

# NeXus Framework at DESY

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# NeXus format and HDF5

- NeXus is a set of rules how data must be organized within a particular format in order to become a valid file.
- Every NeXus file written by us is also a valid HDF5 file!



NeXus

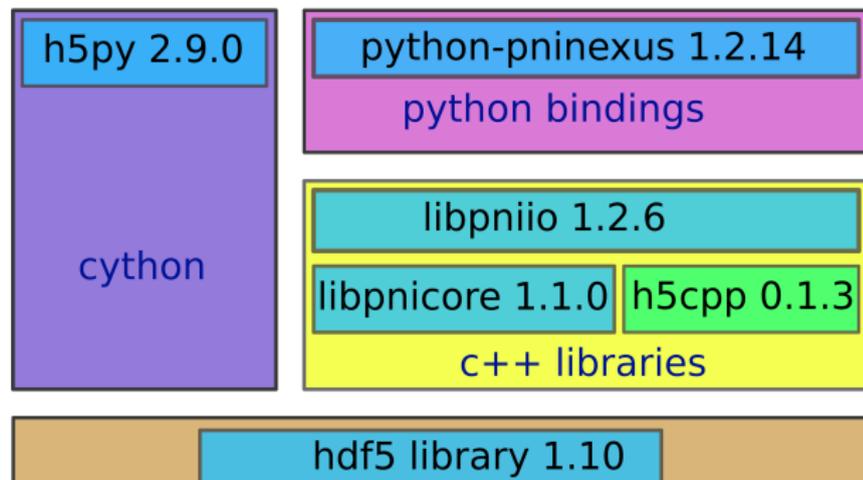
Layer 3: application definitions

Layer 2: base classes

Layer 1: nxgroup, nxfield, nxattribute, nxlink, types

- scalar and multidimensional data within a single file
- data within the file in a tree like manager
- additional attributes can be attached to objects in a file storing metadata which might be required for later analysis

## production



**h5cpp** – c++ wrapper for hdf5 library (ESS/DESY)

**pniio/pnicore** – HL interface and NeXus structure from XML

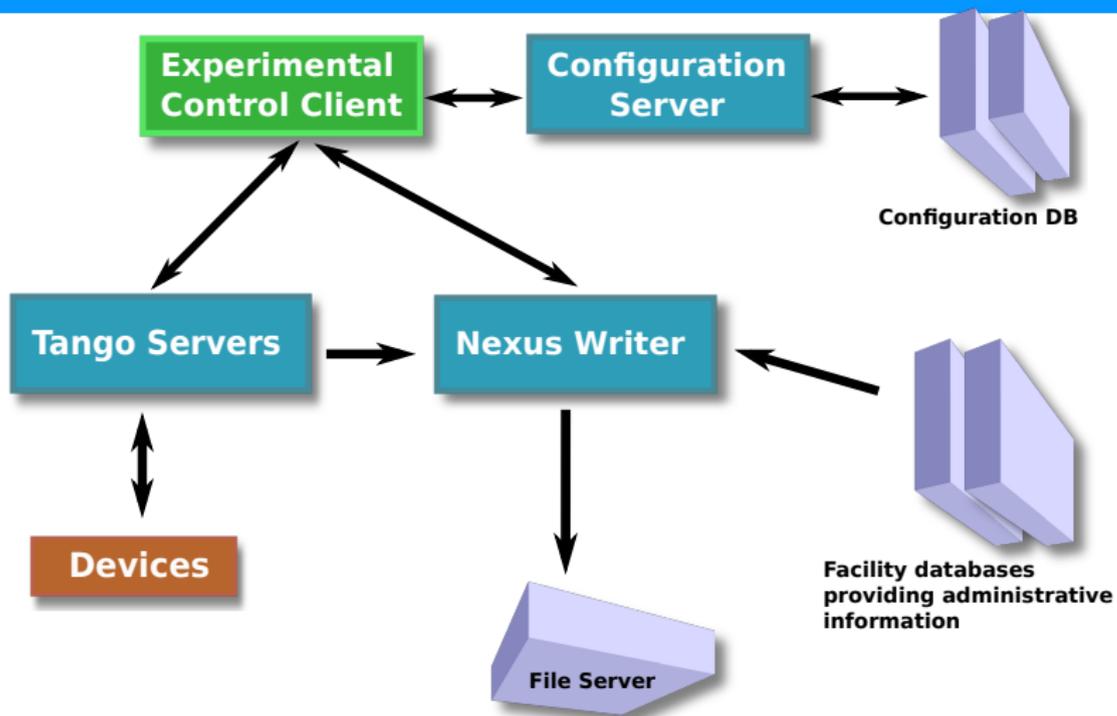
**c++ libraries** used to store fast detector data

