From calibrationresults to Machine readable data, DFMs approach

Temadag om digitale kalibreringscertifikater (DCC)
October 5th 2023

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DFM
Danish National Metrology Institute

DFM receives funding by:
Danish Agency for Institutions and Educational Grants

DFM A/S

NMI:

Denmark joined the Metre Conventionen (1875)
DK is therefore obliged to have a National Metrology Institute (NMI), and realizing the SI units.

GTS:

DFM is one of seven Danish GTS institutes, and provides advanced technology services to Danish companies in form of:

calibrations, testing, validation and standardization.

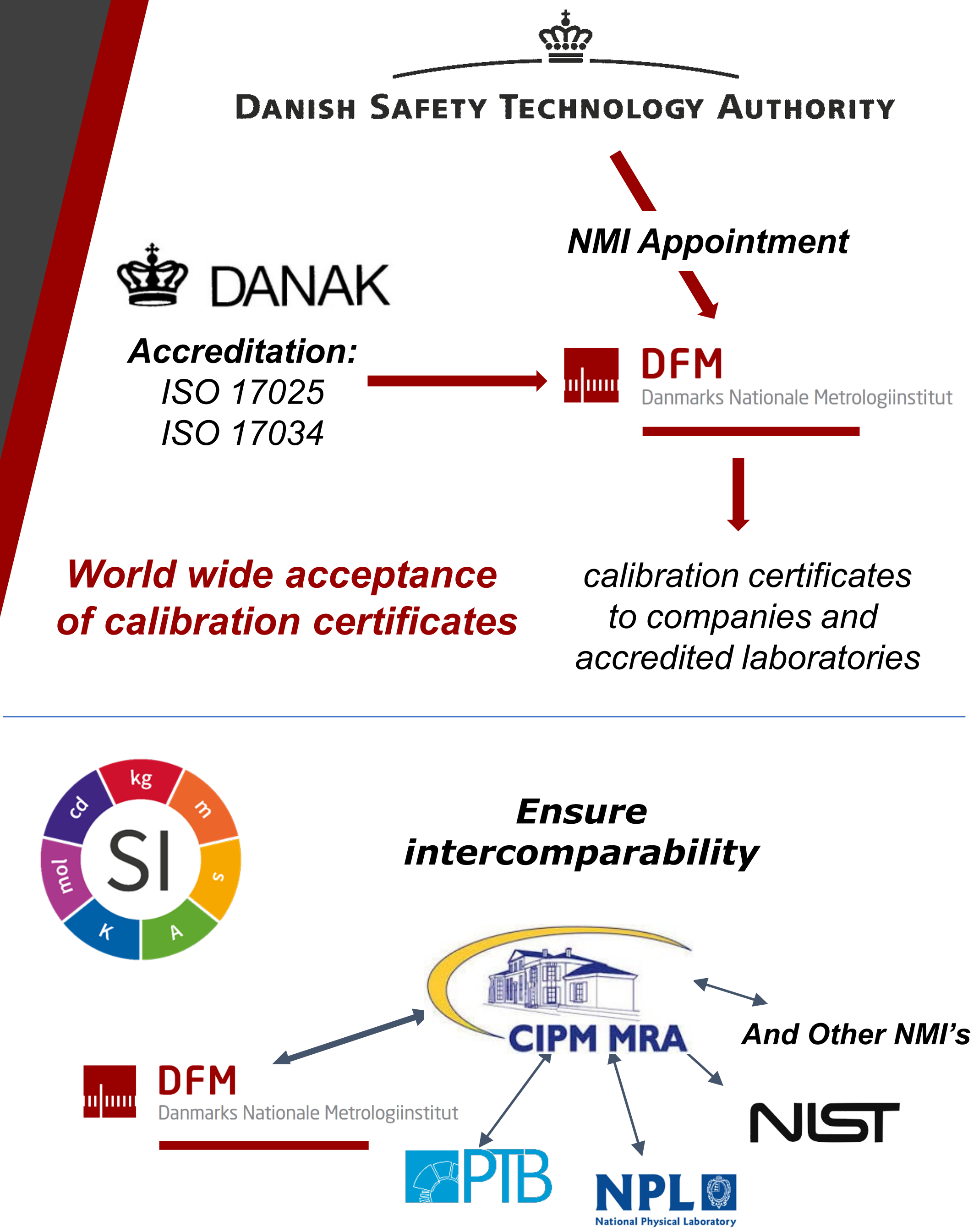
A crossover between academia and industry

DTU:

DFM is 100 % owned by DTU

Staff:

36 people in total, 24 PhDs



DFM Calibration services

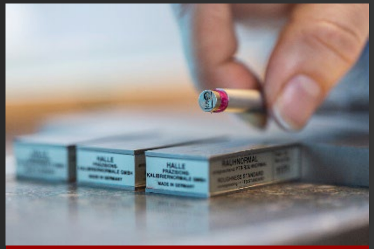
Nano particles
(size, counters)

Length

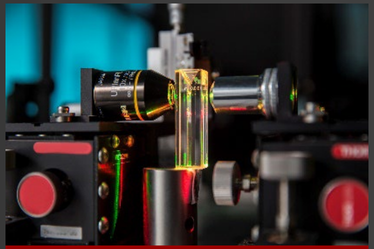
Electricity

Thermometry
(non-contact)

Mass

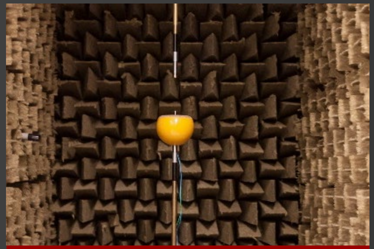


Roughness and
hole plates



Optical
radiometry &
spectro-radiom.

