here the NIST progress and status of these projects with a perspective of some of the key challenges regarding the digital representations of traceability that are presently perceived.

2 THE DIGITAL TRANSFORMATION OF METROLOGY FOR CALIBRATIONS

NIST calibration services is developing an application to produce both human readable and digital calibration reports from calibration data and metadata. Increasing internal efficiency of metrology organizations is one of the advantages to the digital transformation of metrology. To that end, NIST has a strong desire to both support its calibrations customers and increase the efficiency of the calibration services. NIST's stakeholders have expressed the desire to have a consistent format for the calibration reports that NIST produces from its many calibration services. Some of NIST's stakeholders also have need of calibration reports in a digital format. Creating an application that produces a human readable calibration report from calibration data and metadata in a consistent format is a first step toward a digital transformation of NIST's calibration services. Such an application can subsequently be used to produce a digital

calibration report based on, for example, an XML schema.

There are several challenges for this current effort. NIST reports tend to give extensive details on the measurement methodology, the data analysis, the apparatus, and, often, the calibration measurement history. NIST calibrations are traceable to NIST primary standards and are often unique. The technique, procedures, and equipment used give the best quality data at the lowest uncertainty. Consequently, NIST calibration reports have evolved to be customized and unique to each service. Even so, the NIST quality manual complies with reporting requirements of the ISO/IEC 17025:2017, and therefore the data and metadata in the reports do follow a common model. One of the challenges of this project is to define elements for the information contained in the reports that are not specified in the ISO/IEC 17025:2017 and to produce the reports in a consistent format.

Another challenge is pulling the metadata from various sources into the report. NIST customers place orders through an e-commerce system. Much of the customer metadata can be obtained from that system. However, metadata describing the equipment is often missing or incomplete, and so this metadata is typically provided by the technical expert performing the calibration. The technical expert also provides the metadata describing the calibration and calibration data. Presently, most of the NIST-provided data and metadata is stored in non-centralized locations. The calibration data is typically acquired and analyzed automatically with acquisition software such as LabVIEW or Python. In some cases, the analysis is performed separately from the acquisition software in spreadsheets. An application for report generation needs to be able to pull data from these various sources. Options for manual entry must also be included.

We have developed a standard template for calibration reports, but the display of data, such as in tables or graphs, is still under development. With so many unique services, there are many ways to display data. Initially, graphical representation of data will be embedded into the report as an image. Pictures or other graphics depicting equipment or apparatus are also common in NIST reports.

Once the calibration reports are broken into its fundamental elements, producing a NIST digital calibration report (NDCR) is somewhat straight forward. The data model and schema are taken from the DCC XML schema maintained by PTB [3]. Various enhancements are likely to be used by NIST; this is in nascent development and will evolve with the needs of NIST and its stakeholders.

A consideration by NIST throughout this development is security. NIST calibration reports are not public facing document. Business identifiable information is protected. Internally, even the metadata can only be accessed by authorized users with proper credentials.

3 DIGITAL CERTIFICATES OF ANALYSIS FOR REFERENCE MATERIALS AND TRACEABILITY

It was determined that to digitize the certificates of analysis, their information, mainly the values contained, must be stored in a database. For this, these data must be analyzed to classify and structure them in a way that leads to the design of the database and eventually to the design of a standard Digital Reference Material Certificate.

The first classification that was carried out was in a general way according to the types of values contained in the certificate and the mode of certification [4]; the classification was made according to the knowledge of those who handle this information. The classification is shown in Table 1.

Table 1. Value type classifications.

			Certification Mode		
			Batch non-continuous	Batch continuous (lot)	Serialized
Value type	Value and uncertainty	Single value	✓	✓	✓
		Multiple value	✓	n/a	✓
	Sequencing		✓	n/a	n/a
	Formula		✓	✓	✓

A random sample of around 130 certified reference materials (considering the current classification areas in NIST: chemical composition, physical properties, and engineering material) was taken to verify the classification and begin with the analysis of the information contained for a first attempt at database design.

