

Data and Metadata acquisition with NeXus Writer

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Motivation – individual binary image files

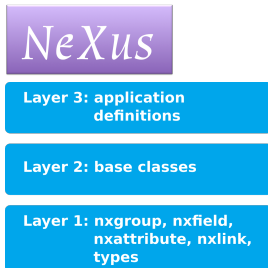
```
user@localhost:~$ ls -r  
run_001.dat  
detector/image_0001.tif  
detector/image_0002.tif  
...  
...  
...  
detector/image_0100.tif
```



- when **the number of image files grows large** the performance of most file systems degenerate
- **to access data in an individual image file** a new file handler has to be created by operating system
- **image and scalar data are stored in different files** which increases the managements efforts to keep related information together by users.

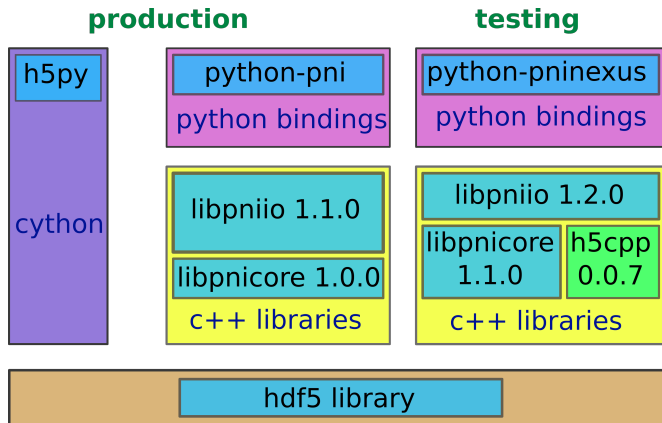
NeXus – attempts to solve all of these problems

- 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



- 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!

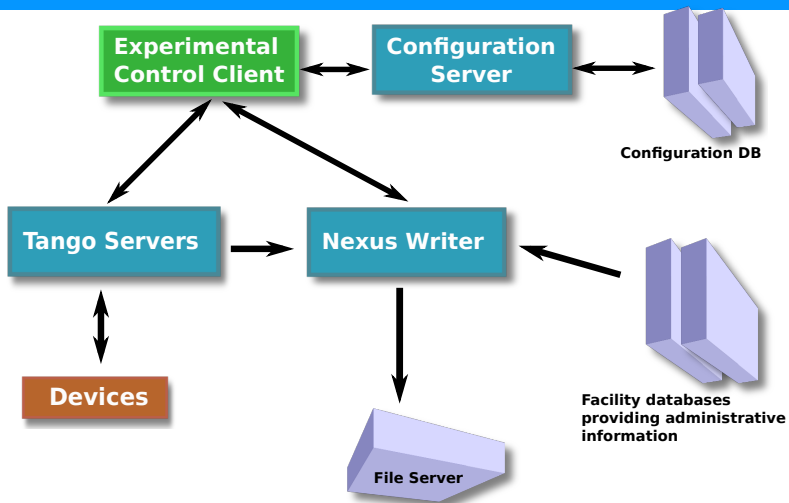
NeXus libraries



h5cpp – new c++ wrapper for hdf5 library
c++ libraries used to store fast detector data
python modules used to store metadata

<https://github.com/pni-libraries/> <https://github.com/ess-dmhc/h5cpp>
deb <http://repos.pni-hdri.de/apt/debian>

Modular structure of the NeXus Framework



<https://github.com/nexdatas/> NeXus Writer uses **pni-libraries** (or h5py)

deb <http://repos.pni-hdri.de/apt/debian>
for **debian stretch**, **jessie**, **wheezy** and **ubuntu 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), a Scan Dir field (/tmp), and a Scan ID field (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 are buttons for Reset, ClearAll, a status indicator 'NOT APPLIED', Apply, Others, Save, Close, and Load.

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

Pilatus1M component

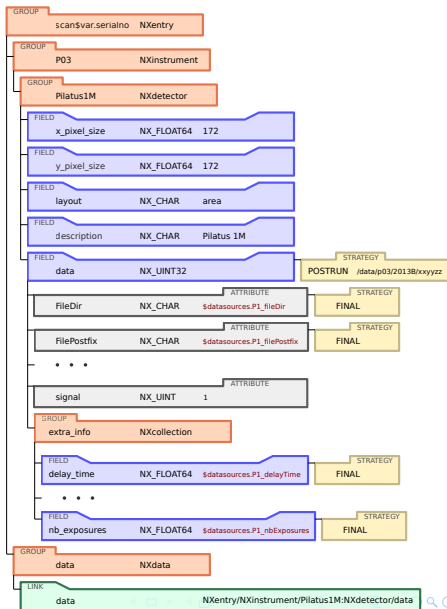
NeXus Semantic

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, ...
- nxscollect 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

The screenshot shows the NeXus Component Selector (expert mode) window. The window title is "NeXus Component Selector (expert mode)". The "Scan File" is "water.nxs, water.fio" and the "Scan Dir" is "/tmp". The "Scan ID" is "498". The "Timer" is "exp_t01" and the "MntGrp" is "img_test01". The "Append Entries" checkbox is checked.

