

NeXus DESY Integration

Jan Kotański

Deutsches Elektronen-Synchrotron



High Data Rate Initiative for
Photons, Neutrons and Ions



HELMHOLTZ
ASSOCIATION



pandata_{europe}

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NeXus Writer Configuration

Components, DataSources and Strategy

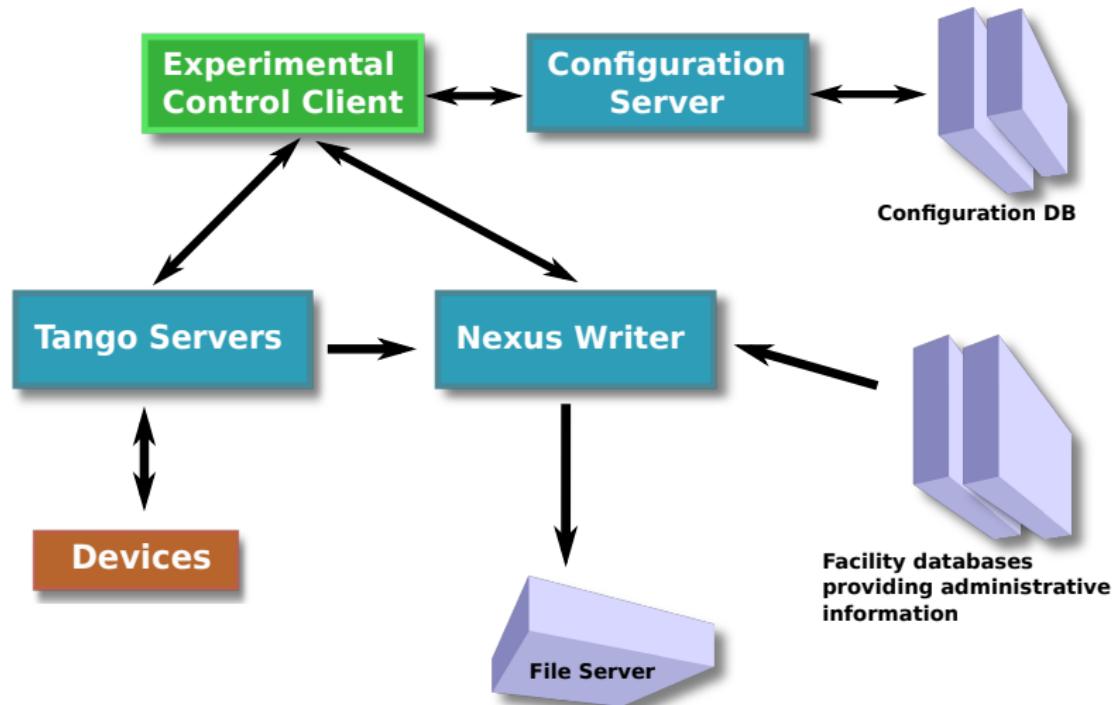
Why NeXus ?

- store all data **in one container** – NeXus file
- full **description** of experiment, **metadata catalogs**
- **data provenance** – sufficient details to allow **reproducibility**
managing, sharing, and reusing data
- application **definitions** for specific experiment types

This way **data** can be managed efficiently



Modular structure of the NeXus Framework



<https://github.com/nexdatas/>
deb http://repos.pni-hdri.de/apt/debian wheezy main

Configuration Components

To store the data we need to know:

- What? – DataSources: CLIENT, TANGO, DB, Python scripts
- When and How? – writing strategy: INIT, STEP, FINAL, POSTRUN
- Where? – NeXus path with physical meaning

Configuration of the hardware devices for the NeXus files is described in Configuration Components and DataSources

Configuration Components:

- identified by their names
- XML Strings in the NXDL format extended by strategy and datasources tags
- their NeXus tree structure assigns to the stored data the proper physical interpretation.

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Configuration Components

The **measurement** \Leftrightarrow **NeXus file correspondence**



experimental setup	\Leftrightarrow	NeXus configuration
hardware device	\Leftrightarrow	component
device attribute	\Leftrightarrow	data source
e.g. counter reading, motor position		

Components correspond to one or more devices and like devices can be switch on/off

- simple components, e.g. counters, MCA, ADC, ...
- composite components, e.g. Pilatus1M, default, ...

