

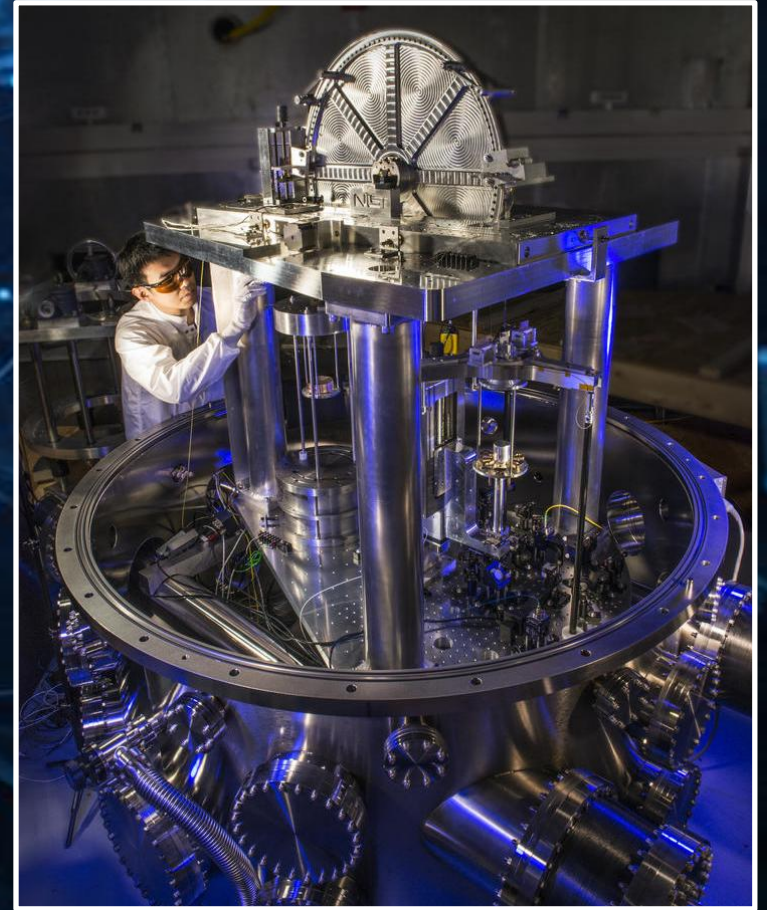
Digital Transformation and NIST's Measurement Services

James Fedchak

Associate Director for Measurement Services
Physical Measurement Laboratory

Digital Transformation of Metrology

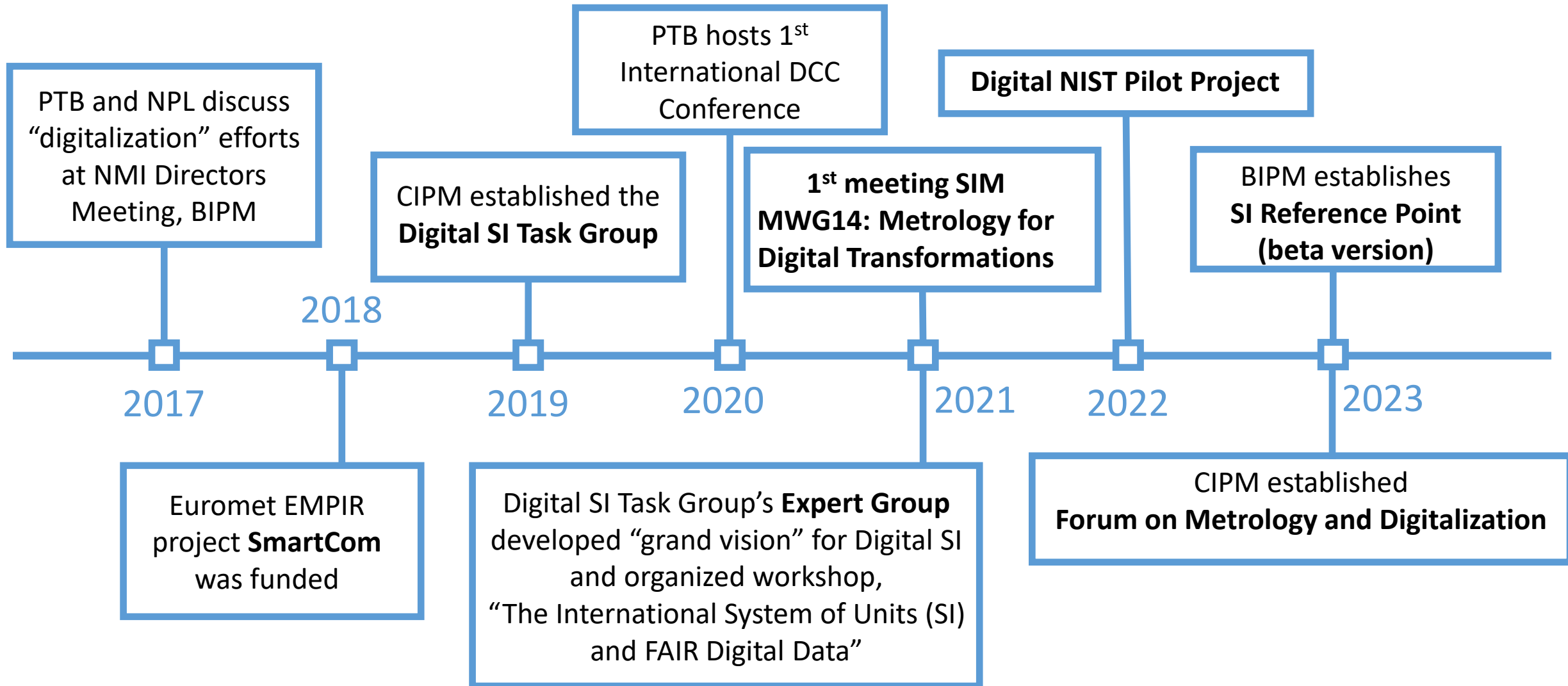
- **The world is clearly being transformed by digital technologies**
- **Examples of Digital Concepts that Metrology can Support:**
 - Industry 4.0/IoT
 - Smart Factories
 - Networked sensors
 - Digital twins
 - Machine learning & AI
 - Remote sensing/calibrations
- **Supportive Digital Metrology Tools**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



