

SECoP@HMC – Data Storage

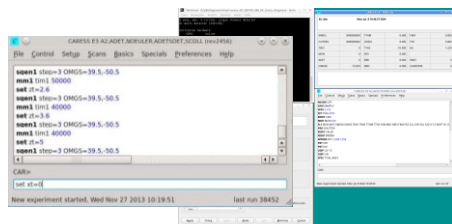
Making sample environment (meta)data understandable



Sample Environment Communication Protocol

HZB

Experiment Control

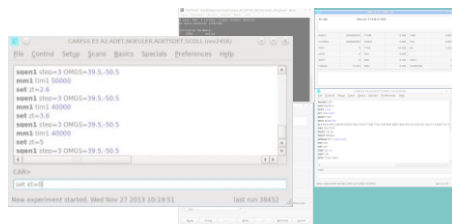


Sample Environment

Sample Environment Communication Protocol

HZB

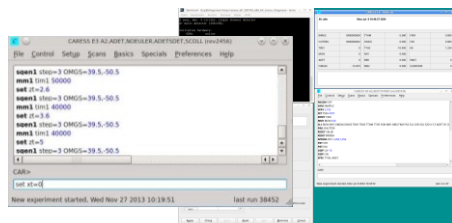
Experiment Control



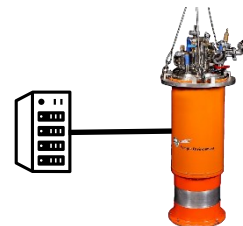
Sample Environment

HZB

Experiment Control
+ SECoP Client



SECoP

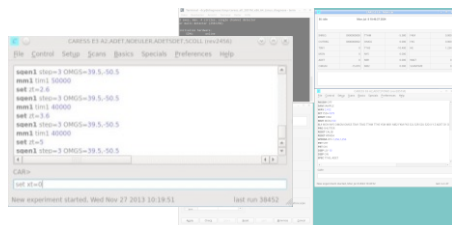


Sample Environment
+ SECoP Server (SENode)

Sample Environment Communication Protocol

HZB

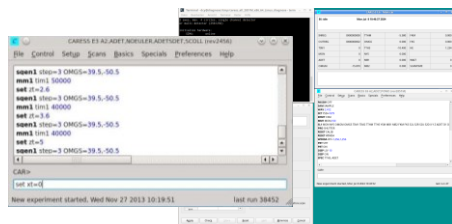
Experiment Control



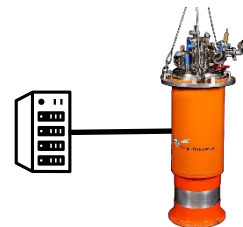
Sample Environment

HZB

Experiment Control
+ SECoP Client



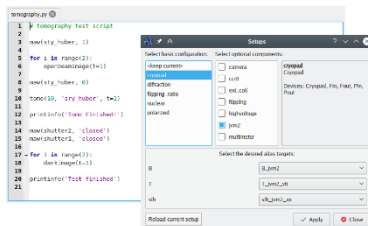
SECoP



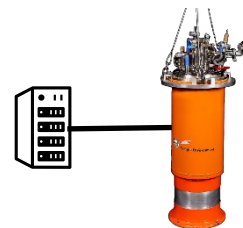
Sample Environment
+ SECoP Server (SENode)

MLZ
Heinz Maier-Leibnitz Zentrum

Experiment Control
+ SECoP Client



SECoP



Sample Environment
+ SECoP Server (SENode)



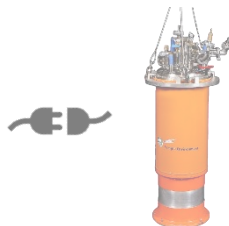
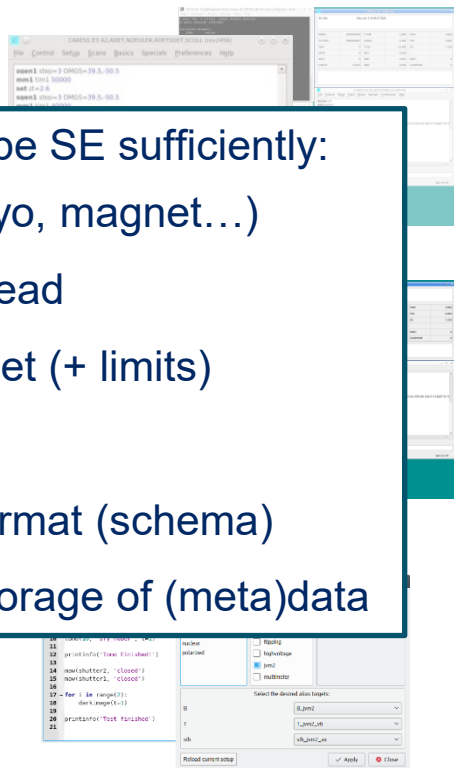
Sample Environment Communication Protocol

HZB

Metadata to describe SE sufficiently:

- Model / kind (cryo, magnet...)
 - Parameters to read
 - Parameters to set (+ limits)
 - Units
- ⇒ Standardised format (schema)
- ⇒ Standardised storage of (meta)data

Experiment Control
+ SECoP Client



Sample Environment

SECoP



Sample Environment
+ SECoP Server (SENode)