Pilatus1M component

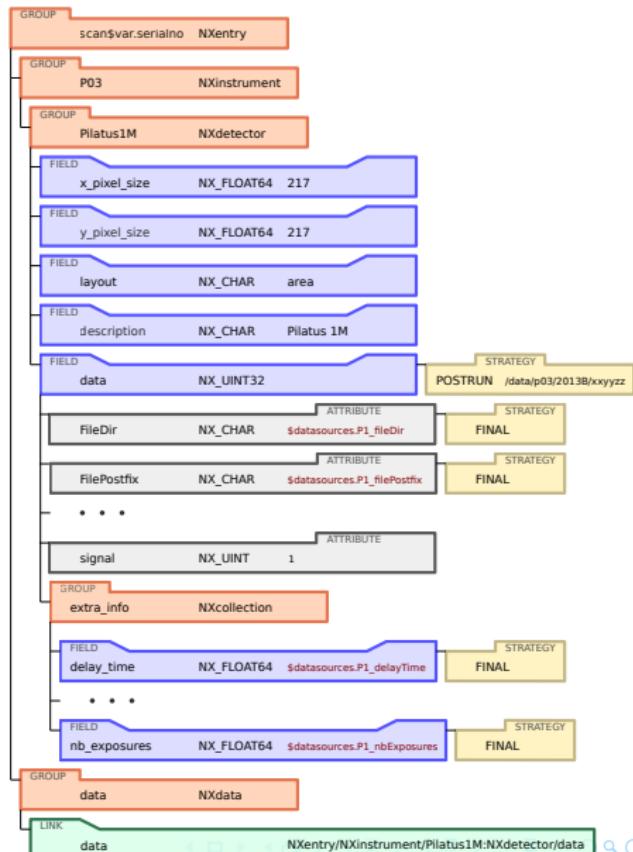
NeXus Semantic

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

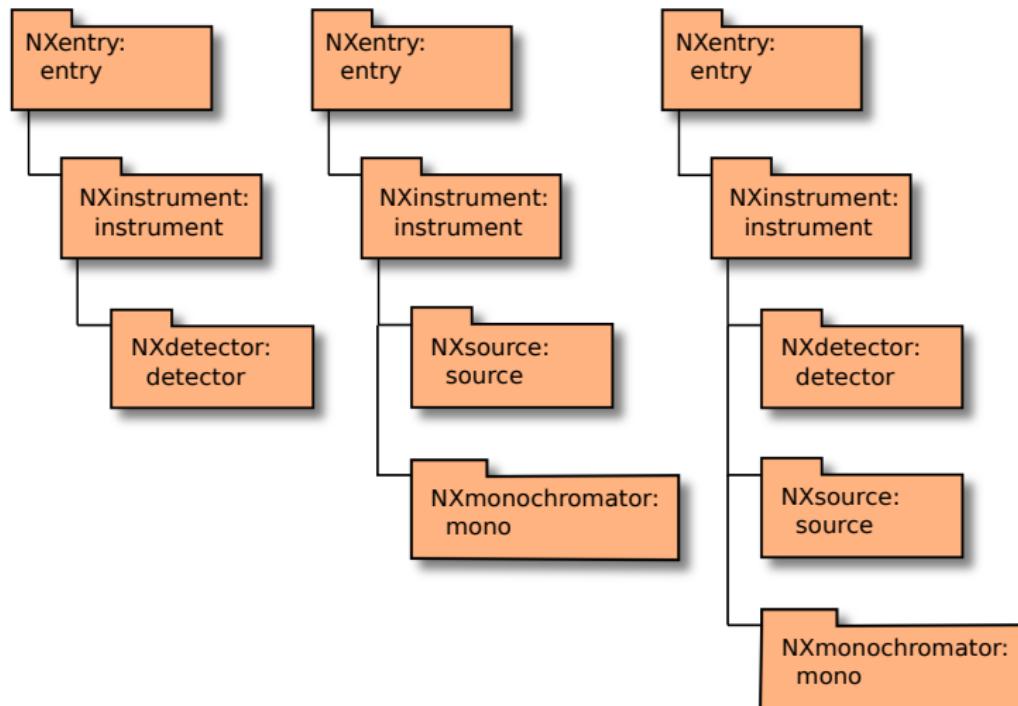
Fields contain **data** with their attributes: **names**, **shape**, **data types** and **unit**.