Electro
chemistry



Acoustics

Nano scale

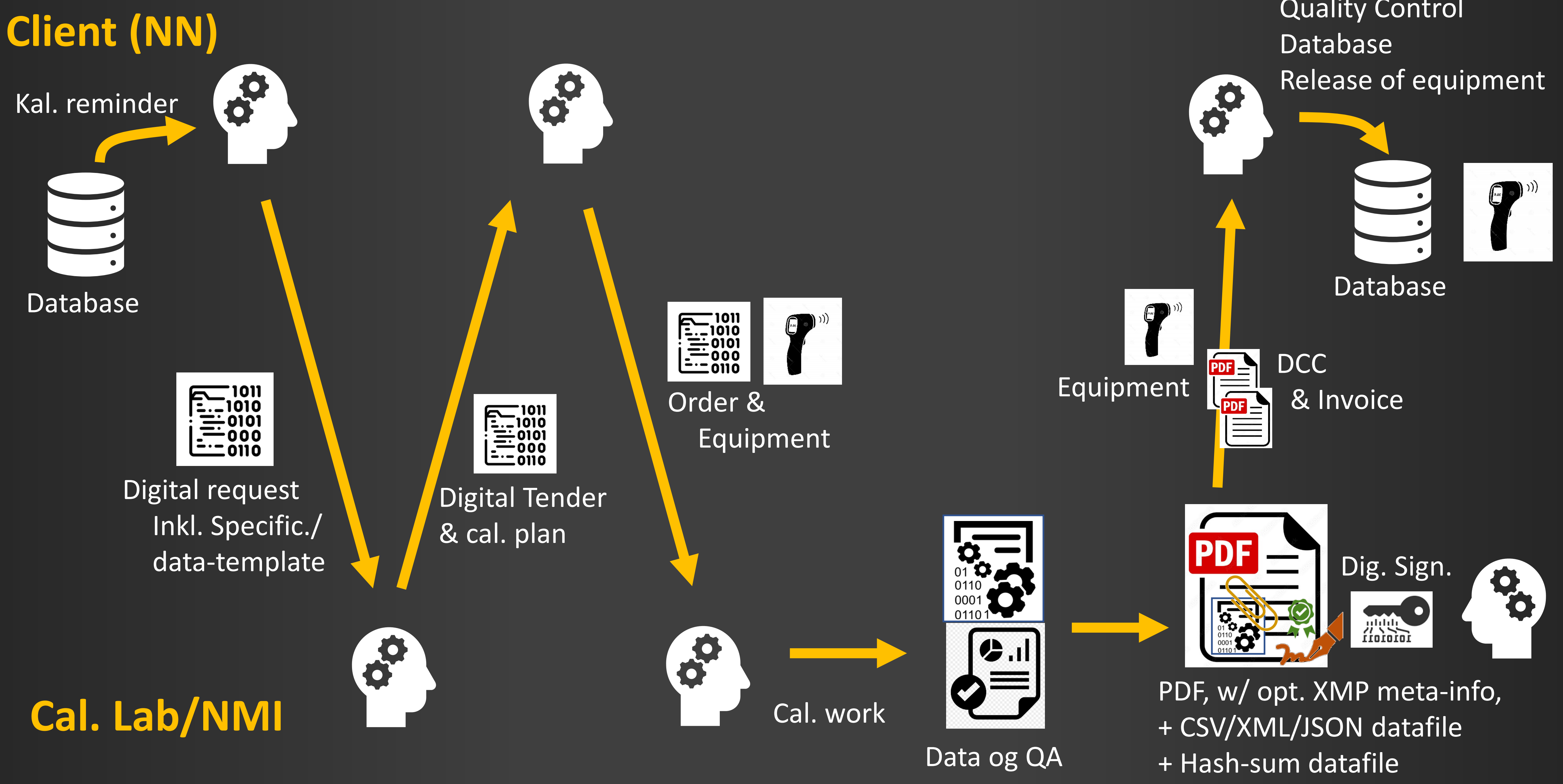
Machine readable Calibration Certificates

DFM's mission: **To support implementation of DCC's that are globally recognized, in order to support efficiency and quality in production companies through automation.**

- Value creation for the customers
  a. Improved data integrity/safety/**quality** (reduction of human errors)
  b. Easier transfer/integration to databases
  c. Efficiency by automation of processes, and streamlining of procedures.
  d. Easier control and adjustment of measurement equipment

- Primarily relevant to
  - Areas with large numbers of calibrations: Temperature, Pressure, IoT sensors
  - Certificates with large amounts of data: CMM, BRDF, acoustics, …

Envisioned workflow for DCC'er



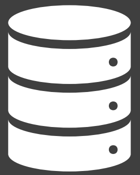
Danish pharma requirements for DCC

A. **Eliminate manual transfer of data from large amounts of certificates.**
B. **A global standard/Harmonisation**: standard = compliance & efficiency, international standards, data interoperability, data integrity, and ***quality***.
C. **Scalable**: Must be userfriendly for Accr. Cal. Labs to easily adopt.
D. **Auditable**: being able to identify errors, IT standards e.g. ISO/IEC 27001, ISO 8000, 16175, & common requirements for reporting (ISO-17025).
E. Accreditation should be reliably identifiable in the DCC
F. Machine interoperable.
G. Preferably be based on PTB's schema work, which has the high recognition in the international metrology community e.g. favoured by NIST, i.e. high likelihood to become a global 'standard'

Client aspect of extracting data from DCC

Often the client only need a few specific informations/data for their QMS in order to release their equipment.

Instrument Database:



- Cert. No
- Supplier Name
- Equipment Id no.
- Calibration date
- Error Results
- Uncertainty(ies)

Incoming

How?

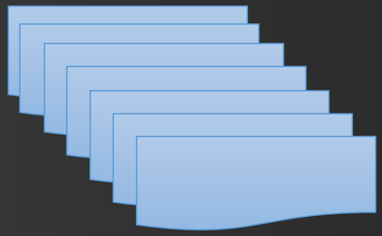
Client database must have registry of:

- All instruments being calibrated.
- what they want to know/extract from a certificate for each instrument.

Measurement Equipment Specification (MES):

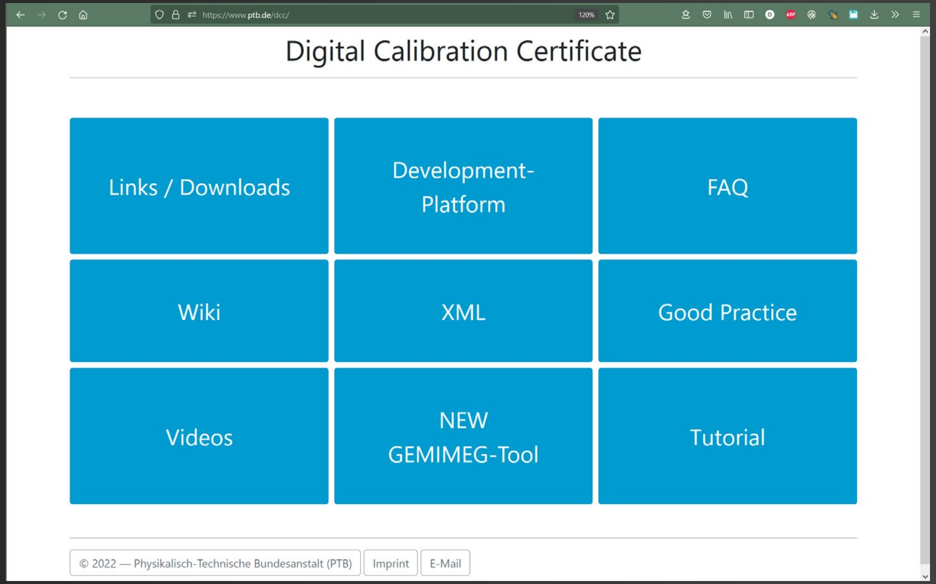
- Applies for similar equipment used for same purpose
- Specifies calibration requirements (Cal. Points, MPEs etc).
- & other info e.g. QA approvals …
- **Mapping table for Data extraction**.