SECoP



Sample Environment
+ SECoP Server (SENode)



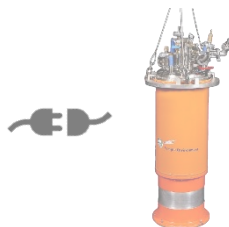
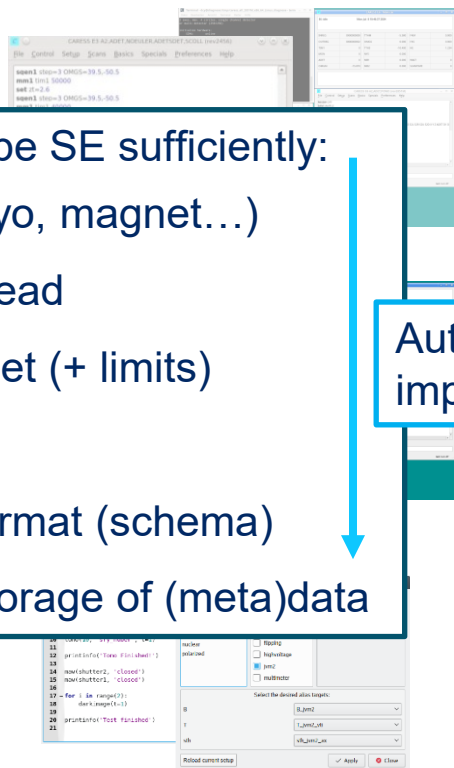
Sample Environment Communication Protocol

HZB

Metadata to describe SE sufficiently:

- Model / kind (cryo, magnet...)
 - Parameters to read
 - Parameters to set (+ limits)
 - Units
- ⇒ Standardised format (schema)
- ⇒ Standardised storage of (meta)data

Experiment Control
+ SECoP Client



Sample Environment

Automatic storage of
important metadata

Sample Environment
+ SECoP Server (SENode)

SECoP



Sample Environment
+ SECoP Server (SENode)

Sample Environment Communication Protocol

```
> describe
< describing .
{
  "description":"TestNode",
  "equipment_id":"HZB_Testnode1",
  "firmware":"SHALL server library (Git 70591a14f66f37b92dcf6386a17159b526fa2913)",
  "modules":
  {
    "temp1":
    {
      "interface_classes":["Writable","Readable"],
      "description":"a meaningful description of the module",
      "accessibles":
      {
        "value":
        {
          "description":"temperature",
          "datainfo":{"type":"double","unit":"K"},
          "readonly":true
        },
        "target":
        {
          "description":"target temperature",
          "datainfo":{"type":"double","unit":"K"},
          "readonly":false
        }
      }
    }
  }
}
```

General description (static parameters)

List of modules (dynamic parameters)
(e.g. a magnet could read/set several temperatures and a magnetic field)

Experiment control can read
current temperature

Experiment control can set
target temperature

SECoP: Meaning

Each module defines what it does:

"meaning": {

"key": "sample temperature",

(human readable)

"link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",

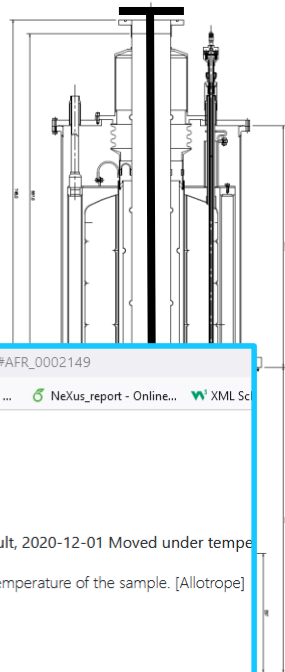
(machine readable)

"function": "temperature_regulation",

(SECoP class)

"importance": 20,

"belongs_to": "sample" }



← → ↻ 🏠 purl.allotrope.org/ontologies/result#AFR_0002149

Perplexity How to Install a Linux ... Meeting eröffnen - Zo... Gerit Guenther / My ... NeXus_report - Online... XML Sc

sample temperature

(http://purl.allotrope.org/ontologies/result#AFR_0002149)

synonyms: 2020-12-01 Changed labels. [Allotrope], sample temperature result, 2020-12-01 Moved under tempe

A sample temperature result is a quality quantification facet that quantifies the temperature of the sample. [Allotrope]

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defined in:

- <http://purl.allotrope.org/voc/afo/REC/2020/12/aft>
- <http://purl.allotrope.org/voc/afo/REC/2021/03/aft>

SECoP: Meaning

Each module defines what it does:

```
"meaning": {
```

```
  "key": "sample temperature",
```

(human readable)

```
  "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",
```

(machine readable)

```
  "function": "temperature_regulation",
```

(SECoP class)

```
  "importance": 20,
```

(artificial parameter)

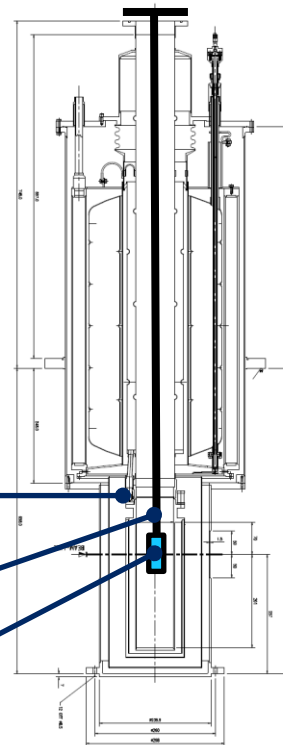
```
  "belongs_to": "sample" }
```

(applies to)

