



Mark Könnecke

Recapitulation of NeXus and NeXus @ PSI



Four Different Things

- Brief intro NeXus
- NeXus at SINQ
- NeXus at SLS
- NeXus at SwissFEL



- Solve the predicament of the traveling scientist
 - Variety of data file formats
 - Often data is distributed across many different files in different formats
- Long term storage of scientific data
- Standardized interfaces between data producers
- Target communities: neutron, X-ray and muSR scattering



What do we Need?

- A physical file format
- Platform independent
- Self describing
- Cater for a wild variety of instrumentation and use cases
- Ontology of well defined names
- Quick visualization



NeXus Adds to HDF5

- HDF-5 as physical file format
 - Platform independent
 - Self describing
 - Public domain
- Rules for organizing domain specific data in an HDF-5 file
- A dictionary of domain specific fields expressed in the form of base classes
- Strict validatable standards in the form of application definitions



- Groups
 - For organizing data in a hierarchy much like a file system
 - NeXus adds a type to groups, prefixed with NX
- Datasets
 - n-dimensional arrays of numbers in a variety of types
- Attributes
 - meta data items to be added to groups and datasets
- Links
 - Like unix filesystem links
 - For organization
 - For linking external data



NeXus Raw Data Structure

entry:NXentry SANS:NXinstrument source:NXsource collimator:NXcollimator detector:NXdetector

user:NXuser sample:NXsample data:NXdata data powder_diffraction:NXsubentry



NeXus Processed Data Structure

entry:NXentry process:NXprocess input:NXparameter output:NXparameter sample:NXsample data:NXdata data



More NeXus Features

- Scan rules
- Crystallographic transformations for positioning components in the McStas coordinate system
- new: NXoff_geometry for describing the geometry of components
 - Working on CSG
- Associating axis with data
- Streaming data acquisition

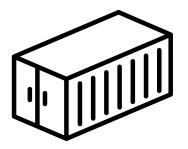


data:NXlog time[] @start_time @scaling_factor value[][][]... cue_timestamp_zero[] cue_index[]



Duality of NeXus

NeXus is a container, I contain everything



NeXus is a validatable standard through Application Definitions



Application Definitions

An application definition defines the minimum content of a file for a given scientific use case

- expressed in NXDL
- available for many scientific use cases already
- NeXus is open to community provided application definitions
- File validation through cnxvalidate available
- Most successful application definition: NXmx



NeXus Summary

- Progress with the adoption of NeXus is slow
 - But when new things are done it is usually done with NeXus
- We have seen people doing a file format themselves and ending up with formats looking very much like NeXus
- Work has started with people from the electron microscope community to expand the use of NeXus
- NeXus is overseen by the NIAC
 - You are invited to join
- www.nexusformat.org



- SINQ has been writing NeXus files since 1996
 - First HDF-4, now HDF-5
- NAPI was developed largely at SINQ
- SINQ got > 2 million files which habe been written, analyzed, and scientific results obtained from
 - Here you have your argument if anyone doubts that NeXus can be made to work
- The NeXus files written at SINQ represent an outdated state of NeXus now
- SINQ has decided to move from SICS to NICOS-3 as experiment control system
 - In the process we will make SINQ NeXus files comply with NeXus application definitions
 - We start with neutron event streaming reusing the ESS architecture



- Most files written via NAPI
- NXDICT
 - Description of the structure
 - Code generates structure from description
 - Scripted
- With NICOS: template based NeXus file generation through h5py
- Many bespoke tools for reducing and analyzing NeXus file data
- Mantid



- There were good intentions to use NeXus...
- Overrun in the rush to get the facility going
- Now:
 - Pollux uses NeXus full-time
 - cSax sometimes
 - EIGER-detector writes NeXus per default
- SLS-2 is coming up
 - We try again with good intentions...
 - New detectors -> more data -> NeXus more attractive



- Decided to do their own stuff, driven by detector manufacturers
 - They also did not have dedicated IT staff for a long time
 - Very dynamic instrumentation
- Still considering to use NeXus to store the machine state
- Insufficient resources to do this



• Questions?