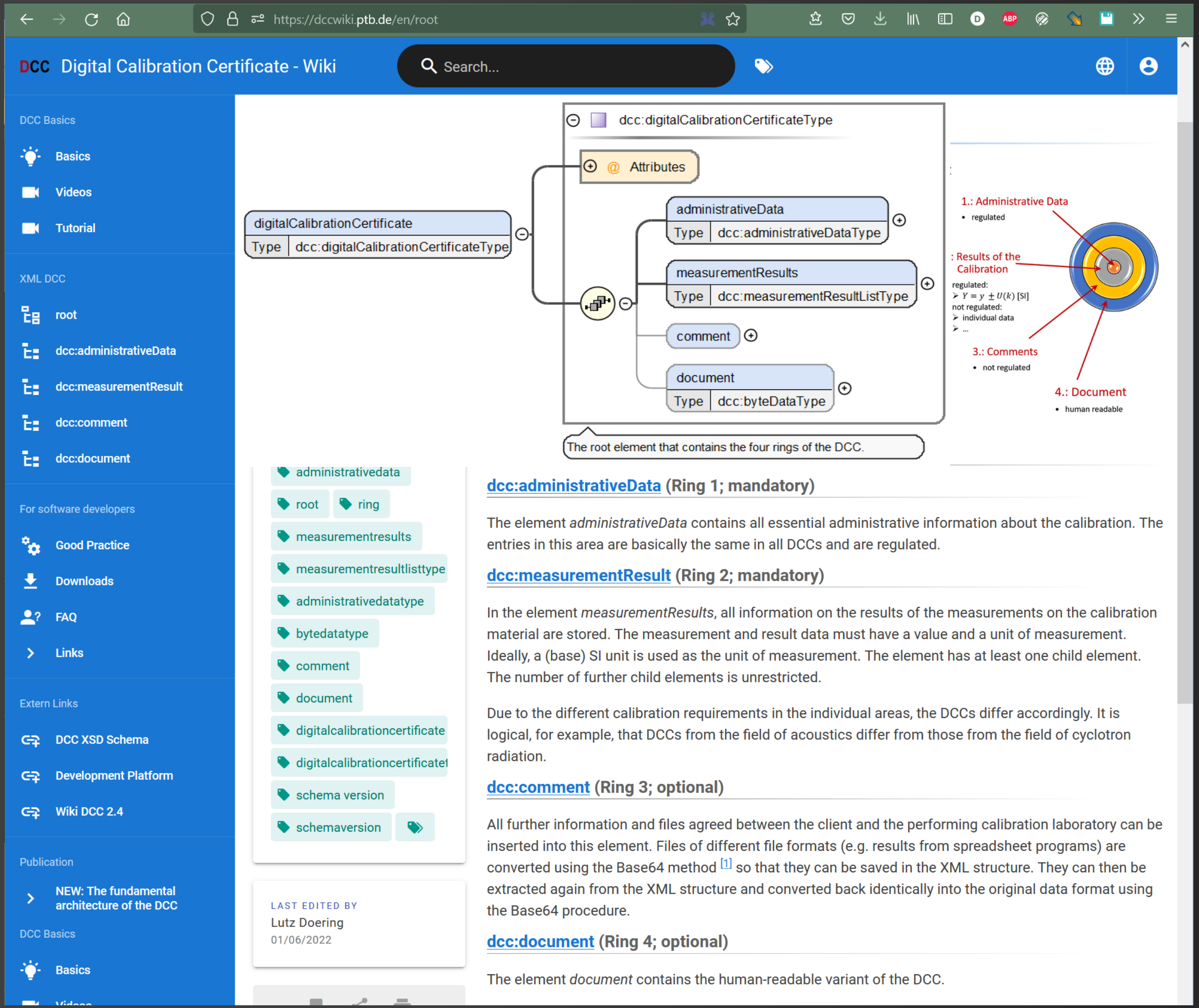
Calibration Task list



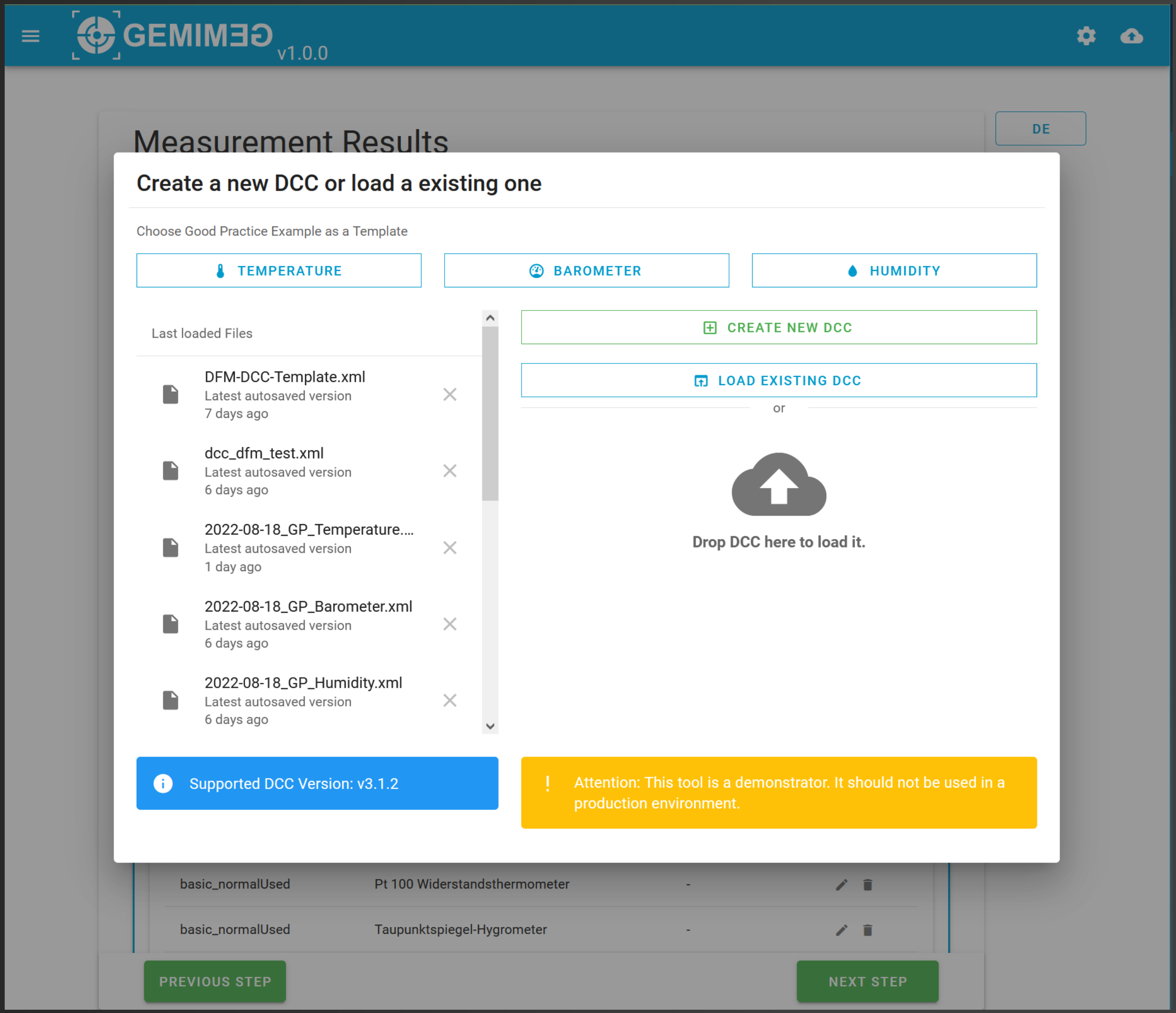
PTB's DCC website and documentation: www.ptb.de/dcc

