NRC·CNRC

NRC.CANADA.CA

Metrology in the Digital Era

Digital Transformation for Quality Infrastructure

World Metrology Day 2022

Ryan M White

National Research Council Canada
Conseil national de recherches Canada

Canada

Overview

Digital Transformation

NRC digitally accessible documents

Digital infrastructure for metrological information

Digital support for *scales of measure*

Introduction

The International System of Units (SI) plays a particular role in the international quality infrastructure

- Confidence in accuracy of measurements
- Global comparability of measurements

Vital to international trade, manufacturing, human health & safety, protection of the environment, global climate studies, and scientific research.

https://www.bipm.org/en/liaison/digital-transformation

Introduction – Digital Transformation

Governments, industry, academia and civil society have been working towards digital transformation

- Establishing systems to collect, aggregate, analyze and interpret digital data
- Introducing networked sensor systems for diverse scientific and industrial applications
- Increasingly sharing data at local, national, regional and international scales
- Increasingly integrating data sources across scientific domains and government siloes.

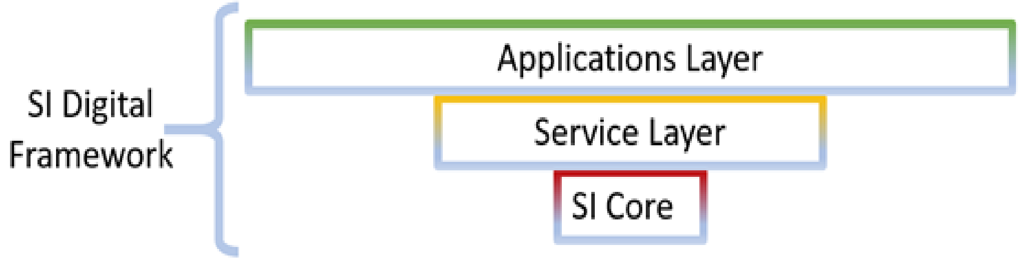
Introduction – Digital SI

Maintain confidence in the accuracy and global comparability of measurement in the digital era

- Creation and adoption of a complete digital representation of the SI, including robust, unambiguous, and machine-actionable digital representations of units of measurement and of measurement results and uncertainties.
- Robust digital infrastructure that ensures low-risk of misinterpretation in the exchange of measurement data in cyber-physical systems.

https://www.bipm.org/en/liaison/digital-transformation

SI Digital Framework



SI Core representation, defined by CIPM

- Digital standards for quantities, units, measurands, measurement models, and uncertainty
- Digital documents for instruments, certificates of calibration and reference material, capabilities
- Digital representation of traceability chains

Services, implemented by NMIs, BIPM and related organizations

- Registers and repositories for digital standards and documents
- Protocols and security for finding, accessing and exchanging measurement information
- Provenance and verifiable quality of key metrological data, e.g. KCDB, JCTLM, NMI products

Applications, broader metrology and research community that rely on the SI

- SI digital framework components in cyber-physical systems, IoT, sensor networks, autonomous systems.
- Support interoperability with the SI

https://www.bipm.org/en/bipm-workshops/digital-si

Measurement Information Infrastructures

Measurement Information Infrastructure (MII)[1]

“*a set of normative standards that unambiguously define data structures, taxonomies, service protocols and security for locating, communicating, and sharing measurement information.*”

[1] NCSLI Measurement Information Infrastructure and Automation Committee

Digital Transformation of QI

Metrology lags behind other sectors – science, academia, finance, …

Metrology can benefit from advances in other sectors

- Agile to adopt common approaches
- Open science & FAIR data
- IOT, automation, smart infrastructure

Digital Signatures

Electronic documents common business practice

- Government sectors have transitioned to electronic documents
- Verifiable electronic signatures are widely supported

National Quality Systems have transitioned to exchanging electronic documents for calibration certificates.

- NRC supports electronic signing
- METRO QMS will soon follow as a requirement

New package for same information

- Keeping pace with common practice but not transformative

Realizing new value for CRMs

Certified reference materials are persistent artifacts of metrology.

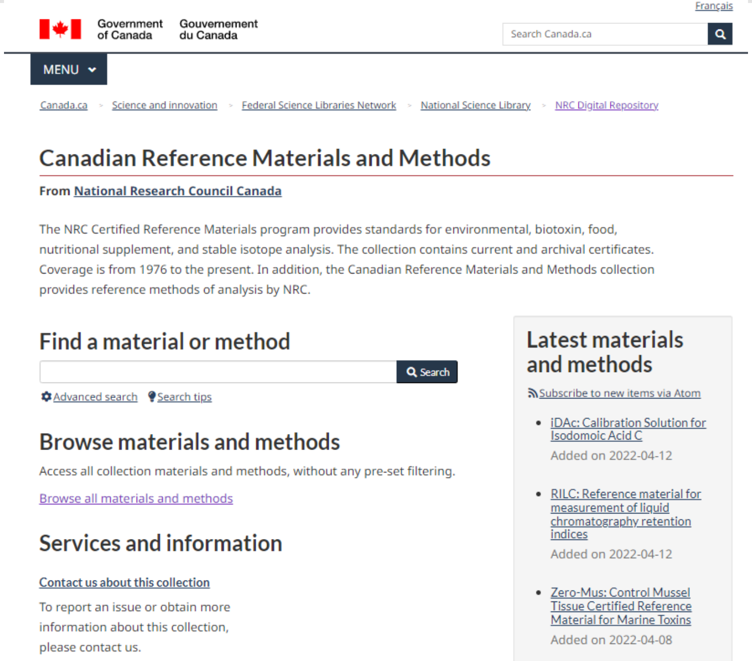
Digital objects for certified reference materials ensures their persistence in the digital domain.

- **Findable -** Standardized metadata
- **Accessible** - Persistent digital object identifiers DOI
- **Provenance** – Linked with Researcher ORCiD

Tailored to metrology

- Certificates of analysis, safety data sheets, additional metadata.
- Digital repository tailored to meet needs of metrology by using existing standards and domain-specific metadata.