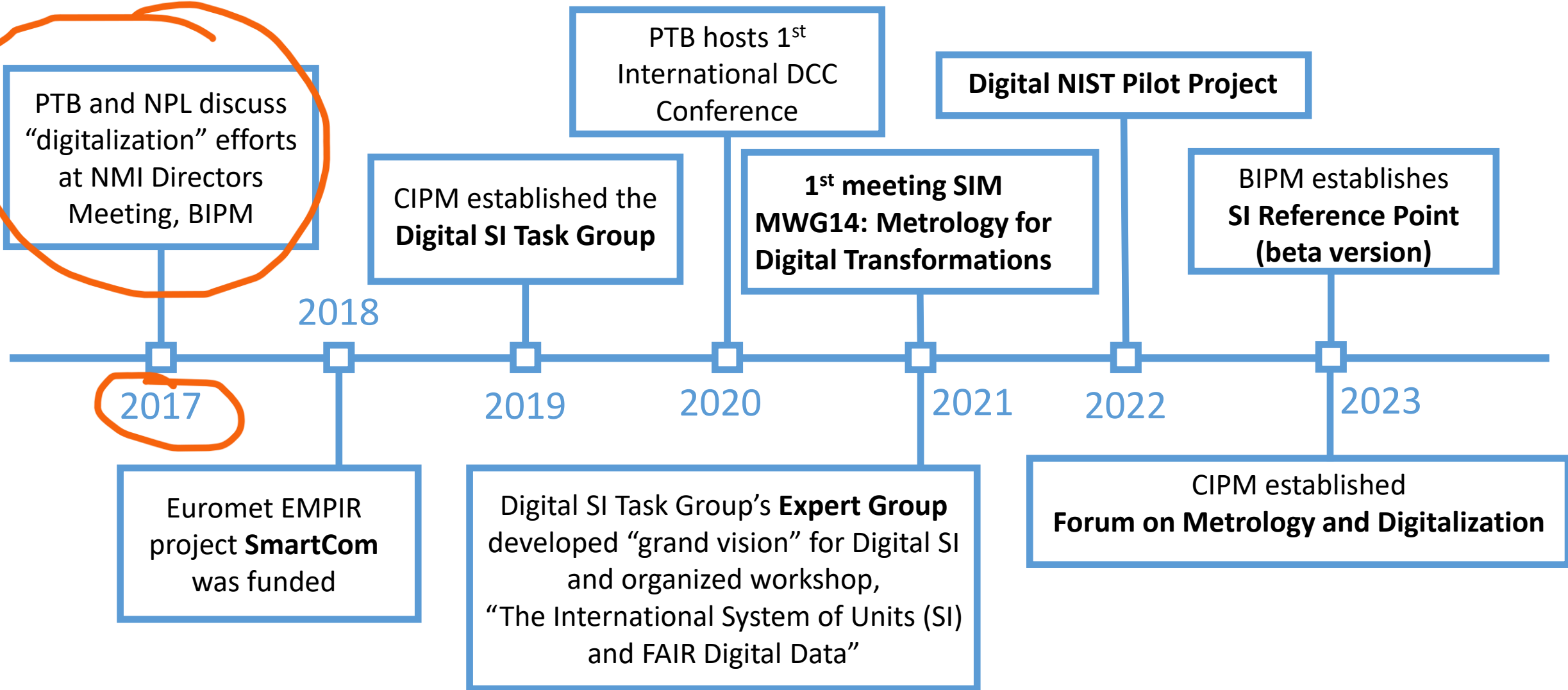


Background Information

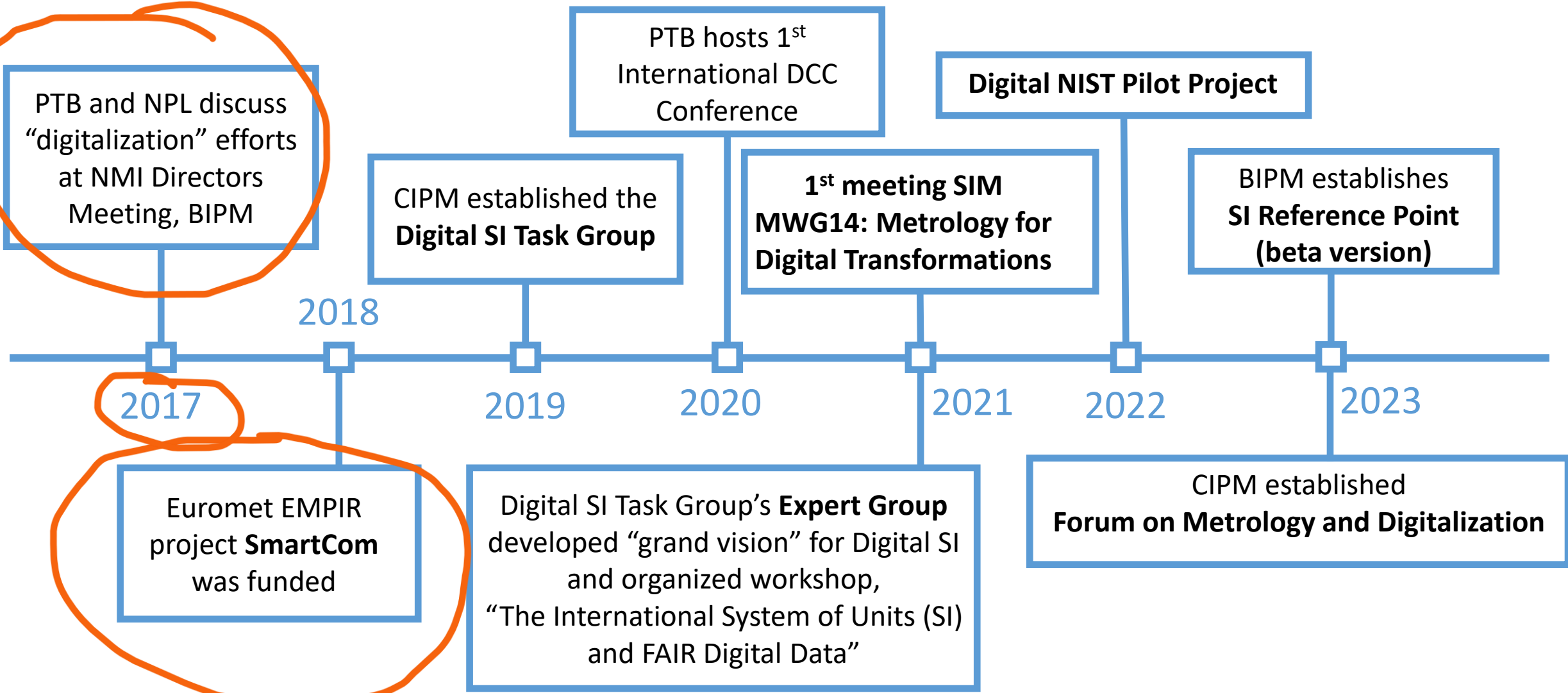
Movement for Digital Transformation of Metrology



