Digital Transformation and NIST's Measurement Services

James Fedchak

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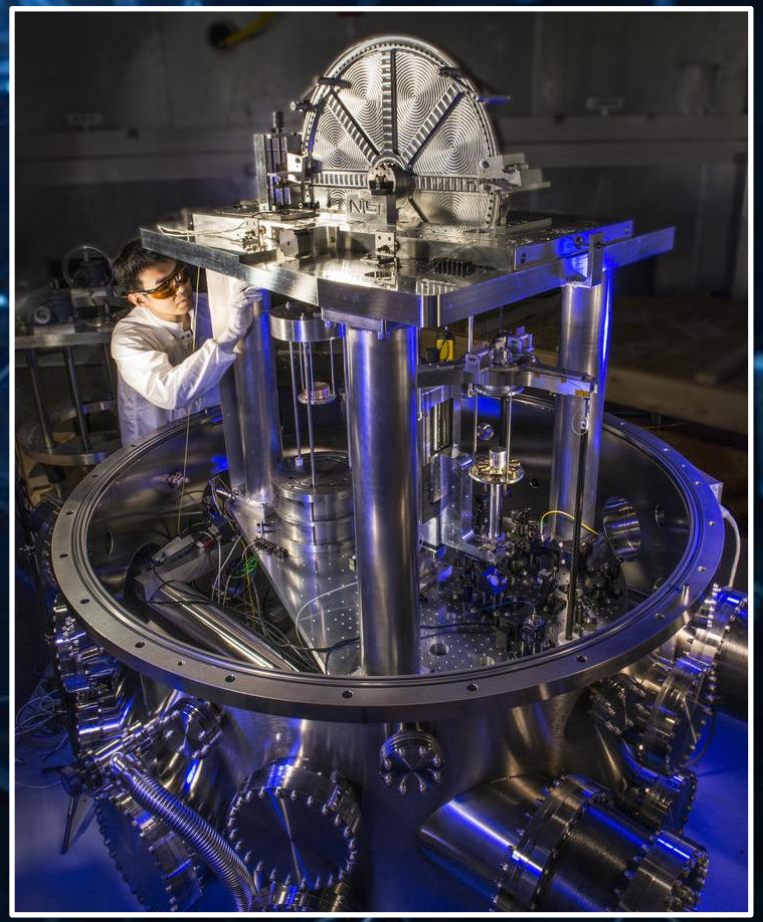
Physical Measurement Laboratory

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

JOINT CIE-USNC & CORM CONFERENCE
Nov 12-14, 2024

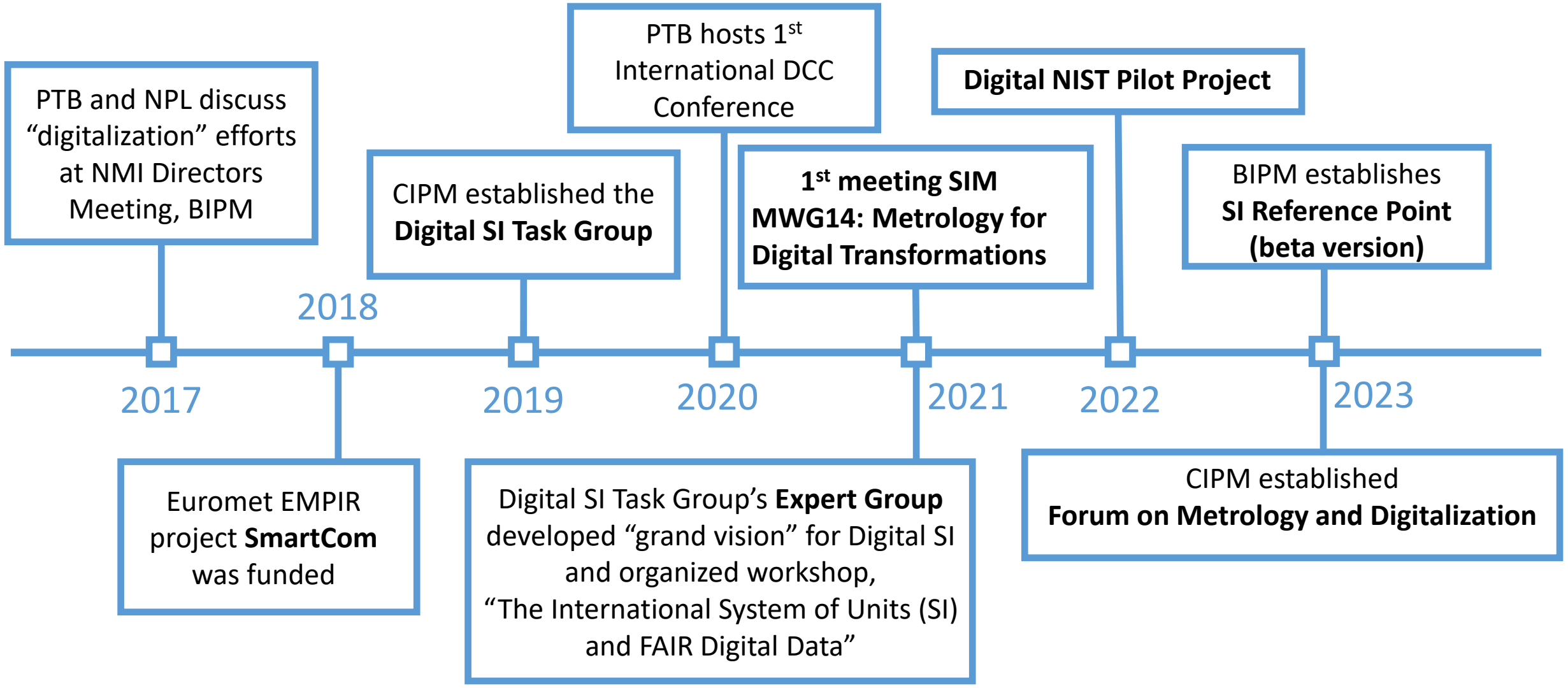
Digital Transformation of Metrology

- **The world is clearly being transformed by digital technologies**
- **Examples of Digital Concepts that Metrology can Support:**
  - Industry 4.0/IoT
  - Smart Factories
  - Networked sensors
  - Digital twins
  - Machine learning & AI
  - Remote sensing/calibrations
- **Supportive Digital Metrology Tools**
  - Digital Calibration Certificates (DCC)
  - Digital Reference Material Certificates
  - Digital Traceability & Provenance Record
  - Digital Calibration Requests
  - Digitized Quality System
  - Semantics