The decision was made to focus, as a first objective, on the analysis and design of the database only for those reference material certificates whose type of value is, according to the general classification, "value and uncertainty" since they represent the bulk of existing SRMs. These are values of the measurands and associated information, such as their unit, uncertainty, traceability, type (certified or non-certified), identification, classification, and conversions. To create the model for reference materials, sample certificates were analyzed. In consultation with people responsible for the content of those

certificates, a specific and structured proposal was designed for this type of reference material certificates. Additional certificates were then added to the analysis and compared against the model design to determine whether they fit the model or the model needed to be adapted. This design includes the following:

- Value of the measurand.
- Unit: expressed as currently stated on the certificate (i.e., could be derived units) but includes information to make a conversion easier if necessary.
- Uncertainty: symmetric and non-symmetric, value of k, level of confidence, and type of uncertainty.
- Type of measurement: certified, non-certified, detection limit.
- Properties of the measurands: such as molar mass, to carry out conversions between mass fraction and concentration; minimum sample size to ensure homogeneity; traceability statements; whether the measurement is on a dry-mass basis; whether the measurement is dependent on a specific method.
- Identification and Synonyms: allowing for multiple ways of identifying what is being measured such as the common name, chemical name, CAS, chemical structure, InChi Key, etc.; all of them can be specified per measurand.
- Groups, allowing infinite ways to group values together such as elements, amino acids, vitamins, fats, tocopherols, etc.
- Statements: additional specific information to the measurand.
- Method(s) for obtaining the value, as well as who performed the measurement.

A test database has been generated with this design and testing carried out with real certificate information within the original sample of 130. The initial tests were satisfactory and now we are working on inserting information beyond that sample.

One of the challenges in the analysis of the reference materials is separating the data from the formatting. For many certificates the values are grouped and presented in ways that are easier for the human reader to understand. For example, a certificate may split the certified values into three separate tables so that Fats, Elements, and Tocopherols are grouped together. However, a good design will accommodate and record appropriate metadata about the value so that the information can be processed, analysed, and grouped in various ways in the future.

Dynamic future uses of certificates can be achieved by focusing the model on the value and its associated data. The values, units, and uncertainties can be evaluated in a systemic and consistent way when the data is stored discreetly. Machine programs can be written to take data from the Digital Reference Material Certificate and combine it with measured data from the user to allow the user to make claims of traceability more easily.

4 SUMMARY

Following a successful pilot project conducted in 2022, in which we confirmed that the PTB Digital Calibration Certificate construct could be adapted for NIST calibration reports and form the basis for NIST reference material certificates of analysis, we are continuing to develop the tools to routinely produce these digital artifacts. We have not yet set a schedule for production, and in any case digital calibration reports and digital reference material certificates will need to be phased in over a period of several years. We also intend to fully modernize NIST's measurement services such that we achieve full traceability to the SI in digital form.

5 REFERENCES

[1] M. Wilkinson et al., "The FAIR Guiding Principles for Scientific Data Management and Stewardship," Nature Scientific Data, vol. 3, article no.160018,2016.DOI: 10.1038/sdata.2016.18

[2] W. D. Camara et al., "Digital NIST: An Examination of the Obstacles and Opportunities in the Digital Transformation of NIST's Reference Materials," Acta IMEKO, vol. 12, no.1, 2023.DOI: 10.21014/actaimeko.v12i1.1403

[3]https://www.ptb.de/dcc/v3.0.0/ [accessed June 2023]

[4] C. R. Beauchamp et al., "Metrological Tools for the Reference Materials and Reference Instruments of the NIST Material Measurement Laboratory," NIST Special Publication 260-136, 2021 edition; National Institute of Standards and Technology, Gaithersburg, MD (2021); available at https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.260-136-2021.pdf [accessed July 2023].