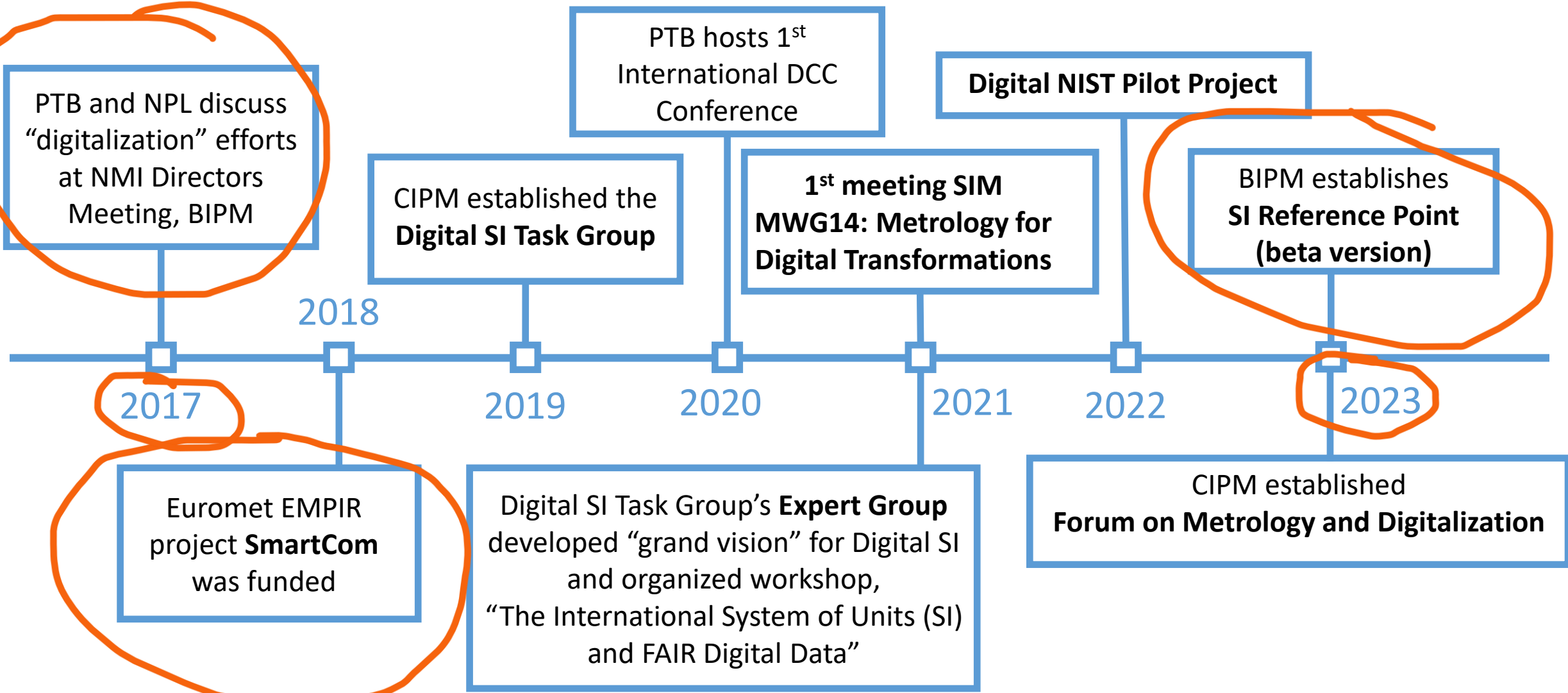
Movement for Digital Transformation of Metrology



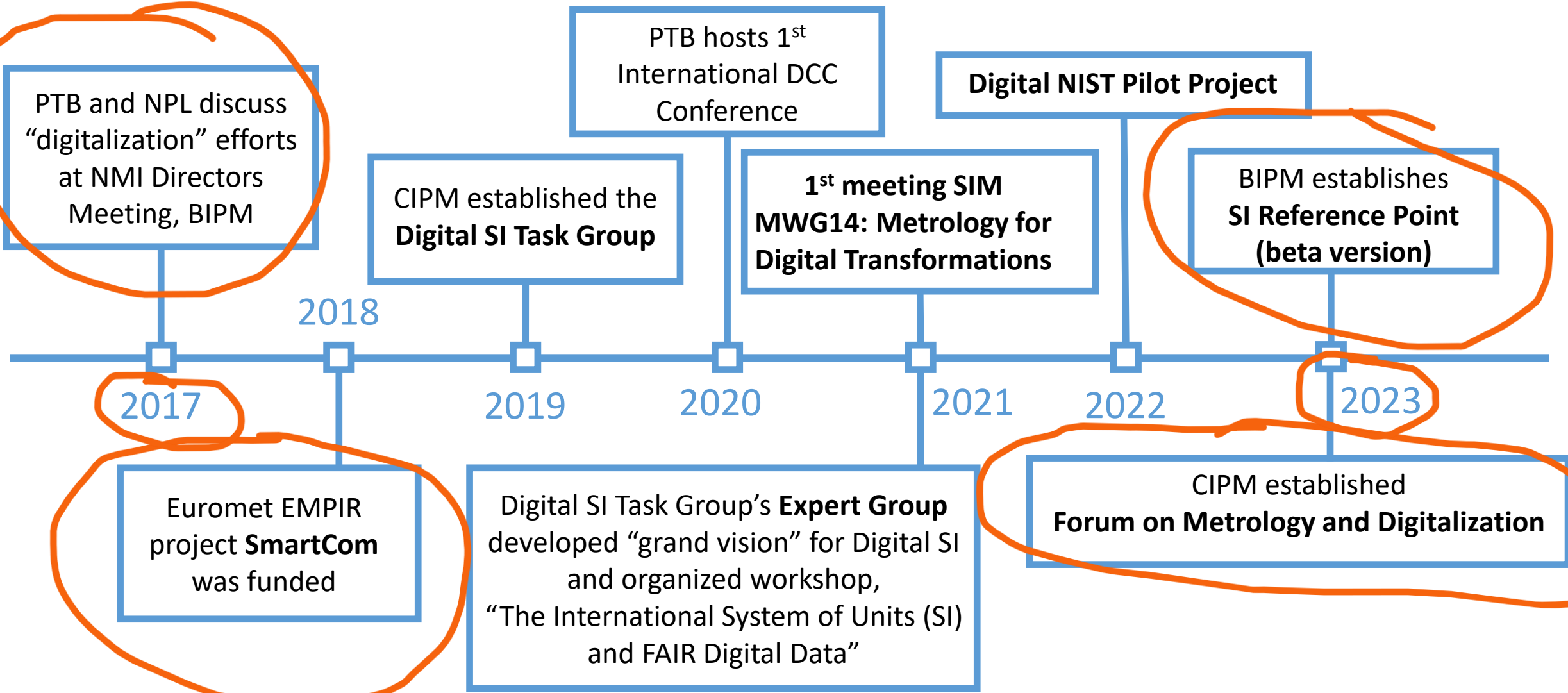
Movement for Digital Transformation of Metrology



Movement for Digital Transformation of Metrology



Movement for Digital Transformation of Metrology



Digital Transformation of Metrology in Europe

Vision: Develop and establish the basis for an unambiguous, universal, safe and uniform communication of metrological data in the Internet of Things (IoT) and Industry 4.0 **17IND02**

need

- worldwide exchange of metrological data, global competition
- chaos and accident prevention
- unambiguity of metrological data
- significant cost reduction (communication costs, bug fixing, liability, device and software adaption)
- digitisation of trade production, metering, homes, buildings, devices, mobility

ground-breaking idea

- universal
- SI-based
- easy and fast implementation
- first digital calibration certification worldwide
- easy integration in existing structures
 - based on SI-units
- covering legal metrology
- 100% praxis oriented
- applicable to all metrological domains

excellence of idea

- worldwide first DCC
- legal metrology oriented
- core competence of NMIs

excellence of the consortium

- driven by leading European NMIs; a worldwide consortium with world market leaders from industry

scientific and technical excellence

- advanced cryptography and data handling concepts using e. g. blockchain or hash chain technology
- research on legal requirements and exchange and conversion of data, mathematical + numerical correctness

excellence

$$2 - \frac{1}{2} \sqrt{4.111 \cdot 10^{-10} + 2.0275 \cdot 10^{-10}} = 2.0275 \cdot 10^{-10}$$

outcome and impact

develop and implement required tools:	communication syntax			
Use/consider conventional concepts:	cloud	RAMI	XML schemes	cryptography
consider regulations and standards:	GUM VIM	SI units	CO-DATA	ISO 17025

worldwide relevance: existing NMI network, multiplier effect

SI-world

2 pilot-applications in two different metrological domains (length-metrology, weighing)

mid-term stakeholder workshop

guidelines "meta-data-format" and "UniTerms in metrology"