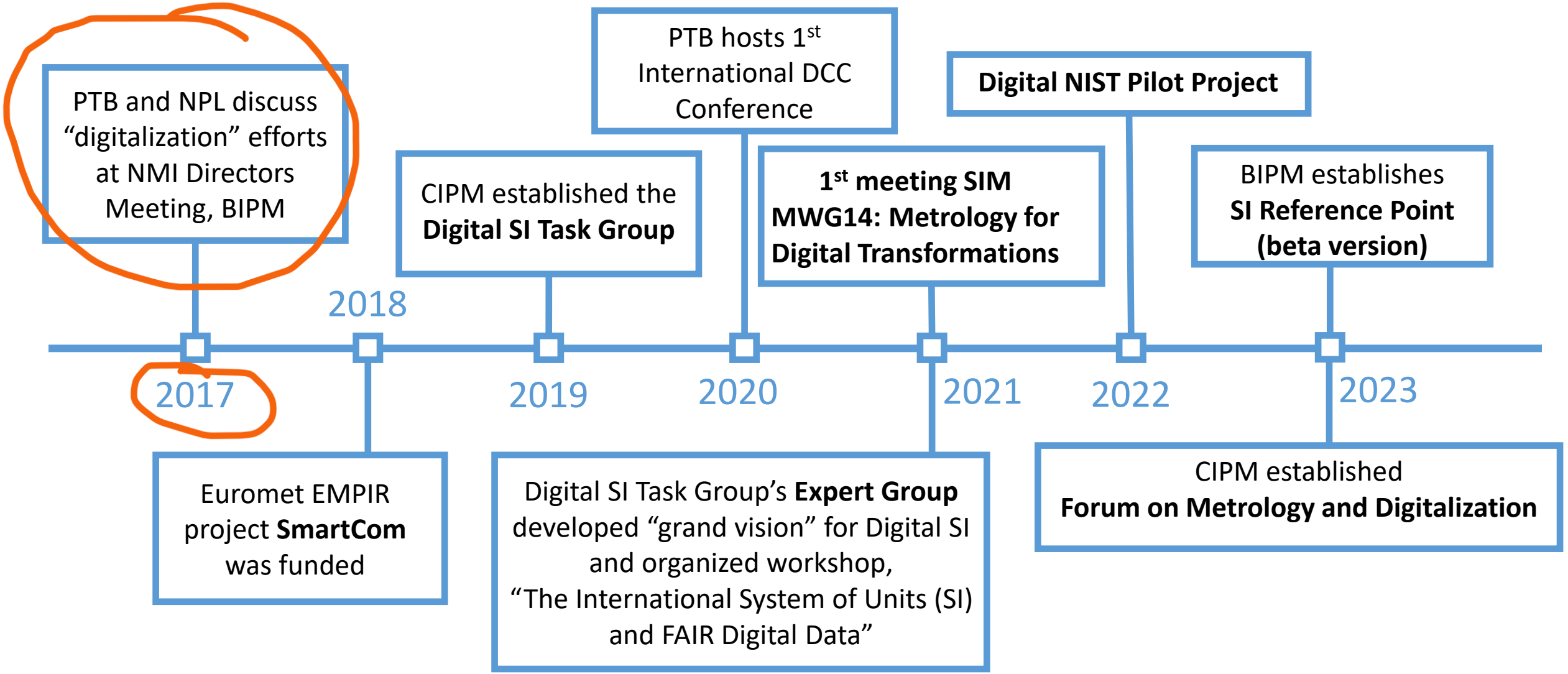


Background Information

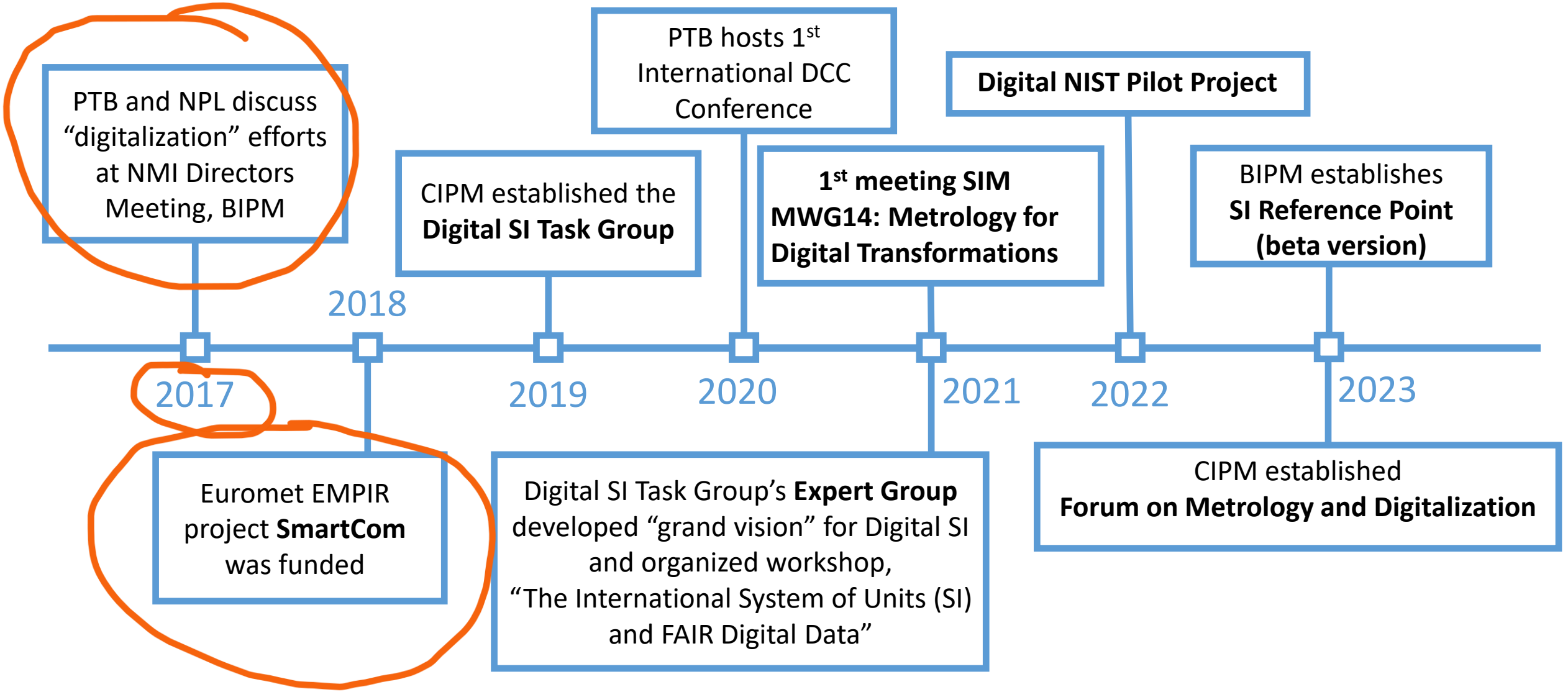
Movement for Digital Transformation of Metrology



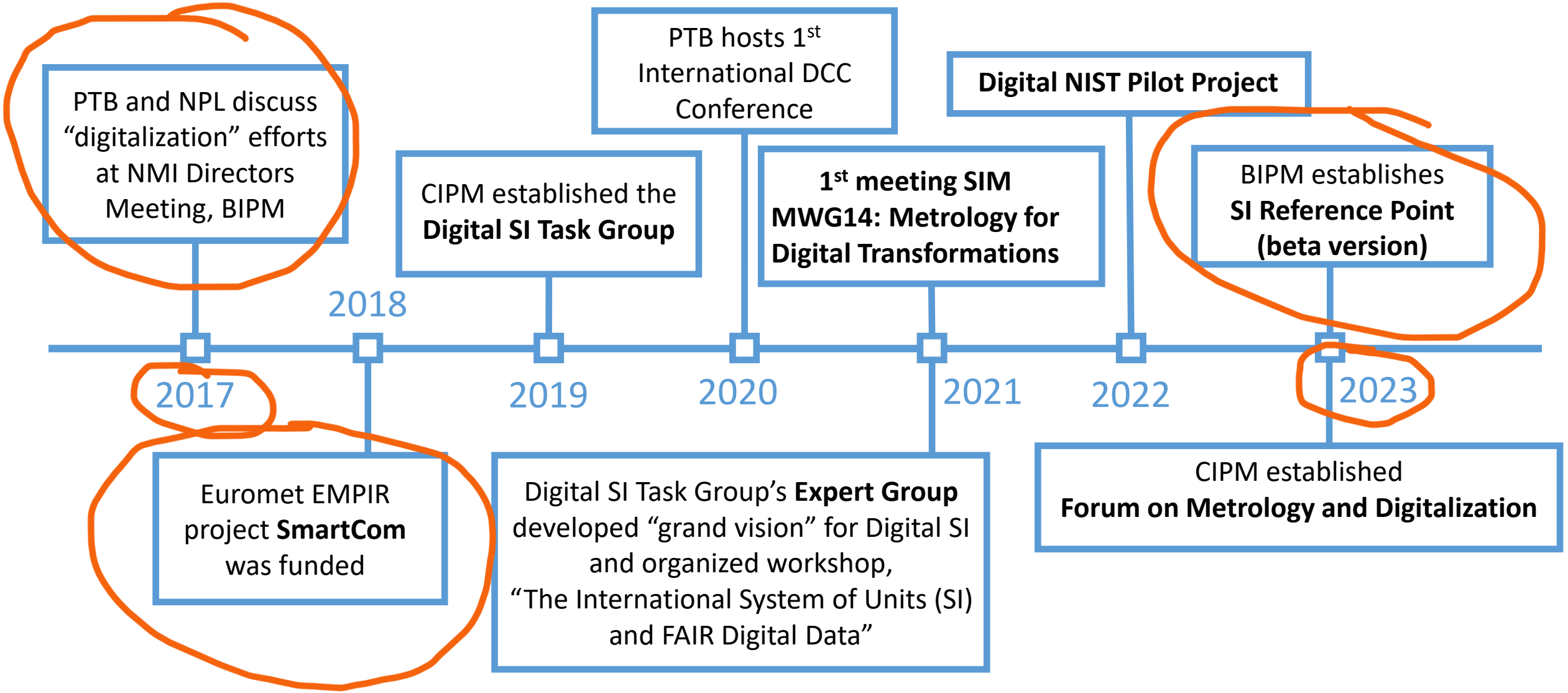
Movement for Digital Transformation of Metrology



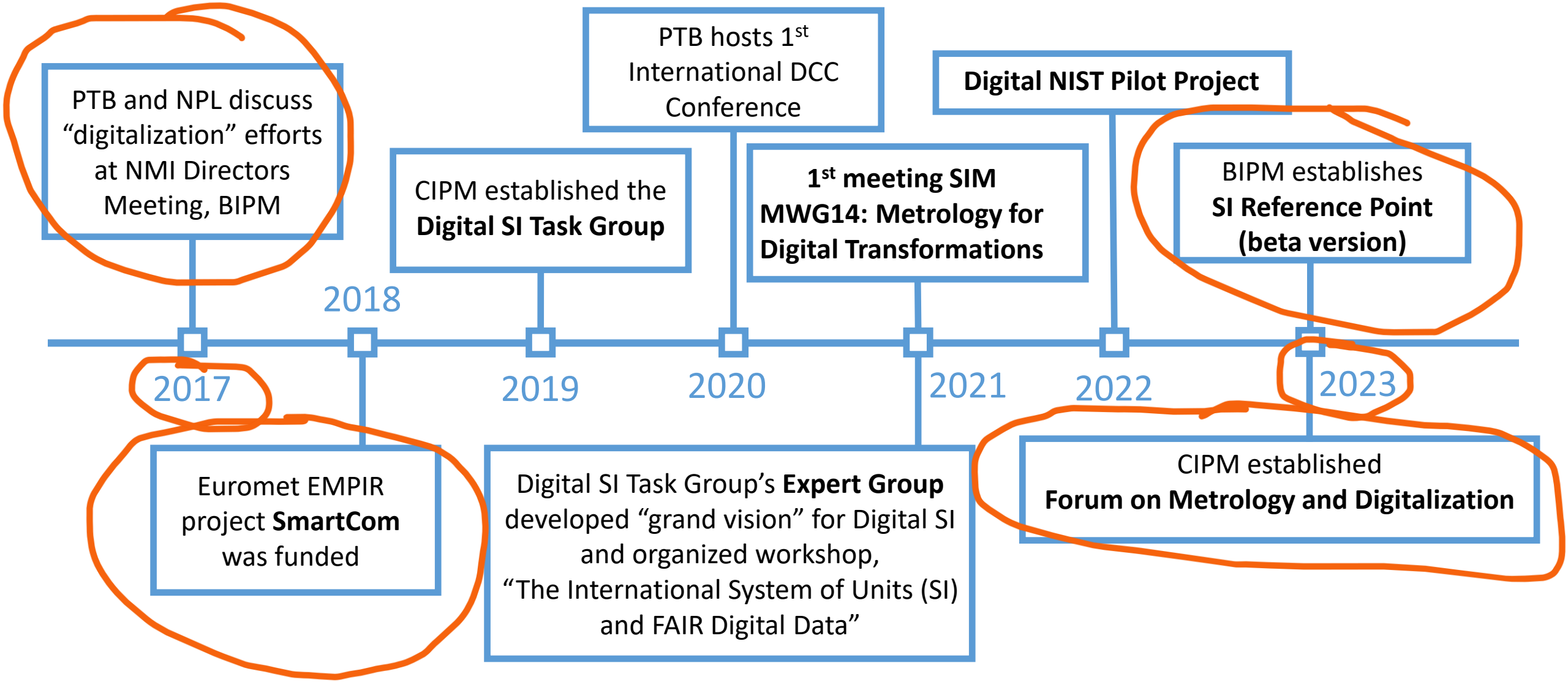
Movement for Digital Transformation of Metrology