SE temperature
(importance 5)

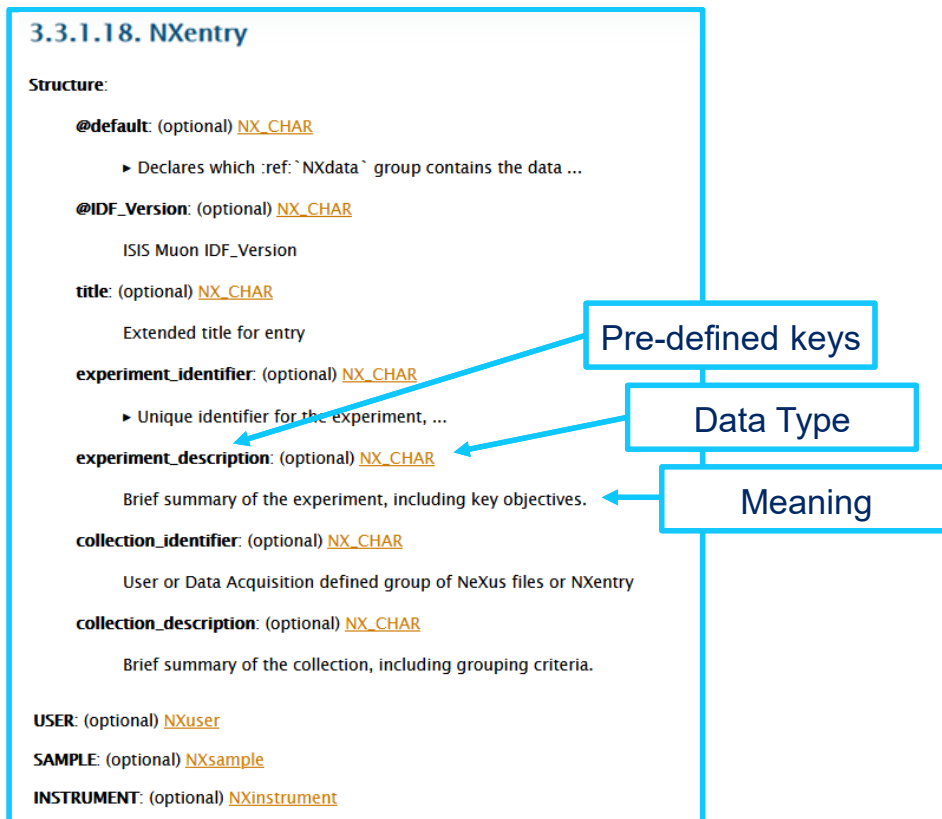
Sample stick temperature
(importance 10)

Sample holder temperature
(importance 20)



NeXus

- Binary file format (HDF5)
- Hierarchical, defined structure
 - Groups
 - Data Fields
 - @Attributes
- Metadata + data create context
- Persistent web description (URL)
- Modular structure (base classes)
- Metadata schema for experimental data



NeXus

- Binary file format (HDF5)
- Hierarchical, defined structure
 - Groups
 - Data Fields
 - @Attributes
- Metadata + data create context
- Persistent web description (URL)
- Modular structure (base classes)
- Metadata schema for experimental data: logic through structure & semantics

3.3.1.18. NXentry

Structure:

@default: (optional) [NX_CHAR](#)

► Declares which :ref:`NXdata` group

@IDF_Version: (optional) [NX_CHAR](#)

ISIS Muon IDF_Version

title: (optional) [NX_CHAR](#)

Extended title for entry

experiment_identifier: (optional) [NX_CHAR](#)

► Unique identifier for the experiment, ...

experiment_description: (optional) [NX_CHAR](#)

Brief summary of the experiment, inc

collection_identifier: (optional) [NX_CHAR](#)

User or Data Acquisition defined gro

collection_description: (optional) [NX_CHAR](#)

Brief summary of the collection, inclu

USER: (optional) [NXuser](#)

SAMPLE: (optional) [NXsample](#)

INSTRUMENT: (optional) [NXinstrument](#)

3.3.1.56. NXuser

Structure:

@default: (optional) [NX_CHAR](#)

► Declares which child group contains a path leading .

name: (optional) [NX_CHAR](#)

Name of user responsible for this entry

role: (optional) [NX_CHAR](#)

► Role of user responsible for this entry. ...