1 brochure "digital communication", 1 handbook about data-validation, 1 pre-normative document on DCCs

implementation

- WP 1 (PTB) data transfer format
- WP 2 (NPL) digital calibration certificate (DCC)
- WP 3 (NPL) online validation
- WP 4 (PTB) conformity assessment in legal metrology
- WP 5 (Aalto) build and validate two demonstrators
- WP 6 (CNL) create practice guides
- WP 7 (PTB) pilot application in weighing

SmartCom

- In 2018, metrology digital transformation efforts in Europe were greatly accelerated by the creation of the funded **Euromet EMPIR project SmartCom**
- PTB and NPL have 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 version="1.0" encoding="UTF-8" standalone="no" ?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:dcc="https://ptb.de/dcc" xmlns:si="https://ptb.de/si"
  <xs:import namespace="https://ptb.de/si" schemaLocation="https://ptb.de/si/v2.1.0/SI_Format.xsd"/>
  <xs:annotation>
    <xs:documentation> DCC - Digital Calibration Certificate Copyright (c) 2019 - 2021 Physikalisch-Technische B
      XSD is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied wa
      by the joint research project EMPIR 17IND02 (title: SmartCom). This project (17IND02) has received funding f
      lighthouse project GEMIMEG-II (GEMIMEG 01 HT20001E) funded by the German Federal Ministry for Economic Affa
    </xs:documentation>
  </xs:annotation>
  <xs:element name="digitalCalibrationCertificate" type="dcc:digitalCalibrationCertificateType"/>
  <xs:complexType name="digitalCalibrationCertificateType">
    <xs:annotation>
      <xs:documentation> The root element that contains the four rings of the DCC. </xs:documentation>
    </xs:annotation>
    <xs:sequence>
      <xs:element name="administrativeData" type="dcc:administrativeDataType"/>
      <xs:element name="measurementResults" type="dcc:measurementResultListType"/>
      <xs:element name="comment" minOccurs="0">
        <xs:complexType>
          <xs:sequence>
            <xs:any namespace="##any" minOccurs="0" maxOccurs="unbounded"/>
          </xs:sequence>
        </xs:complexType>
      </xs:element>
      <xs:element name="document" type="dcc:byteDataType" minOccurs="0"/>
    </xs:sequence>
  </xs:complexType>
  <xs:attribute name="schemaVersion" use="required">
    <xs:simpleType>