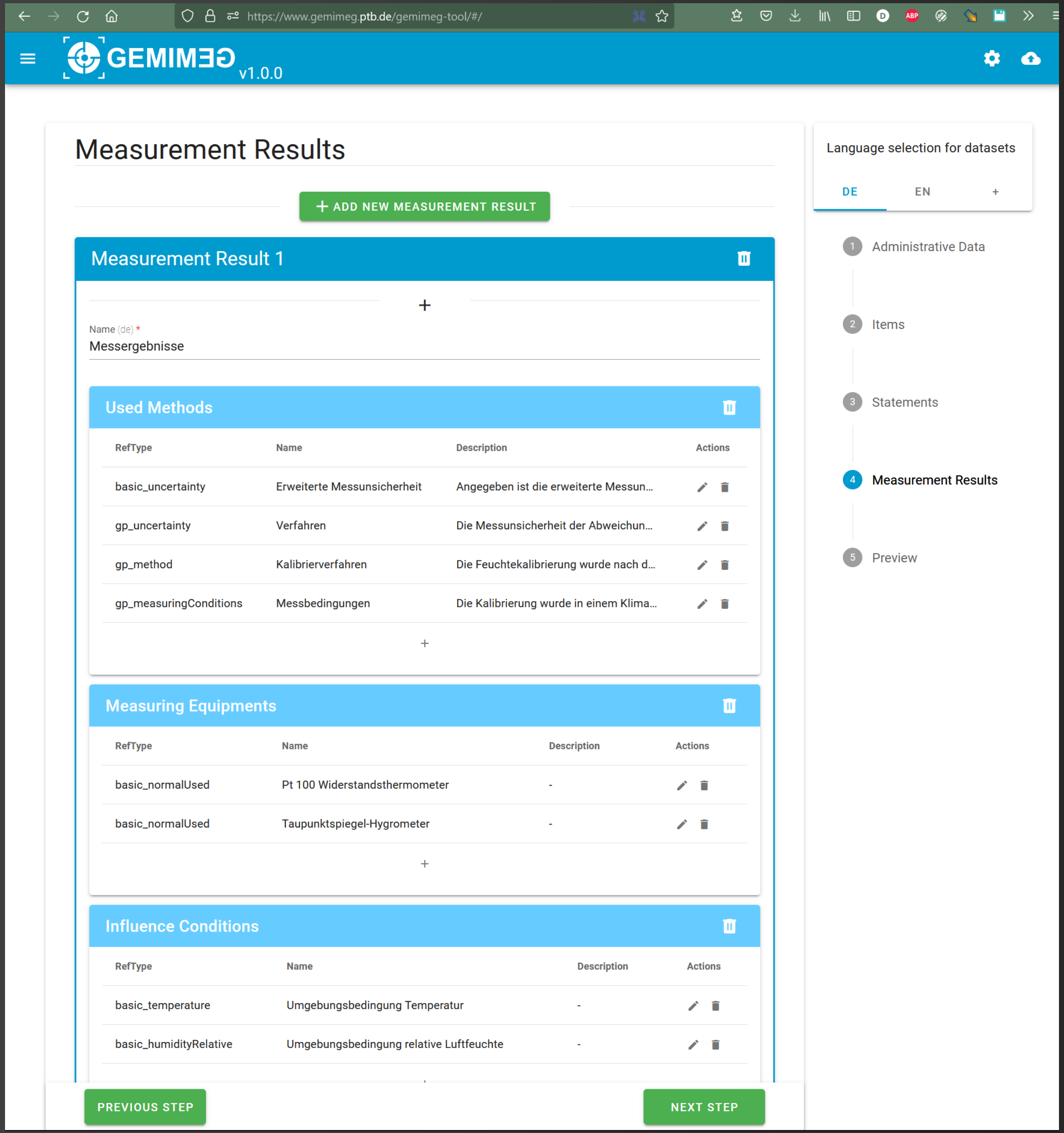
Data types and structure are defined in XML-schema files: dcc.xsd and SI_Format.xsd.
These are also used for validation of created DCC-xml-files.





GEMIMEG Tool





Predefinions are in external documents

PTB
Messen ▪ Forschen ▪ Wissen

search

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Title:	Instructions on how to use the DCC schema to create a digital calibration certificate for weights : Expert Report DKD-E 7-2
Authors:	Members of the Technical Committee Mass and Weighing Instruments of the DKD, Physikalisch-Technische Bundesanstalt (PTB), ISNI: 0000-0002-1140-5252
Contributors:	HostingInstitution: Physikalisch-Technische Bundesanstalt (PTB), ISNI: 0000 0001 2186 1887
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Publisher:	Physikalisch-Technische Bundesanstalt (PTB)
Rights:	https://creativecommons.org/licenses/by-nc-nd/3.0/de/ CC by-nc-nd 3.0
Relationships:	IsVariantFormOf: DOI 10.7795/550.20220419A
Dates:	Available: 2022-04-22 Created: 2022-04
File:	Download File (application/zip) 490.55 kB (502327 Bytes) MD5 Checksum: a766826b6bcd0cae1538a68decd07e43 SHA256 Checksum: 88f45bebfbdd1ab9f1097825062d25e4d1fc56f5df6c4a9a56d566e66f583830
Keywords:	DKD Expert Report ; DCC ; digital calibration certificate ; mass ; weight ; XSD ; SI
Abstract:	Advancing digitalisation does also affect the field of calibration. In view of this development and responding to the needs of industry, the digital calibration certificate (DCC) has been developed. The DCC is an XSD schema file that serves as a kind of template for digital calibration certificates for all measurands in XML format. Its implementation therefore requires further, subject-related specifications. To examine potential applications for the mass calibration of weights and weight sets and to determine the related specifications, the DKD Technical Committee Mass and Weighing Instruments has set up a group of experts who have created the present document. This document describes the contents of the digital calibration certificate for mass calibrations of weights and weight sets. The present document refers to version 3.0.0 of the DCC scheme. For implementation, it is recommended to refer to the latest version of the scheme, currently version 3.1.2. This version is completely downward compatible and allows, among other things, improved indication of references. Given the continuous changes in the field of digital certificates, this report can only reflect the current state of discussions - something to be taken into account in any kind of evaluation or referencing. These changes may refer to changes in the schema file or to higher-level specifications such as coordinated refType attributes. The validity of the remaining regulations remains unaffected. Two xml files are attached to the expert report as examples.
Citation:	Expert report DKD-E 7-2 Instructions on how to use the DCC schema to create a digital calibration certificate for weights, Edition 04/2022, Revision 0, Physikalisch-Technische Bundesanstalt, Braunschweig and Berlin. DOI: 10.7795/550.20220419B