3.3.1.47. NXsample

Structure:

@default: (optional) [NX_CHAR](#)

► Declares which child group contains a path leading ...

name: (optional) [NX_CHAR](#)

Descriptive name of sample

chemical_formula: (optional) [NX_CHAR](#)

► The chemical formula specified using CIF conventions. ...

```
{
  "description": "TestNode",
  "equipment_id": "HZB_Testnode1",
  "firmware": "SHALL server library (Git 70591a14f6",
  "modules":
  {
    "temp1":
    {
      "interface_classes": ["Writable", "Readable"],
      "description": "a meaningful description of t",
      "accessibles":
      {
        "value":
        {
          "description": "temperature",
          "datainfo": {"type": "double", "unit": "K"},
          "readonly": true
        },
        "meaning":
        {
          "key": "sample temperature",
          "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",
          "function": "temperature_regulation",
          "importance": 20,
          "belongs_to": "sample"
        }
      }
    }
  }
}
```

3.3.1.47. NXsample

Structure:

name: (optional) [NX_CHAR](#)

Descriptive name of sample

temperature: (optional) [NX_FLOAT](#) (Rank: anyRank, Dimensions: [1

Sample temperature. This could be a scanned variable

temperature_env: (optional) [NXenvironment](#)

Additional sample temperature environment information

magnetic_field: (optional) [NXlog](#)

magnetic_field.value is a link to e.g. magnetic_field_env.sensor1.value

chemical_formula: (optional) [NX_CHAR](#)

► The chemical formula specified using CIF conventions. ...

```
{
  "description": "TestNode",
  "equipment_id": "HZB_Testnode1",
  "firmware": "SHALL server library (Git 70591a14f6)",
  "modules": {
    "temp1": {
      "interface_classes": ["Writable", "Readable"],
      "description": "a meaningful description of temperature",
      "accessibles": {
        "value": {
          "description": "temperature",
          "datainfo": {"type": "double", "unit": "K"},
          "readonly": true
        }
      },
      "meaning": {
        "key": "sample temperature",
        "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",
        "function": "temperature_regulation",
        "importance": 20,
        "belongs_to": "sample"
      }
    }
  }
}
```

3.3.1.47. NXsample

Structure:

name: (optional) [NX_CHAR](#)

Descriptive name of sample

temperature: (optional) [NX_FLOAT](#) (Rank: anyRank)

Sample temperature. This could be a scanned

temperature_env: (optional) [NXenvironment](#)

Additional sample temperature environment info

magnetic_field: (optional) [NXlog](#)

magnetic_field.value is a link to e.g. magnetic_field_env.sensor1.value

chemical_formula: (optional) [NX_CHAR](#)

► The chemical formula specified using CIF conventions. ...

3.3.1.19. NXenvironment

Structure:

name: (optional) [NX_CHAR](#)

Apparatus identification code/model number; e.g. OC100 011

description: (optional) [NX_CHAR](#)

Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump

SENSOR: (optional) [NXsensor](#)

SECoP ⇒ NeXus

```
{
  "description": "TestNode",
  "equipment_id": "HZB_Testnode1",
  "firmware": "SHALL server library (Git 70591a14f6)",
  "modules": {
    "temp1": {
      "interface_classes": ["Writable", "Readable"],
      "description": "a meaningful description of the module",
      "accessibles": {
        "value": {
          "description": "temperature",
          "datainfo": { "type": "double", "unit": "K" },
          "readonly": true
        },
        "meaning": {
          "key": "sample temperature",
          "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149",
          "function": "temperature_regulation",
          "importance": 20,
          "belongs_to": "sample"
        }
      }
    }
  }
}
```

3.3.1.47. NXsample

Structure:

name: (optional) [NX_CHAR](#)
Descriptive name of sample

temperature: (optional) [NX_FLOAT](#) (Rank: anyRank)
Sample temperature. This could be a scanned value.

temperature_env: (optional) [NXenvironment](#)
Additional sample temperature environment information.

magnetic_field: (optional) [NXlog](#)
magnetic_field.value is a [NXlog](#).

chemical_formula: (optional) [NX_CHAR](#)
The chemical formula of the sample.

3.3.1.19. NXenvironment

Structure:

name: (optional) [NX_CHAR](#)
Apparatus identification code/model number; e.g. OC100 011

description: (optional) [NX_CHAR](#)
Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump

SENSOR: (optional) [NXsensor](#)

3.3.1.49. NXsensor

Structure:

name: (optional) [NX_CHAR](#)
Name for the sensor

value_log: (optional) [NXlog](#)
Time history of sensor readings

measurement: (optional) [NX_CHAR](#)
name for measured signal ...
Any of these values:

- [temperature](#)
- [pH](#)
- [magnetic_field](#)
- [electric_field](#)
- [conductivity](#)
- [resistance](#)
- [voltage](#)

SECoP ⇒ NeXus

```
{
  "description": "TestNode",
  "equipment_id": "HZB_Testnode1",
  "firmware": "SHALL server library (Git 70591a14f6)",
  "modules": {
    "temp1": {
      "interface_classes": ["Writable", "Readable"],
      "description": "a meaningful description of the module",
      "accessibles": {
        "value": {
          "description": "temperature",
          "datainfo": { "type": "double", "unit": "K" },
          "readonly": true
        },
        "meaning": {
          "key": "sample temperature",
          "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149",
          "function": "temperature_regulation",
          "importance": 20,
          "belongs_to": "sample"
        }
      }
    }
  }
}
```

3.3.1.47. NXsample

Structure:

- name:** (optional) [NX_CHAR](#)
Descriptive name of sample
- temperature:** (optional) [NX_FLOAT](#) (Rank: anyRank)
Sample temperature. This could be a scanned value.
- temperature_env:** (optional) [NXenvironment](#)
Additional sample temperature environment information.
- magnetic_field:** (optional) [NXlog](#)
magnetic_field.value is an array of [NXlog](#) objects.
- chemical_formula:** (optional) [NX_CHAR](#)
The chemical formula of the sample.

