

# The Status of NeXus

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# Google “nexus file”

- DNA file
- Amino acid file
- Format for storing neutron, X-ray, and muon scattering data
- ... “a file format designed to contain systematic data for use by computer programs”
- “NEXUS files are the main file format supported by Mesquite, and perhaps will remain the only file format supported fully”
- Phylo team intends to develop “an XML standard to replace the NEXUS file format”

# What is NeXus?

Neutron

e

X-ray

$\mu$  (muon)

science

data format

# 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)

# Principles of NeXus

# 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

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

# Guiding Principles of NeXus

- **Allow different levels of implementation**
- **Provide flexibility of structure**
- **Produce definitions of common instrumentation**
- **Facilitate automated plotting**



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- If it looks too complicated, we're doing something wrong
- The most important thing is that everybody agrees on a standard, not what it is

# Is it based on anything?

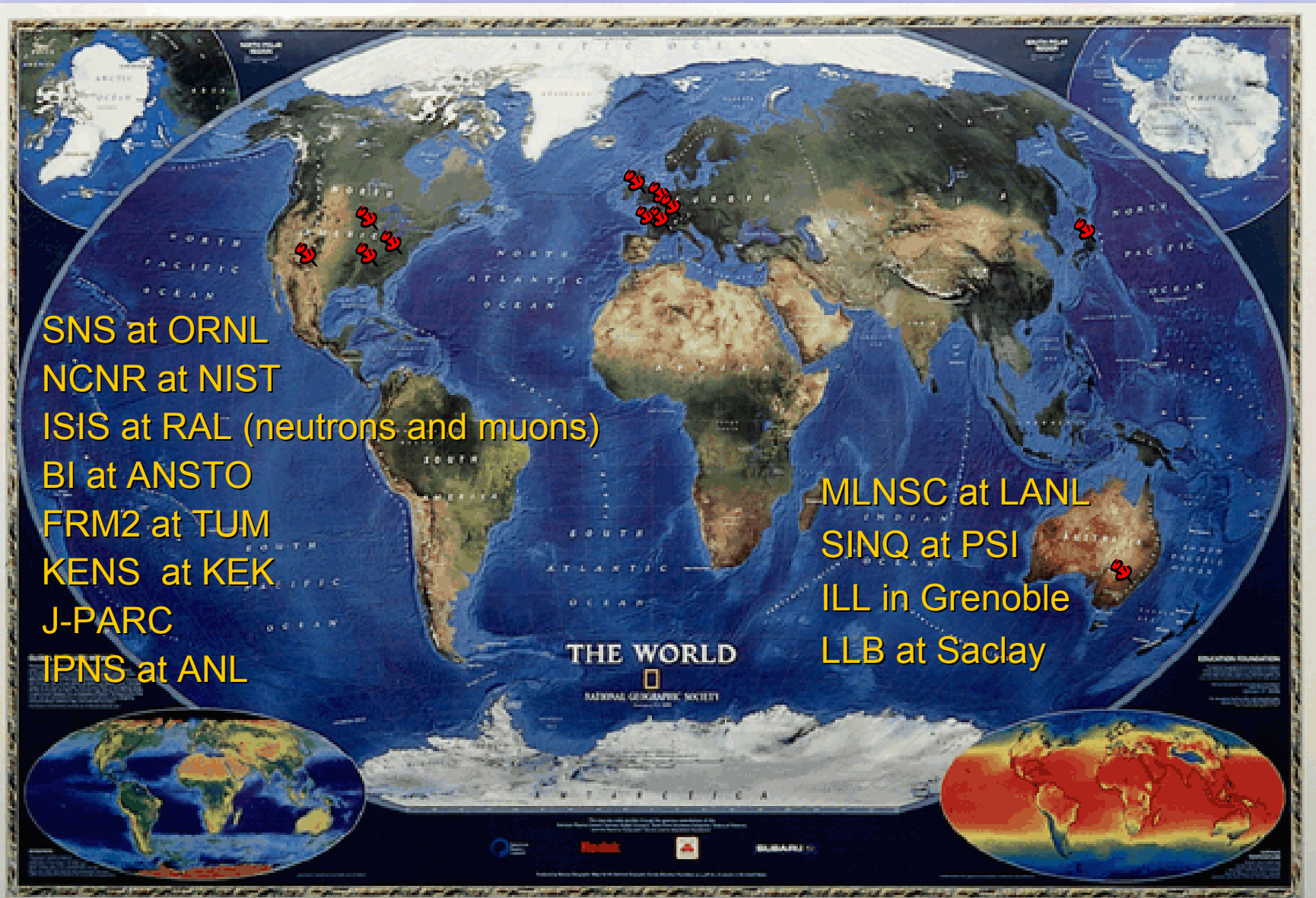
- Hierarchical Data Format (4 and 5)
  - NXOpen(filename,NXACC\_CREATE4,handle)
  - NXOpen(filename,NXACC\_CREATE5,handle)
- eXtensible Markup Language (in progress)
  - NXOpen(filename,NXACC\_CREATEEX,handle)
  
  - NXOpen(filename,NXACC\_RDWR,handle)
  - NXOpen(filename,NXACC\_READ,handle)

# Is it based on anything?

- ISO8601 – date and time
- McStas – coordinate system
- Crystallographic Information File (CIF) – chemical composition and crystallographic information

Where and how is NeXus  
used?