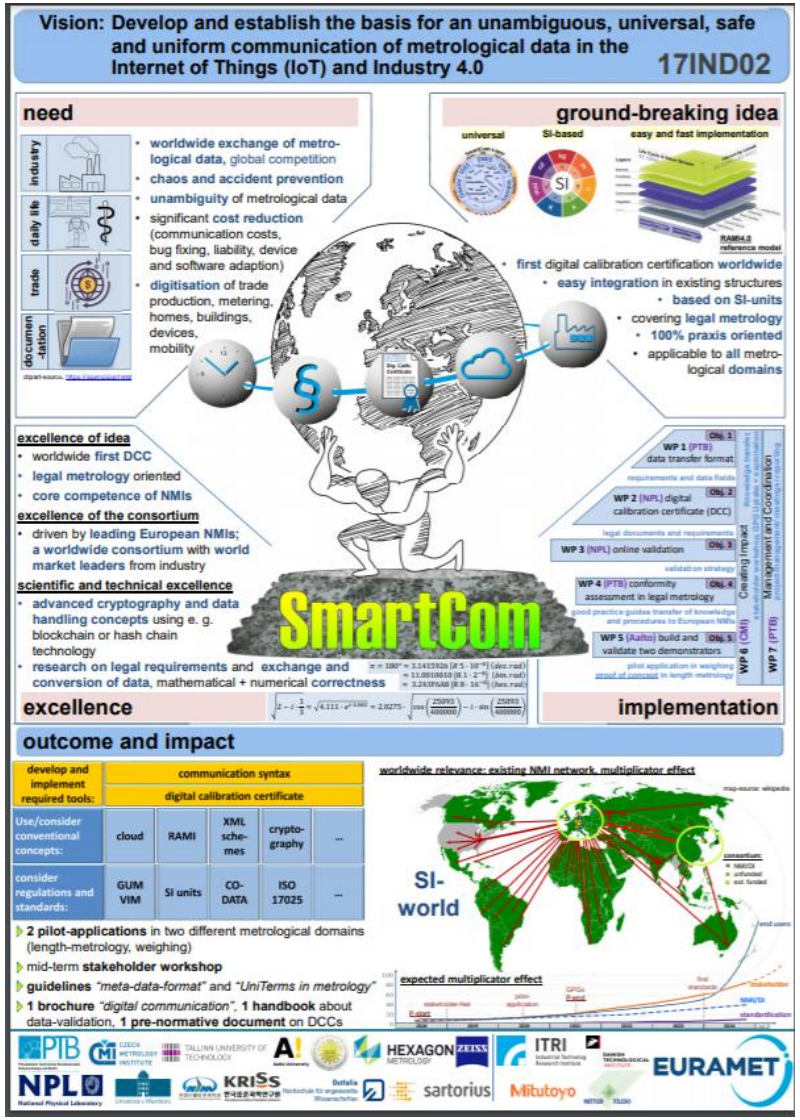
Movement for Digital Transformation of Metrology



Movement for Digital Transformation of Metrology



Digital Transformation of Metrology in Europe



- In 2018, metrology digital transformation efforts in Europe were greatly accelerated by the creation of the funded **Euromet EMPIR project SmartCom**

- PTB and NPL haves been leaders in developing the **Digital Calibration Certificate (DCC)** and the **European Metrology Cloud**
  - Created an XML schema for digital calibration certificates

- Since then, there have been numerous workshops on the digital transformation of metrology
  - Annual **DCC conference** started in 2020 (PTB)
  - https://www.ptb.de/dcc/

What is the DCC?

- PTB & collaborators have been working on the DCC since before 2019
  - On version 3.3.0
- The DCC is an XML schema
  - Schema elements represent all data and metadata in a calibration certificate
  - Satisfies ISO 17025 required elements
- Fundamentally machine readable
  - Eliminates transcription errors
  - Interoperable data and unit formats
- Human readable reports may be directly generated from the DCC

XML is a language for digital data

https://www.ptb.de/dcc/

Key BIPM/CIPM Developments

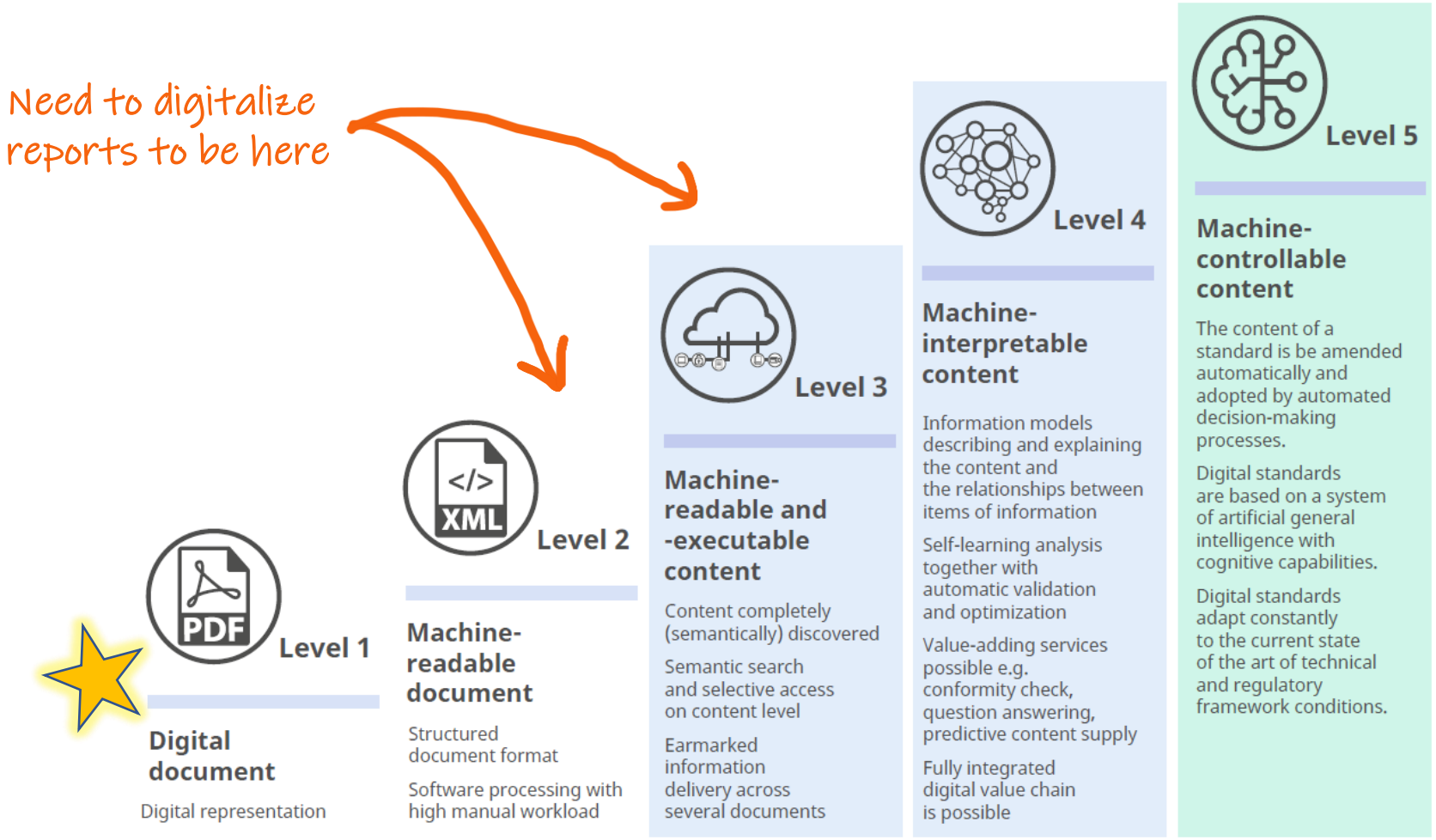
- October 2019: New version of the **BIPM key comparison database, KCDB 2.0**.
  - Web-based user platform, directly linked to database
  - API for CMC queries.
  - Supports the Digital Calibration Certificate (DCC) concept

- BIPM launches **SI Reference Point**
  - Authoritative digital reference for the International System of Units (SI).
  - Provides Permanent Digital Identifiers (PIDs) for SI units

- 2023: 1st meeting CIPM Digital Forum**: FORUM-MD**
  - ad hoc Task Group on **Secure and Trustworthy AI**
  - ad hoc Task Group on **FAIR for Metrology**
  - ad Hoc Task Group on **Metrological Semantics**
  - ad hoc Task Group on **Data Quality in Metrology**
  - ad hoc Task Group on **Harmonizing DCC and DRMC**
  - ad hoc Task Group on **SI-Digital Framework**
  - Other groups on coordination and strategy

NIST Digital Transformation Efforts

Where are we at NIST?



IDIS Whitepaper, “SCENARIOS FOR DIGITIZING STANDARDIZATION AND STANDARDS”, 2021

Digital Transformation of Metrology

We have not had much customer demand for digital certificates or other digital products

Present efforts focus on **increasing internal efficiency** and being ready when demand increases.

Introduction

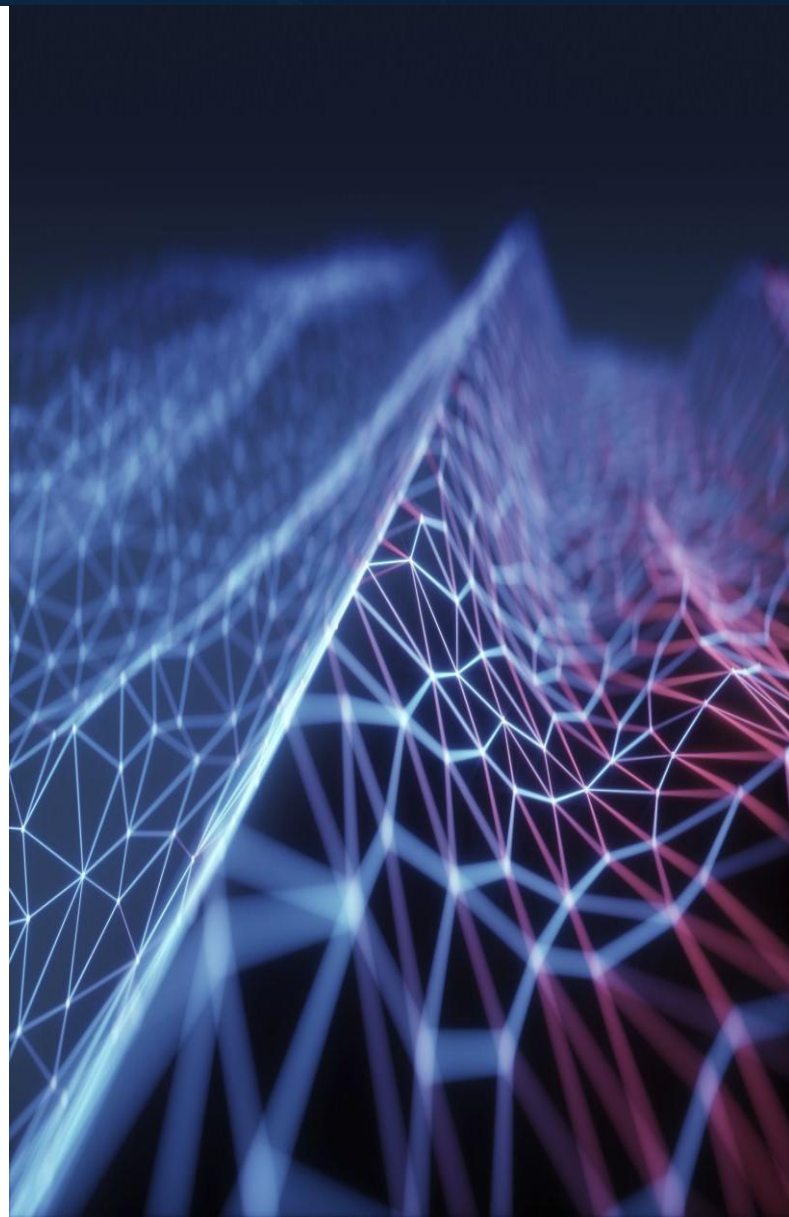
Digital Transformation of Metrology

NIST is still early in its organizational efforts

Presently, 3 main areas of development

- Digital Calibration Reports
- Digital Certificates of analysis
- Digital Traceability