NRC Digital Repository for Canadian Certified Reference Materials


Français

Government of Canada | Gouvernement du Canada

Search Canada.ca

MENU

Canada.ca > Science and innovation > Federal Science Libraries Network > National Science Library > NRC Digital Repository

Canadian Reference Materials and Methods

From National Research Council Canada

The NRC Certified Reference Materials program provides standards for environmental, biotoxin, food, nutritional supplement, and stable isotope analysis. The collection contains current and archival certificates. Coverage is from 1976 to the present. In addition, the Canadian Reference Materials and Methods collection provides reference methods of analysis by NRC.

Find a material or method

Search

Advanced search | Search tips

Browse materials and methods

Access all collection materials and methods, without any pre-set filtering.

Browse all materials and methods

Services and information

Contact us about this collection

To report an issue or obtain more information about this collection, please contact us.

Latest materials and methods

Subscribe to new items via Atom

- iDAc: Calibration Solution for Isodomoic Acid C
  Added on 2022-04-12
- RILC: Reference material for measurement of liquid chromatography retention indices
  Added on 2022-04-12
- Zero-Mus: Control Mussel Tissue Certified Reference Material for Marine Toxins
  Added on 2022-04-08

145 Certified Reference Materials!

- Digital Object Identifiers
- Linked to Researcher ORCiDs
- Indexed metadata
- Certificates of Analysis (English/French)
- Safety Data Sheets (English/French)

Canadian Reference Materials and Methods - NRC Digital Repository - Canada.ca

NRC Digital CRM

iDAc: Calibration Solution for Isodomoic Acid C

From National Research Council Canada

Return to search results | Next result ➡

Alternative title	iDAc : Solution d'étalonnage d'acide isodomoïque C
Downloads	File / Format / Size / Last Updated
	View certificate (English) / PDF / 107 KB / 2022-04-13
	View certificate (French) / PDF / 108 KB / 2022-04-13
	View Safety Data Sheet (English) / PDF / 169 KB / 2022-04-12
	View Safety Data Sheet (French) / PDF / 259 KB / 2022-04-12
DOI	https://doi.org/10.4224/crm.2022.idac.20051028
Author	Thomas, Krista[1] ; Crain, Sheila[1] ; Hardstaff, William[1] ; Chen, Yi-Min[2] ; Quilliam, Michael[1] ; McCarron, Pearse[1]
Name affiliation	1. National Research Council Canada 2. National Cheng-Kung University, Taiwan
Format	3D, Material
Subject	Canadian reference material; isodomoic acid C; domoic acid isomer
Abstract	RM-iDAc is a non-certified calibration solution of iDAc in acetonitrile/water (1:9, v/v).
Publication date	2022-04-12
Publisher	National Research Council Canada
Copyright statement	© 2022 National Research Council of Canada
Access condition	Please visit http://nrc-cnrc.gc.ca/crm to obtain the material http://nrc-cnrc.gc.ca/crm
References	▸ View items (8)
Export citation	Export as RIS
Collection	Canadian Reference Materials and Methods

Isodomoic Acid C

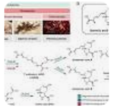
All | Images | Shopping | Videos | News | More | Tools

Page 2 of about 4,970 results (0.33 seconds)

https://www.pnas.org › doi › pnas.2117407119

Domoic acid biosynthesis in the red alga Chondria ... - PNAS

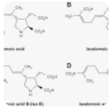
by TS Steele · 2022 — armata extracts, the presence of **isodomoic acid** A and **C** in the algae is yet to be explained biochemically. Although trace quantities of ...



https://www.sciencedirect.com › science › article › pii

Comparative toxicity to mice of domoic acid and isodomoic ...

by R Munday · 2008 · Cited by 45 — Furthermore, the severities of the behavioural changes induced by **isodomoic acids** A, B and **C** were all much lower than that of domoic **acid** itself ...



https://nrc-digital-repository.canada.ca › view › object

iDAc: Calibration Solution for Isodomoic Acid C - NRC Digital ...

Apr 12, 2022 — Subject, Canadian reference material; **isodomoic acid C**; domoic acid isomer. Abstract. RM-iDAc is a non-certified calibration solution of ...

Digital Transformation of QI

Metrology can provide better support for the SI with digital technology

- Increase visibility of services and products
- Realize new value from digitized measurement information
- Sustained viability of the QI in a digital era

Barriers to Success

Digital Transformation can solve existing challenges and foster adoption

- Requires solutions that are fit for purpose
- Consistent vision
- Broad support and interest from the community
- Champions

Barriers to Success

Digitizing existing processes, documents, etc… is not transformative

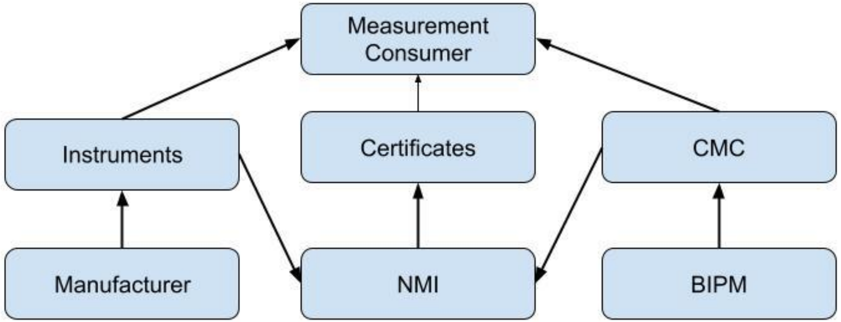
- Only changes the package not the content
- Retains existing manual processes and weakness
- Ambiguity remains that cannot be used by machines
- Inadequate information management

Success Factors

Digital transformation requires rethinking our existing concepts

- Structure information to leverage digital technology
- Building blocks
- Resolve existing challenges
- Value to the end user to make informed decisions

D-SI Documents in Measurement Science



SI Digital Framework Requirements

- Standards (norms)
- Interoperable (unambigious)
- Identifiable (reuse data)
- Extensible (forward/backward compatible)

Digital Documents revolve around measurement information and share common data structures, the basic building blocks.