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

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



Components and their merging

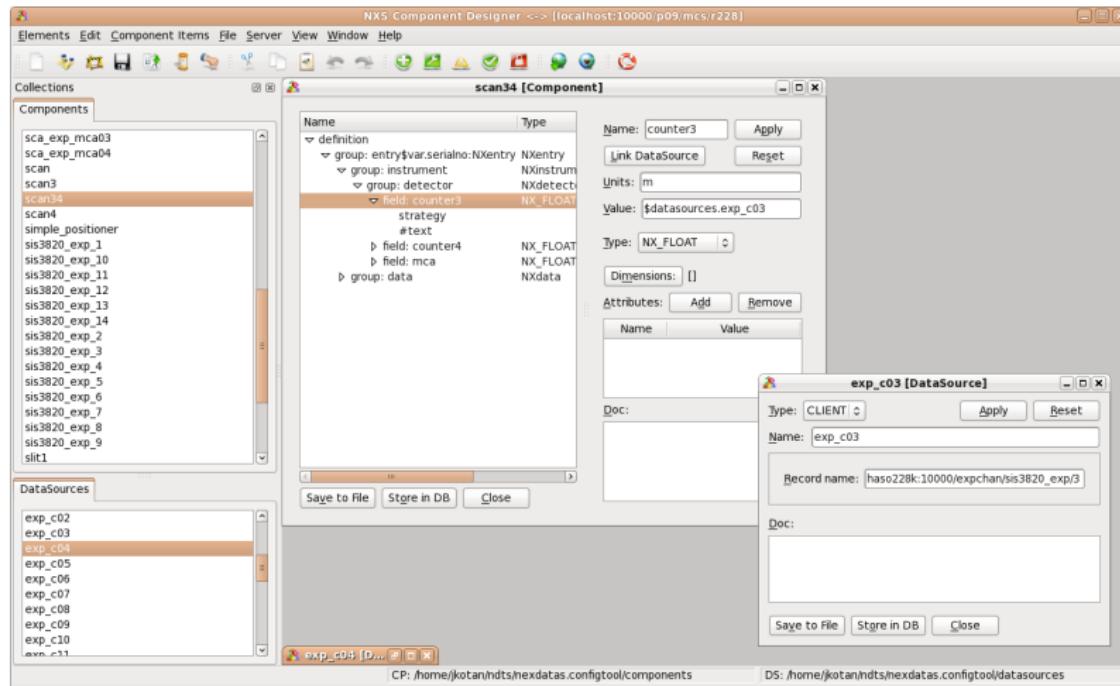


Detector
Component

Default
Component

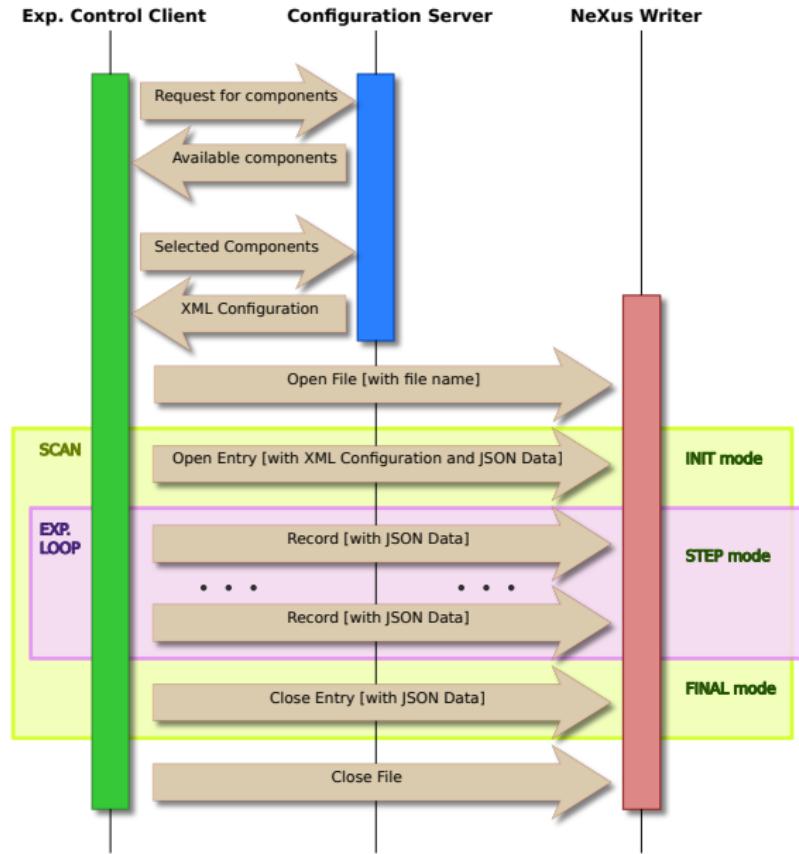
Merged
Components

Component Designer



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

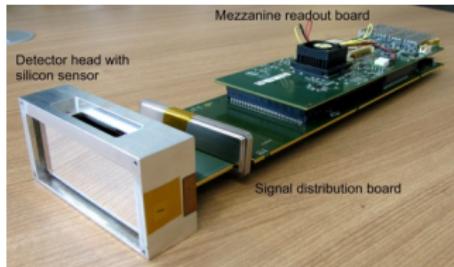
Writing Sequence Diagram



Data Collector

For fast detector data is:

- saved locally by Detector Tango Server,
e.g. lambda detector in HDF5 files
- denoted in components by POSTRUN strategy tag
- merged with data from NeXus Writer
after performed experiment
- merging is done by Data Collector



User Interfaces to NeXus Writer

User Interfaces to NeXus Writer

- NeXus Component Selector with Sardana
NeXus File Recorder with Selector server
extension to Sardana
- Sardana Macros from nxsmacros.py
NeXus File Recorder with Selector server
extension to Sardana
- Other Sardana Macros
NeXus Writer and Configuration Server used directly
Beamline specific
- Python scripts or C++/Java programs
NeXus Writer and Configuration Server used directly
Beamline specific
- NeXus Component Selector with other programs
Direct use of Selector Server
i.e. with Online, user programs

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NeXus Component Selector

Device Selection Editor/View – Detector Components

NeXus Component Selector (expert mode)

Scan File: sarr12.nxs Scan Dir: /tmp MntGrp: mg_data Scan ID: 35 Append Entries

Timer: exp_t01 Detectors Descriptions User Data Configuration

Components		Counters				ADC				VFC				MCA/SCA	
Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.		
<input checked="" type="checkbox"/> detectorA	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> exp_c01	<input checked="" type="checkbox"/> exp_c12	<input type="checkbox"/> exp_c23	<input type="checkbox"/>	<input checked="" type="checkbox"/> exp_adc01	<input checked="" type="checkbox"/>	<input type="checkbox"/> exp_vfc01	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc02	<input type="checkbox"/>	<input checked="" type="checkbox"/> exp_mca01	<input checked="" type="checkbox"/>		
<input type="checkbox"/> pilatus3Q	<input checked="" type="checkbox"/> detectorA: exp_c01, exp_c02, mca	<input type="checkbox"/> exp_c02	<input type="checkbox"/> exp_c13	<input type="checkbox"/> exp_c24	<input type="checkbox"/>	<input type="checkbox"/> exp_adc02	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc03	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc04	<input type="checkbox"/>	<input type="checkbox"/> exp_mca02	<input type="checkbox"/>		
		<input type="checkbox"/> exp_c03	<input type="checkbox"/> exp_c14	<input type="checkbox"/> exp_c25	<input type="checkbox"/>	<input type="checkbox"/> exp_adc03	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc05	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc06	<input checked="" type="checkbox"/>	<input type="checkbox"/> exp_mca03	<input type="checkbox"/>		
		<input checked="" type="checkbox"/> exp_c04	<input type="checkbox"/> exp_c15	<input type="checkbox"/> exp_c26	<input type="checkbox"/>	<input type="checkbox"/> exp_adc04	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc07	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc08	<input type="checkbox"/>	<input type="checkbox"/> exp_mca04	<input type="checkbox"/>		
		<input type="checkbox"/> exp_c05	<input type="checkbox"/> exp_c16	<input checked="" type="checkbox"/> exp_c27	<input checked="" type="checkbox"/>	<input type="checkbox"/> exp_adc05	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc09	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc10	<input type="checkbox"/>	<input type="checkbox"/> sca_exp_mca01_0_200	<input type="checkbox"/>		
		<input type="checkbox"/> exp_c06	<input type="checkbox"/> exp_c17	<input type="checkbox"/> exp_c28	<input type="checkbox"/>	<input type="checkbox"/> exp_adc06	<input type="checkbox"/>	<input checked="" type="checkbox"/> exp_vfc11	<input checked="" type="checkbox"/>	<input type="checkbox"/> exp_vfc12	<input type="checkbox"/>				
		<input type="checkbox"/> exp_c07	<input type="checkbox"/> exp_c18	<input type="checkbox"/> exp_c29	<input type="checkbox"/>	<input type="checkbox"/> exp_adc07	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc13	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc14	<input type="checkbox"/>				
		<input type="checkbox"/> exp_c08	<input type="checkbox"/> exp_c19	<input type="checkbox"/> exp_c30	<input type="checkbox"/>	<input type="checkbox"/> exp_adc08	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc15	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc16	<input type="checkbox"/>				
