The NeXus Data Format for muon Spectroscopy and Neutron or X-ray Scattering

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The Predicament of the Traveling Scientist

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- Cannot read her collaborators data
- Has to keep extra information in yet another form

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- Definition of a standard data format
  - Rules
  - Validation tools
- Promotion of NeXus
  - Documentation
  - NeXus API
  - Outreach to the scientific community

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NeXus Design

- Complete data for typical use
- Extendable, add additional data as you please
- Self describing
- Easy automatic plotting
- Platform independent, public domain, efficient
- Suitable for a wild variety of applications

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NeXus Levels

1. Physical file format and API for accessing files
2. Rules for storing data in files
3. Component and application definitions
4. NeXus Utilities

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Physical File Format

- Portable, self describing, extendable, public domain
- Hierarchical data format, NCSA, HDF-4, later HDF-5
- HDF-5:
  - grouping support
  - on the fly compression
  - reading/writing subsets
  - first dimension appendable
  - Public domain C, F77 access library
  - Used by: NASA, Boing, the weathermen, ...
- XML for those who wish to edit their data

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- NeXus-API hides complex HDF API
- Transparent access to all three supported physical file formats
- ANSI-C implementation
- Bindings: C++, F77, Java, python, IDL, SWIG
- January, 4, 2010: 1311217 files processed at PSI alone

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Threads Versus NeXus

- Planned: NeXus is threadsafe when each thread has its own NXhandle
- A little work needs to be done to arrive there
- BUT: HDF-5 serialises access, no performance gain!
- Parallel HDF5, PHDF, with a different API
- PHDF requires: MPI, MPI-IO, parallel file system
- A new NeXus file driver for PHDF would be required
- Will only be implemented when the community really wants it

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NeXus Objects

- Files
- Groups identified by name and a classname beginning with NX
- Scientific data sets
- Attributes
- Links

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- McStas Coordinate System
- Angle based polar coordinate system
- NEW: full mapping imageCIF - NeXus now possible
- NEW: General axis and transformations

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NeXus General Rules

- NeXus reserves the prefix NX for group names.
- Store as much as possible
- A NeXus file has one to many NXentry groups
- There are two types of entries: raw data and processed data
- Multiple different techniques in one file go into separate NXsubentries
- If there is only one entry, the preferred name is entry, else entry1, entry2... entryn
- If an entry or an NXsubentry conforms to an application definition, the application definitions must be stated in the entries definition field.

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entry:NXentry
- sample:NXsample
- instrument:NXinstrument
  - source:NXsource
  - velocity_selector:NXvelocity_selector
  - detector:NXdetector
    - data[xsize,ysize], signal=1 (1)
- control:NXmonitor
  - data
- data:NXdata
  - link to (1)

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NeXus Processed Data File Structure

entry:NXentry
- sample:NXsample
- processing_name:NXprocess
  - program
  - version
  - parameters:NXparameter
    - raw_file
- data:NXdata
  - data[nx,ny,nz], signal=1

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NEW: NXsubentry

entry:NXentry
- sample:NXsample
- instrument:NXinstrument
- .....
- sas:NXsubentry
  - sample:NXsample
  - instrument:NXinstrument
    - source:NXsource
    - velocity_selector:NXvelocity_selector
    - detector:NXdetector
      - data[xsize,ysize], signal=1 (1)
  - control:NXmonitor
    - data
  - data:NXdata
    - link to (1)

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NEW: NXcollection

entry,NXentry
- measurement:NXcollection
  - positions:NXcollection
    - om
    - two_theta
  - scalars:NXcollection
    - title
    - wavelength
  - data:NXdata
    - detector1
    - mca5

Why the Hierarchy??

- Supports self description and allows short names in components

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Why the Hierarchy??

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- NXentry allows for multiple datasets in the same file
- NXdata supports automatic plotting
- Take care once when writing, use n times

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Rules for Storing Data Items

- Store physical values in C storage order
- Use NeXus components and dictionary names
- Missing names will be quickly accepted by the NIAC
- Names: full words separated by _
- Specify units in same format as used by UDunits
- Application definitions may restrict units

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NEW: Data Storage Exceptions

- There are situations were data has to be dumped as fast as possible in order to keep up with a high data rate. Or to save disk space.
- **Data not in C storage order:** use attributes stride and offset to describe the memory layout of the data.
- **Data needs scaling:**Use a NXformula group to specify a formula in muParser notations plus the parameters and data necessary to do the scaling.
- Details on both methods will be in the NeXus manual