      <xs:restriction base="xs:string">
        <xs:pattern value="3\.1\.2"/>
      </xs:restriction>
    </xs:simpleType>
  </xs:attribute>
</xs:schema>
```

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

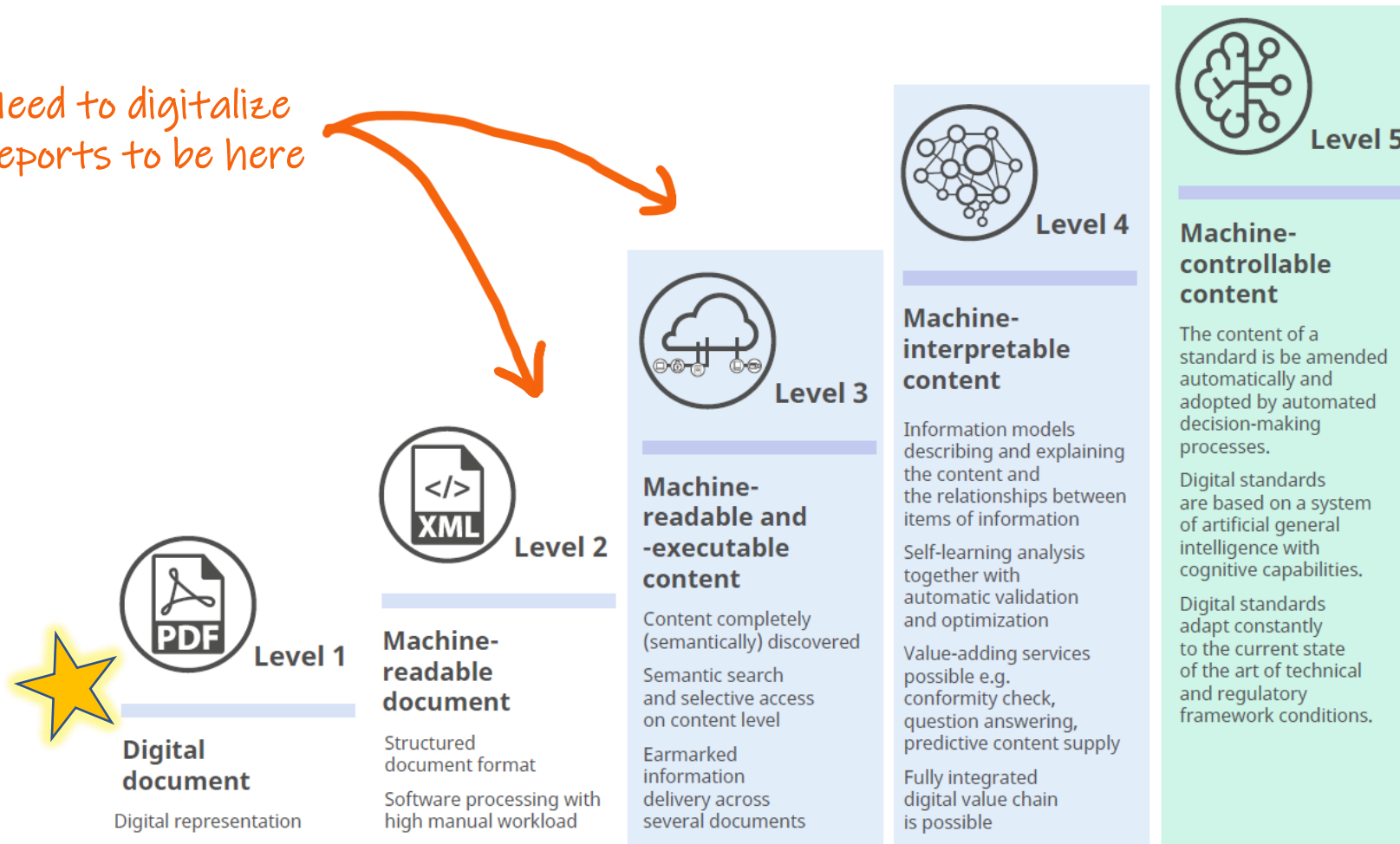




NIST Digital Transformation Efforts

Where are we at NIST?

Need to digitalize reports to be here



IDIS Whitepaper, "SCENARIOS FOR DIGITIZING STANDARDIZATION AND STANDARDS", 2021

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

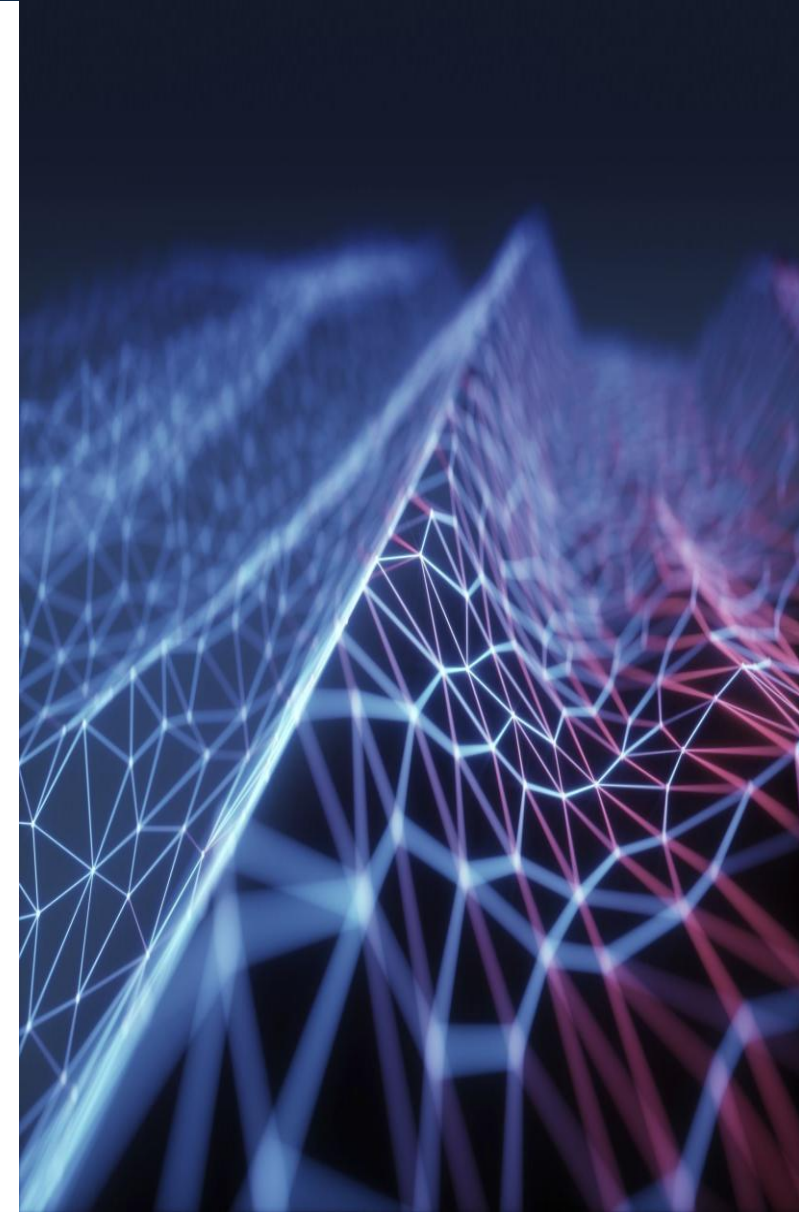
Digital Transformation of Metrology

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

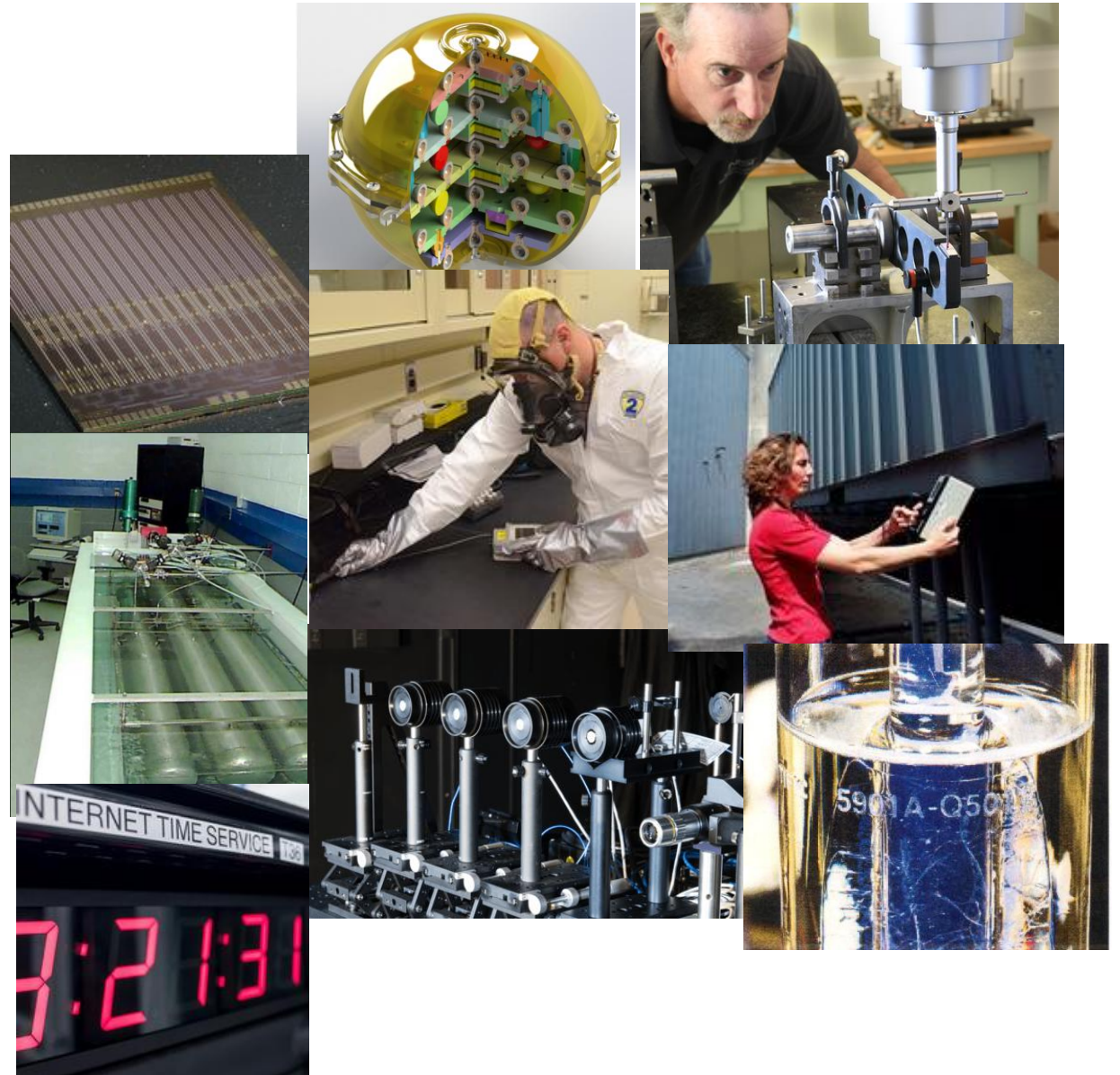


Calibration Services & Challenges

More than 500 Services

Nine Calibration Areas

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



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
Lockheed
Orlando

This standard resistor was calibrated on June 8, 2021 of resistance is based on the results of measurements d calibrated in terms of the quantum Hall effect used a value of the von Klitzing constant $R_K = h/e^2$ is set t 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 $U = 2u_c =$

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

The calibration uncertainty is affected by the measure and calculated using the method described in NIST T4 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: Martina I
112 Colonnade
Ottawa, ON K1P
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 s

Persons performing, analyzing and
Patrick Abbott (Project Lead)

ZEINA
KUBARYCH
For the Director of the National Institute of Standard
Dr. Zeina J. Kubarych, Leader
Mass and Force Group
Quantum Measurement Division
Physical Measurement Laboratory

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

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

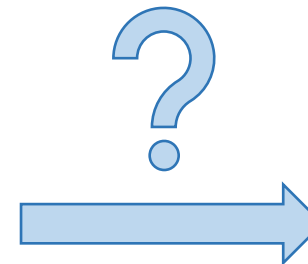
The lamp was calibrated in the new NIST Facility for Automated Spectroradiometric Calibrations (FASCAL 2) using the equipment and procedures described in Ref. [1]. A spectroradiometer utilizing a f -number of 4.8 and a spectral bandwidth of 3.5 nm from 250 nm to 1050 nm and 7 nm from 1050 nm from 2400 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 cm². 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