		<input type="checkbox"/> exp_c09	<input type="checkbox"/> exp_c20	<input type="checkbox"/> exp_c31	<input type="checkbox"/>										
		<input type="checkbox"/> exp_c10	<input type="checkbox"/> exp_c21	<input type="checkbox"/> exp_c32	<input type="checkbox"/>										
		<input type="checkbox"/> exp_c11	<input type="checkbox"/> exp_c22	<input type="checkbox"/>											
Timers															
Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.		
<input checked="" type="checkbox"/> exp_t01	<input type="checkbox"/>	<input type="checkbox"/> exp_c01	<input type="checkbox"/> exp_c12	<input type="checkbox"/> exp_c23	<input type="checkbox"/>	<input checked="" type="checkbox"/> exp_adc01	<input checked="" type="checkbox"/>	<input type="checkbox"/> exp_vfc01	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc02	<input type="checkbox"/>	<input checked="" type="checkbox"/> exp_mca01	<input checked="" type="checkbox"/>		
<input type="checkbox"/> exp_t02	<input type="checkbox"/>	<input type="checkbox"/> exp_c02	<input type="checkbox"/> exp_c13	<input type="checkbox"/> exp_c24	<input type="checkbox"/>	<input type="checkbox"/> exp_adc02	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc03	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc04	<input type="checkbox"/>	<input type="checkbox"/> exp_mca02	<input type="checkbox"/>		
		<input type="checkbox"/> exp_c03	<input type="checkbox"/> exp_c14	<input type="checkbox"/> exp_c25	<input type="checkbox"/>	<input type="checkbox"/> exp_adc03	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc05	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc06	<input checked="" type="checkbox"/>	<input type="checkbox"/> exp_mca03	<input type="checkbox"/>		
		<input checked="" type="checkbox"/> exp_c04	<input type="checkbox"/> exp_c15	<input type="checkbox"/> exp_c26	<input type="checkbox"/>	<input type="checkbox"/> exp_adc04	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc07	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc08	<input type="checkbox"/>	<input type="checkbox"/> exp_mca04	<input type="checkbox"/>		
		<input type="checkbox"/> exp_c05	<input type="checkbox"/> exp_c16	<input checked="" type="checkbox"/> exp_c27	<input checked="" type="checkbox"/>	<input type="checkbox"/> exp_adc05	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc09	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc10	<input type="checkbox"/>	<input type="checkbox"/> sca_exp_mca01_0_200	<input type="checkbox"/>		
		<input type="checkbox"/> exp_c06	<input type="checkbox"/> exp_c17	<input type="checkbox"/> exp_c28	<input type="checkbox"/>	<input type="checkbox"/> exp_adc06	<input type="checkbox"/>	<input checked="" type="checkbox"/> exp_vfc11	<input checked="" type="checkbox"/>	<input type="checkbox"/> exp_vfc12	<input type="checkbox"/>				
		<input type="checkbox"/> exp_c07	<input type="checkbox"/> exp_c18	<input type="checkbox"/> exp_c29	<input type="checkbox"/>	<input type="checkbox"/> exp_adc07	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc13	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc14	<input type="checkbox"/>				
		<input type="checkbox"/> exp_c08	<input type="checkbox"/> exp_c19	<input type="checkbox"/> exp_c30	<input type="checkbox"/>	<input type="checkbox"/> exp_adc08	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc15	<input type="checkbox"/>	<input type="checkbox"/> exp_vfc16	<input type="checkbox"/>				
		<input type="checkbox"/> exp_c09	<input type="checkbox"/> exp_c20	<input type="checkbox"/> exp_c31	<input type="checkbox"/>										
		<input type="checkbox"/> exp_c10	<input type="checkbox"/> exp_c21	<input type="checkbox"/> exp_c32	<input type="checkbox"/>										
		<input type="checkbox"/> exp_c11	<input type="checkbox"/> exp_c22	<input type="checkbox"/>											
Others															
Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.		
<input checked="" type="checkbox"/> BPM_OH	<input checked="" type="checkbox"/>	<input type="checkbox"/> expmi_mot54	<input type="checkbox"/>												
<input type="button" value="Reset"/>	<input type="button" value="ClearAll"/>	APPLIED										<input type="button" value="Apply"/>	<input type="button" value="Close"/>		

Selecting components containing other devices.
One can also disable display for TaurusGUI, e.g. nxsmacrogui.