**python modules** used to store metadata

<https://github.com/pni-libraries/> <https://github.com/ess-dmsec/h5cpp>

deb <http://repos.pni-hdri.de/apt/debian>

# Modular structure of the NeXus Framework



<https://github.com/nexdatas/> NeXus Writer uses `pninexus` bindings (or `h5py`)

deb <http://repos.pni-hdri.de/apt/debian>  
for `debian` `buster`, `stretch`, `jessie` and `ubuntu` `bionic`, `xenial`

# NeXus Component Selector

## Device Selection Editor/View – Detector Components

The screenshot shows the NeXus Component Selector (expert mode) window. The interface includes a Scan File field (water.nxs, water.flo), Scan Dir (/tmp), and Scan ID (498). Below these are fields for Timer (exp\_t01) and MntGrp (mg\_test01). The main area is divided into several sections: 2D detectors, Counter detectors, Timers, Counters, ADC, VFC, MCA/SCA, and Additional. Each section contains a list of components with checkboxes for selection and disablement. A tooltip is visible over the 'detector\_a' checkbox, displaying the text: 'detector\_a: exp\_c01, exp\_c02 [mca]'. At the bottom, there is a 'NOT APPLIED' status bar and buttons for Reset, ClearAll, Apply, Others, Save, Close, and Load.

Select components of Pool channels and other TANGO devices.  
Disable display for TaurusGUI, e.g. nxsmacrogui.

# Pilatus1M component

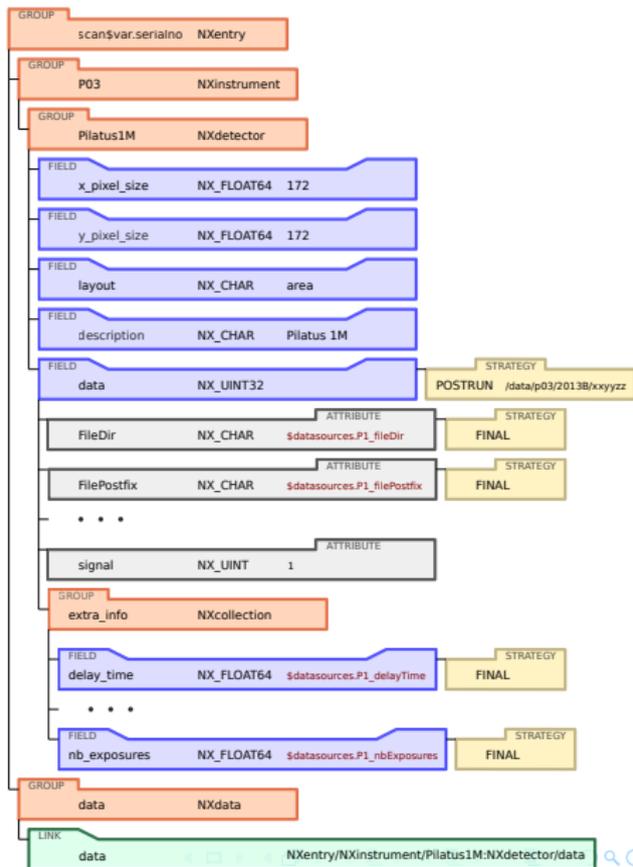
## NeXus Semantic

**Groups** contain **groups**, **fields** and **links**. They generate the hierarchical file structure. They have **names**, associated **attributes** and **types**:  
e.g. NXentry, NXdetector, ...