Creating repositories are a critical part of the first two efforts

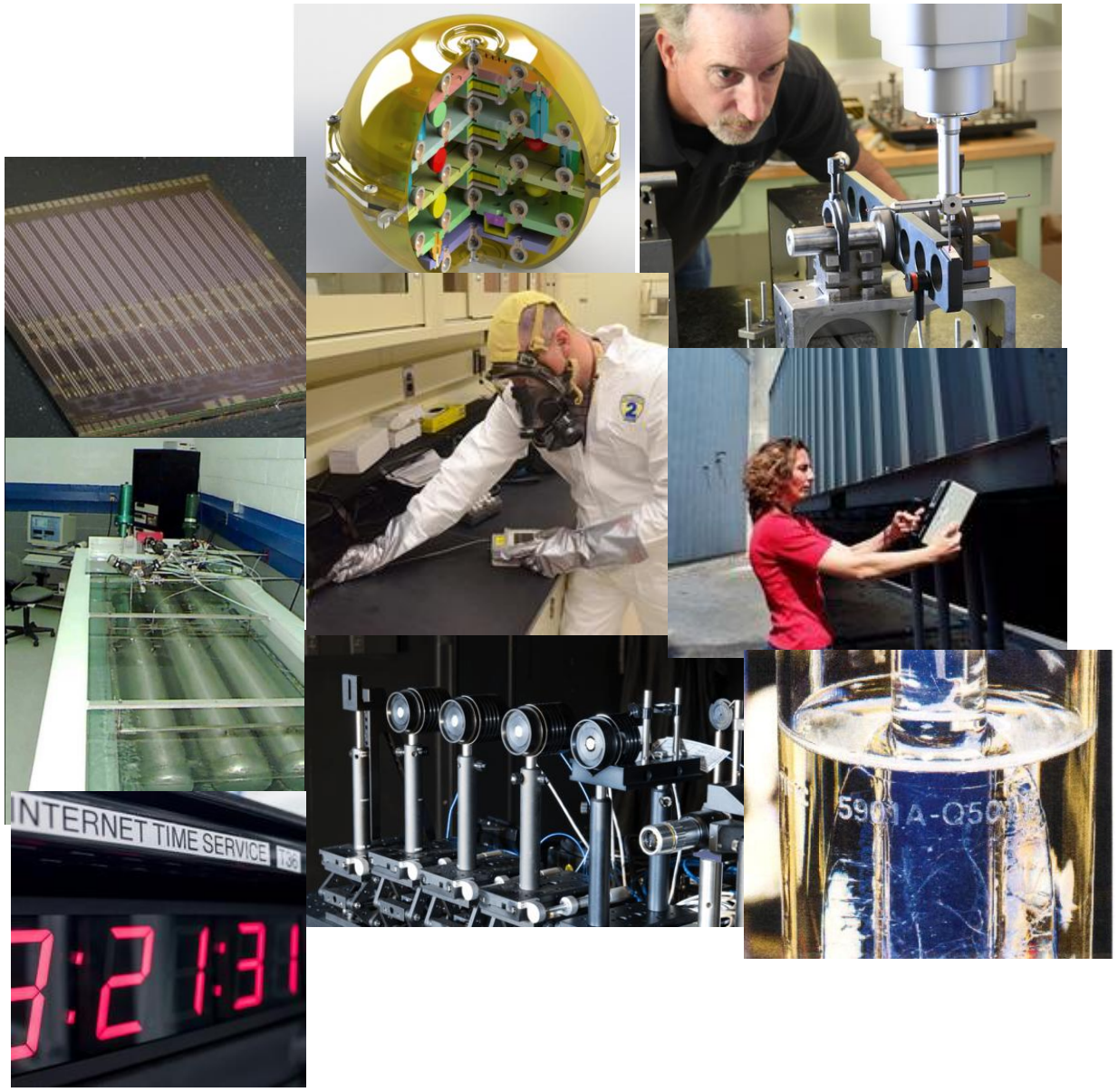


Calibration Services & Challenges

More than 500 Services

<u>Nine Calibration Areas</u>

- Biomedical
- Dimensional
- Electromagnetic
- Environmental Area
- Ionizing Radiation
- Mechanical
- Optical Radiation
- Thermodynamic
- Time and Frequency



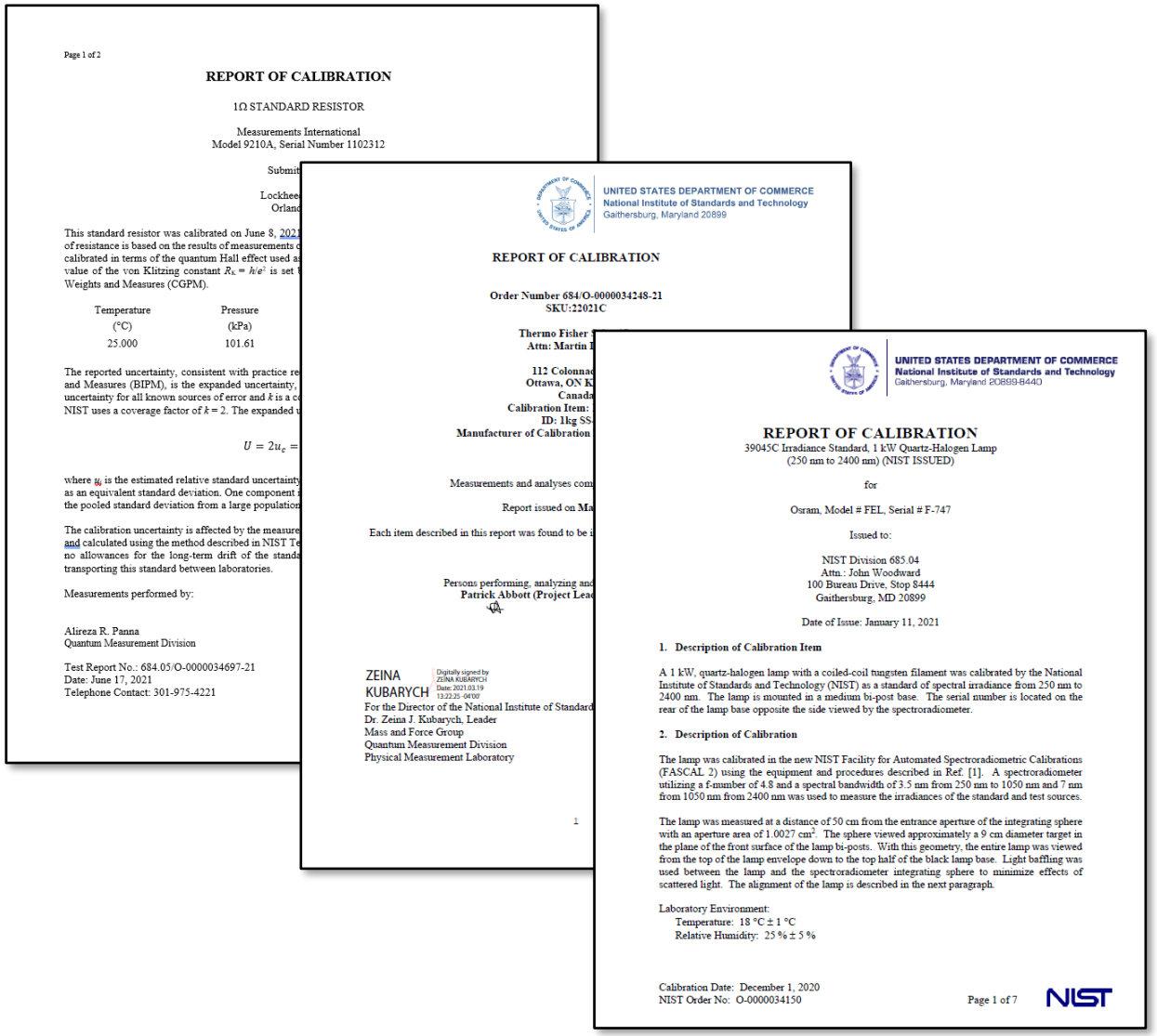
Digital Calibration Reports: Technical challenges

Digital Calibration Reports

Landscape of Technical Challenges

- NIST has over 500 services
- **Every report** seems to be a **different format**
  - NIST reports contain a lot of educational material
  - Often contain data history
- Report **metadata** & **data** comes from **various sources**
  - Customer metadata is collected through our e-commerce system
  - Other data & metadata comes from calibration operators or other databases

First Steps towards Digital Transformation



Page 1 of 2

REPORT OF CALIBRATION

1Ω STANDARD RESISTOR

Measurements International
Model 9210A, Serial Number 1102312

Submit

Lockhee
Orlan

This standard resistor was calibrated on June 8, 2021
of resistance is based on the results of measurements c
calibrated in terms of the quantum Hall effect used as
value of the von Klitzing constant $R_K = h/e^2$ is set
Weights and Measures (CGPM).

Temperature (°C)	Pressure (kPa)
25.000	101.61

The reported uncertainty, consistent with practice re
and Measures (BIPM), is the expanded uncertainty,
uncertainty for all known sources of error and k is a c
NIST uses a coverage factor of $k = 2$. The expanded u

$$U = 2u_c =$$

where u_i is the estimated relative standard uncertainty
as an equivalent standard deviation. One component i
the pooled standard deviation from a large population

The calibration uncertainty is affected by the measure
and calculated using the method described in NIST Te
no allowances for the long-term drift of the standa
transporting this standard between laboratories.