NeXus Component Selector

Device Selection View – Description Components

NeXus Component Selector (expert mode) *

Scan File: sarr12.nxs Scan Dir: /tmp ... Scan ID: 35

Timer: exp_t01 MntGrp: mg_data Append Entries

Detectors Descriptions User Data Configuration

Optional

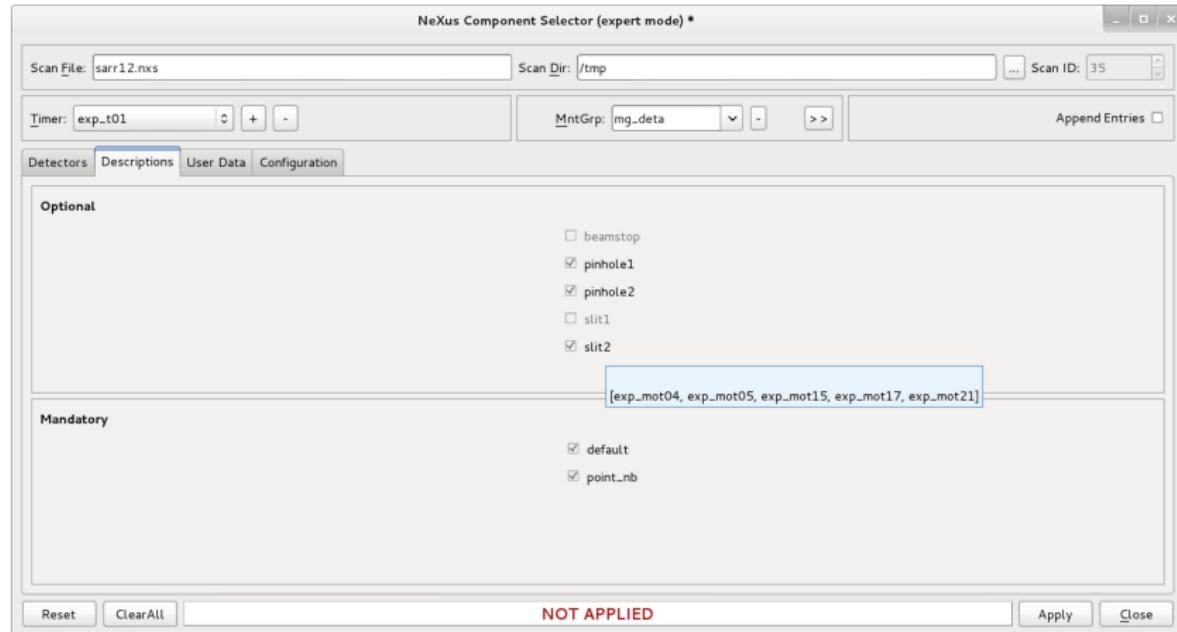
beamstop
 pinhole1
 pinhole2
 slit1
 slit2

[exp_mot04, exp_mot05, exp_mot15, exp_mot17, exp_mot21]

Mandatory

default
 point_nb

Reset ClearAll NOT APPLIED Apply Close



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



NeXus Component Selector

Experiment metadata – User Data

NeXus Component Selector (expert mode) *

Scan File: sarr12.nxs Scan Dir: /tmp ... Scan ID: 35

Timer: exp_t01 MntGrp: mg_data >> Append Entries

Detectors Descriptions User Data Configuration

Name	Value
1 beamtime_id	213231
2 chemical_formula	LBa6
3 sample_name	LBa6
4 title	Measurement of LBa6