**Fields** contain **data** with their attributes: **names**, **shape**, **data types** and **unit**.

**Attributes** are descriptive info for **groups** and **fields**.

**Links** refer to **fields** at different **locations** in the data tree.



# Detector data

## Data from detectors

- 0D and 1D – data in one file
- 2D and fast 1D – strategy depends on vendor software

## Configuration components for detectors

- data in master file during scan:  
0D, MCA, Mythen2, ...
- master file and images file will be linked:  
Lambda, Eiger, ...
- nxscout for integrating TIFs, ... into NeXus file:  
Pilatus, PE, PCO, Mythen1, MarCCD, ...
- dedicated macros for detectors in continuous scans



All-in-one is easier to manage

## Device Selection View – Description Components

NeXus Component Selector (expert mode)

Scan File: water.nxs, water.fio Scan Dir: /tmp Scan ID: 498

Timer: exp\_t01 MntGrp: img\_test01 Append Entries

Detectors Descriptions User Data Configuration

**Optional**

- absorber
- analyzer
- beam\_monitor
- beamstop
- dcm
- diff\_hkl
- diffractometer
- lenses
- mirrors
- pinhole1
- pinhole2
- powerslit1
- powerslit2
- qbpm1
- qbpm2
- slit1
- slit2
- slit3
- slit4
- source
- table\_eh1
- table\_eh2
- undulator
- xrmcd

**Other Optional**

- exp\_mot17
- exp\_mot18
- exp\_mot20
- exp\_mot22
- exp\_mot23
- exp\_mot25
- exp\_mot26
- exp\_mot30
- exp\_mot62
- exp\_mot63

**Mandatory**

- default

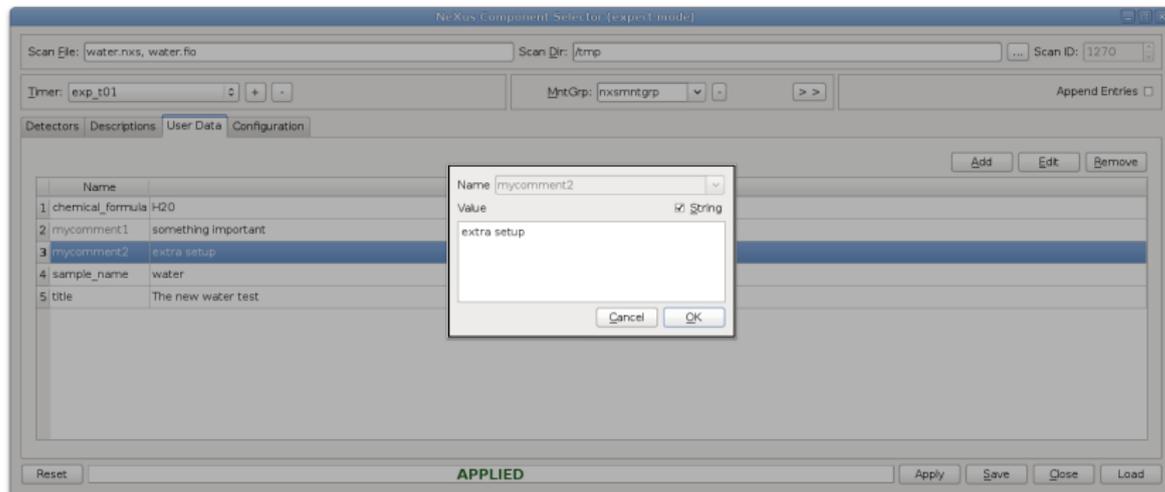
slit1:  
[exp\_mot13, exp\_mot17, exp\_mot20, exp\_mot30, exp\_mot33]

Reset Reset Desc. **APPLIED** Apply Others Save Close Load

Descriptive components are automatically deselected if related to them motors are switch off.