Building Blocks

Units
Scales & Aspects

Quantities
Influences & Measurands

Traceability
Models & Uncertainty

Relationships
Taxonomies, Lineage, Operations

- Support diverse metrological data
- Fully exploit opportunities of digital transformation
- Embed metrological concepts in digital infrastructure
- Global interoperability

→ **MII Taxonomies for Scopes of Accreditation**

Maxwell's system

Maxwell's expression of the value of a quantity

$$Q = \{Q\} \cdot [Q]$$

"If l is the numerical value of a length, it is understood to be expressed in terms of the concrete unit [L], so that the actual length would be fully expressed by l [L]." Maxwell, A Treatise on Electricity and Magnetism

Problems for Digital Transformation

The unit name (or symbol) does not reliably identify a quantity.

Dimensional expression associated with a unit does not reliably identify a quantity.

Unit names are sometimes interchangeable.

Unit conversions do not always use multiplicative scale factors (e.g., degrees Celsius).

Existing digital unit systems have limited capability or provide ad hoc solutions

Unit Names

Torque and energy have the same unit: kg m^2/s^2

- Torque: N·m
- Energy: J
- Information about the kind of quantity is required

Temperature is an intensive quantity whereas temperature difference is extensive.

- Both quantities can be expressed with the same unit.
- Information about the kind of quantity and type of scale is necessary.

Dimensional Expressions

Difficult to distinguish the kind of quantity (aspect) in dimensionless quantities and method-defined measurands (e.g., grain moisture content).

SI unit for refractive index is one, because the dimensional expression is 1. Conversion from one unit system to another involves a conversion factor of 1. Dimensions are not useful to identify the quantity.

Additional challenging use cases

SI Unit for Angle

SI requires angle expressed in radians, yet does not specify whether the range of values is bounded. Typically angles is restricted to a finite range, -pi to pi or 0 to 2pi.

Engineering use case

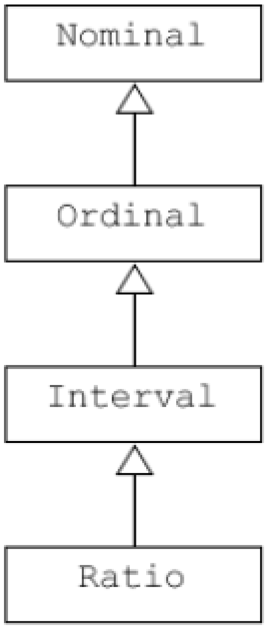
A measure of height above sea level (elevation) may be interpreted with respect to different reference points in different jurisdictions yet referred to simply as the height above sea level. To convert between measures referred to different points, it is necessary to know the relative vertical separation of the reference points.

Digital support for *scales of measure*

- Units must be qualified by the type of scale; ratio, interval, ordinal, etc…
- Reliable identification of the aspect (kinds of quantity)
- Reliable conversion between alternative expressions

Scale types

- **Ratio**: conversion factor
- **Interval**: Affine transforms (offset and scale factor)
- **Ordinal**: Monotonically increasing functions
- **Nominal**: Permutation



S.S. Stevens **On the theory of scales** Science, 103 (2684) (1946), pp. 677-680

M-Layer

digital support for scales of measure

General metrology information basis (M-Layer)

- Aspect[1] – generalized “quantity”
- Scale - Unit and type of scale
- Numerical (typically) value

[1] VIM3 1.2 kind of quantity – aspect common to mutually compatible quantities

Example

Simple (traditional) expression

$$x = 10 \text{ kg}$$

M-Layer expression

x = {10}, [kg, ratio], <mass>

M-layer captures an aspect (mass), a value (10), and a scale composed of the unit (kg) and the scale-type (ratio).

The mass aspect of x is 10 when expressed in kilograms on a ratio scale.

Examples of scales

- [interval quantity, degree Celsius]
- [ratio quantity, degree Celsius]
- [ratio quantity, metre]; [ratio quantity, centimeter]
- [ratio quantity, metre-per-second]
- [ordinal quantity, Rockwell C hardness]
- [ordinal quantity, Richter scale]
- [nominal, sex of human]
- [nominal, ISO country code]

M-Layer Proposal

1. Aspect being expressed, e.g. length, temperature

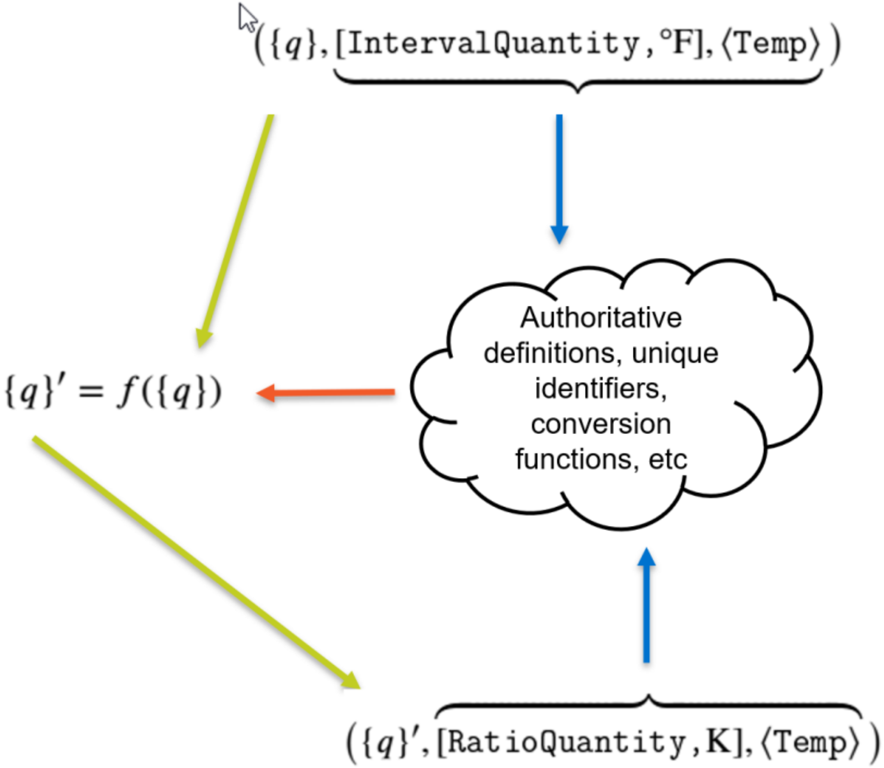
2. Extended unit, combines the unit with the type of scale

