# NeXus at DESY Photon Science

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# **PETRA III Beamlines**



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# NeXus libraries

#### production



h5cpp – c++ wrapper for hdf5 library (ESS/DESY) pninexus – HL interface and NeXus structure from XML

c++ libraries used to store fast detector data python3 modules used to store metadata

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

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# Configuration: Components and Datasources

#### Datasources are created automatically from user configuration

component templates <u>nxscreate</u> <u>components</u>

#### • Standard component templates common all for beamlines:

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

• Beamline specific component templates diffractometer, mirrors, pcostage, microscope, samplehexapod, samplepiezo, saxstage, laser, interferometer, crl, lenshexapod, cryostage, ...

Advantages:

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

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# NeXus component

#### Component describes

- which datasources to read (TANGO, CLIENT, PYEVAL, DB)
- in which time of the scan to read datasources (INIT, STEP, FINAL, POSTRUN)
- where in the NeXus file to write data
  as well all releated metadata (defines physical meaning)

### The components are in NXDL-like format



# 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 bullseye, **buster**, stretch and ubuntu focal, bionic

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#### **Device Selection – Detector Components**

NeXus Component Selector (expert mode) * _ u >									×				
Scan <u>Fi</u> le: water.nxs, w	ater.fi	D				Scan <u>D</u> ir:	/tmp	)				Scan ID: 498	
Imer: exp_t01 v + •							•	> >		Append E	intries 🗆		
Detectors Descriptions	User	Data Configura	tion										
2D detectors		Counters						ADC		VFC		MCA/SCA	
Sel. Dis	s.	Sel.	Dis. Se	el.	Dis. S	el.	Dis.	Sel.	Dis.	Sel.	Dis.	Sel.	Dis.
🔲 lambda 🛛		∉ exp_c01	9	exp_c12		exp_c23		exp_adc01		<pre>exp_vfc01</pre>		✓ exp_mca01	<b>e</b>
🗉 pilatus1M 🛛		₽ exp_c02		exp_c13		exp_c24		exp_adc02		exp_vfc02		exp_mca02	
🗆 pilatus300k 🗌		∉ exp_c03	<b>e</b> .	exp_c14	0.0	exp_c25		✓ exp_adc03	×	exp_vfc03		exp_mca03	
		∉ exp_c04	<b>e</b> .	exp_c15	0.0	exp_c26		✓ exp_adc04	×	exp_vfc04		exp_mca04	
Counter detectors		exp_c05		exp_c16		€ exp_c27	s.	✓ exp_adc05	×	exp_vfc05			
Sel. Dis	s.	🗆 exp_c06		exp_c17		exp_c28		exp_adc06		exp_vfc06		Additional	
detector_a	1	🔲 exp_c07		exp_c18		exp_c29		exp_adc07		exp_vfc07		Additional	
detector_a: e	exp_cC	01, exp_c02 c08		exp_c19		exp_c30		exp_adc08		exp_vfc08		Sel.	Dis.
[Imca]	_	exp_c09		exp_c20		exp_c31						exp_moto3	
Timers		🗆 exp_c10		exp_c21		exp_c32						exp_mot04	
Sel. Dis	5.	🗆 exp_c11		exp_c22								exp_morro	
exp_to1 ∈												✓ insertion_gap	×
□ exp_t02 □												insertion_taper	
Reset ClearAll				NOT		PLIED				Apply Oth	ers	Save Gose	Load

Select components of Pool channels and other TANGO devices.

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# NeXus Component Selector

#### **Device Selection – Description Components**

		NeXus (	omponent Selector (expert mode)	- ¤ ×
Scan <u>Fi</u> le: water.nxs,	water.fio		Scan <u>D</u> ir: /tmp	Scan ID: 498
Timer: exp_t01	× + -		MntGrp: mg_test01 V ->>	Append Entries 🕞
Detectors Description	ns User Data Configuratio	n		
Optional				Other Optional
	🗹 absorber	✓ mirrors	✓ slit2	∉ exp_mot17
	🗹 analyzer	✓ pinhole1	⊮ slit3	∉ exp_mot18
	✓ beam_monitor	🔲 pinhole2	'slit4	∉ exp_mot20
	𝗭 beamstop	✓ powers!	t1 🐨 source	∉ exp_mot22
	⊮ dcm	S powers	t2 📝 table_eh1	∉ exp_mot23
	' diff_hki	𝓝 qbpm1	⊮ table_eh2	∉ exp_mot25
	✓ difftractometer	✓ qbpm2	S undulator	∉ exp_mot26
	✓ lenses	i slita	ise xmcd	✓ exp_mot30
		slit1:	mot13 exp mot17 exp mot20 exp mot30 e	vp_mot331
		Look		€ exp_mot63
Mandatory				
		✓ default		
Reset Reset De	sc.	APPLI	ED	oly Others Save Gose Load