```
<result refType="measured_resistance">
  <name>
    <content lang="en">Measured Resistance</content>
  </name>
  <data>
    <list>
      <quantity refType="measured_resistance">
        <name>
          <content lang="en">Measured Resistance</content>
        </name>
        <real xmlns="https://ptb.de/si">
          <value>1.00000389</value>
          <unit>\ohm</unit>
          <expandedUnc>
            <uncertainty>0.04</uncertainty>
            <coverageFactor>2</coverageFactor>
            <coverageProbability>0.95</coverageProbability>
          </expandedUnc>
        </real>
      </quantity>
    </list>
  </data>
</result>
```

First Steps towards Digital Transformation

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

Page 1 of 2

REPORT OF CALIBRATION

This standard resistor was calibrated in terms of resistance based on the results of measurements made at the National Institute of Standards and Technology (NIST) using the von Klitzing constant, R_K , and the von Klitzing constant, R_K , and the von Klitzing constant, R_K .

Temperature (°C)	Pressure (kPa)
25.000	101.61

The reported uncertainty, consistent with practice and Measures (BIPM), is the expanded uncertainty, U , for all known sources of error and k is a coverage factor of $k = 2$. The expanded uncertainty is given by $U = 2u_c$, where u_c is the estimated relative standard uncertainty as an equivalent standard deviation. One component of the pooled standard deviation from a large population of measurements is affected by the measurement and calculated using the method described in NIST Technical Note 1331, "Guidelines for the long-term drift of the standard 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 20899-8443

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

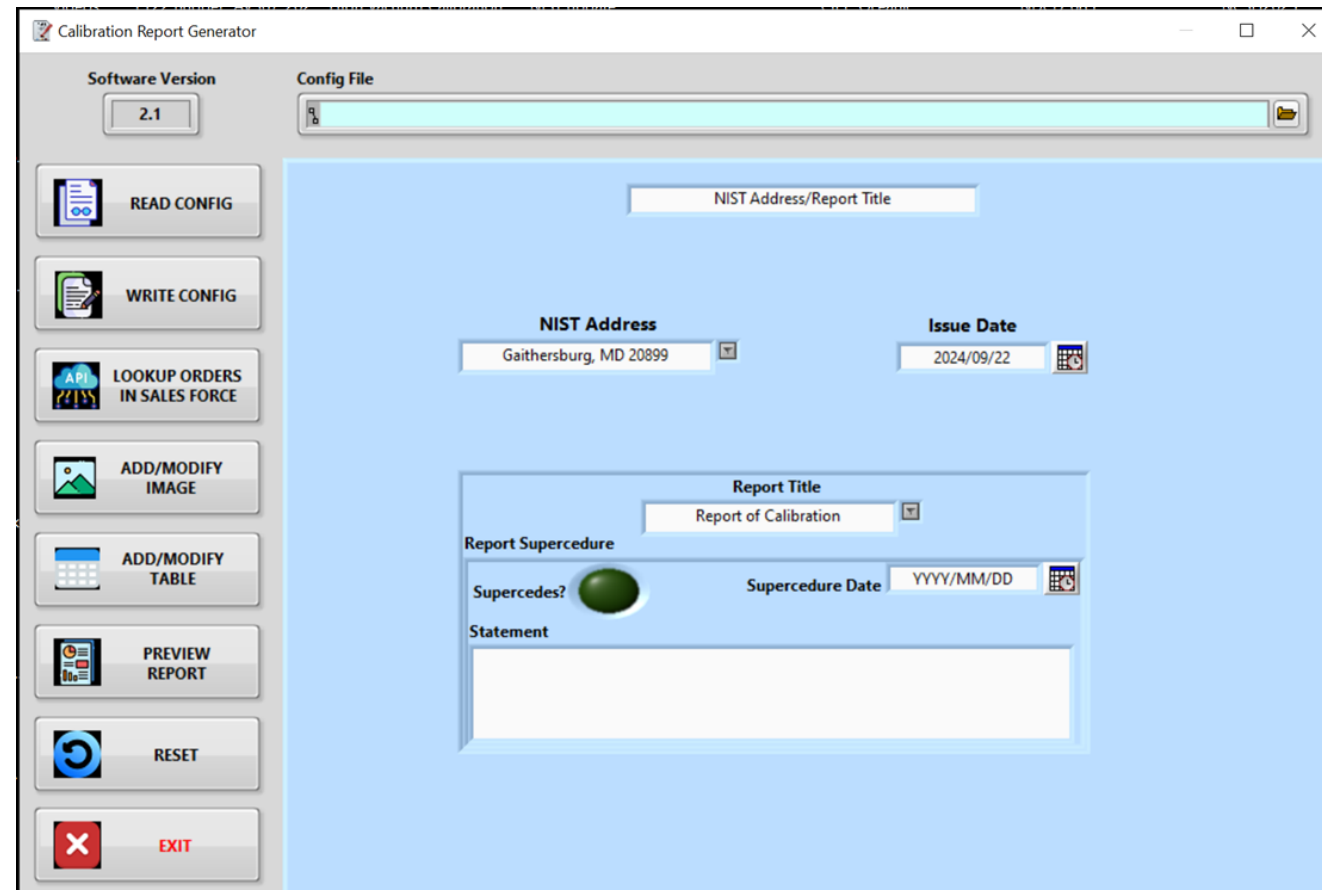
Calibration Date: December 1, 2020
NIST Order No: O-0000034150

Page 1 of 7

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<result refType="measured_resistance">
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  </name>
  <data>
    <list>
      <quantity refType="measured_resistance">
        <name>
          <content lang="en">Measured Resistance</content>
        </name>
        <real xmlns="https://ptb.de/si">
          <value>1.00000389</value>
          <unit>\ohm</unit>
          <expandedUnc>
            <uncertainty>0.04</uncertainty>
            <coverageFactor>2</coverageFactor>
            <coverageProbability>0.95</coverageProbability>
          </expandedUnc>
        </real>
      </quantity>
    </list>
  </data>
</result>
```


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



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.