Measurements performed by:

Alireza R. Panna
Quantum Measurement Division

Test Report No.: 684.05/O-0000034697-21
Date: June 17, 2021
Telephone Contact: 301-975-4221

UNITED STATES DEPARTMENT OF COMMERCE
National Institute of Standards and Technology
Gaithersburg, Maryland 20899

REPORT OF CALIBRATION

Order Number 684/O-0000034248-21
SKU:22021C

Thermo Fisher
Attn: Martin

112 Colonna
Ottawa, ON K
Canada
Calibration Item:
ID: 1kg SS
Manufacturer of Calibration

Measurements and analyses com

Report issued on Ma

Each item described in this report was found to be i

Persons performing, analyzing and
Patrick Abbott (Project Lead

ZEINA KUBARYCH
Digitally signed by ZEINA KUBARYCH
Date: 2021.03.19 13:22:25 -04'00'
For the Director of the National Institute of Standard
Dr. Zeina J. Kubarych, Leader
Mass and Force Group
Quantum Measurement Division
Physical Measurement Laboratory

1

UNITED STATES DEPARTMENT OF COMMERCE
National Institute of Standards and Technology
Gaithersburg, Maryland 20899-8440

REPORT OF CALIBRATION
39045C Irradiance Standard, 1 kW Quartz-Halogen Lamp
(250 nm to 2400 nm) (NIST ISSUED)

for

Osram, Model # FEL, Serial # F-747

Issued to:

NIST Division 685.04
Attn.: John Woodward
100 Bureau Drive, Stop 8444
Gaithersburg, MD 20899

Date of Issue: January 11, 2021

1. Description of Calibration Item

A 1 kW, quartz-halogen lamp with a coiled-coil tungsten filament was calibrated by the National Institute of Standards and Technology (NIST) as a standard of spectral irradiance from 250 nm to 2400 nm. The lamp is mounted in a medium bi-post base. The serial number is located on the rear of the lamp base opposite the side viewed by the spectroradiometer.

2. Description of Calibration

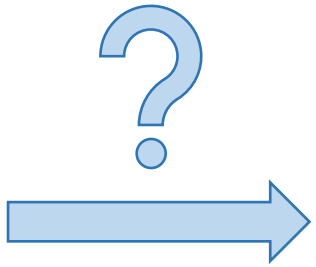
The lamp was calibrated in the new NIST Facility for Automated Spectroradiometric Calibrations (FASCAL 2) using the equipment and procedures described in Ref. [1]. A spectroradiometer utilizing a f-number of 4.8 and a spectral bandwidth of 3.5 nm from 250 nm to 1050 nm and 7 nm from 1050 nm from 2400 nm was used to measure the irradiances of the standard and test sources.

The lamp was measured at a distance of 50 cm from the entrance aperture of the integrating sphere with an aperture area of 1.0027 cm^2. The sphere viewed approximately a 9 cm diameter target in the plane of the front surface of the lamp bi-posts. With this geometry, the entire lamp was viewed from the top of the lamp envelope down to the top half of the black lamp base. Light baffling was used between the lamp and the spectroradiometer integrating sphere to minimize effects of scattered light. The alignment of the lamp is described in the next paragraph.

Laboratory Environment:
Temperature: 18 °C ± 1 °C
Relative Humidity: 25 % ± 5 %

Calibration Date: December 1, 2020
NIST Order No: O-0000034150

Page 1 of 7 NIST



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        </name>
        <real xmlns="https://ptb.de/si">
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          </expandedUnc>
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</result>
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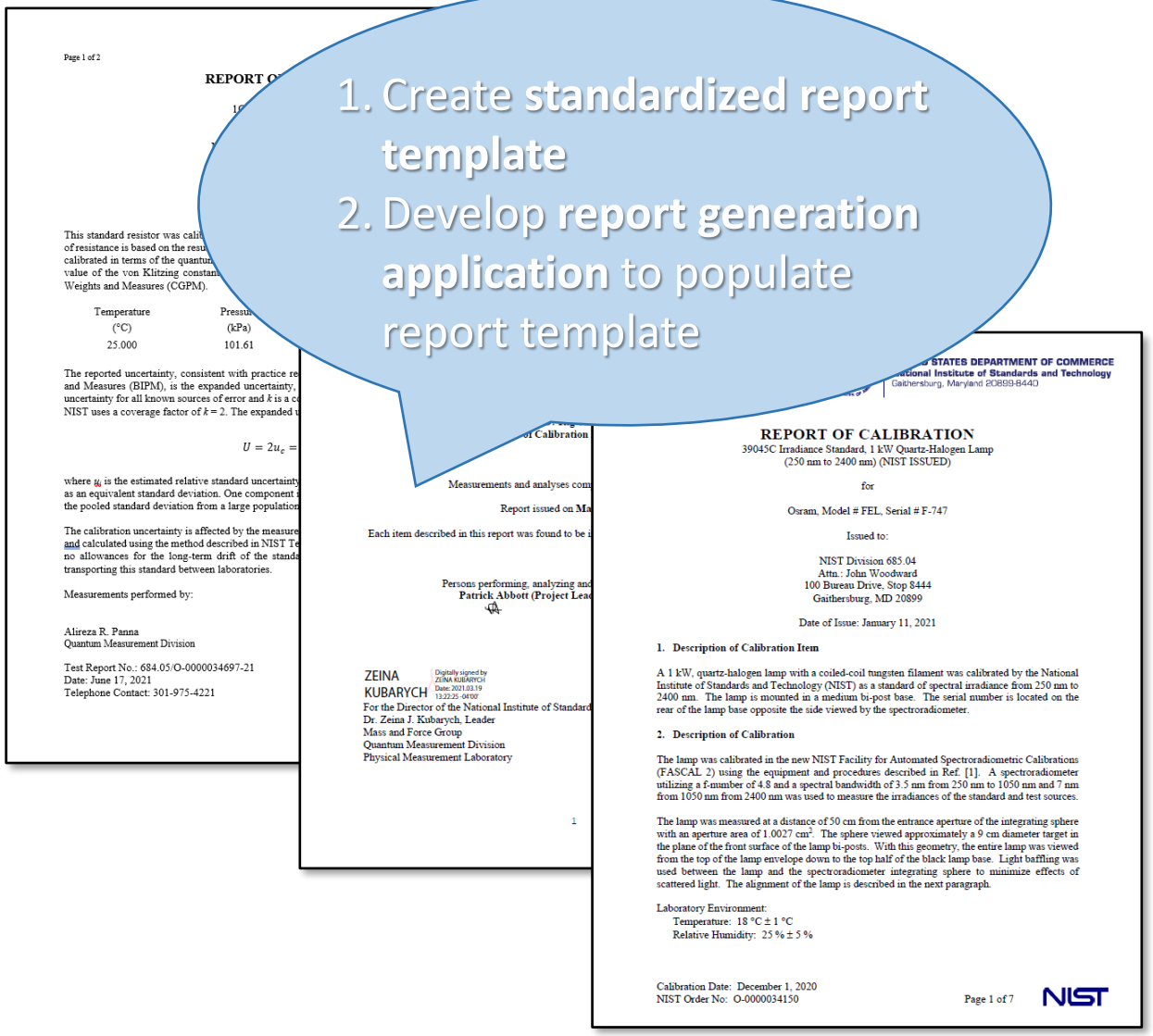
First Steps towards Digital Transformation

1. Create **standardized report template**
2. Develop **report generation application** to populate report template



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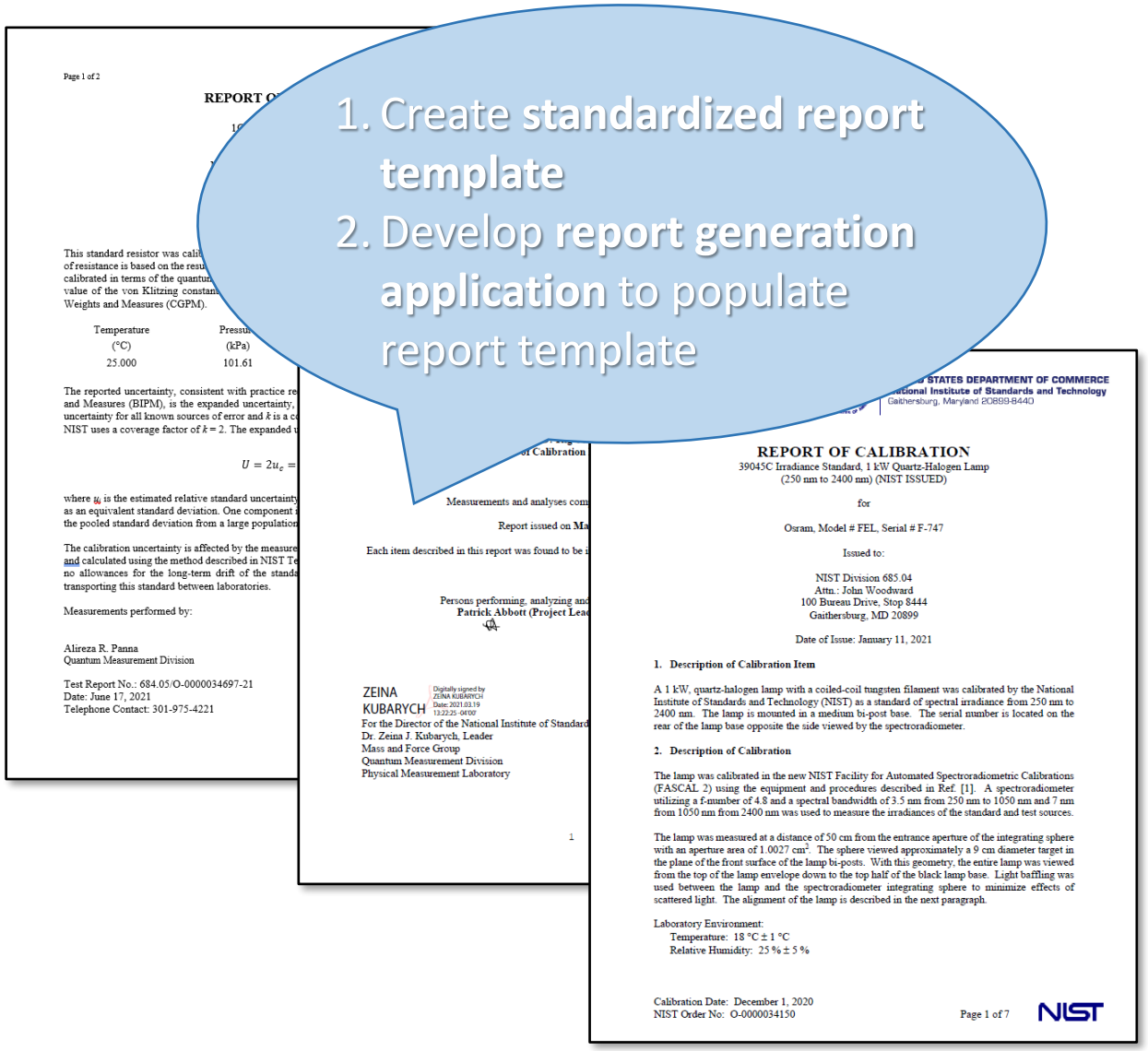
First Steps towards Digital Transformation