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

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### Spock with NeXus Sardana Recorder

#### User scan in spock with the exp\_mot03 motor.

Ð				IF	ython: home/jk	otan			٩	=	-	•	×
n09/door/baso228ik 01 [2]. ascan evo mot03 0 10 16 0 1													
Operatio	n will be sa	ved in /tmp	/scan [Sc	anIdl.fio	(fio from F	CO FileRe	corder)						
Operatio	n will be sa	ved in /tmp	/scan 000	10.nxs (nx)	from NXS I	leRecord	der)						
Scan #10	started at	Mon Mar 7	13:15:11	2022. It w	ill take at	least 0:0	0:10.037980						
#Pt No	exp mot03	exp mca01	exp c01	exp c05	exp c07	exp t01	dt						
Θ	Θ	(2048.)	11.7244	28,9639	91,4073	0.1	2.93764						
1	0.625	(2048,)	97.3422	8.22722	32.6115	0.1	3.94519						
2	1.25	(2048,)	186.923	1.53491	8.10139	0.1	4.94577						
3	1.875	(2048,)	238.24	0.19974	1.38327	0.1	5.94517						
4	2.5	(2048,)	201.647	0.0024720	0.18817	3 0.1	6.9314						
5	3.125	(2048,)	113.264	9.60994	0.0344282	0.1	7.94553						
6	3.75	(2048,)	42.2399	38.4604	0.0158475	0.1	8.93514						
7	4.375	(2048,)	10.5086	97.4677	0.0457621	0.1	9.94498						
8	5	(2048,)	1.70074	155.785	2.22103	0.1	10.9344						
9	5.625	(2048,)	18.9255	157.116	37.9432	0.1	11.9361						
10	6.25	(2048,)	57.0528	99.9306	149.054	0.1	12.9361						
11	6.875	(2048,)	107.005	40.0908	132.242	0.1	13.9458						
12	7.5	(2048,)	124.834	10.1164	26.5476	0.1	14.9385						
13	8.125	(2048,)	90.4417	43.3001	26.1402	0.1	15.9343						
14	8.75	(2048,)	40.7437	105.797	56.5867	0.1	16.9366						
15	9.375	(2048,)	11.3776	180.699	83.9238	0.1	17.9372						
16	10	(2048,)	2.02956	215.669	85.2412	0.1	18.9376						
<b>Operatio</b>	n saved in /	tmp/scan_00	010.fio (	fio)									
<b>Operatio</b>	n saved in /	tmp/scan_00	0010.nxs (	nxs)									
Scan #10	ended at Mo	n Mar 7 13	8:15:30 20	22, taking	0:00:19.31	2633. Dea	d time 91.2%	(motion	dead	time	62.7	%)	
p09/door	/haso228jk.0	1 [3]:											