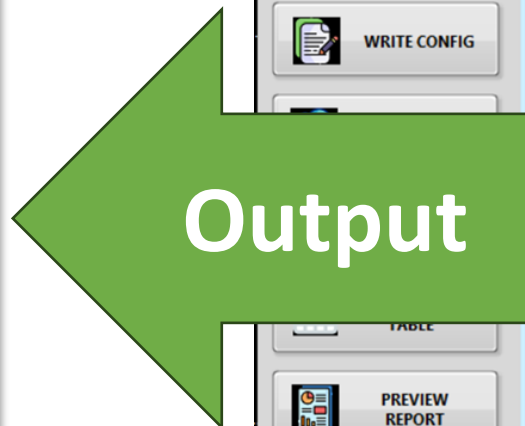
NIST Calibration Service:	Title Service ID(s)/SKU(s)
Measured Quantity(s):	Measurand Line 1 Measurand Line 2
Calibration Item(s):	Name NIST No.: Number Manufacturer: Name Model No.: Number Serial No.: Number Designation No.: Number Date of receipt: YYYY-MM-DD
Submitted by:	Customer/Company Name Name 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

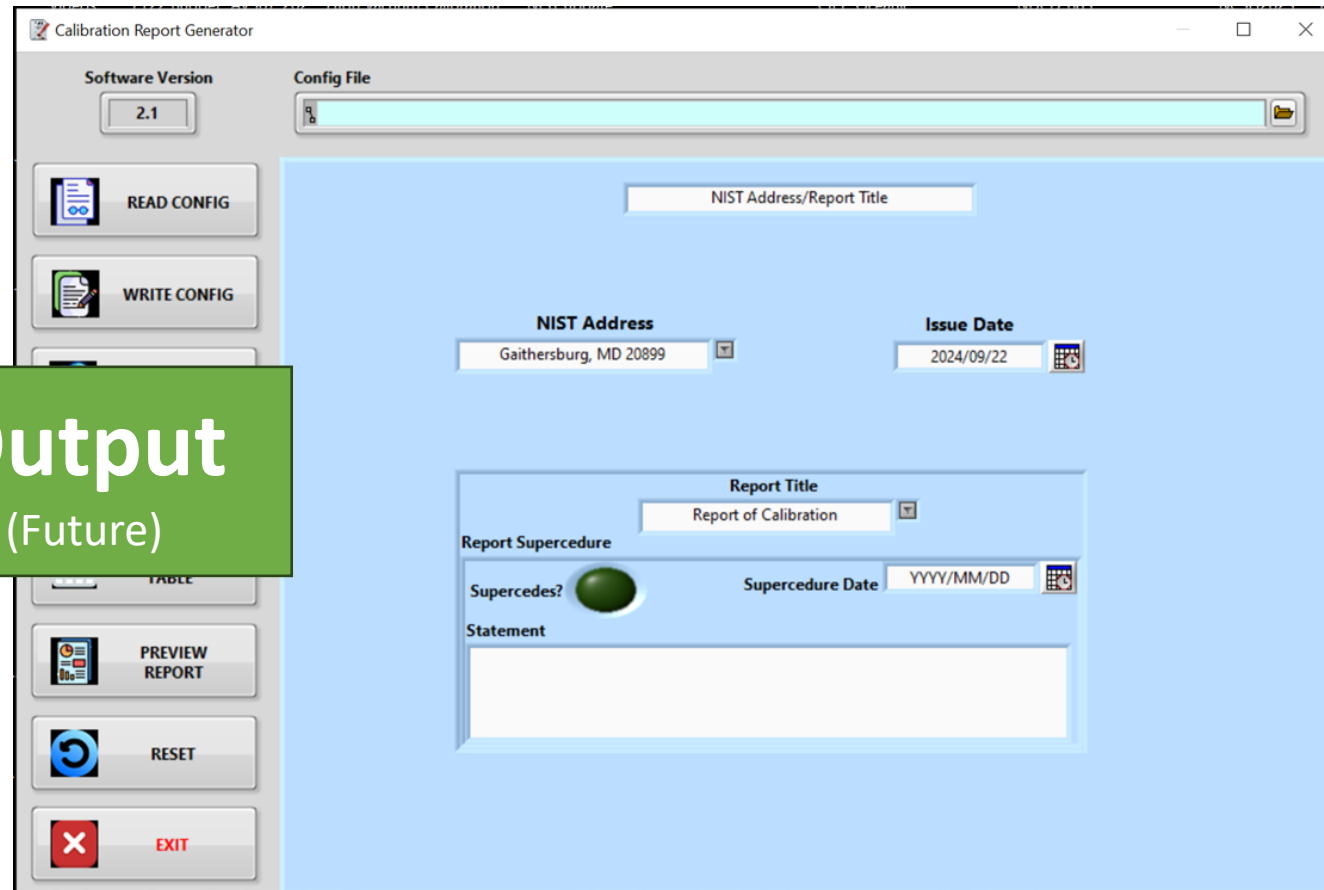
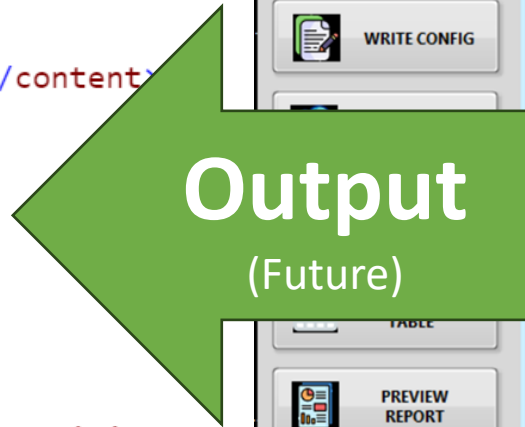
Page U of V



“Beta” version of application

Advantages of Report Generation Application

```
<result refType="measured_resistance">
  <name>
    <content lang="en">Measured Resistance</content>
  </name>
  <data>
    <list>
      <quantity refType="measured_resistance">
        <name>
          <content lang="en">Measured Resistance</content>
        </name>
        <real xmlns="https://ptb.de/si">
          <value>1.00000389</value>
          <unit>\ohm</unit>
          <expandedUnc>
            <uncertainty>0.04</uncertainty>
            <coverageFactor>2</coverageFactor>
            <coverageProbability>0.95</coverageProbability>
          </expandedUnc>
        </real>
      </quantity>
    </list>
  </data>
</result>
```



“Beta” version of application

>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 led 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

- 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

QVTLRESGPALVKPTQTLTLTCTFSGFSLSTAGMSVGVIRQPPGKALEWLADIWDDKKHYNPSLKDRLTIS
KDTSKNQVVLKVTNMDPADTATYYCARDMIFNFYFDVWVGQTTVTVSS ASTKGPSVFPLAPSSKSTSGGTA
ALGCLVKDYFPEPVTVSWNSGALTSGVHTFPAVLQSSGLYSLSSVTVTPSSSLGTQTYICNVNHKPSNTKVD
KRV EPKSCDKTHTCPPCP **APELLGGPSVFLFPPPKDTLMISRTPEVTCVVVDVSHEDPEVKFNWYVDGV**
EVHNAKTKPREEQYNSTYRVVSVLTVLHQDWLNGKEYKCKVSNKALPAPIEKTI SKAKGQPREPQVYTLPPS
REEMTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTTTPVLDSDGSFFLYSKLTVDKSRWQQGNVFNCS
VMHEALHNHYTQKSLSLSPGK

