

# NIAC Meeting Minutes – (14/5/2007)

## ALS, Berkeley

5 - 6 October 2007

### ***present :***

L.Lerousse (RAL), J.Suzuki (J-Parc), A.Götz<sup>1</sup> ESRF), P.Peterson<sup>2</sup> (SNS), P.Jemian (ANL), M.Koennecke (PSI), F.Akeroyd (CCLRC), S.Campbell (DLS), T.Proffen (LANL), N.Hauser (ANSTO), M.Drochner (KFI Julich), M.McKerns (CalTech), P.Klosowski (NIST), J-U.Hoffman (HMI)

***The meeting was held directly after the NOBUGS 2006 conference at the same venue. Thanks to Pete Jemian for doing the local organising, Pete Peterson for helping him and Przemek Klosowski for providing funding***

### ***ILL Meeting Minutes***

The following points arose from the ILL February 2006 Meeting Minutes :

- ACTION – A.Gotz to submit article on NIAC meeting to Synchrotron and Neutron News
- ACTION – a big THANKS to Freddie Akeroyd for all his work on the moving the NeXus wiki to the new nexusformat.org domain, which is being hosted by CCLRC
- ACTION – everyone to check that the contents of the Argonne web server ([www.nexus.anl.gov](http://www.nexus.anl.gov)) have been correctly transferred
- ACTION – move nexus, nexus-developers and nexus-committee mailing list from anl.gov to nexusformat.org (try to preserve archive if possible)
- Mark Koennecke has sent the scan DTD to Andy Gotz
- NXcharacterisation needs to be revived
- Freddie Akeroyd has briefly looked in Plone as an alternative to Mediawiki, but concluded that MediaWiki is simpler and has all the functionality we need for now.

Renew members

The following members were renewed :

- Nick Hauser - ANSTO

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1 secretary

2 president

- Ray Osborn - IPNS ?
- Jiro Suzuki – J-PARC (replaces Toshiya Otomo)

The following new members were welcomed :

- Jens-UweHoffman (HMI)
- Paul Kienzle (NIST, representing the DANSE project)

## ***NXarchive***

L.Lerousse presented the NXarchive definition. It is being used by the ICAT data file cataloguing project being developed by ISIS, SNS, and Diamond. The NXarchive definition is being used for data archiving and for data mining. The first NXentry info is mandatory.

QUESTION : should publications be in the Nexus file? NXarchive definition sub-group will discuss this.

It was decided that the NXarchive definition is not ready for voting yet and it was sent back to the proposers to make a new proposal.

## ***Base classes***

- NXpositioner was discussed. M.Koennecke and R.Osborn voiced their concern about the existence of this class.

## ***SANS Instrument***

A long discussion was held about the SANS instrument. The question was raised whether we should have separate SANS and SAXS instrument definitions. Another question was raised whether we need a new base class for velocity selector. No conclusions were proposed for voting.

## ***ILL/ESRF proposal***

A.Gotz presented the joint ILL/ESRF proposal (cf. attached text). The proposal was discussed. It

was concluded that one of the points in the proposal to adopt a general (name,value) part approach is not in the spirit of NeXus (a hierarchy of containers where similar values are grouped together). A number of the other points were addressed by the meeting and decisions taken e.g. separating base classes and instrument definitions, freezing Nexus 1.0, adopting McStas geometry.

## **General Discussion**

The following points were raised during the general discussions :

1. Instrument definitions must be done
2. Axis indexing must be from left to right ... ???does this refer to [i,j] etc. in instrument definitions for arrays?
3. There is a need to show how to ratify instruments which are being proposed
4. Nexus 3.0 will probably be object oriented ... definitions ratified at this meeting will be NeXus 2.0
5. Base classes must not be changed
6. We should finish doing the best we can and not wait anymore
7. Monochromatic powder diffraction definition is missing info for GSAS
8. A question was raised whether NXinstrument should be stored with Nxdata ? ?????
9. NXsource should include the radiation type
10. There was a discussion about ScanRaw and which order to store scan area detector data in. The possibility of storing data in multiple files was accepted to accommodate instruments which generate large volumes (gigabytes to terabytes).
11. N.Hauser reported back on the ImgCIF meeting he and T.Proffen attended. There was an interest in the ImgCIF meeting to co-exist with NeXus. ImgCIF want to go to schema. Nexus community could provide some help here.
12. A request was made for money. Who can finance projects ? It was decided to make an NSF proposal.