# NeXus Component Selector

## Experiment metadata – User Data



To describe the experiment completely some of the **CLIENT data** have to be **provided** by the **user**

# Spock with NeXus Sardana Recorder

## User scan in spock with the exp\_mot07 motor.

```
Terminal
File Edit View Search Terminal Help
p09/door/haso228k.01 [3]: ascan exp_mot07 0 1 20 0.1
Operation will be saved in /tmp/sarr12_00038.nxs (nxs)
Scan #38 started at Tue Sep 22 11:30:34 2015. It will take at least 0:00:02.200012
Moving to start positions...

#Pt No  exp_mot07  exp_adc01  exp_c01  exp_c02  exp_c04  exp_c27  exp_mca01  exp_t01  exp_vfc06  p03 motor expmi.31  Position  dt
#Pt No  exp_mot07  exp_adc01  exp_c01  exp_c02  exp_c04  exp_c27  exp_mca01  exp_t01  exp_vfc06  motor  expmi.31  Position  dt
0      0      -0.047619  14.2737  194.118  -0.0102757  81.0833  (2048,)  0.1  2.851e+08  42.5  2.69412
1      0.05  -1.85714  24.907  169.267  93.3115  26.5114  (2048,)  0.1  2.295e+08  42.5  3.17904
2      0.1  -2.64286  81.2282  64.6847  76.786  2.91691  (2048,)  0.1  1.032e+08  42.5  3.55215
3      0.15  -1.78571  116.605  0.00987697  24.0581  85.4986  (2048,)  0.1  8.031e+08  42.5  3.93055
4      0.2  0.692308  73.7028  -0.0071638  2.86908  140.2  (2048,)  0.1  2.552e+08  42.5  4.30403
5      0.25  1.14286  20.4691  0.0338292  0.0846919  108.416  (2048,)  0.1  5.668e+08  42.5  4.71271
6      0.3  0.47619  2.4889  0.101939  -0.0185421  39.578  (2048,)  0.1  2.928e+08  42.5  5.33755
7      0.35  1.71429  0.103017  42.1995  0.210651  6.82285  (2048,)  0.1  8.141e+08  42.5  5.798
8      0.4  -0.461538  0.0170992  102.016  10.5632  0.601225  (2048,)  0.1  6.075e+08  42.5  6.1855
9      0.45  -1.64286  -0.0275928  14.3158  78.6786  0.291925  (2048,)  0.1  5.529e+08  42.5  6.55229
10     0.5  -2.07692  0.0405144  61.9118  73.5049  4.72761  (2048,)  0.1  1.37e+07  42.5  6.93391
11     0.55  1.73333  4.6877  121.521  8.57693  37.8267  (2048,)  0.1  5.168e+08  42.5  7.29245
12     0.6  -1  92.1075  108.35  0.144767  135.406  (2048,)  0.1  5.23e+07  42.5  7.67615
13     0.65  -0.357143  244.429  43.9304  36.4597  217.8  (2048,)  0.1  6.631e+08  42.5  8.0511
14     0.7  0.214286  0.253492  8.08141  141.424  157.636  (2048,)  0.1  4.511e+08  42.5  8.42511
15     0.75  -0.5  2.73178  100.702  199.585  0.0362168  (2048,)  0.1  8.09e+08  42.5  8.80014
16     0.8  -2.57143  17.6445  88.9136  102.393  6.09374  (2048,)  0.1  4.842e+08  42.5  9.1725
17     0.85  -0.785714  57.0967  41.4813  19.115  86.2354  (2048,)  0.1  4.633e+08  42.5  9.54844
18     0.9  1.21429  93.7693  10.2586  1.30535  97.1395  (2048,)  0.1  5.173e+08  42.5  9.92166
19     0.95  -2.5  85.5538  2.12824  0.119238  17.2362  (2048,)  0.1  6.78e+07  42.5  10.4497
20     1  2.35714  6.16448  0.193503  0.856645  0.217808  (2048,)  0.1  7.569e+08  42.5  10.8052

Operation saved in /tmp/sarr12_00038.nxs (nxs)
Scan #38 ended at Tue Sep 22 11:30:45 2015, taking 0:00:11.037453. Dead time 81.0% (motion dead time 30.7%)

p09/door/haso228k.01 [4]:
```

For NeXus Recorder the file extension is `.nxs`

# lavue: Live Image Viewer in SWMR mode

The screenshot displays the 'laVue: Live Image Viewer (on haso228k)' window. The interface is divided into several sections:

- Image Source:** Source: Nexus File; File: /kotan/files/watertest\_00564.nxs; Field: /entry/data/detector; Stacking: 0; Status: Connected (green bar); Stop button.
- Image preparation:** Subtract bkg (checkbox); Background image: no image selected; Transformation: none.
- Intensity display scaling:** sqrt (selected), linear, log.
- Display levels and colors:** sqrt scale! (checkbox checked); Automatic levels (checkbox checked); Minimum value: 0.00; Maximum value: 38.04; Color gradient: reversegrey.
- Image statistics:** Scaling: linear; Maximum: 1447.0000; Mean: 54.7005; Variance: 1753.0483.