RM 8671 Light Chain Amino Acid Sequence

DIQMTQSPSTLSASVGRVTITCSASSRVGYMHWYQQKPGKAPKLLIYDTSKLAGVPSRFRSGSGSGTEFTLT
ISSLPDDFATYYCFQSGSGYPFTFGGGTKVEIK RTVAAPSVFIFPPSDEQLKSGTASVVCLLNNFYPREAKV
QWKVDNALQSGNSQESVTEQDSKSTYLSSTLTLSKADYEKHKVYACEVTHQGLSSPVTKSFNRGEC

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.

$$\lambda = -1.97313 \times 10^{-3} + 1.99227 \times 10^{-5} \rho + 1.07923 \times 10^{-4} T \pm 1.0 \% (k = 2)$$

- 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

Go to Search

SRM: 1401

Srm Number	Batch	Name
1401		Trace Metals in Frozen Human Blood

Identifications Lot Certificate Groups Mixtures Files

Lot

Lot	Parts																											
1	<table border="1"><thead><tr><th>Quantity In Unit</th><th>Part Id</th><th>Title</th><th>Title short</th><th>Title certificate</th><th>Nominal Amount</th><th>Amount</th><th>Unit</th><th>Source</th></tr></thead><tbody><tr><td>2</td><td>A</td><td>Level 1</td><td>Level 1</td><td>Level 1</td><td>false</td><td>1.6</td><td>mL</td><td>SRM</td></tr><tr><td>2</td><td>B</td><td>Level 2</td><td>Level 2</td><td>Level 2</td><td>false</td><td>1.6</td><td>mL</td><td>SRM</td></tr></tbody></table>	Quantity In Unit	Part Id	Title	Title short	Title certificate	Nominal Amount	Amount	Unit	Source	2	A	Level 1	Level 1	Level 1	false	1.6	mL	SRM	2	B	Level 2	Level 2	Level 2	false	1.6	mL	SRM
Quantity In Unit	Part Id	Title	Title short	Title certificate	Nominal Amount	Amount	Unit	Source																				
2	A	Level 1	Level 1	Level 1	false	1.6	mL	SRM																				
2	B	Level 2	Level 2	Level 2	false	1.6	mL	SRM																				

New Serial Number

New Part

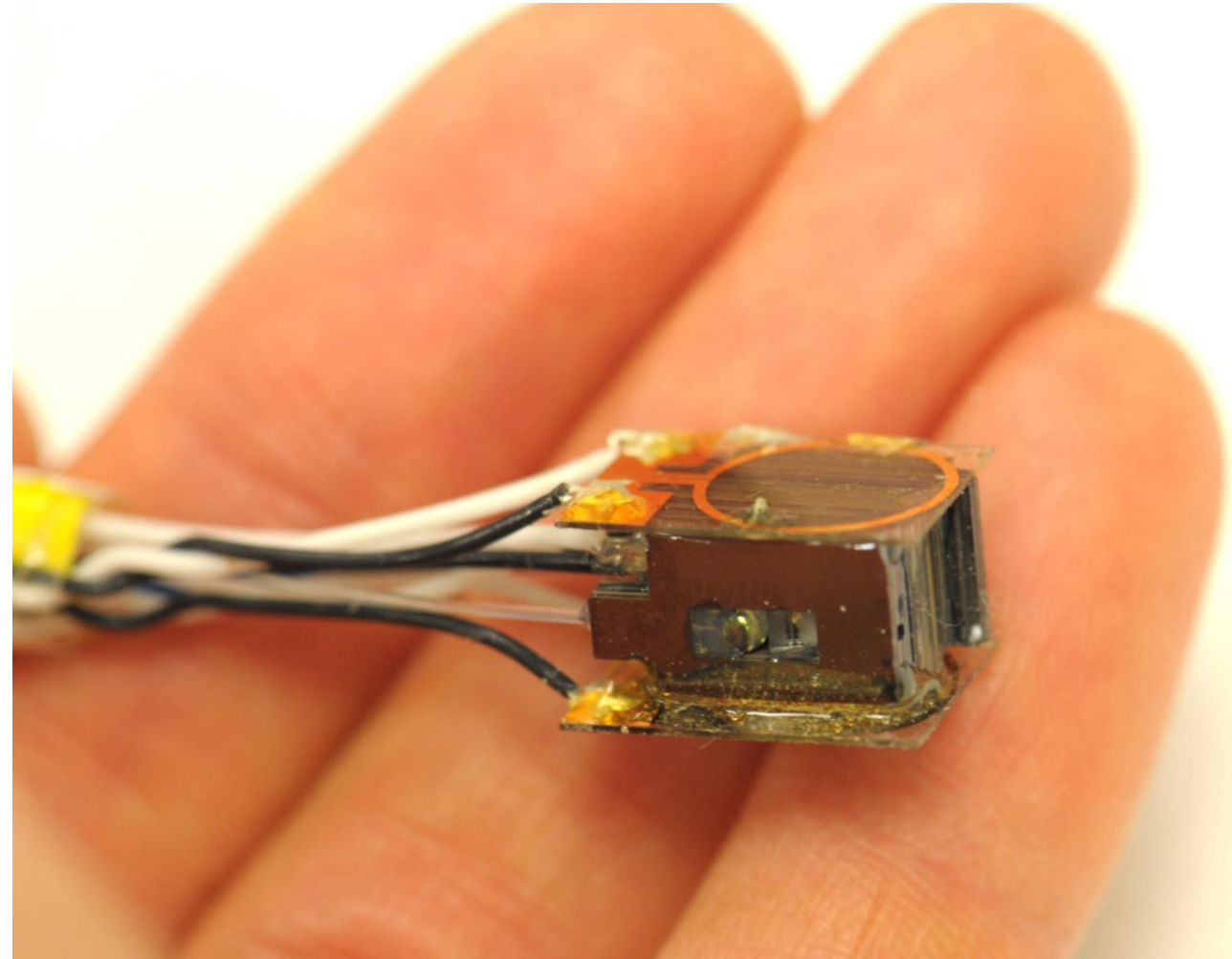
Value Sequences Formula

Values New Value

Value type	Value sub type	Operator	Value	Unit	Significant figures	Period of validity	Details												
Certified	Certified		2.89	µg/L	3	2024-12-01	<p>Group Identifications Basis Conversion Sample size</p> <p>Traceability Uncertainty / Coefficient of variation Statements Methods</p> <p>Part Mixture Reference Time Properties References</p> <p>Identifications</p> <table border="1"><thead><tr><th>Identification</th><th>Identification Type</th><th>Description</th><th>Reference</th></tr></thead><tbody><tr><td>Chromium</td><td>Chemical name</td><td></td><td>0</td></tr><tr><td>Cr</td><td>Symbol</td><td></td><td>0</td></tr></tbody></table>	Identification	Identification Type	Description	Reference	Chromium	Chemical name		0	Cr	Symbol		0
Identification	Identification Type	Description	Reference																
Chromium	Chemical name		0																
Cr	Symbol		0																

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.





- 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

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Scientists, Statisticians, other NIST Experts

The END

Thank you!