3.3.1.19. NXenvironment

Structure:

- name:** (optional) [NX_CHAR](#)
Apparatus identification code/model number; e.g. OC100 011
- description:** (optional) [NX_CHAR](#)
Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump
- SENSOR:** (optional) [NXsensor](#)

3.3.1.49. NXsensor

Structure:

- name:** (optional) [NX_CHAR](#)
Name for the sensor
- value_log:** (optional) [NXlog](#)
Time history of sensor reading
- measurement:** (optional) [NX_CHAR](#)
name for measured signal ...
Any of these values:
 - [temperature](#)
 - [pH](#)
 - [magnetic_field](#)
 - [electric_field](#)
 - [conductivity](#)
 - [resistance](#)
 - [voltage](#)

3.3.1.30. NXlog

Structure:

- time:** (optional) [NX_NUMBER](#) {units=[NX_TIME](#)}
Time of logged entry. The times are relative to the "start" attribute ...
- @start:** (optional) [NX_DATE_TIME](#)
- @scaling_factor:** (optional) [NX_NUMBER](#)
- value:** (optional) [NX_NUMBER](#) {units=[NX_ANY](#)}
Array of logged value, such as temperature. If this is ...

SECoP ⇒ NeXus

```
{
  "description": "TestNode",
  "equipment_id": "HZB_Testnode1",
  "firmware": "SHALL server library (Git 70591a14f6)",
  "modules": {
    "temp1": {
      "interface_classes": ["Writable", "Readable"],
      "description": "a meaningful description of the module",
      "accessibles": {
        "value": {
          "description": "temperature",
          "datainfo": {
            "type": "double",
            "unit": "K",
            "readonly": true
          },
          "meaning": {
            "key": "sample temperature",
            "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149",
            "function": "temperature_regulation",
            "importance": 20,
            "belongs_to": "sample"
          }
        }
      }
    }
  }
}
```

3.3.1.47. NXsample

Structure:

- name:** (optional) [NX_CHAR](#)
Descriptive name of sample
- temperature:** (optional) [NX_FLOAT](#) (Rank: anyRank)
Sample temperature. This could be a scanned value
- temperature_env:** (optional) [NXenvironment](#)
Additional sample temperature environment information
- magnetic_field:** (optional) [NXlog](#)
magnetic_field.value is an [NXlog](#)
- chemical_formula:** (optional) [NX_CHAR](#)
The chemical formula of the sample

3.3.1.19. NXenvironment

Structure:

- name:** (optional) [NX_CHAR](#)
Apparatus identification code/model number; e.g. OC100 011
- description:** (optional) [NX_CHAR](#)
Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump
- SENSOR:** (optional) [NXsensor](#)

3.3.1.49. NXsensor

Structure:

- name:** (optional) [NX_CHAR](#)
Name for the sensor
- value_log:** (optional) [NXlog](#)
Time history of sensor reading
- measurement:** (optional) [NX_CHAR](#)
name for measured signal ...
Any of these values:
 - [temperature](#)
 - [pH](#)
 - [magnetic_field](#)
 - [electric_field](#)
 - [conductivity](#)
 - [resistance](#)
 - [voltage](#)

3.3.1.30. NXlog

Structure:

- time:** (optional) [NX_NUMBER](#) {units=[NX_TIME](#)}
Time of logged entry. The times are relative to the "start" attribute ...
- @start:** (optional) [NX_DATE_TIME](#)
- @scaling_factor:** (optional) [NX_NUMBER](#)
- value:** (optional) [NX_NUMBER](#) {units=[NX_ANY](#)}
Array of logged value, such as temperature. If this is ...

SECoP ⇒ NeXus

```
{  
  "description": "TestNode",  
  "equipment_id": "HZB_Testnode1",  
  "firmware": "SHALL server library (Git 70591a14f6)",  
  "modules":  
  {  
    "temp1":  
    {  
      "interface_classes": ["Writable", "Readable"],  
      "description": "a meaningful description of the module",  
      "accessibles":  
      {  
        "value":  
        {  
          "description": "temperature",  
          "datainfo": {"type": "double", "unit": "K"},  
          "readonly": true  
        },  
        "meaning":  
        {  
          "key": "sample temperature",  
          "link": "http://purl.allotrope.org/ontologies/result#AFR_0002145",  
          "function": "temperature_regulation",  
          "importance": 20,  
          "belongs_to": "sample"  
        }  
      }  
    }  
  }  
}
```

3.3.1.47. NXsample

Structure:

name: (optional) [NX_CHAR](#)
Descriptive name of sample

temperature: (optional) [NX_FLOAT](#) (Rank: anyRank)
Sample temperature. This could be a scanned value.

temperature_env: (optional) [NXenvironment](#)
Additional sample temperature environment information.

magnetic_field: (optional) [NXlog](#)
magnetic_field.value is an NXlog.

chemical_formula: (optional) [NX_CHAR](#)
The chemical formula.