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Associating Axis and Data, Preferred method

entry:NXentry
    data:NXdata
        data[nx,ny,nz], signal=1, axes=x_axis,y_axis,z_axis
        x_axis[nx]
        y_axis[ny]
        z_axis[nz]

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- Preserve original dimensionality of detector, if possible
- Time-of-flight becomes last dimension
- Highly irregular detectors:

```
entry:NXentry
        instrument:NXinstrument
                detector:NXdetector
                        data[ndet], signal=1
                        polar_angle[ndet], axis=1
                        azimuthal_angle[ndet]
                        distance[ndet]
```

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- Come in all shapes and sizes
- Captured by rules:
  - Store all varied parameters as arrays of length NP at the appropriate place in the NeXus hierarchy
  - For multi detectors, NP, number of scan points is always the first dimension
  - In NXdata: create links to counts and varied variables

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Scan Example 1: rotating sample

entry:NXentry
- sample:NXsample
  - rotation_angle[NP], axis=1 (1)
- instrument:NXinstrument
  - detector:NXdetector
    - data[NP],signal=1 (2)
- control:NXmonitor
  - data[NP]
- data:NXdata
  - link to (1)
  - link to (2)

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Scan Example 2: complex scan in Q

entry:NXentry
- sample:NXsample
  - rotation_angle[NP], axis=1 (1)
  - phi[NP], axis=1 (2)
  - chi[NP], axis=1 (3)
  - h[NP], axis=1 (4), primary=1
  - k[NP], axis=1 (5)
  - l[NP], axis=1 (6)
- instrument:NXinstrument
  - detector:NXdetector
    - data[NP],signal=1 (7)
    - polar_angle[NP],signal=1 (8)
- data:NXdata
  - link to (1)
  - link to (2)
  - link to (...)
  - link to (8)

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Scan Example 3: sample rotation, area detector

```
entry:NXentry
        sample:NXsample
                rotation_angle[NP], axis=1 (1)
        instrument:NXinstrument
                detector:NXdetector
                        data[NP,xsize,ysize],signal=1 (2)
        control:NXmonitor
                data[NP]
        data:NXdata
                link to (1)
                link to (2)
```

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- This is rastering a sample at different wavelengths, positions etc.
- Same treatment as scans, NP replaced by NR number of raster points
- For the common case of rastering on a 2D grid one can store [nx,ny,detdim]. Be aware, though, that this causes problems if the rasterisation is aborted in mid operation.

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NeXus Component and Application Definitions

- Component definitions: dictionaries of allowed field names for the various NeXus groups
- Application Definitions
  - Define what has to be in a NeXus file for a certain application
  - Defines standards
  - Another view: Contract between file producers and users about what has to be in a NeXus file for a well defined purpose
  - Validation by NXvalidate
- Written in NeXus Definition Language, NXDL

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All Base Classes

NXaperture
NXattenuator
NXbeam_stop
NXbeam
NXbending_magnet
NXcharacterization
NXcollimator
NXcrystal
NXdata
NXdetector
NXdisk_chopper
NXentry
NXenvironment
NXevent_data
NXfermi_chopper
NXfilter
NXflipper
NXgeometry
NXguide
NXinsertion_device
NXinstrument
NXlog
NXmirror
NXmoderator
NXmonitor
NXmonochromator
NXnote
NXorientation
NXparameters
NXpolarizer
NXprocess
NXsample
NXsensor
NXshape
NXsource
NXtranslation
NXuser
NXvelocity_selector

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Application Definition Process

1. Construct an application definition with advice from the NIAC
2. You can also inherit from and extend an existing definition
3. Cure for a year; data should be produced in the new format in this time
4. After curation and review: this is the standard for this application type.

- No promises, but the NIAC may do it for you
  - Description of experiment
  - Minimum set of data items necessary form common use
  - Example data

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Four Steps

1. Think! what ought to go into the file
2. Map this into the NeXus file structure
3. Cast this mapping into a NXDL file
4. Standardize your application definition together with the NIAC

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Think!

- What has to go into the file?
- Minimum data necessary for common usage scenarios
- Haggle it out with your community
- Coverage ratio: > 80 % of use cases

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Map to NeXus

- Consider into which NeXus group an item might belong
- Look in the base class for a suitable data field
- Link the data items required for the default plot into NXdata

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From an application definition to a real NeXus file

- The structure defined by the application definition is the minimum

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  - Look at each of your instruments components and the matching NeXus base class
  - Add whatever you feel like adding or the instrument scientists wants to have
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- Remember: Adding more fields does not break application definition compliance!