DKD	Instructions on how to use the DCC schema to create a digital calibration certificate for weights https://doi.org/10.7795/550.20220419B	DKD-E 7-2	
		Edition:	04/2022
		Revision:	0
		Page:	13 / 46

Main element	Sub-element	Explanation	Sample value
measurementResult (refId: weightABC1234)	*name*	Name of the result (multilingual text)	Mass calibration Weight ABC1234
	description	Description of the result (multilingual text, optional)	Mass calibration after revision of the piece of weight
	usedMethods	Description of the methods (optional)	see chapter 4.1
	usedSoftware	Description of the evaluation software used (optional)	1 - ∞ *software* (child elements: *name*, *release*, *description*)
	measuringEquipment	Description of the measuring equipment (optional)	see chapter 4.3
	influenceConditions	Description of measurement results (optional)	see chapter 4.2
	results	Results	see chapter 4.4
	measurementMetaData	Additional information (optional)	see chapter 4.5

Table 4: Example of contents in the element *measurementResult*

List of identified possible *refTypes* especially in the results part (usable in the elements *influenceCondition* – chapter 4.2, results – chapter 4.4 und *measurementMetaData* – chapter 4.5):

- *humidity*
- *temperature*
- *airpressure*
- *volume*
- *density*
- *mass*
- *conventionalWeighingValue*
- *min*
- *max*
- *nominalValue* (only to be used in the *result* element)
- *measurementValue* (only to be used in the *result* element)
- *referencedValue*
- *measurementDeviation* (only to be used in the *result* element)
- *meanValue*

4.1 Sub-element *usedMethods*

The element *measurementResult* contains the sub-element *usedMethods* to describe the calibration methods used. This sub-element consists of any number of child elements *usedMethod*; each of these child elements contains a name and a description.

DCC-Good Practice : Enabling machine interpretability?

```xml
<dcc:quantity refType="basic_referenceValue">
    <dcc:name>
        <dcc:content lang="de">Bezugswert</dcc:content>
        <dcc:content lang="en">Reference value</dcc:content>
    </dcc:name>
    <si:hybrid>
        <si:realListXMLList>
            <si:valueXMLList>306.248 373.121 448.253 523.319 593.154</si:valueXMLList>
            <si:unitXMLList>\kelvin</si:unitXMLList>
        </si:realListXMLList>
        <si:realListXMLList>
            <si:valueXMLList>33.098 99.971 175.103 250.169 320.004</si:valueXMLList>
            <si:unitXMLList>\degreecelsius</si:unitXMLList>
        </si:realListXMLList>
    </si:hybrid>
    <dcc:measurementMetaData>
        <dcc:metaData refType="basic_calibrationValue">
            <dcc:declaration>
                <dcc:content lang="de">Kalibrierpunkt</dcc:content>
                <dcc:content lang="en">Calibration value</dcc:content>
            </dcc:declaration>
            <dcc:data>
                <dcc:quantity>
                    <si:hybrid>
                        <si:realListXMLList>
                        <si:valueXMLList>306 373 448 523 593</si:valueXMLList>
                        <si:unitXMLList>\kelvin</si:unitXMLList>
                        </si:realListXMLList>
                        <si:realListXMLList>
                        <si:valueXMLList>32.85 99.85 174.85 249.85 319.85</si:valueXMLList>
                        <si:unitXMLList>\degreecelsius</si:unitXMLList>
                        </si:realListXMLList>
                    </si:hybrid>
                </dcc:quantity>
            </dcc:data>
        </dcc:metaData>
    </dcc:measurementMetaData>
</dcc:quantity>
```

Special attributes for defining the content, and protocols for data arrangement.

Language support

Calibration data in different units

Interpretation integrity of queried data

Xpath is the common tool for querying xml's, but it is weaknesses.

- **Complexity**: Challenging to understand, especially when dealing with nested structures. Writing and debugging becomes time-consuming and error-prone.
- **Fragile**: sensitive to changes in the document structure or layout. Even minor modifications can cause failure.

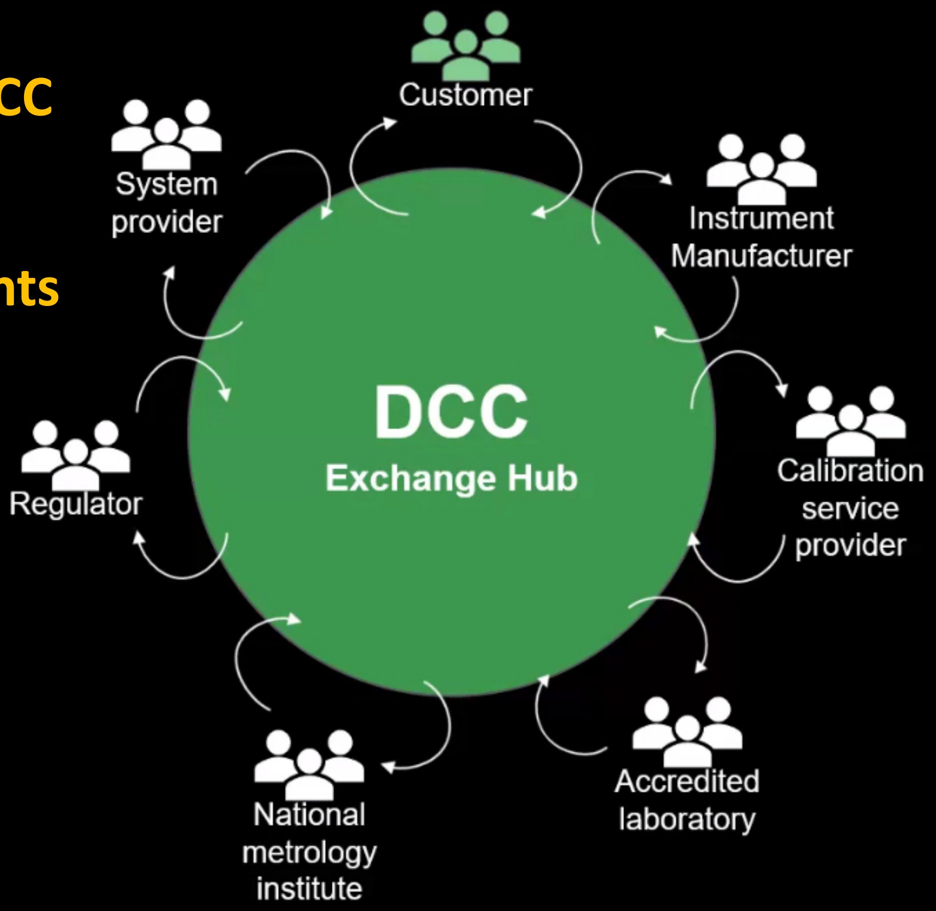
```
/dcc:digitalCalibrationCertificate/dcc:measurementResults/dcc:measurementResult/dcc:results/dcc:result[1]/dcc:data/dcc:list/dcc:quantity[2]/si:hybrid/si:realListXMLList[2]/si:valueXMLList

/dcc:digitalCalibrationCertificate/dcc:measurementResults/dcc:measurementResult/dcc:results/dcc:result[1]/dcc:data/dcc:list/dcc:quantity[2]/si:hybrid/si:realListXMLList[2]/si:expandedUncXMLList/si:uncertaintyXMLList
```

Scalability

DCC's needs to solve a many-to-many data transfer problem.

