

# The Status of NeXus

Neutron  
e  
X-ray  
 $\mu$  (muon)  
science  
data format

Thomas Proffen  
tproffen@lanl.gov



## Abbreviated Timeline

- Jon Tischler (ORNL) proposed an HDF-based format as a standard for data storage at APS (August 1994)
- Mark Koennecke (PSI) made a similar proposal using netCDF for the European neutron scattering community while working at ISIS (June 1994)
- This was the basis for the current design which was developed at SoftNeSS 1995 (at NIST) and SoftNeSS 1996 (at ANL)
- NeXus Abstract Programmer Interface (NAPI) released (August 1996)
- Przemek Klosowski (NCNR) produced a first draft of the NeXus proposal drawing on ideas from both sources (October 1996)
- SINQ at PSI started writing NeXus files to store raw data (July 1997)
- MLNSC at LANL started writing NeXus files to store raw data (summer 2001)
- NeXus International Advisory Committee (NIAC) formed and first meeting held at CalTech (October 2003)
- Ratifying base classes (March – September 2004)
- SINQ at PSI has created 391,789 NeXus files, ~65GB of data (October 7, 2004, 09:30 MESZ)
- MLNSC at LANL has created ~35,000 NeXus files (October 2004)
- Second NIAC meeting held at PSI (October 2004)

## NIAC Members

- Freddie Akeroyd, ISIS RAL
- Stephen Cotrell, ISIS RAL
- Matthias Drochner, DIDO (FRJ-2) FZ-Juelich
- Ron Ghosh, ILL
- Andy Gotz, ESRF
- Nick Hauser, BI ANSTO
- Jason Hodges, SNS ORNL
- Przemek Klosowski, NCNR NIST
- Mark Koennecke, PSI
- Peter Link, FRM2 TUM
- Ray Osborn, IPNS ANL (chair)
- Toshiya Otomo, KENS and J-PARC KEK
- Peter Peterson, SNS ORNL (executive secretary)
- Thomas Proffen, MLNSC LANL

## Advantages of a Common Data Format

- **Reduce need for local expertise**
- **Reduce number of conversion utilities**
- **Reduce redundant software development**
- **Increase cooperation in software development**
- **Increase sophistication of visualization software**
- **Increase functionality of generic software**

## Criteria for Data Format

- o It must be portable
- o It must be self-describing
- o It must be extensible
- o It must be flexible in data organization
- o It must be efficient in data storage
- o It must be available in the public domain

## Is it based on anything?

- o **Hierarchical Data Format** (4 and 5)
  - NXopen(filename,NXACC\_CREATE4,handle)
  - NXopen(filename,NXACC\_CREATE5,handle)
- o **eXtensible Markup Language** (API 3.0)
  - NXopen(filename,NXACC\_CREATEX,handle)
  - NXopen(filename,NXACC\_RDWR,handle)
  - NXopen(filename,NXACC\_READ,handle)

## Who is committed to NeXus

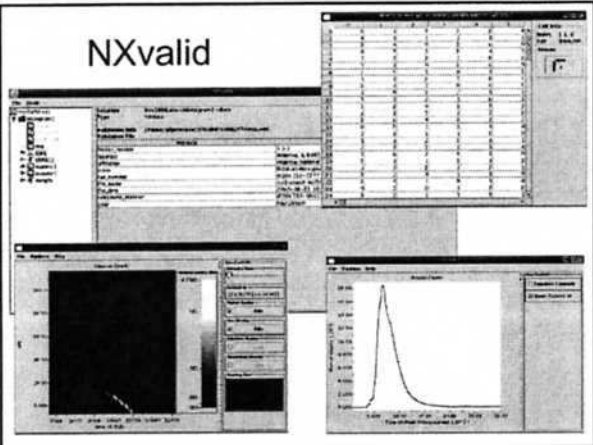


## List of Base Classes

- o NXroot → NXentry
  - NXuser
  - NXsample
    - o NXenvironment
      - NXanalyzer
  - NXinstrument
  - NXdata
  - NXmonitor
  - NXevent\_data
  - NXprocess
    - o NXnote
- o NXbeam
- o NXlog
- o NXgeometry
  - NXtranslation
  - NXorientation
  - NXshape
- o NXnote

- o NXroot → NXentry → NXinstrument
  - NXsource
  - NXmoderator
  - NXcrystal
  - NXdisk\_chopper
  - NXfeml\_chopper
  - NXvelocity\_selector
  - NXguide
  - NXcollimator
  - NXaperture
  - NXfilter
  - NXattenuator
  - NXpolarizer
  - NXflipper
  - NXmirror
  - NXdetector
  - NXbeam\_stop

## NXvalid



## Storage of large data sets

- Peter Peterson (SNS):

The XML base was given birth out of the cry by the reactor and x-ray people for their ASCII data. "Binary" information is stored as "NX\_CHAR", but care should be taken to set the "whitespace matters" flag upon opening the file. If the "binary" information is numbers, just say it and they will be stored that way. **The limit on the what you put in an xml based file is your patience** (it takes significantly longer to read and write, only noticed with bigger files), and the amount of disk space you have (the files are much bigger as well). Here we use xml-based NeXus to store instrument geometry information in a way that the scientists can touch, but NXtranslate can scoop up without effort. **I encourage everybody to use HDF5-based files unless they have a good reason to use something else.**

## NXtranslate

- Anything to NeXus converter
- Uses an XML-based translation file to determine where to get information from
- Additional information can be supplied in the translation file directly
- CLI to encourage batch usage
- Simple macro language to allow translating several files using one translation file
- Can already read from NAPI available files and portions of IPNS runfiles

## From Pre-NeXus to NeXus