# Who is committed to NeXus



# Existing HDF4/5 tools

- HDFLook – HDF based plotter (???)
- Java HDF Viewer (NCSA)
- Scientific Data Browser – view data over the web (NCSA)

# NeXus Built NeXus Utilities

- NXbrowse – CLI tool to interactively explore NeXus files
- NXdir – CLI tool that lists contents of NeXus file and convert selected portions to ASCII
- NXtoDTD – Creates a definition file from an existing NeXus file
- NXtoXML – Writes an XML version of an existing NeXus file
- NXtranslate – anything to NeXus converter NXvalid – GUI tool to interactively explore, plot, and validate NeXus files
- NXtree – Create a html based tree view of NeXus files
- NXvalid – GUI tool to view and validate NeXus files



# Tools and Utilities

- addit, subi – programs to add or subtract powder data and write files suitable for Rietveld programs (SINQ)
- Amortool – simple CLI tool for Reflectometer data analysis (SINQ)
- anatric, cami4pcd – four circle diffractometer data analysis (SINQ)
- BerSANS – data analysis for SANS through adapter (SINQ)
- DANSE – **D**ata **A**nalysis Architecture for **N**eutron **S**cattering Experiments (CalTech)
- DAVE (future) - **D**ata **A**nalysis and **V**isualization **E**nvironment (NCNR)
- fit – home grown fitting program (SINQ)
- GumTree – scientific workbench for instrument control (BI)
- hdfb.sav and h5b.sav – browser for any 1D/2D/3D data saved in HDF (APS)
- ISAW – **I**ntegrated **S**pectral **A**nalysis **W**orkbench (IPNS)
- LAMP – **L**arge **A**rray **M**anipulation **P**rogram (ILL)
- KUPLOT – General purpose plotting program (MLNSC)
- McStas – instrument modeling program (SINQ/ILL)
- Nathan – TOF data analysis for FOCUS (IDL based) (SINQ)
- NDS – NeXus data server, publish NeXus files on TCP/IP, read only (SINQ)
- ninx – inx (ILL) adapted to read FOCUS TOF files (SINQ)
- NNDB – Java program to browse NeXus files published through NDS (SINQ)
- NXviewer – OpenDave based viewer (FRM2)
- OpenGenie – General purpose neutron and muon scattering data reduction and analysis tool (ISIS)
- Redas – data analysis for Reflectometer, based on Scilab (SINQ)
- Scilab – general matlab like data analysis tool - with a NeXus interface for that (SINQ)
- UDA and WIMDA – General purpose muon scattering analysis packages (ISIS)

What is happening with  
NeXus?

**“Dedicated Worker”**

# NIAC Terms of Reference

The purpose of the NeXus International Advisory Committee is to supervise the development and maintenance of the NeXus common data format for neutron, x-ray, and muon science.

This purpose include, but is not limited to, the following activities.

1. To establish policies concerning the definition, use, and promotion of the NeXus format
2. To ensure that the specification of the NeXus format is sufficiently complete and clear for its use in the exchange and archival of neutron, x-ray, and muon data.
3. To receive and examine all proposed amendments and extensions to the NeXus format. In particular, to ratify proposed instrument and group class definitions, to ensure that the data structures conform to the basic NeXus specification, and to ensure that the definitions of data items are clear and unambiguous and conform to accepted scientific usage.
4. To ensure that documentation of the NeXus format is sufficient, current, and available to potential users both on the internet and in other forms.
5. To coordinate with the developers of the NeXus Application Programming Interface to ensure that it supports the use of the NeXus format in the neutron, x-ray, and muon communities, and to promote other software development that will benefit users of the NeXus format.
6. To coordinate with other organizations that maintain and develop related data formats to ensure maximum compatibility.