The "Descriptions" tab is selected, showing a list of components under "Optional" and "Mandatory" sections. The "Optional" section is divided into two columns. The first column contains: absorber, analyzer, beam_monitor, beamstop, dcm, diff_hkl, diffractometer, lenses. The second column contains: mirrors, pinhole1, pinhole2, powerslit1, powerslit2, qbpm1, qbpm2, qbpm3, slit1. The third column contains: slit2, slit3, slit4, source, table_eh1, table_eh2, undulator, xrmcd. The "Mandatory" section contains: default.

The "Other Optional" section contains: exp_mot17, exp_mot18, exp_mot20, exp_mot22, exp_mot23, exp_mot25, exp_mot26, exp_mot30, exp_mot62, exp_mot63.

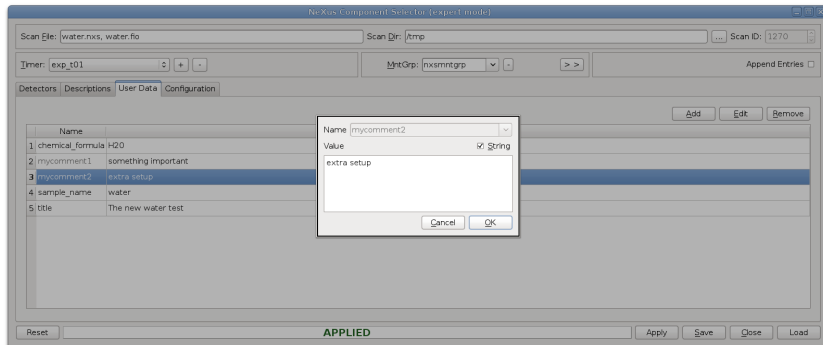
A tooltip is visible over the "slit1" component, displaying the text: "slit1: [exp_mot13, exp_mot17, exp_mot20, exp_mot30, exp_mot33]".

The "APPLIED" button is highlighted in green. Other buttons include "Reset", "Reset Desc.", "Apply", "Others", "Save", "Close", and "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...

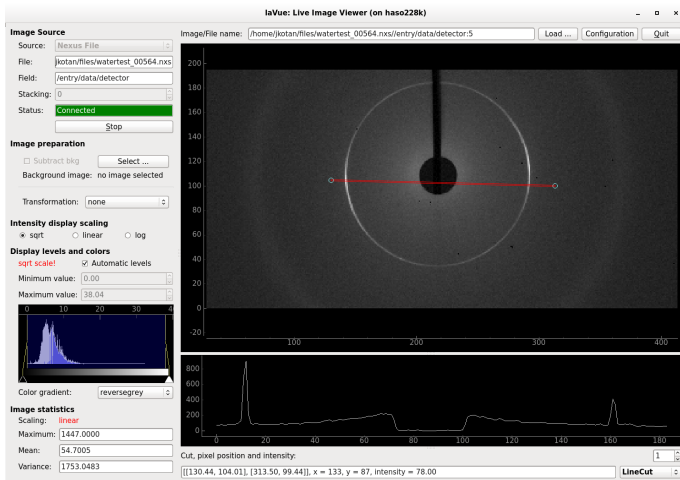
#Pt No  exp_mot07  exp_adc01  exp_c01  exp_c02  exp_c04  exp_c27  exp_mca01  exp_t01  exp_vfc06  p03 motor expmi.31  Position  dt
#Pt No  exp_mot07  exp_adc01  exp_c01  exp_c02  exp_c04  exp_c27  exp_mca01  exp_t01  exp_vfc06  Position  dt
0      0      -0.047619  14.2737  194.118  -0.0102757  81.0833  (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



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

Components are created by the `nxcreate` script from component templates

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

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

- **Beamline specific components**

Advantages:

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

Component Designer

The screenshot displays the NX5 Component Designer interface. The main window is titled "scan34 [Component]" and shows a tree view of the component structure. The "DataSources" panel on the left lists various data sources, with "exp_c04" selected. A configuration dialog for "counter3" is open, showing fields for Name, Units, Value, and Type. A second dialog for "exp_c03 [DataSource]" is also open, showing fields for Type, Name, Record name, and Doc. The status bar at the bottom indicates the current path (CP) and data source path (DS).

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%
```


NeXus is ready-to-use



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