## **Votes**

Here are the results of the votes which were taken :

1. NXMonoPowder – 1 AGAINST, rest FOR

2. NXGenericScan – results ?!
3. NXPositioner – 1 ABSTENTION, rest FOR
4. NXTOF – 2 ABSTENTIONS, rest FOR ??? Do you mean TOFRAW or something else? TOFRAW was ratified in Grenoble though
5. Axes = 1 – all FOR ??? is this 2. from above general discussion?
6. Geometry definitions will follow the McStass conventions – all FOR
7. NXMonitor – 1 ABSTENTION rest FOR

## **Decisions**

1. At the end of this meeting all classes which have been ratified will be collectively referred to as Nexus 2.0
2. Nexus 3.0 refers to the next version of Nexus. It was left open for discussion how best to implement the next version of Nexus e.g. uses object oriented technology or not
3. P.Klosowski will continue to be in charge of the FAQ
4. When scan data is stored in one file the scan variable should be the slowest varying variable. This is an effect from how HDF4/5 work.
5. NXsample is not mandatory to have counting time
6. There is a need to resurrect NXtimer
7. NXdata does not necessarily contain real data – it provides info for plotting
8. Nexus community to collaborate with ImgCIF
9. NXarchive proposers to rework the NXarchive class and present the new version when ready
10. Base class and instrument definitions will be stored in separate areas of the repository in the future
11. Change all units to EDU standard units
12. Don't store CCD efficiency as part of NXdetector

See <http://www.nexusformat.org/Instruments> for latest status

## **Actions**

The following actions were identified :

1. *M.Koennecke* to make a picture of his geometry
2. *Tech Group* to change FLOAT32 to FLOAT
3. *???* to put NXGenericScan text in manual
4. *P.Kienzle, N.Hauser and P.Peterson* will look into making an NSF proposal to request for money
5. *A.Gotz* to add missing items for ccd detectors to NXdetector
6. *Tech Group* to find a solution to the linking problem for when you need the source and target names to be different.
7. *P.Peterson* to explain how to change a definition
8. *P.Peterson* to write up the versioning mechanism
9. *P.Kienzle* to provide an example of a Tscan
10. *P.Kienzle* to make a proposal for NXScan
11. *P.Kienzle* to make a list of all units used in NeXus
12. *P.Kienzle* to make a proposal for a measurement type scan
13. *P.Peterson + P.Kienzle* to make a proposal fro NXcharacterisation
14. *Tech Group* to provide an example file of using NXlog instead of NXtimer
15. *F. Akeroyd* to move *NeXus code and definitions from CVS to Subversion* (*svn.nexusformat.org*)
16. *F. Akeroyd* to move *NeXus mailing lists from anl.gov to lists.nexusformat.org*
17. *F. Akeroyd* to provide a *Mediawiki extension for rendering definitions held in Subversion onto a Wiki page in a tabular format on the fly*
18. *ALL: some definitions exist only on the WIKI, some are in source control (Subversion); they should all be moved into Subversion*
19. *P. Peterson* tag current version of *NeXus definitions as version 1.0.*

# NeXus – ILL and ESRF proposal

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This document presents conclusions and proposals from the NeXus ILL+ESRF Local Advisory Committee (NLAC).