#### For NeXus Recorder the file extension is .nxs

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# Metadata in NeXus

•	jkotan@haso2	28jk: ~				Q = _ = ×
haspp06ctrl% nxsconfig geometry dcm_mono						
Component: 'dcm mono'						
nexus_path	source_name	units	trans_type	trans_vector	trans_offset	depends_on
scan/instrument/dcm_mono/crystal1/usage						
scan/instrument/dcm_mono/crystall/type						
scan/instrument/dcm mono/crystal1/reflection	dcm mono reflection					
scan/instrument/dcm mono/crystal1/depends on						[transformations/lat]
scan/instrument/dcm_mono/crystal1/transformations/lat	monoy	mm	translation	100		chi
scan/instrument/dcm_mono/crystal1/transformations/chi	dcm_chi1	deg	rotation	001		phi
scan/instrument/dcm_mono/crystall/transformations/phi	dcm_phi	deg	rotation	010		//transformations/bragg
scan/instrument/dcm_mono/crystal1/chemical_formula						
scan/instrument/dcm_mono/crystal2/usage						
scan/instrument/dcm_mono/crystal2/type						
scan/instrument/dcm_mono/crystal2/reflection	dcm_mono_reflection					
scan/instrument/dcm_mono/crystal2/depends_on						[transformations/chi]
scan/instrument/dcm_mono/crystal2/transformations/chi	dcm_ch12	deg	rotation	001		theta
scan/instrument/dcm_mono/crystal2/transformations/theta	dcm_th2	aeg	rotation	010		perp
scan/instrument/dcm_mono/crystal2/transformations/perp	dcm_perp	mm	translation	0 1 0		para ( (transformations (bragg
scan/instrument/dcm_mono/crystal2/transformations/para	uciii_para		transtation	001		//transformations/bragg
scan/instrument/dcm_mono/transformations/bragg	dem bragg	deg	rotation	-100		inck]
scan/instrument/dcm_mono/transformations/blagg	mono jackl	mm	translation	0 1 0		JUCKI
scan/instrument/dcm_mono/transformations/jack1	mono_jack2	mm	translation	010		
scan/instrument/dcm_mono/transformations/jack2	mono_jack2	mm	translation	010		
scan/instrument/dcm_mono/transformations/table	monojacks	mm	translation	0 1 0		
scan/instrument/dcm_mono/collection/exit_offset	dcm_exitoffset	mm				
scan/instrument/dcm mono/collection/unit calibration	dcm mono unitcalibration	deg/mm				
scan/instrument/dcm mono/collection/crystal	dcm mono crystal	-				
scan/instrument/dcm_mono/collection/energyfmb	energy fmb	eV				
have of stals.						

#### Motor positions in NXtransformations Other data not defined by NeXus in NXcollection

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# DESY FS is testing SciCat

- $\bullet$  Scientific data organized into datasets ( $\sim$  our scans)
- Datasets annotated with administrative and flexible scientific metadata
  (Dataset.scientificMetadata, Instrument.customMetatdata, Sample.sampleCharacteristics – nested dictonaries)
- Infrastructure for publishing the data, DOI generation provided



• Both open access and embargoed data supported (i.e. openly accessible after a specified time period)

# Metadata ingestion

- Proposal/Beamtime metadata with fixed keywords automatic ingested from our DOOR server
- The definition of scientific meta data is fully flexible,
- e.g. NeXus based HDF5 files, extracted from instrument.

```
"scientificMetadata": {
"beamlineParameters": {
    "monostripe": "Ru/C",
    "ring_current": {
        "value": 0.402246,
        "units": "A"
    },
    "beam energy": {
        "value": 22595,
        "units": "eV"
},
"detectorParameters": {
    "objective": 20,
    "scintillator": "LAG 20um",
    "exposure_time": {
        "value": 0.4,
        "units": "s"
           ESS example
```

At DESY we can

- 1) ingest NeXus files via:
  - filter out 1D/2D data
  - dump to JSON

with keywords taken from NeXus names

- ingest to SciCat
- 2) let users to run a script

to ingest additional metadata

Similarly: Instrument.customMetatdata, Sample.sampleCharacteristics

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# SECoP@HMC project

SECoP – Sample Environment Communication Protocol

Helmholtz Metadata Collaboration – develops and implements novel concepts and technologies for a sustainable handling of research data through high-quality metadata.

#### Work packages:

- WP1: Standards for Sample Environment metadata in SECoP (K. Kiefer, HZB)
- WP2: Standards for storage of Sample Environment metadata (T. Kracht, DESY)
- WP3: Implementation into experimental control systems (G. Brandl, FZJ)
- WP4: Outreach, Dissemination & Training (T. Herrmannsdörfer, HZDR)

https://github.com/SampleEnvironment/SECoP

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Mapping the SECoP meta data into NeXus/HFD5 structure, i.e. NXsample, NXsensor, NXenvironment, NXtransformations, NXcollection



- Define a NeXus/HDF5 structure for the sample environment metadata
- Try to find a solution compliant with NIAC
- Develop a SECoP metadata collector for the Petra-3 experiment control system, Tango/Sardana
- Create a Tango-SECoP adaptor
- Define a process for creating vocabularies

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# NeXus is production





#### Advantages

- full description included, metadata and data
  - Od 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
- NeXus configuration components allow to fit sophisticated NeXus structure into specific experiment and beamline

# NeXus is production





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# Thank You !