Add Edit Remove

Dialog

Name: title

Value: Measurement of LBa6 String

Cancel OK

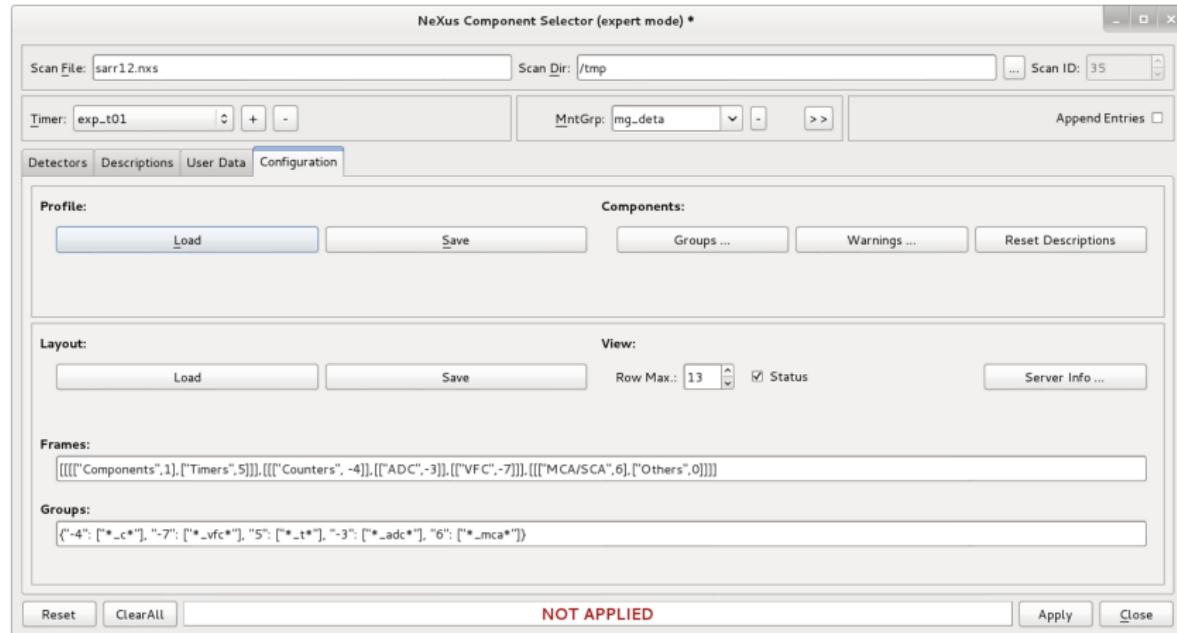
Reset ClearAll NOT APPLIED Apply Close

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



NeXus Component Selector

Preferences for Layout and Profile – Configuration



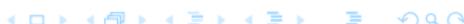
Loading or saving in a file a selected profile.
Changing the Detectors layout.

Spock with NeXus Sardana Recorder

User scan in spock with the exp_mot04 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...
          p03
          motor
expm1.31
#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  2.869898  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  182.016   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   1.30953   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



NeXus Macros - from nxsmacros.py

lsprof or **nxsprof** - lists the current profile (mntgrp)

nxsettimers - sets the current profile timers

nxsadd - selects the given detector components

nxsrn - deselects the given detector components

nxsclr - removes all detector components from the current profile

nxsetappentry - sets the append entry flag for the current profile

nxsetudata - sets the given user data

nxsunsetudata - unsets the given user data

nxsadddesc - adds the given description components to the current profile

nxsrmdesc - removes the given description components from the current profile

nxsupdatedesc - updates a selection of description components

nxsetprof - sets the active profile

nxsrmpf - removes the current profile

nxslsprof - lists all available profiles

nxsls - lists all available components to select

nxslstimers - lists all available timers

nxslscp - lists configuration server components

nxslsds - lists configuration server datasources

nxslsdevtype - list all defined device types

nxshow - describes the given component

nxsav - saves the current profile to the given file

nxsload - loads a profile from the given file



Client code example – Python script

```
from PyTango import DeviceProxy
# create configuration from components
cserver = DeviceProxy("p09/nxsconfigserver/01")
cserver.CreateConfiguration(["ten_channnel_detector", "slits", "beamstop"])
writer = DeviceProxy("p09/nxsdatawriter/01")
writer.Init()
writer.FileName = "/tmp/my_scan.nxs"
writer.OpenFile()

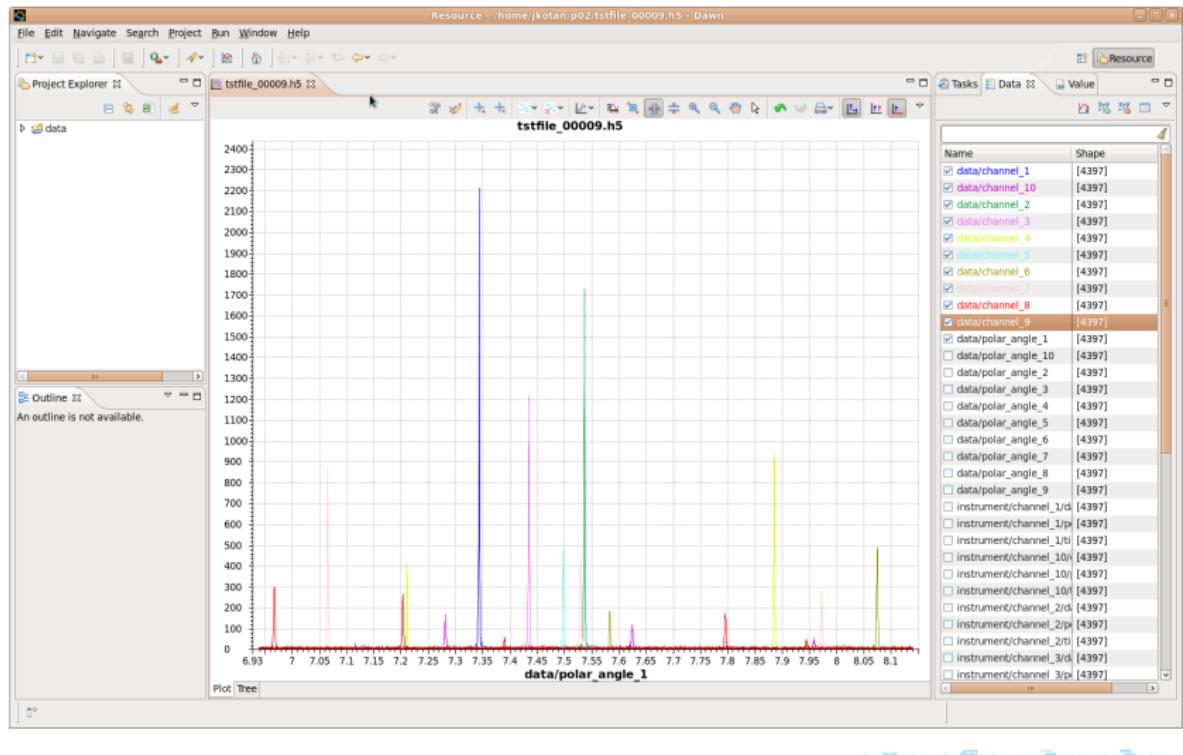
# send XMLString for a new scan
writer.XMLSettings = cserver.XMLString
# write init data (strategy INIT)
writer.JSONRecord = '{"data":{"parameterA":0.2}}'
writer.OpenEntry()

# experiment main loop
# (write data with strategy STEP)
for i in range(100):
    writer.Record(
        '{"data":{"exp_c01":%s, "exp_c02":%s}}' % (i*0.1, i*1.2))

# write final data (strategy FINAL)
# - close the entry - close the file
writer.JSONRecord = '{"data":{"parameterB":0.3}}'
writer.CloseEntry()
writer.CloseFile()
```