3. Register of conversions

Each aspect is unique

Each extended unit is unique

Tripartite expression: ({numerical value}, [scale, unit], <Aspect>)



Summary

Digital documents in the measurement economy incorporate M-layer

- Adequate digital support *scales of measure.*
- Core component of the SI Digital Framework

Current efforts

- Continue to model M-Layer
- Refine M-layer concepts
- Examining existing digital systems for interoperability with M-layer
- Engage with metrology community on use cases

Upcoming seminars

Digital Metrology and related subjects

- Traceability in Digital Systems, Blair Hall, MSL, New Zealand
- NCSLI committee Measurement Information Infrastructure and Automation, Mark Kuster, NCSL
- Digital CRMs and the NRC Digital Repository

Upcoming Events

[SciDataCon and International Data Week 2022]

[DCC Summer School]

[NCSLI Workshop & Symposium 2022]

[IMEKO TC6: First International Conference on Metrology and Digital Transformation]

References

CIPM Digital SI Grand Vision

Joint Statement of Intent - Digital Transformation (bipm.org)

Stop squandering data: make units of measurement machine-readable

MII Initiative Knowledge Base - MII Initiative (wikidot.com)

Metrological Support for Quantities and Units in Digital Systems

Representing metrological traceability in digital systems

NRC Digital Repository for Certified Reference Materials

Researchers: Do you have an ORDiD?

BACKUP

Digital Transformation Efforts

CIPM Task Group on the Digital SI – largely focused on generating awareness within the International Quality Infrastructure on basic requirements.

NCSLI Committee on Measurement Information Infrastructure and Automation – Trailblazers for digital transformation. Developing digital documents for the measurement economy. Mature Scope of Accreditation product. More recently, collaboration on support for quantities and units in digital systems.

PTB – Broad digitization strategy across the German NMI. Chair of CIPM Digital SI, promotion of XML-based calibration report.

NIST – Emphasis on open science infrastructure and adoption of existing standards to improve interoperability of metrology products. Developed the International Metrology Resource Registry. Recent funding for the Digital NIST project.

SIM M4DT – Development of new services via digital transformation. Aligned with PTB strategy on digitalization.

NRC – Digital Metrology sector and member of CIPM Digital SI. Integrated digital services with NRC KITS digital repository.

CIPM Task Group Digital-SI

Digital Representation of physical quantities and measurement data

Redefinition of the SI based on fundamental constants creates new opportunity to advance the field of metrology into the digital era.

- Digital representation of the SI, *D-SI*, is required to support the digital transformation of the international Quality Infrastructure
  - Develop and establish a data exchange framework based on the SI described in the SI brochure.
  - Propose suitable actions towards making the SI brochure machine readable.
  - Coordinate efforts across stakeholders.

SIM Metrology for Digital Transformation

Promote adoption of digital technologies to improve NMI services.

- Digital Calibration Certificates
- Automation of Laboratory Processes
- Metrology for Industry 4.0
- Cloud Technologies
- Agile Projects

Digital Representation of Units of Measure (DRUM) - CODATA, The Committee on Data for Science and Technology

Digital representation of units of measure(ment) (physical quantities) (DRUM) across domains is a significant problem relative to the interoperability of data and it needs to be addressed immediately.

- Recommendation of Units of Measurement (UoM) representation systems for different use cases.
- Guidelines for annotation of data with UoM in digital systems.
- Best practices for adopting the recommended DRUM system.
- Metrology 101 – introduction to concepts in metrology
- Units of Measure interoperability service operated by NIST

Use cases for expressing SI units

Speed

The SI unit for speed is meter-per-second. To convert an expression in meter-per-second to a different unit for speed, the numerical value in the expression will be rescaled by a conversion factor that depends on the size of the divisions on both scales.

Meter-per-second belongs to the category of ratio scales because conversion requires rescaling by a simple conversion factor.

The dimensional expression L/T can be used to evaluate the conversion factor for speed if conversion factors for the base units—length and time—are already known.

Activity

The SI unit for the activity of a radioactive substance has two legitimate names: becquerel and per-second. Conversion of a value of activity from the SI unit to a non-SI unit (e.g., curie or rutherford) can be carried out using a conversion factor.

Becquerel belongs to the category of ratio scales because conversion requires rescaling by a simple conversion factor.

The dimensional expression 1/T can be used to evaluate the conversion factor for activity. The conversion factor is inversely proportional to the conversion factor for the base unit time and proportional to the number of events (unity for the becquerel, 3.7×10^{10} for the curie and 10^{6} for rutherford).

Use cases for expressing SI units

Celsius relative temperature

When a temperature difference is expressed in degrees Celsius, zero degrees corresponds to zero on any other ratio scale for temperature difference. To convert a temperature difference in degrees Celsius to any ratio scale for relative temperature (kelvin, for example) requires information about the size of divisions on the two scales (Celsius and kelvin divisions are equivalent).

Celsius temperature difference belongs to the category of ratio scales because requires rescaling by a simple conversion factor.

Celsius absolute temperature

When absolute temperature is expressed in degrees Celsius, the value zero is offset by 273.15 degrees from zero on ratio scales for thermodynamic temperature. To convert from temperature in degrees Celsius to any ratio scale for thermodynamic temperature (kelvin, for example) requires information about the value of this offset and the size of divisions on the two scales (Celsius and kelvin divisions are equivalent).

Celsius temperature belongs to the category of interval scales because information about an offset and the size of the divisions used to express the value is need for conversions.

Use cases in engineering

Height above sea level

A measure of height above sea level (elevation) may be interpreted with respect to different reference points in different jurisdictions yet referred to simply as the height above sea level. To convert between measures referred to different points, it is necessary to know the relative vertical separation of the reference points.