Requirements for DCC exchange system is comparable to the interface requirements for a relational database.

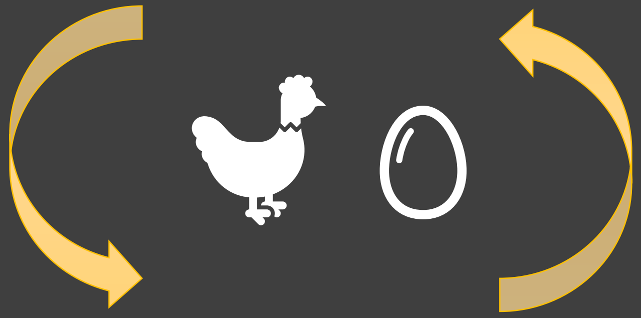


Databases (e.g. SQL) are most commonly designed as relational structures rather than Hierachical structures

Main challenge

Extraction of data from DCC

- *How to identify what data that is available*
- *How to extract the data relevant to the user*



- *How does the DCC structure best support that data is findable and extractable.*
- *How easy is it for the cal.lab. to adjust for different orders.*

Structure of the DCC

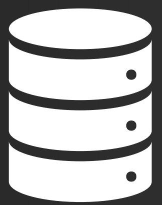
- *Restrictive structure ->*
  - *The structure cannot support all scenarios and customer requests.*

- *Flexible structure ->*
  - *Lots of implementation at the customer end to ensure valid extraction of data.*
  - *The Cal. Lab. has to support too many customer requirements.*
  - *Potential loss of data integrity*

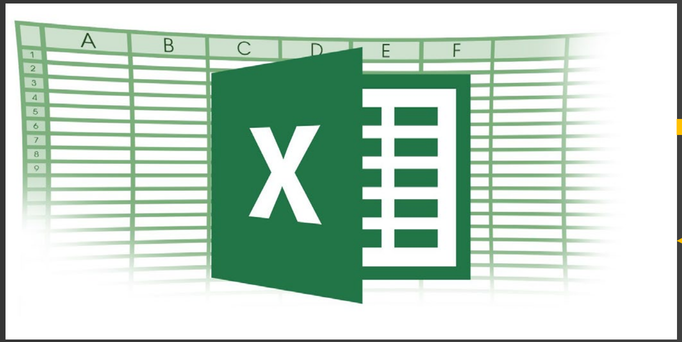
A Restrictive Harmonized Protocol / Standard is needed

Our own basic need in order to work with DCC:

Calibration
Worksheet
Database



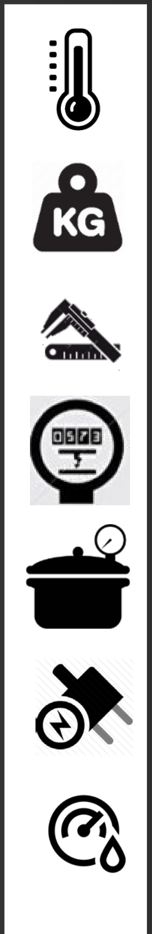
User
Interface



Generate
DCC

Load/query
DCC

Broad coverage



Temperature

Mass, volume, density

Geometry

Flow

Pressure

Electric

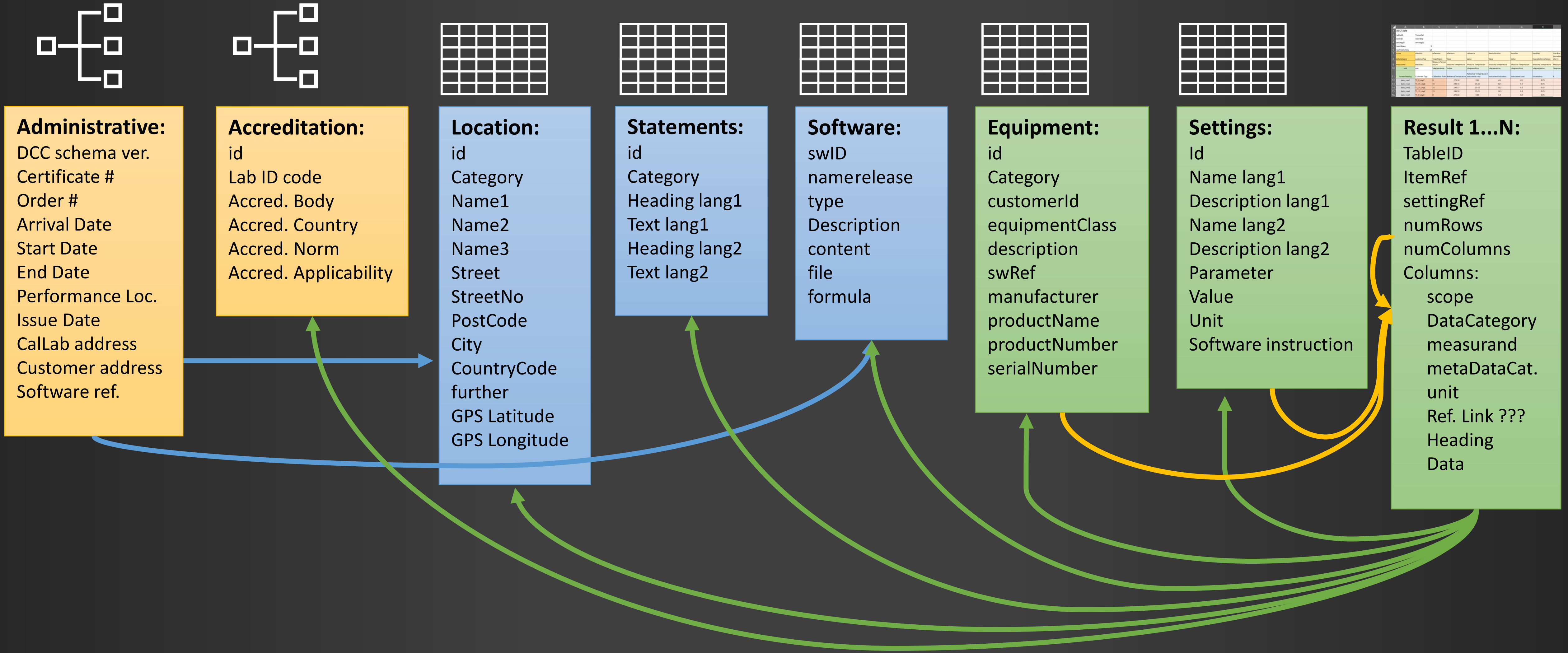
Humidity, Force, torque

If you can do it with Excel you can do it with any software

- Generating DCC: actually quite easy
- Making a general algorithm to load/query data: **quite difficult** due to flexibility of complex tree structure

Relational database architecture applied to DCC

As in a relational database – the data is structured into tables with predefined columns.
All row entries in the tables have unique identifiers – which can be reference /linkedto as required or needed.
Id's in the equipment, settings and results, are agreed with client and needed as parameters when doing a data lookup.



