

Minutes of the NeXus International Advisory Committee Meeting
Bishop's Lodge, Sante Fe, NM
April 26-28, 2005

In attendance:

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Thomas Proffen	tproffen@lanl.gov

Members of the NeXus International Advisory Committee (NIAC):

Freddie Akeroyd	ISIS Pulsed Neutron Facility, UK
Stuart Campbell ²	Diamond Light Source, UK
Stephen Cottrell	ISIS Pulsed Muon Facility, UK
Matthias Drochner ²	Forschungszentrum Juelich, Germany
Ron Ghosh	Institut Laue Langevin, France
Andy Goetz ²	European Synchrotron Radiation Facility, France
Nick Hauser ²	Bragg Institute, Australia
Przemek Klosowski	NIST Center for Neutron Research, USA
Mark Koennecke	SINQ, Switzerland
Harmut Gilde ²	FRM2, Germany
Nick Maliszewskyj ¹	NIST Center for Neutron Research, USA (Technical Committee Chair)
Ray Osborn	Intense Pulsed Neutron Source, USA (Chair)
Toshiya Otomo	J-PARC, Japan
Peter Peterson	Spallation Neutron Source, USA (Executive Secretary)
Thomas Proffen	Lujan Neutron Scattering Center, USA

¹ non-voting member² did not attend

Tuesday, April 26, 2005

Welcome and Introductions

The NIAC recorded its thanks to Peter Peterson and Thomas Proffen for organizing the meeting.

Review of NIAC 2004 Minutes

ACTION ITEM: Przemek Klozowski will continue to compile questions and answers for the frequently asked questions (FAQ) document on the NeXus web-site.

Nick Maliszweskyj as technical chair will release NAPI 3.0 at the end of the meeting.

NXcharacterize and NXprocess will use external linking scheme.

ACTION ITEM: Peter Peterson will work on NXuser and isotopes.

Busing-Levy and UB need to discuss during instrument definitions. Discussion of whether it is necessary is not resolved.

Review of XML base of the NAPI.

Plugin architectures and NXtranslate.

Short discussion of NXU routines.

Lunch: Discussion of subclassing. Decision was to put it off until later.

Discussion of translation tables.

VOTE: Approve minutes of the meeting [9 for, 0 against]

Open Discussion

Discussion of NXdata and NXdetector, and their uses. It was reiterated that NXdata is a mechanism for plotting. In general the NXdata will consist of links to other locations in the file to find more information specific to the NXdata and its plotting axes.

Discussion of linking to external information such as characterization measurements. A suggestion was made to use the attributes from NXtranslate, but the group agreed that a whitepaper will be created suggesting a particular syntax.

Revisit inheritance discussion.

Review triple axis (TAS) definition. The discussion frequently visits the idea of an "NXscan" and how it should be stored in the file.

Dinner: Discussion of agenda for Wednesday

Wednesday, April 27, 2005

Steve Miller presents information on the DICOM standard for medical imaging

DICOM is used in medical imaging mostly for reduced (image) data, but also defines a standard for storing raw data from devices. Links to more information on DICOM: <http://medical.nema.org>, <http://medical.nema.org/dicom/2004.html>, <http://www.hl7.org>.

Discussion of publishing definitions for specific instruments.

Split into groups

TOFNPD

See resulting definition

Triple Axis and Reflectometry

0. NXscan

This is a class which would be very useful especially in step scanning instruments allowing the set-up phase to be recorded. It would have a simplified structure primarily containing only NXdata, and the stepped component. This would allow easy visualization of the phase of the experiment, perhaps with an NXnote of result!

NXentry

 NXscan

 NXdata

 NXinstrument or NXsample

 scanned item

 NXnote

1. Triple axis

ILL (E. Farhi) had provided a fairly complete set of example scans for Nick Maliszewskyj to examine and to base his original xml file.

Most points were brought to the main meeting.

Derived scan variables should be placed in "sample" qh qk ql, dE

Mono/analyzer includes d-spacing and hkl; angles are relative to preceding component - the sign conventions actually give the correct scattering geometry in the general case. qv Nick Maliszewskyj.