## NeXus "raison d'etre"

1. NeXus is an *exchange format* to all n,X,muon scattering techniques in large facilities.
  - This implicitly limits the scope of NeXus to all that is *common* to these techniques, while excluding instrument/technique peculiarities. Further descriptions (instrument details) are in principle out of scope, but may be specified as extensions to the basis requirements.
2. The scientific *data* set is intrinsically the most important to physicists, compared with the exact instrument definition (which is essentially relevant for instrument debugging and simulation purposes). The official 'base' NeXus format should focus on the former rather than the latter.
3. NeXus must be *easy to use*.
  - This means that there is an efficient API (and this is the case, thanks Mark K.)
4. At the same time, NeXus should be flexible enough to potentially evolve from HDF and XML towards other physical storage format (Open Document, ...)
5. NeXus must be *appealing* for people to voluntarily use it (in programs).
  - This means that the format structure must be clear, simple and easy to understand. This is probably the most important point, otherwise it will push people to develop their own NeXus format, or event use their own non-NeXus format (based on HDF or not)
6. The NeXus web server must present usage examples and distribute associated software.
7. NeXus must be *flexible and expandible*.
  - This means that there should be a recommended mechanism for extension of the 'base' NeXus into 'proprietary' NeXus. At the same time, a clear statement must be done concerning a limited number of absolute requirements, as well as 'official' recommandations for extensions.
8. The scientific *Data must be immediately visible* in the NeXus structure, as well as *essential parameters* for the data analysis. This means that the NXData must be directly in the NXentry, that essential parameters should be as well there (in an NXparameters class, see below). Further information (NXinstrument, ...) is optional.

## Format requirements

### Proposal R1: Simplified NeXus hierarchy

The base NeXus format should contain the following hierarchy:

NXentry	NXdata
	NXsample
	NXparameters

Other classes should be mentioned as optional, even though NXmonitor and NXuser are recommended.

### Proposal R2: simplified NXdata

- rename 'long\_name' into 'label' in 'variable'
- suppress 'first\_good' and 'last\_good'
- add a 'range' attribute to 'variable' so that it can be given as a regularly sampled range.

### Proposal R3: scanning mechanism (dim <= 3)

For low dimensionality data sets (dim <= 3), the scan may be stored as a array in the NXdata, with associated axis.

### Proposal R4: scanning mechanism (general): NXgroup

As an alternative, or for higher dimensionality, each scan step is stored as a single NXdata, with one 'master' NXgroup describing how to assemble scan steps into series. The assembling mechanism is to be discussed further.

### Proposal R5: the NXparameters class

As an alternative to the NXinstrument, which brings usually too much information as required for a basic data analysis, a new NXparameters class should be defined next to the NXdata, and gather 'important' parameters to be used by scientists.

The NXparameter is a kind of 'abstract' of NXinstrument. The list of these parameters should be defined per class of instrument, based on requirements from existing data analysis programs (FullProf, INX, Sqw, Dave, Isaw, Nathan, ...), to be discussed further.

## Format extensions (optional)

### Proposal E1: NXinstrument is optional

The NXinstrument class is optional. No NXinstrument class should be specifically defined as

'official'. However, some examples per class of instrument will be available to programmers. Indeed, as all instruments are essentially unique, no description can cope with all of them.

The usage of NXinstrument usually concerns instrument simulations (McStas, Vitess, NISP, ResTrax, IDEAS, ...) as well as exact configuration (e.g. for repeating experiment and debugging purposes).

### **Proposal E2: NXinstrument vs NXdata and redundancy**

If present, NXinstrument should contain all the relevant information concerning the instrument parameters. In order to prevent redundancy for the data set (in detector and NXdata), the usage of links is required.

A NXsample class should better appear in the NXinstrument as a link to the NXentry/NXsample. One or more NXmonitor class should better appear in the NXinstrument as a link to the NXentry/NXmonitor.

### **Proposal E3: positioning and distances**

The 'official' mechanism for distance/geometry specification is NXgeometry. It derives from McStas positioning system. Other distance specification attributes defined within NXinstrument objects should be avoided.

### **Proposal E4: no object definition**

The usage of objects and inheritance is not envisaged as it brings too much complexity in the associated definitions. We rather promote a simplification of the existing NeXus.

### **Proposal E5: grouping of equivalent elements**

The NXgroup class could be used to assemble other items than scan steps in order to define super-classes, e.g. sets of detectors and monochromators.