3.3.1.19. NXenvironment

Structure:

name: (optional) [NX_CHAR](#)
Apparatus identification code/model number; e.g. OC100 011

description: (optional) [NX_CHAR](#)
Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump

SENSOR: (optional) [NXsensor](#)

3.3.1.49. NXsensor

Structure:

name: (optional) [NX_CHAR](#)
Name for the sensor

value_log: (optional) [NXlog](#)
Time history of sensor readings.

measurement: (optional) [NX_CHAR](#)
name for measured signal ...
Any of these values:

- [temperature](#)
- [pH](#)
- [magnetic_field](#)
- [electric_field](#)
- [conductivity](#)
- [resistance](#)
- [voltage](#)

3.3.1.30. NXlog

Structure:

time: (optional) [NX_NUMBER](#) {units=[NX_TIME](#)}
Time of logged entry. The times are relative to the "start" attribute ...

@start: (optional) [NX_DATE_TIME](#)

@scaling_factor: (optional) [NX_NUMBER](#)

value: (optional) [NX_NUMBER](#) {units=[NX_ANY](#)}
Array of logged value, such as temperature. If this is ...

SECoP ⇒ NeXus

```
{
  "description": "TestNode",
  "equipment_id": "HZB_Testnode1",
  "firmware": "SHALL server library (Git 70591a14f6)",
  "modules": {
    "temp1": Module
  }
  {
    "interface_classes": ["Writable", "Readable"],
    "description": "a meaningful description of the module",
    "accessibles": {
      "value": Parameter
    }
    {
      "description": "temperature",
      "datainfo": { "type": "double", "unit": "K" },
      "readonly": true
    },
    "meaning": {
      "key": "sample temperature",
      "link": "http://purl.allotrope.org/ontologies/result#AFR_0002145",
      "function": "temperature_regulation",
      "importance": 20,
      "belongs_to": "sample"
    }
  },
}
```

3.3.1.47. NXsample

Structure:

name: (optional) [NX_CHAR](#)
Descriptive name of sample

temperature: (optional) [NX_FLOAT](#) (Rank: anyRank)
Sample temperature. This could be a scanned value.

temperature_env: (optional) [NXenvironment](#)
Additional sample temperature environment information.

magnetic_field: (optional) [NXlog](#)
magnetic_field.value is an array of [NXlog](#) objects.

chemical_formula: (optional) [NX_CHAR](#)
The chemical formula of the sample.

3.3.1.19. NXenvironment

Structure:

name: (optional) [NX_CHAR](#)
Apparatus identification code/model number; e.g. OC100 011

description: (optional) [NX_CHAR](#)
Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump

SENSOR: (optional) [NXsensor](#)

3.3.1.49. NXsensor

Structure:

name: (optional) [NX_CHAR](#)
Name for the sensor

value_log: (optional) [NXlog](#)
Time history of sensor readings.

measurement: (optional) [NX_CHAR](#)
name for measured signal ...
Any of these values:

- temperature
- pH
- magnetic_field
- electric_field
- conductivity
- resistance
- voltage

3.3.1.30. NXlog

Structure:

time: (optional) [NX_NUMBER](#) {units=[NX_TIME](#)}
Time of logged entry. The times are relative to the "start" attribute ...

@start: (optional) [NX_DATE_TIME](#)

@scaling_factor: (optional) [NX_NUMBER](#)

value: (optional) [NX_NUMBER](#) {units=[NX_ANY](#)}
Array of logged value, such as temperature. If this is ...

3.3.1.8. NXcollection

Description:

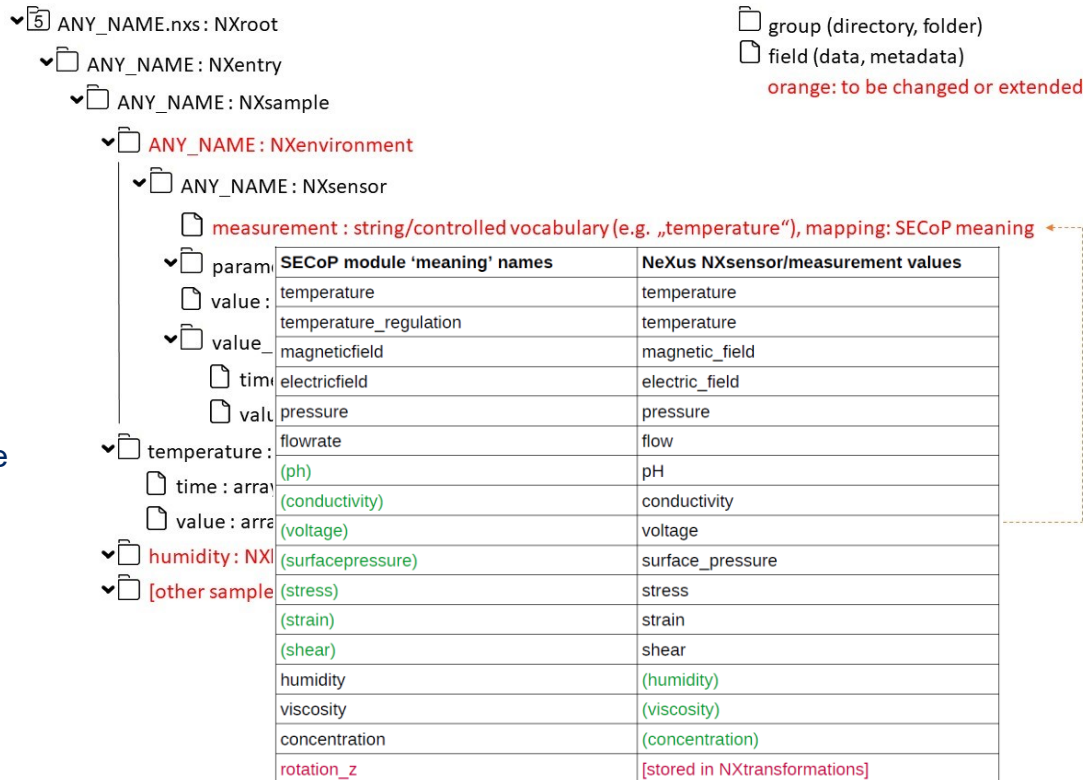
► An unvalidated set of terms, such as the description of a beam line. ...