Mark Koennecke and Nick Maliszewskyj then prepared a specimen example file

2. NXmonoref Paul Kienzle, Ron Ghosh

New requirements could include a tag in NXentry with the intent of the experiment, with attributes of measurement style sample conditions, etc to enable quick browser tables to be built up in GUIs etc and help automating treatment (searchable name/value pairs?)

SLIT

This might be established independently of NX aperture; "opening" is a needed derived value; sample is centrally aligned so left/right values may be individually adjusted. Slit designs are crucial to resolution.

3. Generic SAS (Nick Maliszewskyj), Toshiya Otomo, Steve Cottrell, Ron Ghosh

The starting points were from SANS (Mark Koennecke) and generic SAS (Steve King (ISIS)), who should be thanked for introducing contributions from Nick Terrill and Mark Malfois(DIAMOND) as demonstrating inclusion of synchrotrons in 17 pages of XML and comments.

Classes for Insertion Devices have still to be defined (ACTION Andy Goetz, ESRF)

Steve Cottrell brought operational knowledge of the spallation source (affects NXmonitor i.e. the flux normalizations depend on integrated beam current (charge)), modes of operation etc., all of which have impact on the SAS measurement, but, unlike reflection, do not require a completely different file layout as between mononref and tofnref.

Toshiya Otomo showed examples from KEK, again demonstrating that high quality results are to be expected for JPARC.

Between us we answered a number of questions posed by King/Terril/Malfois, but it still remains for me to complete this comparison and distil a template etc. I hope to finish before the end of this month, including seeking responses from Steve King et al.

Lunch: Breakout groups continue discussions of instrument definitions

Meet as full group

Presentation of TOFNPD time focus and rietveld

VOTE: Describe links in the metaDTD as NAPILink. [9 for, 0 against]

Presentation of MONONTAS. During the presentation it is suggested that there is enough information for automated simulations of instruments in the NeXus file.

Split into groups

NXcharacterization and Instrument Definition Inheritance

Radically different definitions should be stored in different NXentries.

Inheritance will be done in the metaDTD only. This will be denoted by a tag at the top of the metaDTD, “conforms_to”, which will have a list of definition tags that this definition will also follow. Tags that exist in the other definitions are missing from the definition with the “conforms_to” tag.

There will be a new utility function that will check if a given definition conforms to another. The syntax is:

```
int NXUconforms_to(definition,version,URL, definition,version,URL);
```

The group noted a desire to have a mechanism for storing parametric studies of processed data.

Dinner: Discussion of NXcharacterization

To store information about characterization measurements the NXentry will reference another complete NXentry using the external linking mechanism. In the meta-DTD the referenced NXentry will exist at the NXentry level, with the definition tag made explicit.

Thursday, April 28, 2005

Propose ratifying base classes on May 27, 2005 with public comment allowed until May 20, 2005.

Meet as full group

Discussion of disallowing components in definitions. Consensus is that it should not be allowed.

Decision to create a special group to decide conventions for definition names, URL/URI, and versions. The group will consist of [not defined].

VOTE: Allow “*” and “?” in definitions to denote groups and fields that are desirable, but not necessary. [9 for, 0 against]

VOTE: Approve the inheritance mechanism determined on the previous day. [9 for, 0 against]

VOTE: NXcharacterization proposal determined on the previous day. [9 for, 0 against]

Presentation of the MONOTAS definition.

Presentation of the TOFDGS definition.

Discussion of what “simple plotting” means

The discussion centered on the variety of interpretations of the term “simple plotting”.

It was determined that the term was being used in two separate contexts:

Trivial plotting: This is the original design principle of a single NXdata. There are instructions on how to plot an n-dimensional block of information. Possible additional features of such a plot is to allow changing the axis and “signal” arrays to be on a logarithmic scale.

Simple plotting: More sophisticated plots that use information frequently found in the NeXus file outside of an NXdata. The majority of these plots require the geometry of the detectors (position and extent) in addition to what is found in the NXdata. Examples of simple plots were:

- Multiple NXdata combined in the same image
- 3D view of the data on the instrument
- The data transformed to physical coordinates using parameters supplied in the file
- An NXdata divided by another
- An NXdata subtracted from each other

Lunch: Eleana Pourmal presents an update on HDF

Among the salient points of the talk was the announcement that HDF is no longer going to be part of NCSA. Instead they are forming a not-for-profit company called The HDF Group (THG). The license for HDF will remain BSD, and the group will continue to work with NCSA. The other big announcement is that THG is working towards ANSI standardization of HDF5.