# 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

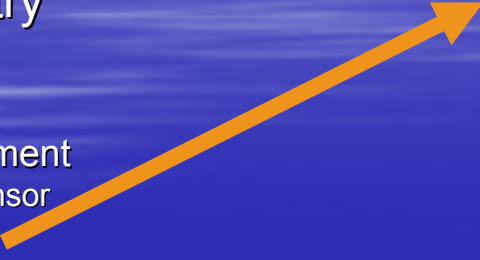
# Instrument Editors

- **Monochromatic Neutron/X-ray Powder Diffractometer (NXmononxpd)**
- Monochromatic Neutron/X-ray Reflectometer (NXmononxref): Paul Kienzle, NCNR NIST
- **Monochromatic Neutron/X-ray Single Crystal Diffractometer (NXmononxscd)**
- Monochromatic Neutron/X-ray Small Angle Scattering Diffractometer (NXmononxsas): Ron Ghosh, ILL
- Monochromatic Neutron/X-ray Triple-Axis Spectrometer (NXmononxtas): Nick Maliszewskyj, NCNR NIST
- Spin Echo: Robert Georgii, FRM2 TUM
- Time-of-flight Direct-Geometry Spectrometer (NXtofndgs): Toby Perring, ISIS RAL
- Time-of-flight Inverse-Geometry Spectrometer (NXtofnigs): Martyn Bull, ISIS RAL
- Time-of-Flight Powder Diffractometer (NXtofnpd): Peter Peterson, SNS ORNL
- Time-of-flight Reflectometer (NXtofnref): Rob Dalglish, ISIS RAL
- **Time-of-Flight Single Crystal Diffractometer (NXtofnscd)**
- Time-of-flight Small Angle Scattering Diffractometer (NXtofnsas): Steve King, ISIS RAL

# What has caused problems?

- Installation problems (HDF and NAPI)
- Lack of [instrument] definitions
- “What if someone puts in bad information?”
- Inertia: “I already have something that works”
- It is an unusable, ten year old standard
- “I don’t want to write software just to look at my data”

# List of Base Classes

- NXroot → NXentry
    - NXuser
    - NXsample
      - NXenvironment
        - NXsensor
    - NXinstrument
    - NXdata
    - NXmonitor
    - NXevent\_data
    - NXprocess
      - NXnote
  - NXbeam
  - NXlog
  - NXgeometry
    - NXtranslation
    - NXorientation
    - NXshape
  - NXnote
- 
- NXroot → NXentry → NXinstrument
    - NXsource
    - NXmoderator
    - NXcrystal
    - NXdisk\_chopper
    - NXfermi\_chopper
    - NXvelocity\_selector
    - NXguide
    - NXcollimator
    - NXaperture
    - NXfilter
    - NXattenuator
    - NXpolarizer
    - NXflipper
    - NXmirror
    - NXdetector
    - NXbeam\_stop



# NXsample contents

- chemical formula
- concentration
- density
- description
- electric field
- magnetic field
- mass
- name
- NXbeam
- NXgeometry
- preparation date
- pressure
- relative molecular mass
- sample orientation (UB)
- scattering length density
- stress field
- temperature
- unit cell
- unit cell class
- unit cell group
- volume fraction

# Connecting NXdata to NXdetector

- One NXdetector for each NXdata
- Relevant axes will be in NXdetector as well (time-of-flight and counts) connecting through linking

# Processed Data

- NXprocess
  - NXnote
    - author
    - date
    - mime type
    - original filename
    - description
    - data

# Some NeXus Software

# NXvalid

**NXvalid**

File Node

- Ircs3000.nxs
  - Histogram1
    - analysis
    - end\_time
    - start\_time
    - title
    - data
    - LRMECS
    - monitor1
    - monitor2
    - sample