Proposal to introduce new attribute types

At the int. DCC conference 2023 DFM recommended to split **refId** and **refTypes** into more specific types.
We investigated this and came up with the following attribute splitting:

- **tableID**: This is equivalent to a resultID. It could be a product id by the cal.lab. or be assigned by customer.
- **itemRef**: This refers to the item being calibrated/testet.
- **settingsRef**: This refers to the setttings being applied on the item being calibrated/testet.
- **metaDataCategory:** Distinguish Data and Metadata
- **scope**: Specifies what the Information is about : item, reference, itemBias (relation btw. item & reference), datainfo
- **dataCategory**: Value, TargetValue, ExpandedUncertainty, …, accreditationApplies, Other
- **measurand**: Defines what kind of physical property is measured (a finite list e.g. using BIPM service categories or NSCLI-MII)
- **unit**: e.g. \kelvin, \kilogram, \metre, …
- **row**: index to point to a specific datapoint in the array.

A. **All 9 attributes has a finite set of predefined possible values, defined either by users or by schema (last 4 types)**

B. **Constitutes a finite set of query options:**
(TableID, ItemRef, SettingsRef, MeataDataCategory, scope, dataCategory, measurand, unit, row)

C. **Any combination attribute-parameter values is unique and provides:**
   A. **a relation between entities in DCC as well as**
   B. **a unique location of where to find the data.**
   C. **The XML tree depth is fixed for each of the parameters**

Finite options for attribute values are predefined in the Schema:

metaDataType

Data
UsedReferenceId
UsedMethodId
UsedEquipmentId
customerTag
laboratoryTag
accreditationException
TimeStamp
Exception
Statement

scopeTypes

-
reference
itemIndication
itemBias
environment

dataCategoryType

-
Value
TargetValue
ToleranceLimitUpper
ToleranceLimitUpper
AcceptanceLimitUpper
AcceptanceLimitUpper
Conformity
repeatability
Other
accreditationApplies
ExpandedUncertainty
UncertaintyCoverageFactor_k
UncertaintyCoverageProbability

measurandType

-
Measure.Conductance
Measure.Conductivity
Measure.Current.AC
Measure.Current.AC.Sinewave
Measure.Current.AC.Squarewave
Measure.Current.AC.Trianglewave
Measure.Current.DC
Measure.Density.Mass.Gas
Measure.Density.Mass.Liquid
Measure.Density.Mass.Solid
Measure.Force
Measure.Humidity.Absolute
Measure.Humidity.Relative
Measure.Frequency
…

Demo 1 – An Excel User Interface

- search(TempCal, itemID1, settings01, reference, Value, temperature, \kelvin, T3_15_degC) -> 288.16
- search(TempCal, itemID1, settings01, itemBias, ExpandedUncertainty, temperature, \degreecelcius, T3_15_degC) -> 0.05
- search(TempCal, itemID1, settings01, itemBias, itemIndication, temperature, \degreecelcius, T3_25_degC) -> 25.2

	A	B	C	D	E	F	G	H	
1	DCCTable								
2	tableID	TempCal							
3	itemID	itemID1							
4	settingID	setting01							
5	numRows	5							
6	numColumns	12							
7	scope	dataInfo	reference	reference	reference	itemIndication	itemBias	itemBias	itemBias
8	dataCategory	customerTag	TargetValue	Value	Value	Value	Value	ExpandedUncertainty	Uncertain ctor_k
9	measurand	metaData	Measure.Temperature	Measure.Temperature	Measure.Temperature	Measure.Temperature	Measure.Temperature	Measure.Temperature	Measure.
10	unit	nan	\degreecelcius	\kelvin	\degreecelcius	\degreecelcius	\degreecelcius	\degreecelcius	\degreece
11	humanHeading	Customer Tags	Calibration Point	Reference Temperature	Reference Temperature in instrument units	Instrument indication	Instrument Error	Uncertainty	k
12	data_row1	T0_0_degC	0	273.16	0.01	-0.1	-0.1	0.05	
13	data_row2	T1_15_degC	15	288.16	15.01	15.1	0.1	0.05	
14	data_row3	T2_25_degC	25	298.17	25.02	25.2	0.2	0.05	
15	data_row4	T3_15_degC	15	288.16	15.01	15.3	0.3	0.05	
16	data_row5	T4_0_degC	0	273.16	0.01	0.0	0.0	0.05	

Client aspect of extracting data from DCC

Instrument Database:

- Cert. No
- Supplier Name
- Equipment Id no.
- Calibration date
- Error Results
- Uncertainty(ies)

DCR generated by client

Table: tableId=nn125 refId=item2

dcc:column								
Sub elements	Column attributes	columns						
	metaType	main	CalibrationPoint	main	main	main	main	
	colType	customerTag	referenceResult	referenceResult	referenceResult	DUTIndication	DUTBias	
	measurandType	identification	temperatureAbsolute	temperatureAbsolute	temperatureAbsolute	temperatureAbsolute	temperatureDifference	
dcc:heading			*Calibration Point*	*Reference Temperature*	*Reference Temperature in instrument units*	*Instrument indication*	*Instrument Error*	
si:unit			\degreecelcius	\kelvin	\degreecelcius	\degreecelcius	\degreecelcius	
XMLList		T0_0_degC	0					
		T1_15_degC	15					
		T2_25_degC	25					
		T3_15_degC	15					
		T4_0_degC	0					

DCR send to Cal. Lab.

DCC generated Cal. Lab.