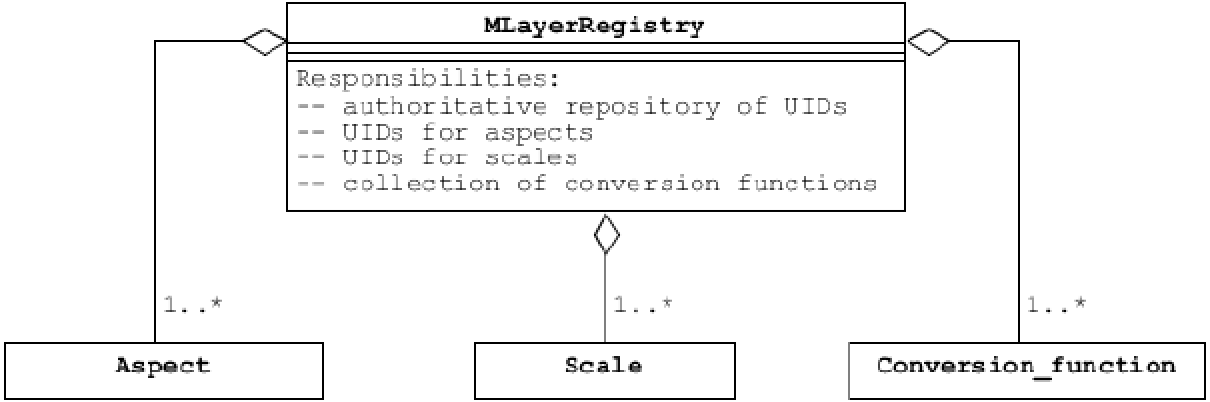
Height above sea level belongs to the category of interval scales because information about the relative separation of offsets and the size of the divisions used to express the value are needed for conversions.

Examples scale, unit and aspect

Examples of <q> and [q] together (SI only)

- [Ratio, degree Celsius] <TemperatureDifference>
- [interval, degree Celsius] <Temperature>
- [Ratio, kelvin] <Temperature>
- [Ratio, radian] <Angle>
- [Ratio, metre-per-metre] <Angle>
- [Ratio, newton-metre] <Torque>
- [Ratio, kilogram-metre-squared-per-second-squared] <Torque>
- [Ratio, kilogram-metre-squared-per-second-squared] <Energy>
- [Ratio, percent] <Relative-humidity>

Measurement Information Registry

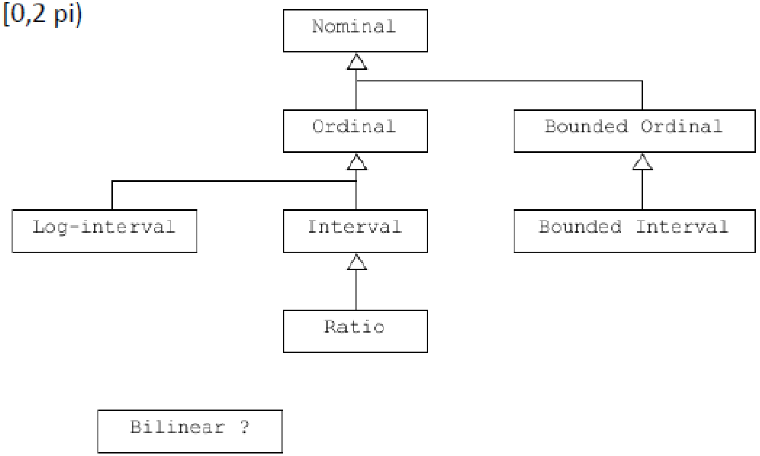


The M-layer would comprise an authoritative register of unique identifiers for aspects, scales (units), and conversion functions. (Blair Hall (MSL) and M. Kuster)

Support beyond SI

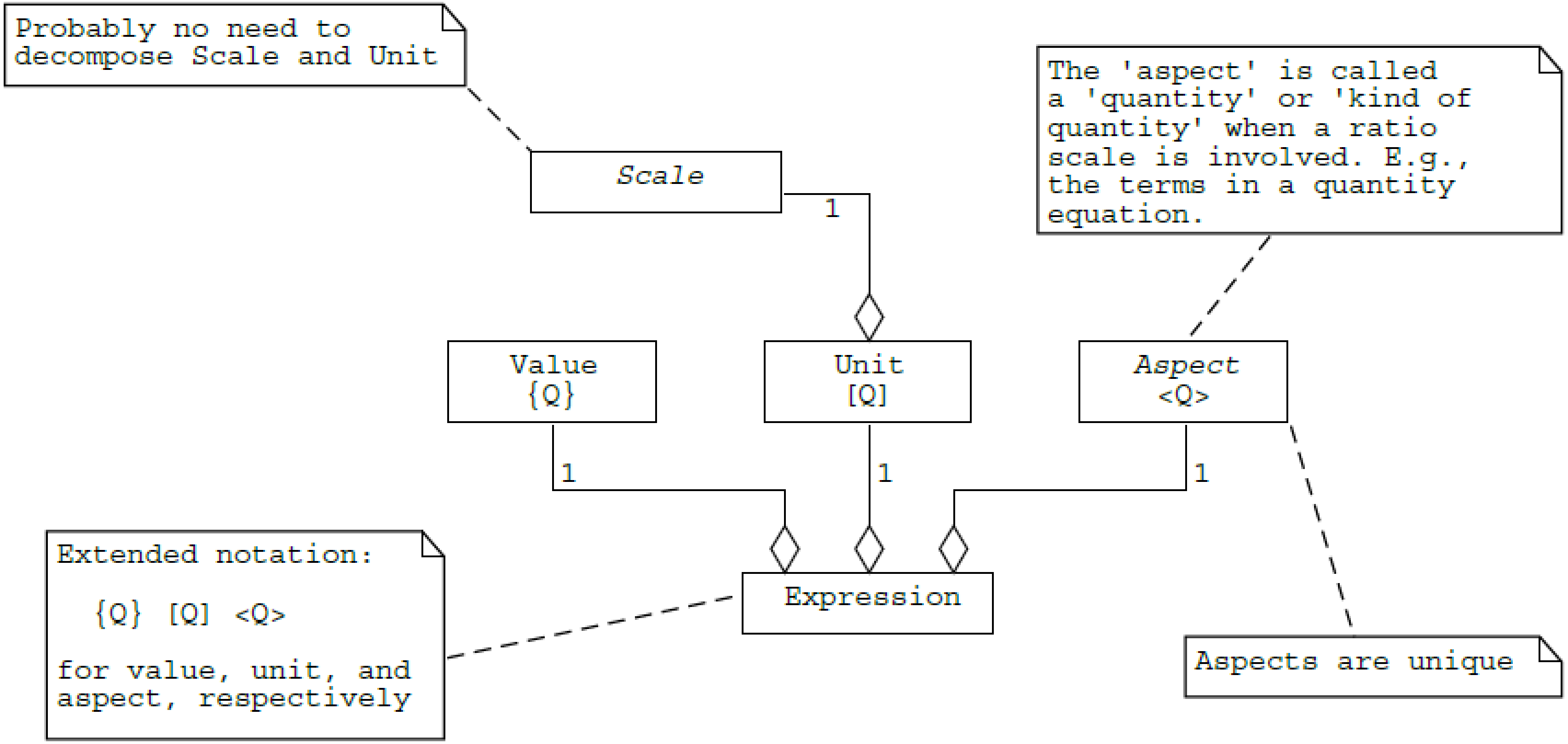
More levels needed for edge cases (not necessarily SI)