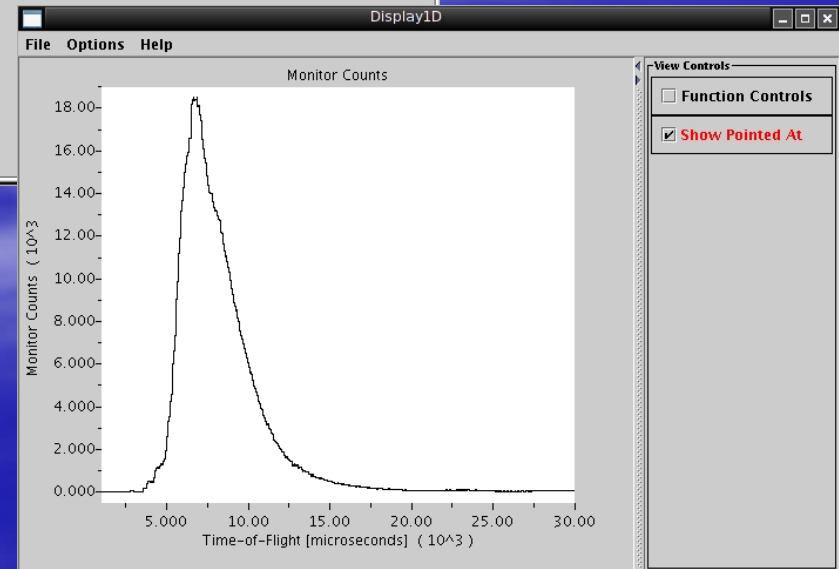
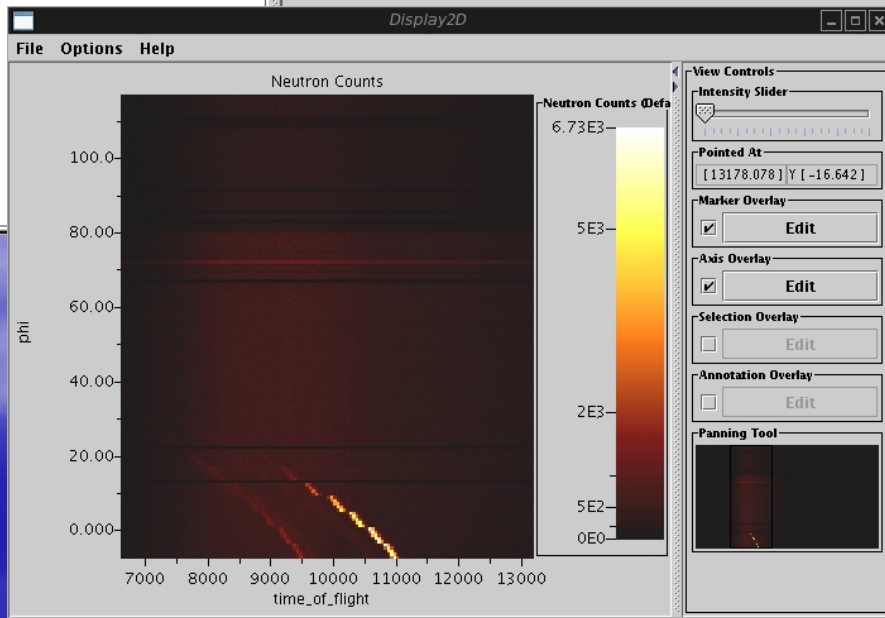
Location: Ircs3000.nxs → Histogram1 → data  
 Type: NXdata  
 Validation Info: /home/pfpeterson/NXvalid/valid/NXentry.xml  
 Validation File

Attribute	
NeXus_version	1.3.2
address	Argonne, IL 6043
affiliation	Argonne National
email	ROsborn@anl.gov
fax_number	(630) 252-7777
file_name	sys\$scratch:Ircs3
file_time	2000-08-23 10:
telephone_number	(630) 252-9011
user	Ray Osborn

Ircs3000.nxs → Histogram1 → data → data[148,580]

	0	1	2	3	4	5	6
0	0	1	5	2	2	4	
1	4	1	1	1	1	1	
2	2	4	0	2	0	0	
3	8	7	3	5	4	2	
4	2	2	2	2	0	2	
5	3	1	0	2	0	0	
6	2	6	3	0	1	2	
7	1	1	2	2	0	1	
8	2	3	1	0	0	5	
9	1	0	2	2	1	1	
10	3	1	2	1	0	1	
11	3	2	0	1	3	3	
12	3	1	3	1	2	2	
13	2	0	4	2	1	2	
14	0	5	1	1	1	0	
15	2	1	1	1	5	0	
16	1	1	2	2	1	1	
17	2	3	2	1	1	4	
18	2	0	2	3	1	0	
19	5	1	1	1	1	3	
20	1	3	2	1	3	1	
21	2	2	4	1	1	0	
22	3	0	1	0	1	0	
23	0	2	0	1	2	2	
24	2	2	1	1	3	1	

Cell Info  
 Index [ i, j ]  
 Key [row,col]  
 Mutate



# NXdir

<code>-p &lt;value&gt;</code>	Path inside the file to look in
<code>-o/+o</code>	Print (or not) the value of selected nodes
<code>-l --max-array [value]</code>	Number of array elements that are printed
<code>-t --tree-mode &lt;value&gt;</code>	Select the formatting of the tree
<code>--path-mode &lt;value&gt;</code>	Select whether paths are write with names/classes
<code>--data-mode &lt;value&gt;</code>	How data is printed
<code>--printline &lt;value&gt;</code>	How data is printed wrt tree
<code>--write-data &lt;filename&gt;</code>	Select an output file to write data

# 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

# More Information

NeXus homepage

<http://www.nexus.anl.gov>

Input on definitions. Visit the swiki at

<http://www.neutron.anl.gov.:8080/NeXus>