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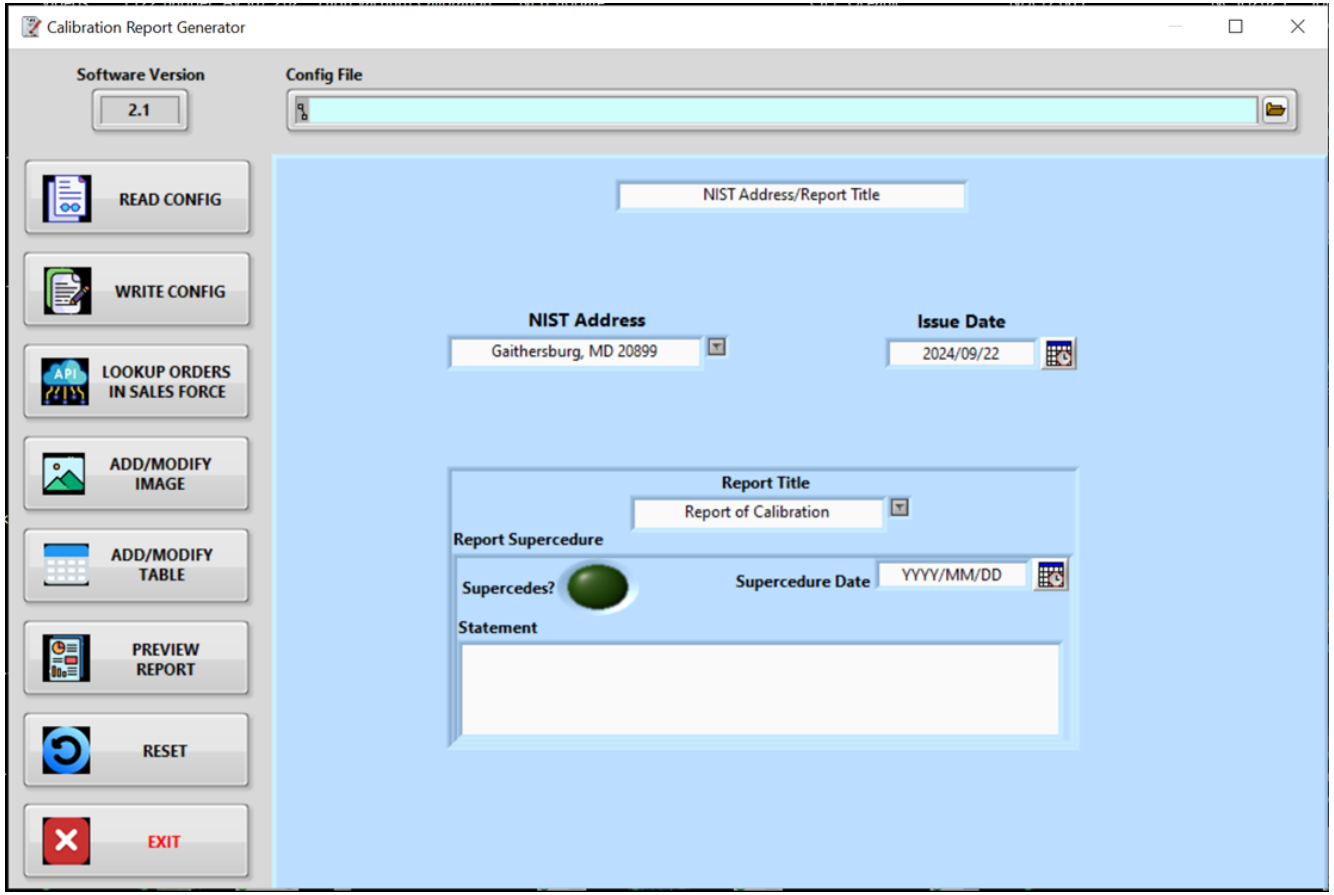
            <coverageFactor>2</coverageFactor>
            ...y>0.95</coverageProbability>
```

3. Report **elements** are easily identified, **digitalized**, and mapped to DCC schema

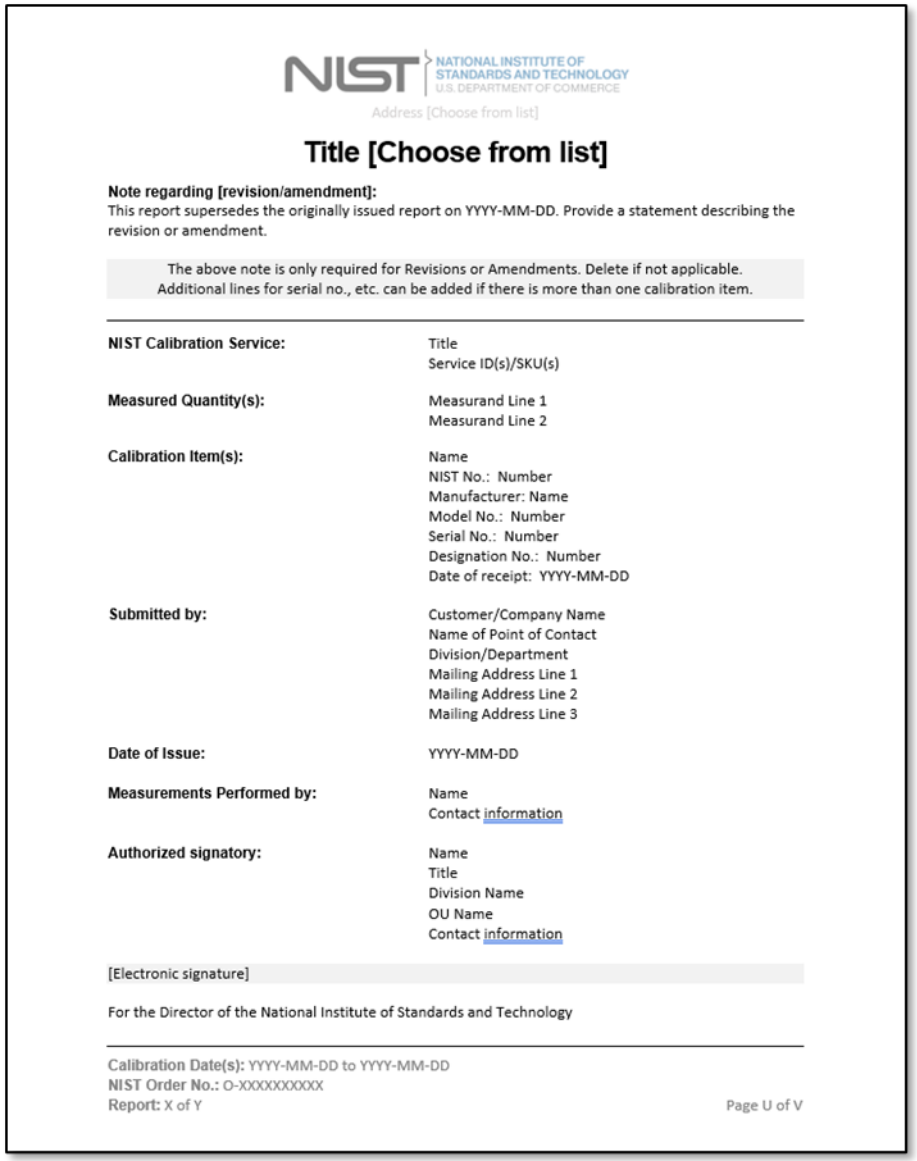
Advantages of Report Generation Application

- Import customer metadata from e-commerce
- Import content from previous calibration reports, such as Calibration Method Description
- Import/copy data and figures from results spreadsheets or other databases
- Outputs Word file that can be edited as needed
- Reduces transcription and copy-paste errors
- Facilitates future efforts to map report content to DCC schema



"Beta" version of application
Thanks to John Qunitavalle

Advantages of Report Generation Application



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U.S. DEPARTMENT OF COMMERCE

Address [Choose from list]

Title [Choose from list]

Note regarding [revision/amendment]:
This report supersedes the originally issued report on YYYY-MM-DD. Provide a statement describing the revision or amendment.

The above note is only required for Revisions or Amendments. Delete if not applicable.
Additional lines for serial no., etc. can be added if there is more than one calibration item.

NIST Calibration Service:	Title Service ID(s)/SKU(s)
Measured Quantity(s):	Measurand Line 1 Measurand Line 2
Calibration Item(s):	Name NIST No.: Number Manufacturer: Name Model No.: Number Serial No.: Number Designation No.: Number Date of receipt: YYYY-MM-DD
Submitted by:	Customer/Company Name Name of Point of Contact Division/Department Mailing Address Line 1 Mailing Address Line 2 Mailing Address Line 3
Date of Issue:	YYYY-MM-DD
Measurements Performed by:	Name Contact information
Authorized signatory:	Name Title Division Name OU Name Contact information

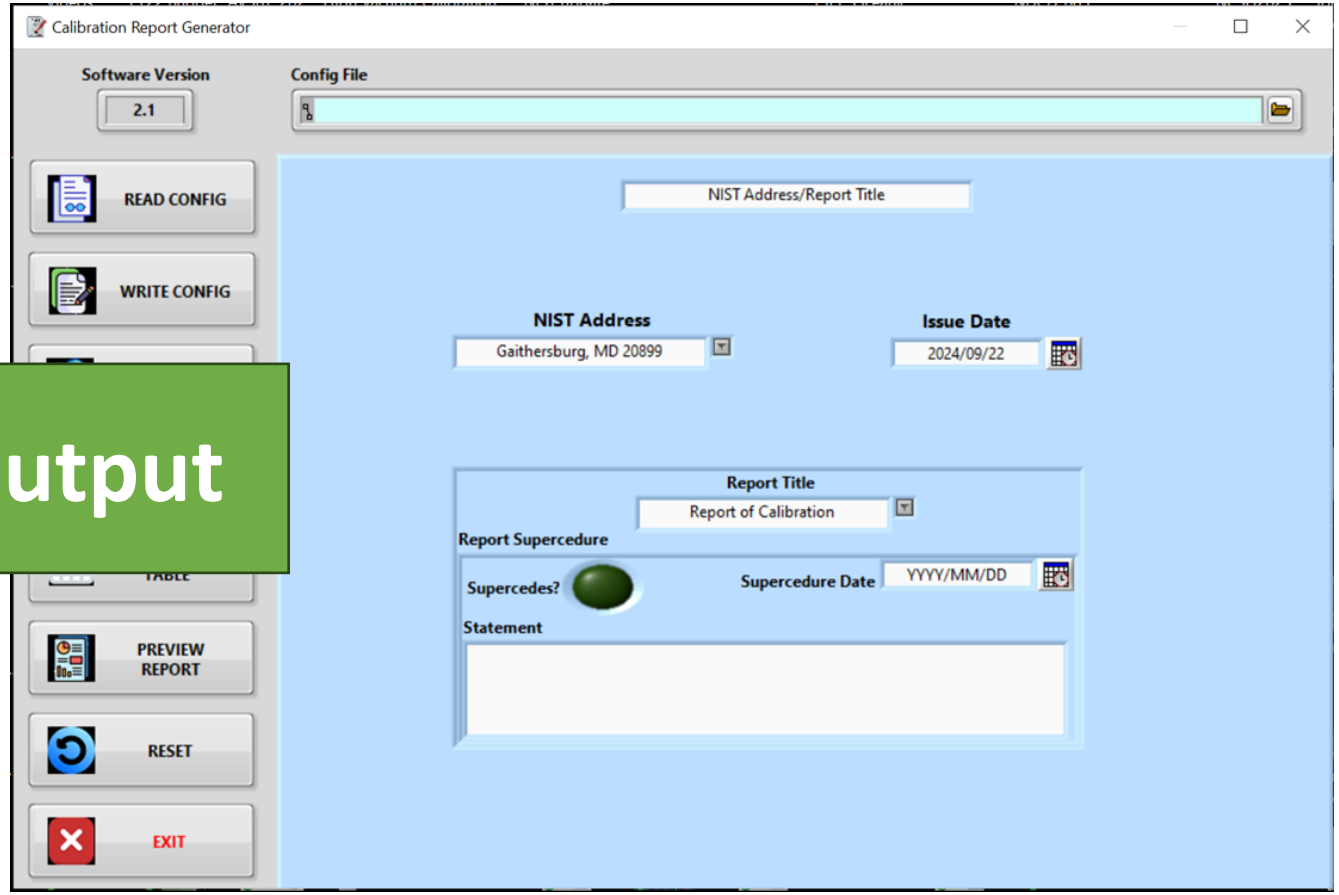
[Electronic signature]

For the Director of the National Institute of Standards and Technology

Calibration Date(s): YYYY-MM-DD to YYYY-MM-DD
NIST Order No.: O-XXXXXXXXXX
Report: X of Y

Page U of V