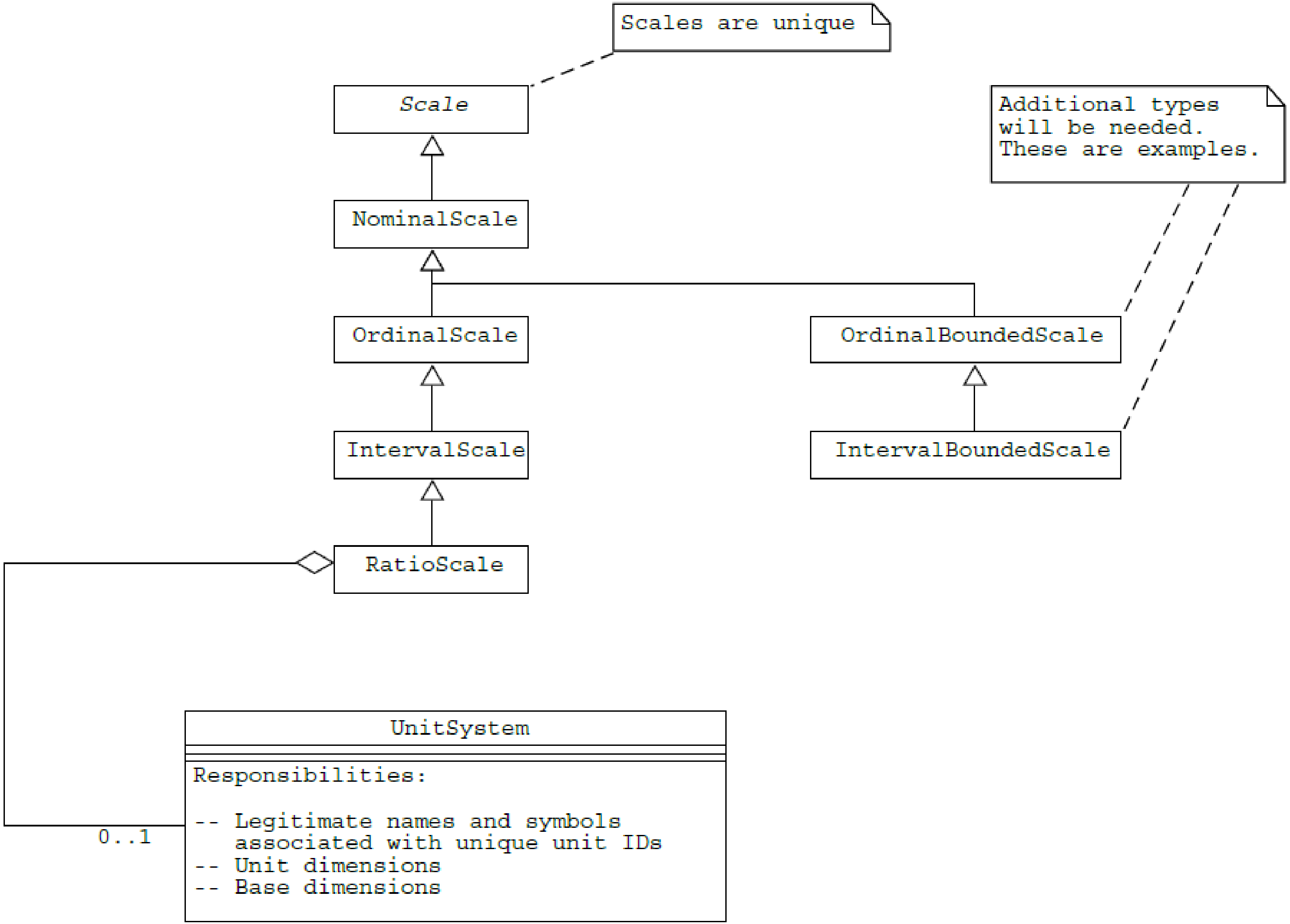
- [Log-interval, dBm] <Power>
- [Bounded-interval, radian] <Angle> % e.g.: (-pi, pi], [0,2 pi)
- [Bounded-ordinal, compass bearing] <Angle>
- [Ordinal, degree Celsius] <Temperature>



Comments:

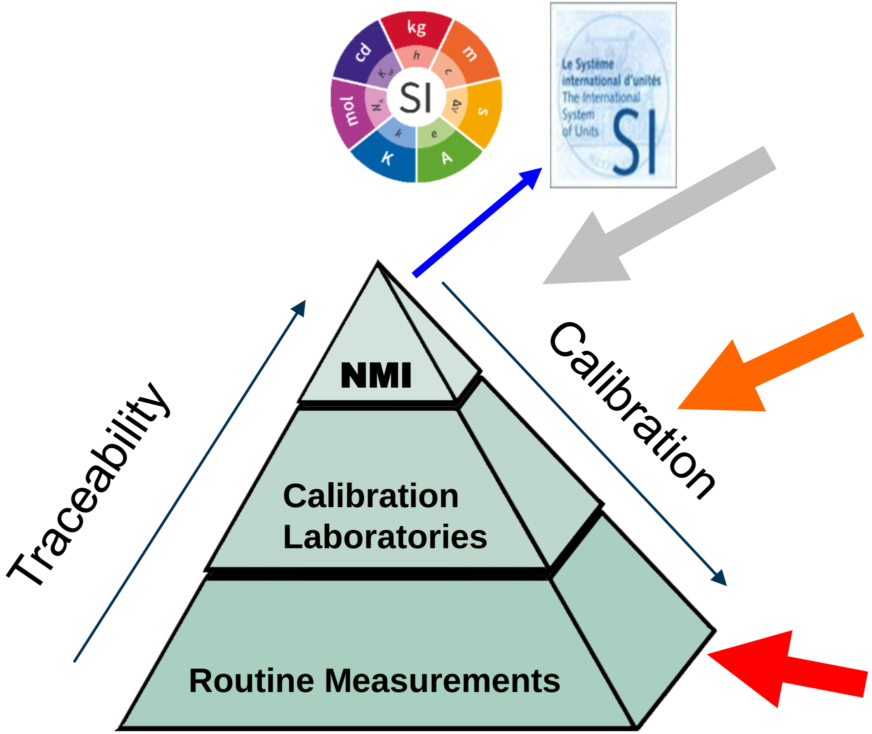
- Each [q] is uniquely identified, so we could have more than one instance of [Bounded-interval, radian] <Angle>, each with different limits.
- The log representations are an example of non-linear transformations of the aspect values. Bilinear transforms are another. Not sure if it is a good idea to accept them (i.e., is the aspect really the same?). However, they are in common use.


Probably no need to
decompose Scale and Unit
Scale
1
The 'aspect' is called
a 'quantity' or 'kind of
quantity' when a ratio
scale is involved. E.g.,
the terms in a quantity
equation.
Value
{Q}
Unit
[Q]
Aspect
<Q>
1
1
1
Extended notation:
{Q} [Q] <Q>
for value, unit, and
aspect, respectively
Expression
Aspects are unique


Scales are unique
Scale
NominalScale
Additional types
will be needed.
These are examples.
OrdinalScale
OrdinalBoundedScale
IntervalScale
IntervalBoundedScale
RatioScale
UnitSystem
Responsibilities:
-- Legitimate names and symbols
associated with unique unit IDs
-- Unit dimensions
-- Base dimensions
0..1

Traceability to the SI

Traceable quality, but not traceable in terms of influences

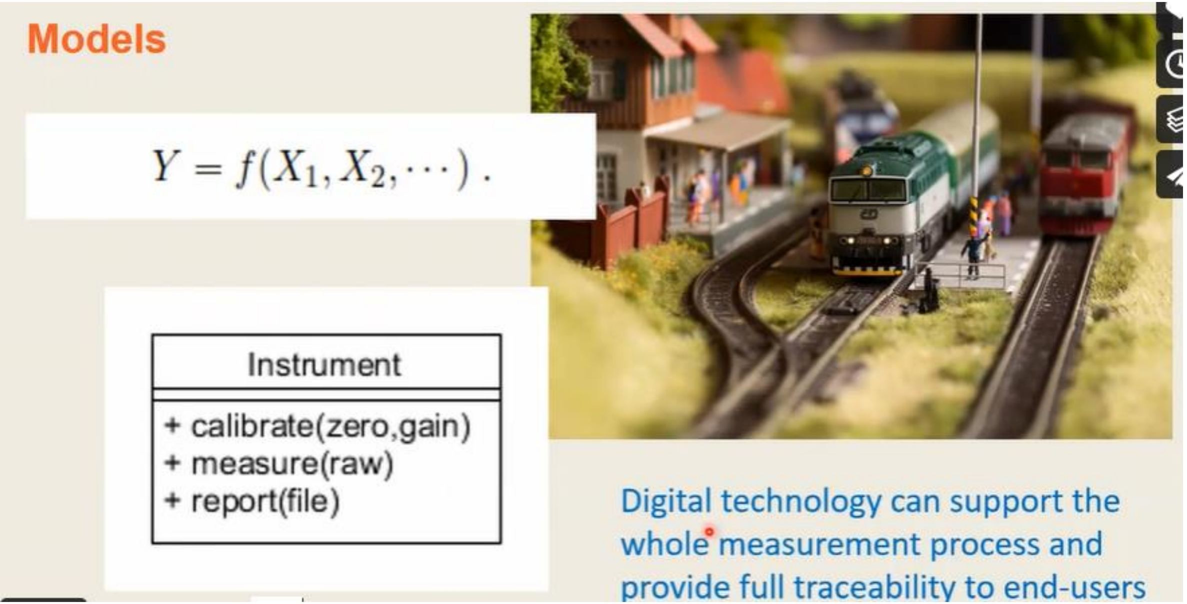


Custody of national standards; responsibility to disseminate

Responsible for calibrating measurement equipment and standards in relation to national standards