Table: tableId=nn125 refId=item2

dcc:column							
Sub elements	Column attributes	columns					
	metaType	main	CalibrationPoint	main	main	main	main
	colType	customerTag	referenceResult	referenceResult	referenceResult	DUTIndication	DUTBias
	measurandType	identification	temperatureAbsolute	temperatureAbsolute	temperatureAbsolute	temperatureAbsolute	temperatureDifference
dcc:heading			*Calibration Point*	*Reference Temperature*	*Reference Temperature in instrument units*	*Instrument indication*	*Instrument Error*
si:unit			\degreecelcius	\kelvin	\degreecelcius	\degreecelcius	\degreecelcius
XMLList		T0_0_degC	0	273.16	0.01	-0.1	-0.1
		T1_15_degC	15	288.16	15.01	15.1	0.1
		T2_25_degC	25	298.17	25.02	25.2	0.2
		T3_15_degC	15	288.16	15.01	15.2	0.2
		T4_0_degC	0	273.16	0.01	0.0	0.0

Mapping table

DB_ID	DCC_LOC
Cert. No	XPath1/…
Meas.val.	XPath2/…
Equip. ID	XPath3/…
Result1	TableID,itemID, scope, category, measurand, unit, (row)
Uncert1	TableID, itemID, scope, category, measurand, unit, (row)

DCC Send to Client

DCC API

Mapping is used to import data from DCC

- Cert. No
- Supplier Name
- Equipment Id no.
- Calibration date
- Error Results
- Uncertainty(ies)

Instrument Database:

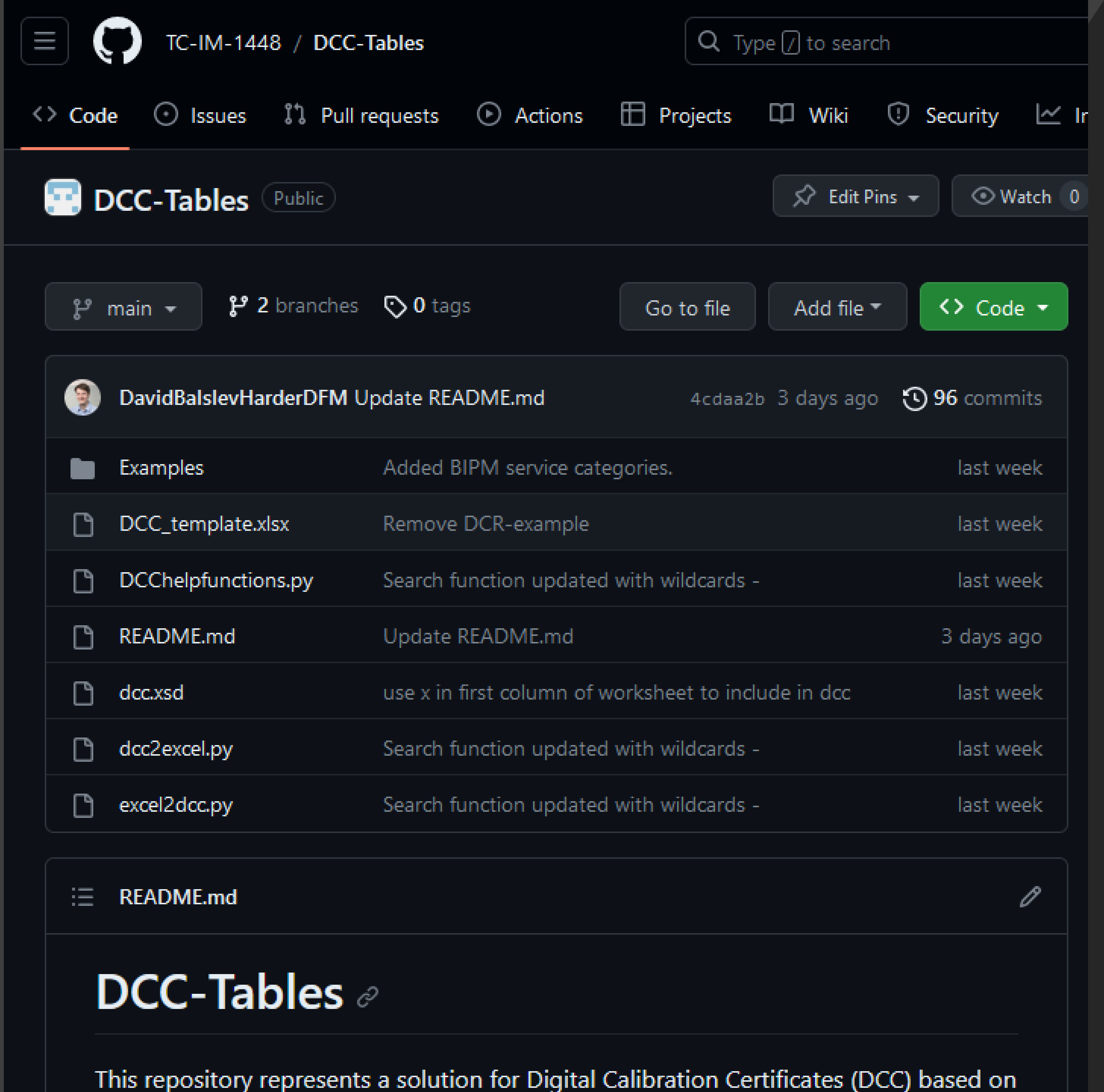
Implementation is available:

https://github.com/TC-IM-1448/DCC-Tables

dcc.xsd - Schema file.

3 python files implementing

- the necessary functions to interface with Excel
- A python API to query data from DCC's



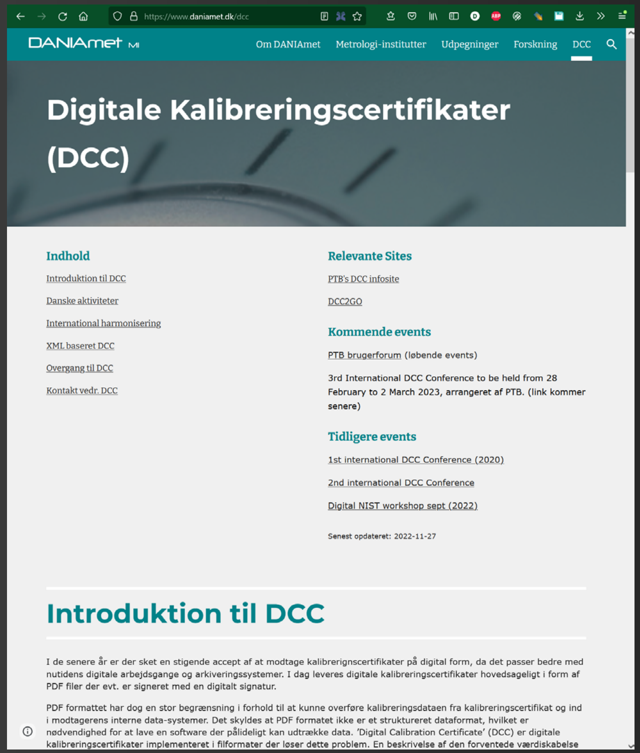
Next steps

International Harmonisation discussed in EURAMET Project TC-IM 1448 WP1.

Testing of DCC Tables and comparison to DCC 3.X is initiating this autumn. In collaborations between DFM, DTI FORCE Technology and Danish pharma-industry (Novo Nordisk) as well as accredited labs e.g. DANDIAG (pipettes).

DCC2GO: https://github.com/DCC2GO-Project

Keep updated on the danish webpage to coordinate and disseminate information about DCC to Danish stakeholders.



www.daniamet.dk/dcc

Thank You

To TI for hosting todays event.

To Danish collaborators, TI, FORCE, Novo Nordisk, DANDIAG etc.

To International collaborators at PTB, TC-IM 1448, DCC2GO and other fora.

To audience for listening.

Contact: David Balslev-Harder (dbh@dfm.dk)