Everything else

SECoP ⇒ NeXus

Required modifications:

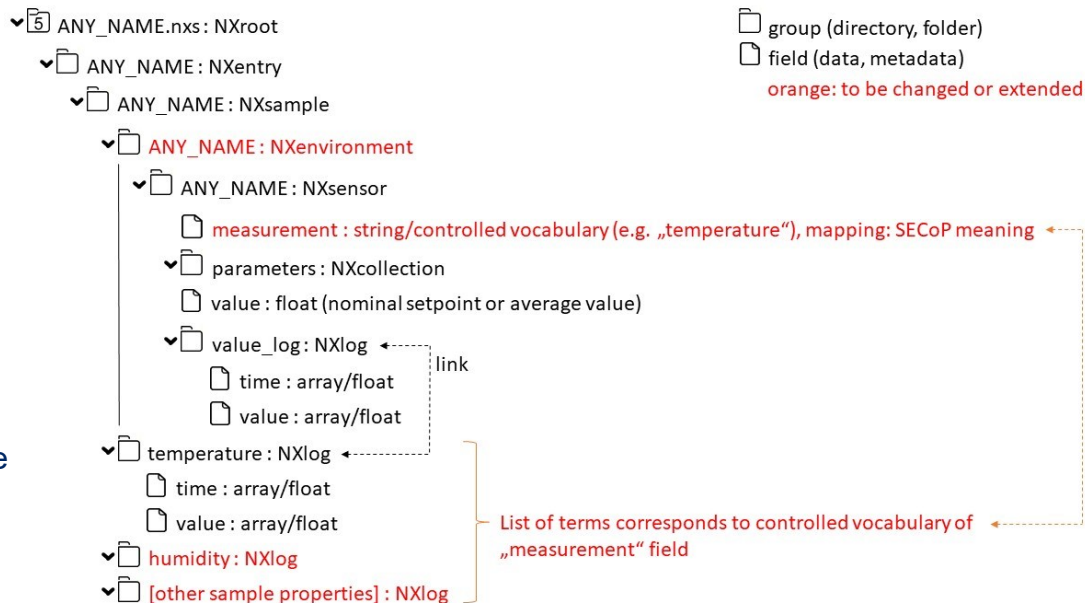
- Extension of 'measurement' field ('humidity', 'viscosity', and 'concentration')
- Add corresponding fields to NXsample
- Adding 'NXenvironments' according to 'measurement' fields (currently only temperature_env and magnetic_field_env are allowed)
- Allow any 'NXenvironment' (ANY_NAME : NXenvironment)



SECoP ⇒ NeXus

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SECoP ⇒ NeXus: Implementation

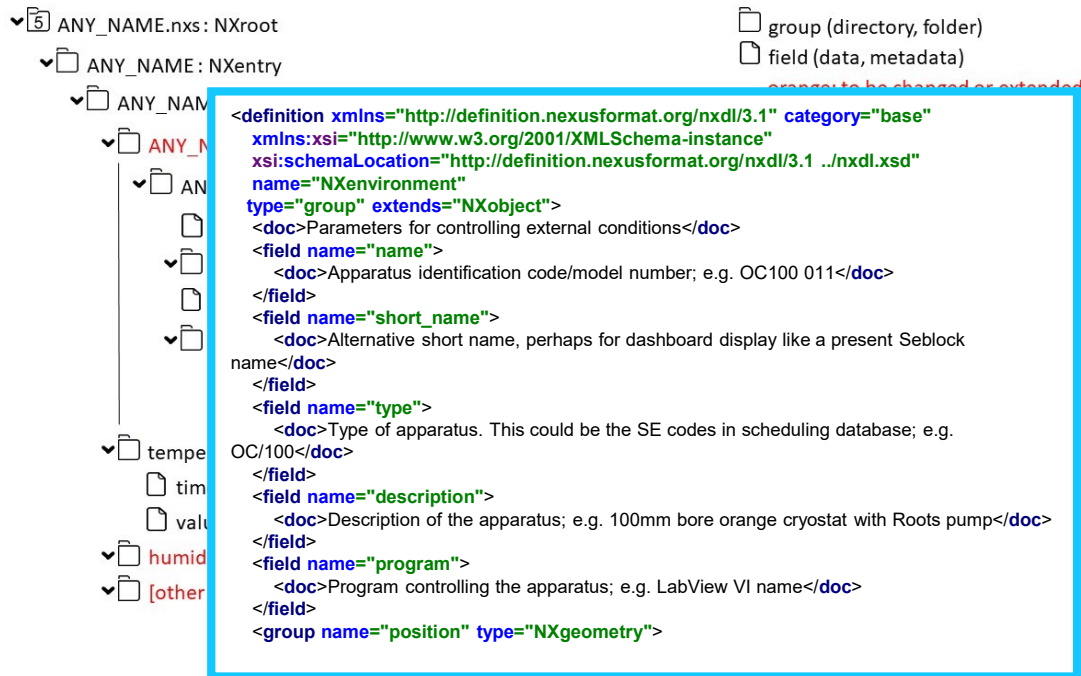
How to implement changes?