The main display area shows a circular detector image with a red line cut across it. Below the image is a plot of the intensity profile along the cut. The plot shows a sharp peak at approximately x=10 and another smaller peak at approximately x=160. The x-axis is labeled from 0 to 180, and the y-axis is labeled from 0 to 800.

At the bottom of the window, there is a text field showing the cut parameters: 'Cut, pixel position and intensity: [[130.44, 104.01], [313.50, 99.44]], x = 133, y = 87, intensity = 78.00'. A 'LineCut' button is also visible.

Single-Writer/Multiple-Reader mode

<https://github.com/jkotan/lavue/> or [deb http://repos.pni-hdri.de/apt/debian](http://repos.pni-hdri.de/apt/debian)

# Component templates



- **Standard component templates** common all for beamlines:

default, bevertimeid, source, undulator, dcm, slit, absorber, beamstop, chcut, keithley, pinhole, qbpm, samplehkl, ...

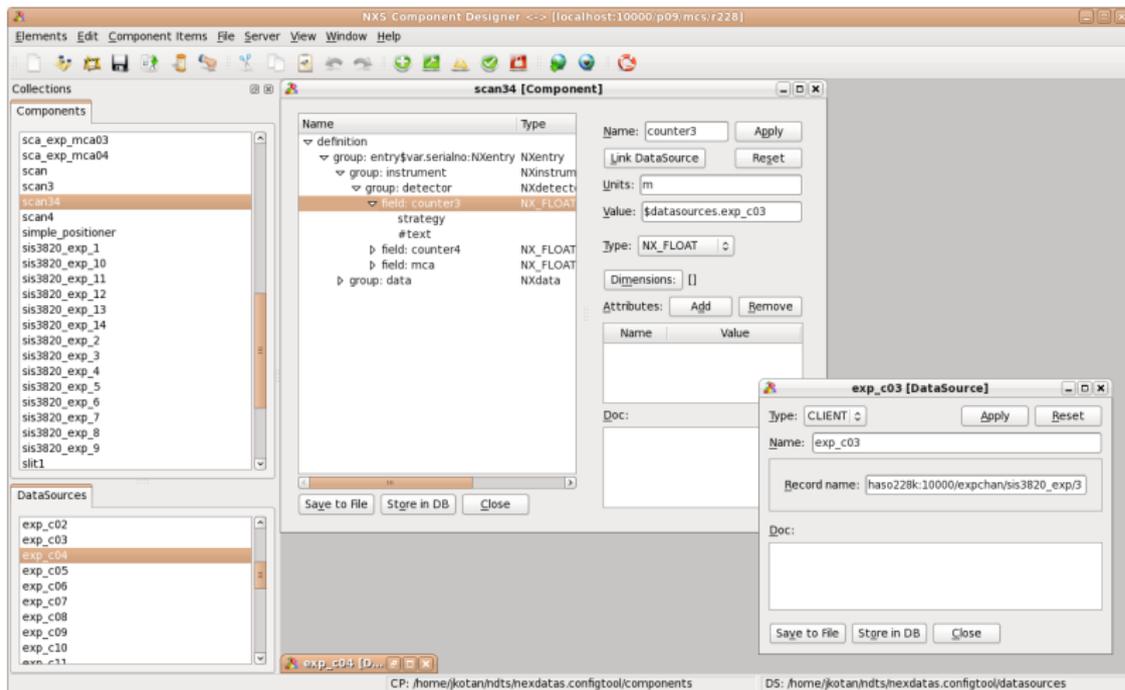
- **Beamline specific components**

diffractometer, mirrors, pcostage, microscope, samplehexapod, samplepiezo, saxstage, laser, interferometer, srl, lenshexapod, cryostage, ...