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NEW: Available NeXus Application Definitions

- NXarchive
- NXreftof
- NXtas
- NXtomophase
- NXxnb
- NXtomoproc
- NXindirectof
- NXsastof
- NXtofsingle
- NXmonopd
- NXsas
- NXtofraw
- NXxeuler
- NXxrot
- NXtofsingle
- NXiqproc
- NXsqom
- NXxas
- NXrefscan
- NXscan
- NXtomo
- NXxkappa
- NXiqproc
- NXdirectof
- NXlauetof
- NXtofraw
- NXxasproc

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Challenge 3 a standard requires scarce scientific programming resources for adoption

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Data Format Benefits

Benefit 1 By using a discoverable data format like NeXus, XML, HDF-5, people can at least figure out what is in the data file.

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Benefit 6 Application Definitions

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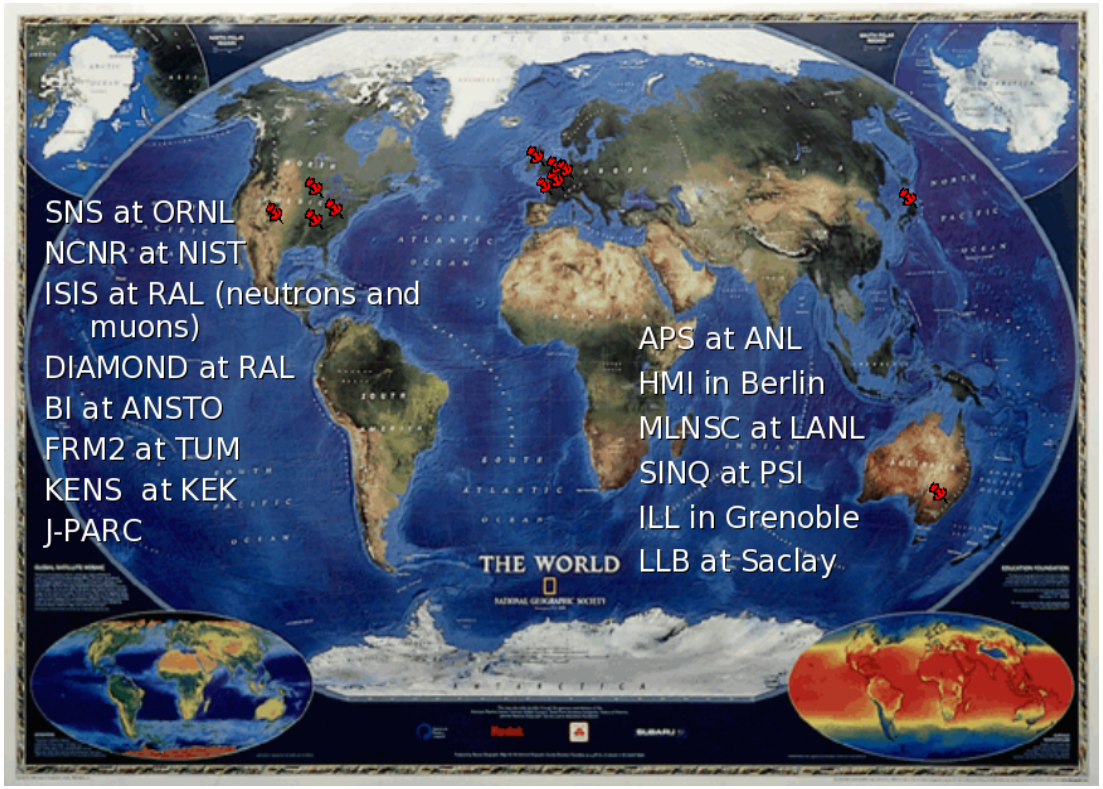
Who commits to NeXus?



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What You Can Do with NeXus

1. Store and archive data from a wild variety of instruments
2. Store processed data
3. Store a complete workflow from raw data to publication ready data in several NXentries in one file
4. Store a set of related experiments in one file
5. Define strict and validatable standards

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NeXus Outlook

- New systems tend to use NeXus
- No competitor for a general purpose data format
- Planned:
  - Refine application definitions together with communities
  - Release application definitions and NXvalidate
  - Update manuals and the NeXus WWW-site
  - www.nexusformat.org, embarrasingly outdated, download manual

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