Output



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Advantages of Report Generation Application

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            <coverageProbability>0.95</coverageProbability>
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</result>
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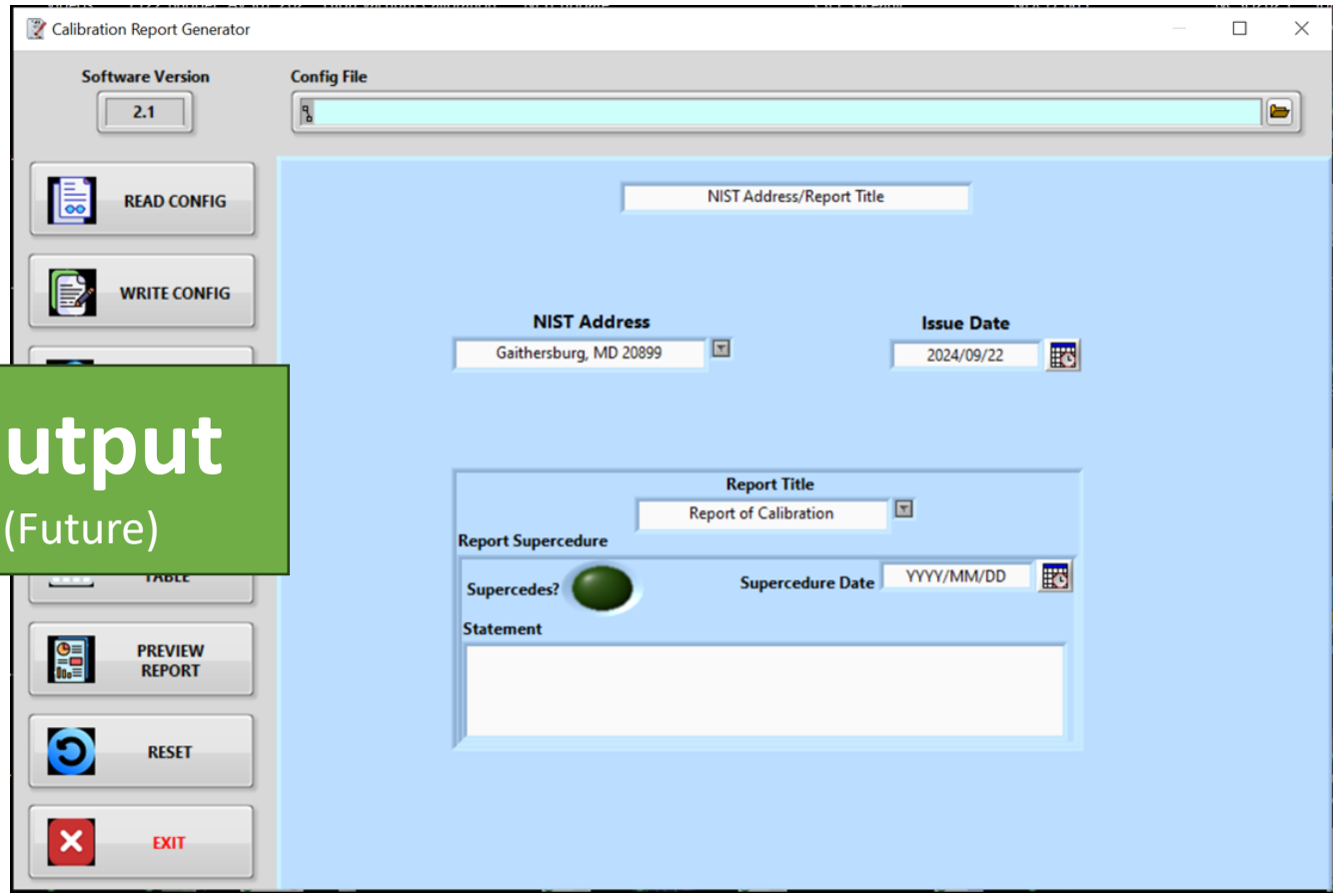
Output
(Future)



"Beta" version of application

NIST Standard Reference Materials (SRM)

>1100 SRM Products

- Ferrous Metals
- Nonferrous Metals
- Microanalysis
- High Purity Materials
- Health and Industrial Hygiene
- Inorganics
- Primary Gas Mixtures
- Fossil and Alternative Fuels
- Organics
- Food and Agriculture
- Geological Materials and Ores
- Ceramics and Glasses
- Cement
- Engine Wear Materials
- Forensics
- Ion Activity
- Polymeric Properties
- Thermodynamic Properties
- Optical Properties
- Radioactivity
- Electrical Properties
- Metrology, Liquids and Glasses
- X-Ray Diffraction
- Sizing
- Surface Finish
- Fire Research
- Nanomaterials
- Miscellaneous Performance Engineering Materials

Digital Reference Materials Certificate (DRMC)

What Goes in a DRMC?
The DRMC has many similar elements as the DCC, but it has many other elements as well

Effort let by Dinis Camara

Based On:

ISO 17034

ISO Guide 31/ISO 33401:2024

NIST Quality Manual

NIST Policy

Customer Input

Current Draft of Schema

- Organization Identification
- Reference Material Identification
- Material Information
  - Unit Description
  - Usage Information
  - Measurement Information
  - Additional Information
- Context
- Provenance
- References

Types of Values

- **Values with uncertainties**
- **Sequences**
- **Formulas**

Table 1. Certified Mass Fraction Value for SRM 2454a Hydrogen in Titanium Alloy

Constituent	Mass Fraction (mg/kg)	95 % Coverage Interval (mg/kg)
Hydrogen (H)	216.0	207.6 to 224.4

RM 8671 Heavy Chain Amino Acid Sequence

QVTLRESGPALVKPTQTLTLTCTFSGFSLSTAGMSVGWIRQPPGKALEWLADIWWDDKKHYNPSLKDRLTIS
KDTSKNQVVLKVTNMDPADTATYYCARDMIFNFYFDVWGQGTTVTVSS ASTKGPSVFPLAPSSKSTSGGTA