1. Extension of NeXus standard:

- NXDL description of changes
- Proposal to NIAC through representatives

2. Meanwhile:

- Make modified NXDL available via PID (e.g. at Zenodo)
- Refer from NeXus field 'definition_local' to modified NXDL



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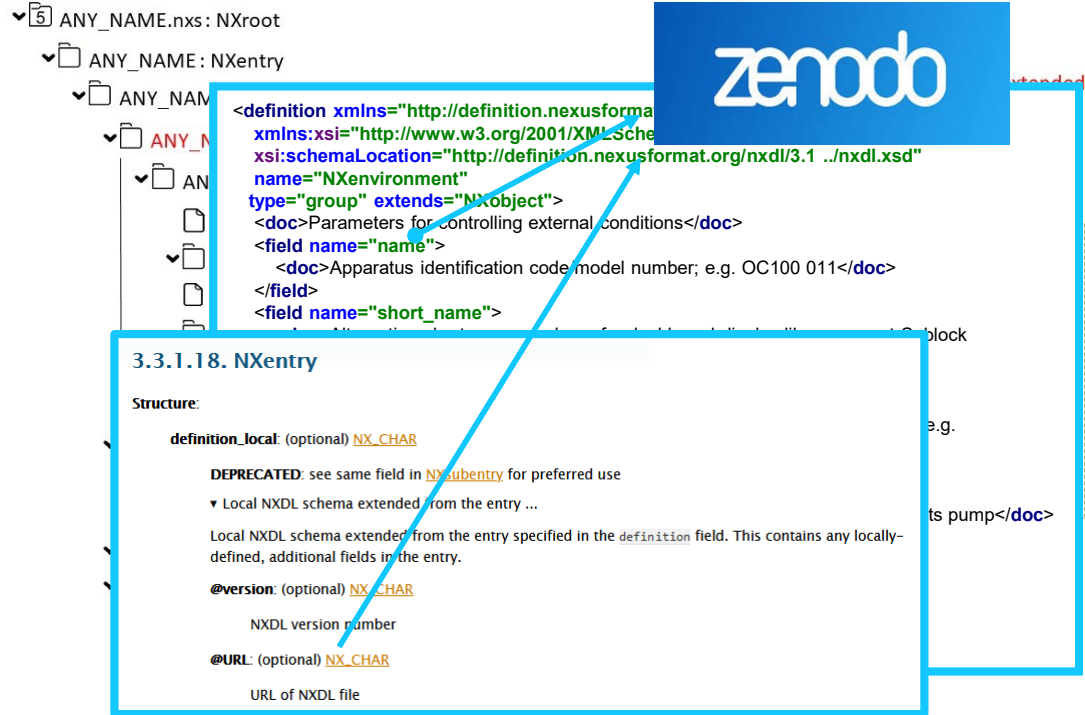


Diagram illustrating the relationship between the NeXus XML schema and its documentation:

- XML Schema (Left):** Shows the definition of `NXEnvironment` (type="group", extends="NXobject"). It includes fields `name` (documentation: Apparatus identification code model number; e.g. OC100 011) and `short_name`.
- Documentation (Right):** Shows the section **3.3.1.18. NXentry** under the heading **Structure:**. It describes the `definition_local` field (optional `NX_CHAR`), which is deprecated and refers to the `definition` field. It also describes the `@version` field (optional `NX_CHAR`) and the `@URL` field (optional `NX_CHAR`).
- Zenodo:** A blue box with the Zenodo logo is positioned above the XML schema, indicating that modified NXDLs are available via PID (e.g., at Zenodo).

SECoP: Meaning

Each module defines what it does:

"meaning": {

 "key": "sample temperature",

 "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",

 "function": "temperature_regulation",

 "importance": 20,

 "belongs_to": "sample" }

The screenshot displays the Protégé ontology editor interface. The left pane shows a hierarchical tree of classes, with 'sample temperature' selected and highlighted in blue. The right pane shows the details for the 'sample temperature' class, including its URI, annotations, and description.

Class Details:

- URI:** http://purl.allotrope.org/ontologies/result#AFR_0002149
- Annotations:**
 - rdfs:label:** sample temperature
 - 'preferred label':** sample temperature
 - definition:** A sample temperature result is a quality quantification facet that quantifies the temperature of the sample. [Allotrope]
 - 'alternative label':** sample temperature (datum)
- Description:** sample temperature
- Equivalent To:** (none listed)
- SubClass Of:** temperature