First data on P02.1 viewed in Dawn

High Resolution Powder Diffraction Beamline: p02sweep.py script



Mandatory Metadata (MMD)

Metadata common to all DESY experiments.

NeXus field or attribute path	ICAT field	Remark
/NXentry/experiment_identifier	Investigation	a unique beamtime ID
/NXentry/title	Investigation.Summary	description of the experiment
/NXentry/NXinstrument/name	Instrument.Fullname	name of the beamline
/NXentry/NXinstrument/name@short_name	Instrument.Name	short name of the beamline
/NXentry/NXinstrument/NXsource/name	Facility.Fullname	accelerator name
/NXentry/NXinstrument/NXsource/name@short_name	Facility.Name	short name for the accelerator
/NXentry/NXsample/name	Sample.Name	name of the sample
/NXentry/NXsample/chemical_formula	Samplename. Molecularformula	the sample chemical formula
/NXentry/start_time	Instrument.Start_Date	start time of the scan
/NXentry/end_time	Instrument.End_Date	end time of the scan

MMD sufficient for an **identification** of the file contents.

They are used by **ingestion procedure** inserting files into the metadata catalogue.

External Recorders

User interface for selecting recorders

External Recorders in Sardana

- Currently DESY uses its own Sardana version with added NeXus Recorder
- In the future Sardana will have **External Recorders**:
 - interface for adding new recorders
 - new recorders are installed as a python module
 - RecorderPath MacroServer property defines a path to new recorders



User interface of External Recorders

- What should be the strategy of recorder selection?
 - file extensions, e.g. .h5, .nxs, .fio, .spec
 - environment variable, e.g. ScanRecorder = 'FIO_FileRecorder', 'NXS_FileRecorder'
 - configuration file or built-in variable, e.g.

```
SCAN_RECORDER_MAP = {'.fio': 'FIO_FileRecorder', '.nxs': 'NXS_FileRecorder'}
```
- file extensions, ScanRecorder or both (priority)?
- SCAN_RECORDER_MAP ? Where? Filled automatically?



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Summary – NeXus Storage Software

Managing data in DESY Volatile Environments

- Creating **fully describing** files
- Configuration in **components** and **datasources**
- User Interfaces to NeXus Writer:
 - Selector GUI + Sardana, Sardana Macros (w/ or w/o Selector), Selector + Python/C++/Java apps, Python scripts
- Deployment:
 - roll-out software (IT staff)
 - provide information about experiment (Beamline Scientists)
 - provide components (IT staff)
 - select devices/components in Selector GUI and run scan (Users)
- External Recorders will simplify installation of NeXus Writer extensions

Summary – NeXus Storage Software

Managing data in DESY Volatile Environments

- Creating **fully describing** files
- Configuration in **components** and **datasources**
- User Interfaces to NeXus Writer:
 - Selector GUI + Sardana, Sardana Macros (w/ or w/o Selector), Selector + Python/C++/Java apps, Python scripts
- Deployment:
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Thank You