Testing laboratories, manufacturers…

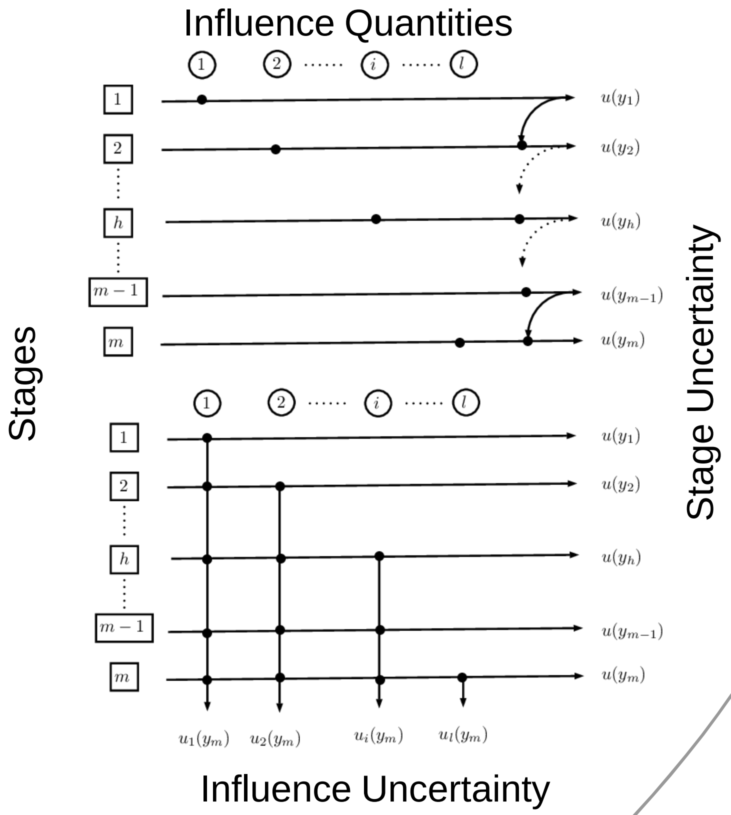
Measurement Models



Traceable Influences

Traceable Quality

Traceable Influences



Digital Calibration Certificate

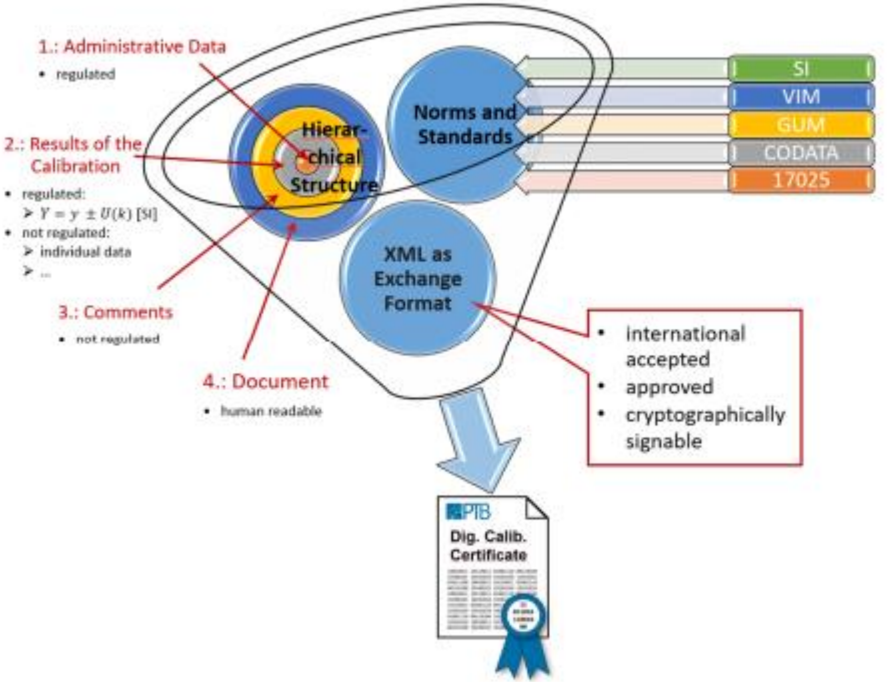
Digitalisation of Calibration Certificates

XML-based format and implementation

- Storage and communication format for calibration data and metadata.
- Aim to increase efficiency and reduce human errors.
- PTB effort towards standardisation.

Challenges and approaches

- Digitization of traditional document – new wrapper, old content.
- Lacks support for quantities and units.
- No new value generated for traceability.
- Suitable for direct exchange but not a building block.



FAIR Data

FAIR Guiding Principles

Data should be Findable

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

Data should be Accessible

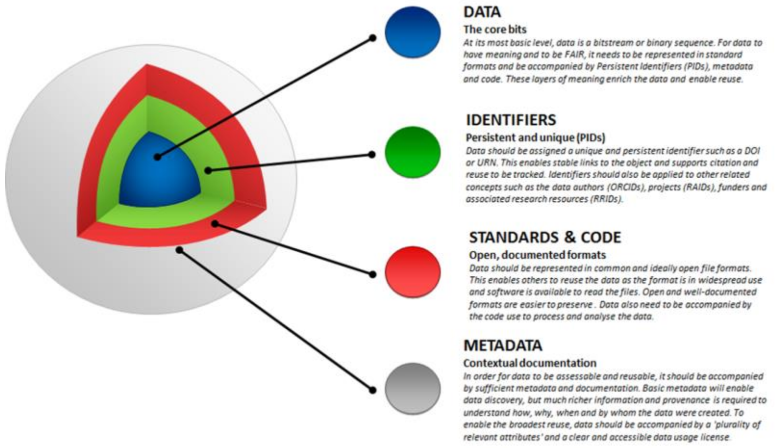
- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
- A2. metadata are accessible, even when the data are no longer available

Data should be Interoperable

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include qualified references to other (meta)data

Data should be Re-usable

- R1. meta(data) are richly described with a plurality of accurate and relevant attributes



Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al.* The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* 3, 160018 (2016). https://doi.org/10.1038/sdata.2016.18

CCU – Missteps in Digital Transformation

Proposed redefinition of quantity

property of a phenomenon, body or substance that can be compared by ratio or by order to others of the same kind.

Obvious problems

- Seemingly considers only physical quantities on ratio scales can be handled correctly by computers.
- Use of ‘ratio’ could be included if quantity is restricted to expressions of quantities on ratio scales and order would need to be removed.
- For quantities on other scales, the quantities would need to be qualified by the class of scale, e.g. ordinal, interval, etc…

IUPAC response

- Implies that ordinal properties are quantitative;
- Leaves in limbo quantitative properties for which differences are meaningful but ratios are not;
- Provides no guidance for how to categorize properties that may be quantitative from one viewpoint, and ordinal from another.

Conceptual metrological models resolve these problems! M-layer is a suitable basis.

NRC·CNRC

NRC.CANADA.CA •

THANK YOU

Ryan White • Digital Metrology • ryan.white@nrc-cnrc.gc.ca