## Advantages:

- Create components of the same type with different motors
- Change motors by changing script parameters

# Component Designer



The Configuration Client Tool allows to create configuration components as well as datasources (for IT staff)

## provides relation between components and datasources

```
File Edit View Search Terminal Help
```

```
haspp08% nxconfig info slit1
```

```
Component: 'slit1'
```

```
source_name source_type nexus_type shape strategy source
```

```
-----  
sl1h TANGO NX_FLOAT INIT haspp08mono:10000/p08/motor/exp.04/Position  
sl1v TANGO NX_FLOAT INIT haspp08mono:10000/p08/motor/exp.02/Position  
sl1hc TANGO NX_FLOAT INIT haspp08mono:10000/p08/motor/exp.05/Position  
sl1vc TANGO NX_FLOAT INIT haspp08mono:10000/p08/motor/exp.03/Position
```

```
haspp08% nxconfig info default
```

```
Component: 'default' ['defaultsample', 'defaultinstrument']
```

```
Component: 'defaultsample'
```

```
source_name source_type nexus_type shape strategy source
```

```
-----  
sample_name CLIENT NX_CHAR INIT sample_name  
chemical_formula CLIENT NX_CHAR INIT chemical_formula
```

```
Component: 'defaultinstrument'
```

```
source_name source_type nexus_type shape strategy source
```

```
-----  
beamtime_id PYEVAL NX_CHAR INIT  
\start_time CLIENT INIT start_time  
start_time CLIENT NX_DATE_TIME INIT start_time  
end_time CLIENT NX_DATE_TIME FINAL end_time  
title CLIENT NX_CHAR INIT title
```

```
haspp08%
```

shows physical information related to component fields

```
jkotan@haso228k:/home/jkotan
File Edit View Search Terminal Help
haspp09% nxscnfig geometry dcm
Component: 'dcm'

nexus_path          source_name  units  trans_type  trans_vector  trans_offset  depends_on
-----
entry/instrument/dcm/crystal1/usage
entry/instrument/dcm/crystal1/type
entry/instrument/dcm/crystal1/reflection
entry/instrument/dcm/crystal1/depends_on
entry/instrument/dcm/crystal1/transformations/dcm_lat  mx      mm      translation  1 0 0      [transformations/dcm_lat]
entry/instrument/dcm/crystal1/transformations/dcm_yaw  myaw    mm      rotation     0 1 0      dcm_yaw
entry/instrument/dcm/crystal2/usage
entry/instrument/dcm/crystal2/type
entry/instrument/dcm/crystal2/reflection
entry/instrument/dcm/crystal2/depends_on
entry/instrument/dcm/crystal2/transformations/dcm_roll2  mchi2   deg     rotation     0 0 1      [transformations/dcm_roll2]
entry/instrument/dcm/crystal2/transformations/dcm_pitch  mth2    deg     rotation     0 1 0      dcm_pitch
entry/instrument/dcm/crystal2/transformations/dcm_perp   dcm_perp mm      translation  0 1 0      dcm_perp
entry/instrument/dcm/crystal2/transformations/dcm_para   dcm_parallel mm      translation  0 0 1      dcm_para
entry/instrument/dcm/crystal2/transformations/dcm_parallel  dcm_parallel mm      translation  0 0 1      ../../transformations/dcm_bragg
entry/instrument/dcm/transformations/dcm_bragg           dcm_bragg deg     rotation     -1 0 0      dcm_z1
entry/instrument/dcm/transformations/dcm_z1              mj1     mm      translation  0 1 0
entry/instrument/dcm/transformations/dcm_z2              mj2     mm      translation  0 1 0
entry/instrument/dcm/transformations/dcm_z3              mj3     mm      translation  0 1 0
entry/instrument/dcm/transformations/mtable              mtable  mm      translation  0 1 0
entry/instrument/dcm/energy                              mnchmtr eV
entry/instrument/dcm/collection/energyfmb                energyfmb eV

haspp09%
```



## Advantages

- full description included, metadata and data
  - 0d and 1D data in one file  
(for 2D: external links or post-collection)
  - beamline description, e.g. motor positions in INIT mode
  - user comments included, per scan
- NeXus configuration components allow to fit sophisticated NeXus structure into specific experiment and beamline
- Standard component templates simplify beamline configuration