ALGCLVKDYFPEPVTVSWNSGALTSGVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYICNVNHKPSNTKVD
KRV *EPKSCDKTHTCPPCP* **APELLGGPSVFLFPPKPKDTLMISRTPEVTCVVVDVSHEDPEVKFNWYVDGV**
EVHNAKTKPREEQYNSTYRVVSVLTVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPS
REEMTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTTPPVLDSDGSFFLYSKLTVDKSRWQQGNVFSCS
VMHEALHNHYTQKSLSLSPGK

RM 8671 Light Chain Amino Acid Sequence

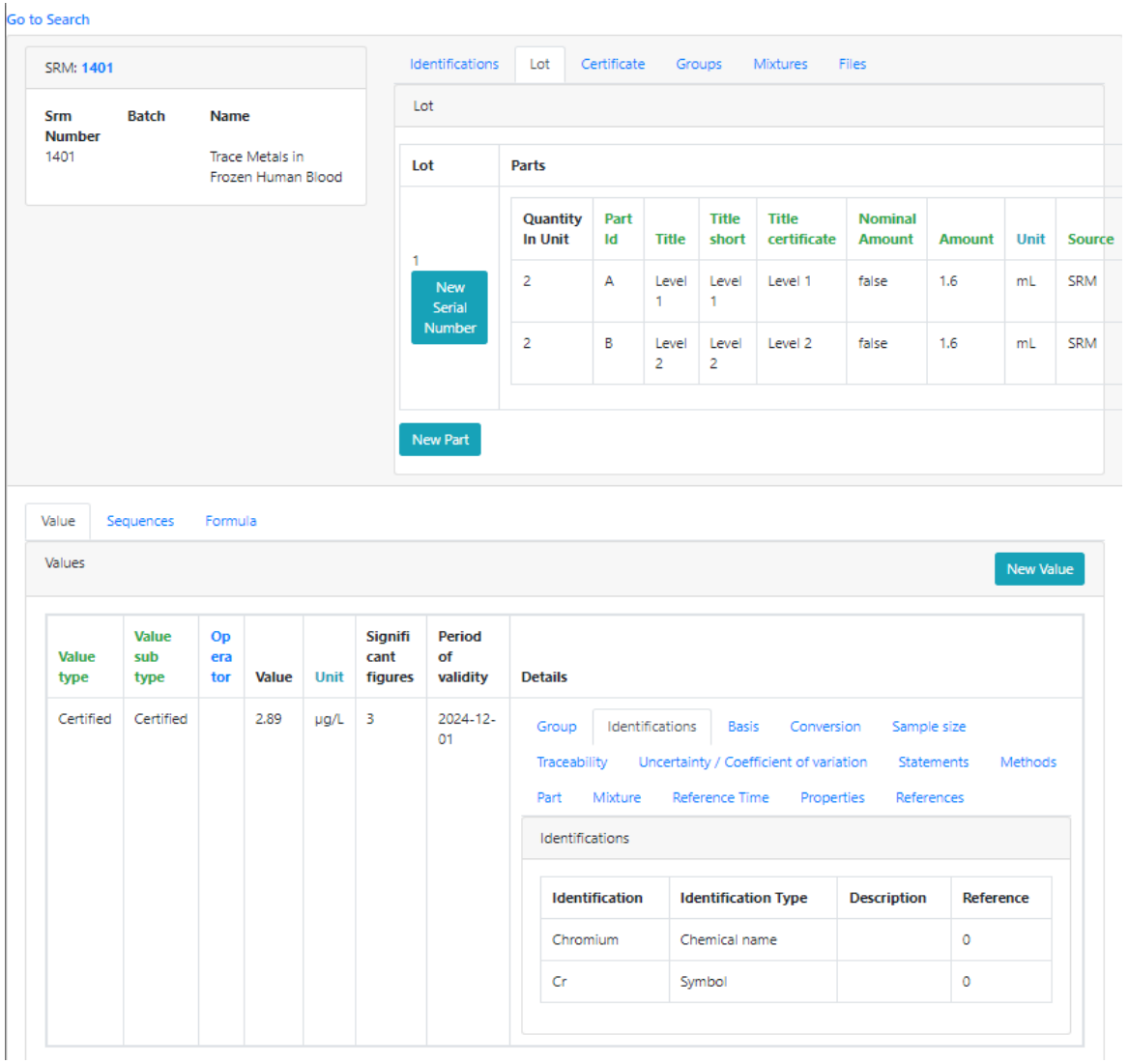
DIQMTQSPSTLSASVGDRVTITCSASSRVGYMHWYQQKPGKAPKLLIYDTSKLASGVPSRFSGSGSGTEFTLT
ISSLQPDDFATYYCFQGSGYPFTFGGGTKVEIK RTVAAPSVFIFPPSDEQLKSGTASVVCLLNNFYPREAKV
QWKVDNALQSGNSQESVTEQDSKDSTYSLSSTLTLSKADYEKHKVYACEVTHQGLSSPVTKSFNRGEC

Figure A1. Primary amino acid sequence for RM 8671 with variable fragment antigen-binding (Fab) region in normal font, constant Fab region underlined, hinge region in italics, and Fc region in bold.

$$\lambda = -1.97313\times10^{-3} + 1.99227\times10^{-5}\rho + 1.07923\times10^{-4}T \pm 1.0\ \%\ (k=2)$$

Database Creation

- Create a repository which accommodates Values (Numbers), Sequences, and Formulas
- Accommodates both reported values and additional values in certificates
- Integrate with current IT applications and DBs
- Version 1

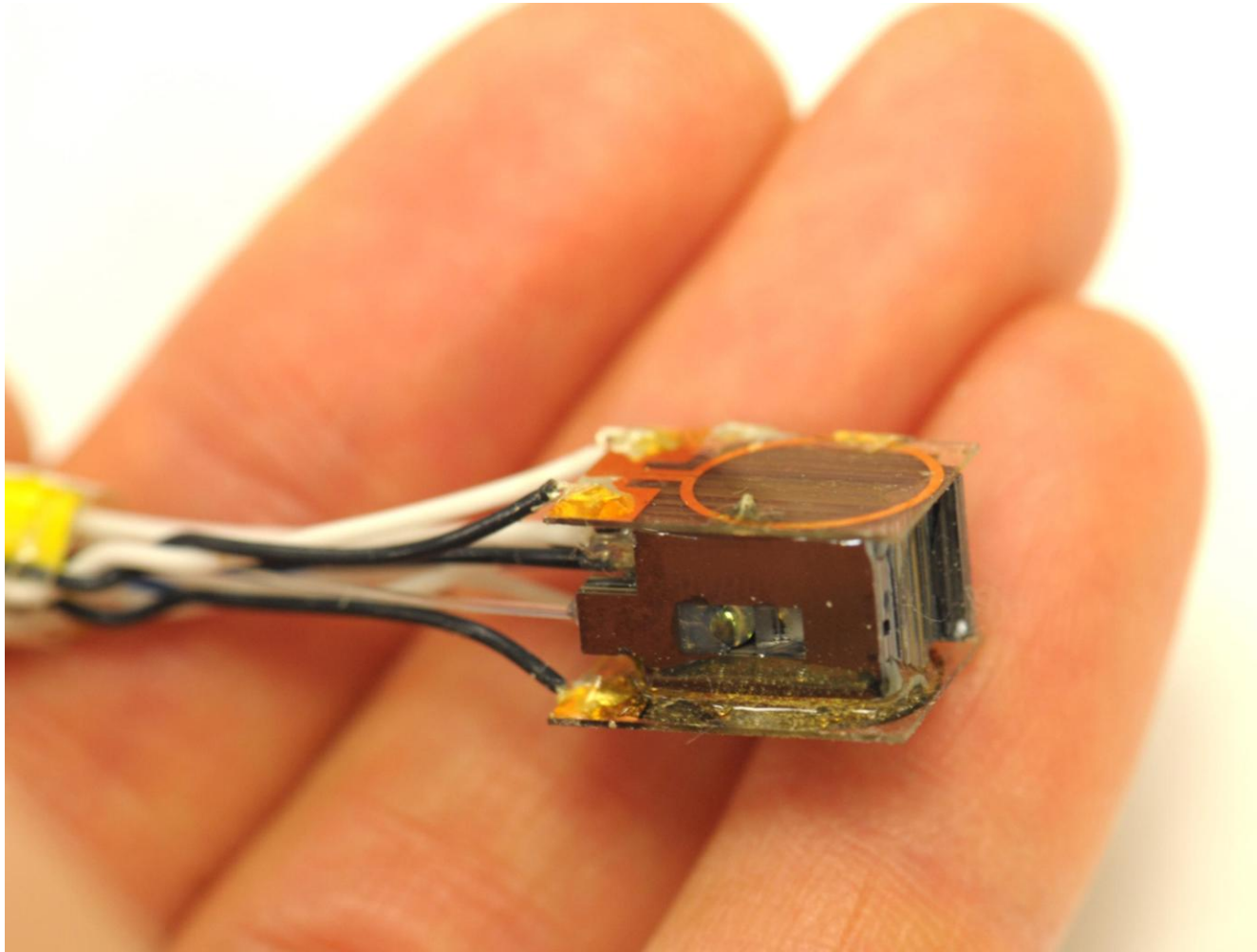


Traceability

NIST has vested interested in digital traceability

- Digital Traceability concepts could be key to the NIST on a Chip Program
  - Intrinsic SI-traceable standards
  - Deployed or embedded

- No formal program yet for digitalization.



Future

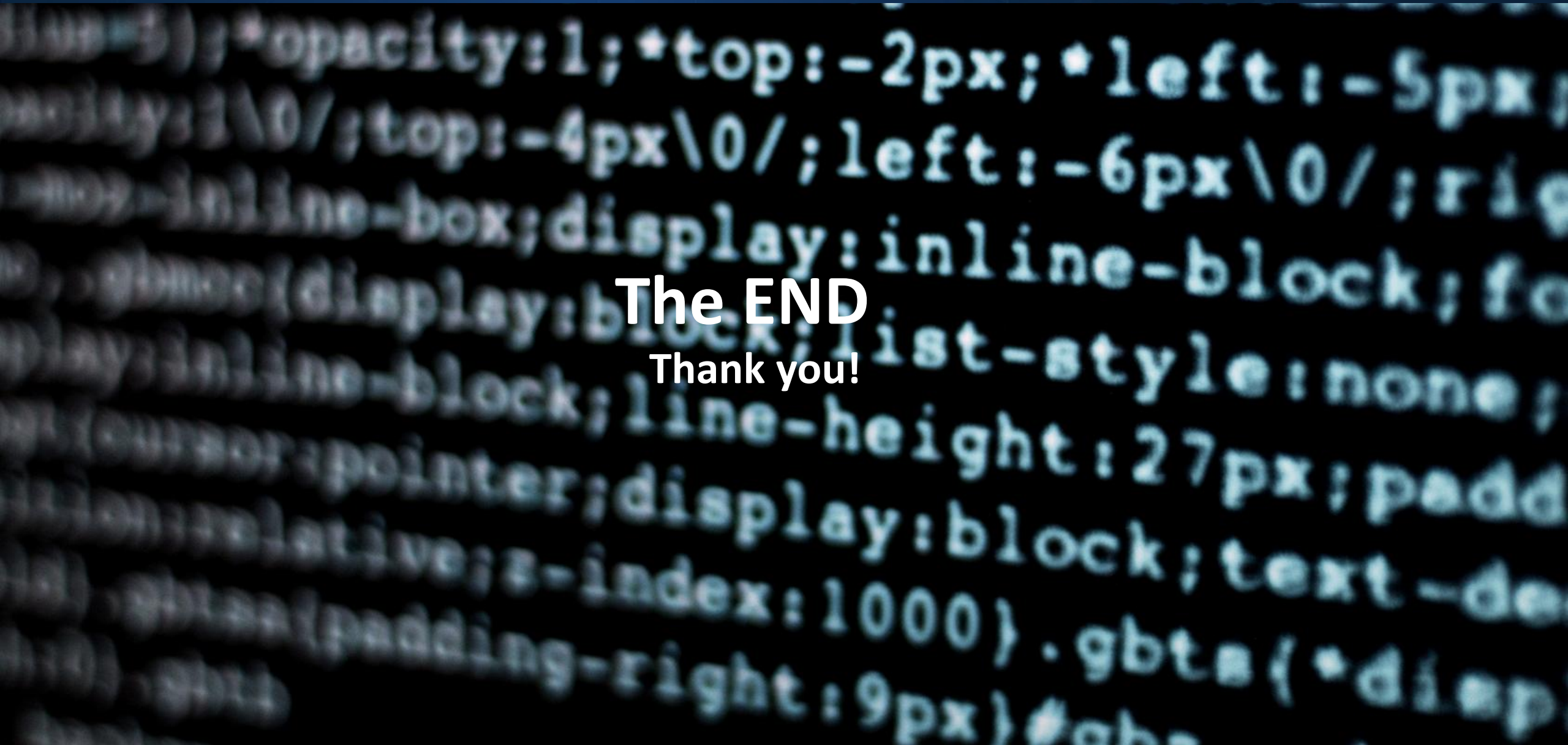
- Continue to develop automatic calibration report generation
  - Produce digital reports
- Develop internal repositories to increase internal efficiency
- Develop repository and schema for reference materials
- Develop models for digital traceability
- Future ideas:
  - Digitizing the quality system
  - Digital calibration requests

Acknowledgements

Digital NIST Team:

Dinis Camara
Benjamin Long
Robert Hanisch
Catherine Rimmer
Steven Choquette
Katya Delak
Itzel Domínguez Mendoza (CENAM)
James Fedchak
Catherine Cooksey
John Quintavalle

Scientists, Statisticians, other NIST Experts


The END
Thank you!