Technical Group Meeting

Preparing for new NAPI release

Changes from 2.0

XML support (mxml)

NXSetNumberFormat - needed for XML

NXU utility API (C)

NXOpenPath

NXOpenGroupPath

NXOpenSourceGroup

NX_BINARY definition

C, F77, java, SWIG

Prospective new release tag is 3.0beta

Testing in preparation for release

- Tests and documentation
 - Automatic testing
 - Peer Review of Code
 - Freddie Akeroyd
 - Uwe Fliges
 - Mark Koennecke
 - Peter Peterson
 - Jens Kruger
- Install Dependencies
 - 1) jpeg, zlib, (gzip)
 - 2) HDF & format libraries
 - 3) NAPI
- Platforms supported
 - Win32 (i686)
 - msi packages (VC .net, Visual FORTRAN)
 - Linux (i686)
 - rpm (gcc/g77)
 - deb
 - Linux (AMD64)
 - OSX ? (fink)
- Repositories
 - Separate documentation from sources in CVS repository
 - Move SWIG wrappers to contrib directory
 - New applications and wrappers go to contrib directory
- Tests
 - Self tests (writing & reading)
 - Hard self tests needed mainly for C API
 - Tests of reading existing files
 - Acceptance tests
 - Performed on all supported platforms
 - Read all existing examples (XML, HDF5, HDF4)
 - Write test file
 - Read test file - compare against what we wrote
 - Beef: libtool tests are sh scripts
 - We need real binaries
 - Fix test suite (FAA - action item)
- Process
 - Bug reports
 - We could use tracking software
 - Possibilities: bugzilla & rt
 - Freddy Akeroyd running bugzilla server
- Miscellany
 - HDF team is now an independent HDF Group (THG)
 - THG assuming responsibility for IDL DLM wrappers (RSI)
 - hdfview (THG) is a java tool for visualizing hdf files
 - THG will work with users to help them get what they need

Action items

- Fix test suite (FAA)
- Code review of core code tree (long term need)
- Discuss how to move items from contrib to distribution
- NCM generate formalized testing plan
- Schedules
 - Fixing test suite
 - Testing on Win32, Linux, OSX
 - Release of 3.0beta

Meet as Full Group for Discussion of documentation

It was decided that there will be 5 documents:

Technical Reference – Describes the metaDTD format and has base class definitions as well as instrument definitions. Edited by Peter Peterson.

NeXus API Reference – Describes, in detail, the NeXus API. Edited by Mark Koennecke.

User Reference – Describes how to use the NeXus API and NeXus Utility API to read and write NeXus files. Edited by Przemek Klosowski.

Plan for testing and releasing the NeXus API. Edited by Nick Maliszewskyj.

Not technically a document, but in addition to the documents listed above, there will be example files that conform to the definitions in the Technical Reference.

Action Item: Peter Peterson will archive the base class definitions and instrument definitions in CVS.

Action Item: Freddie Akeroyd will create a new CVSROOT for documentation (shared with definitions).

Action Item: Mark Koennecke will synchronize the European mirror of the NeXus web site.

Discussion of how open the nexus-committee@anl.gov mailing list is. The decision is that anyone can ask to join it, but only committee members can make unmoderated posts.

General Discussion

The NIAC thanks Steve King for his hard work on the Small Angle Scattering (SAS) definition.

Action Item: Nick Hauser (with Mark Koennecke) work on a NeXus talk for ICNS.

It is suggested that NIAC produces a project plan with a list of people working on various tasks to give the community a better understanding of how NeXus develops and provide incentive to facilities to give more formal support to NeXus.

Discussions about getting more involvement from the synchrotron community. The first two to approach (that are not already involved) are API and Brisbane. It is suggested that NIAC members go to the facilities to give a talk on NeXus and to personally invite people from the facilities to attend the next NIAC meeting.

Dinner: The location and dates for the next NIAC meeting is discussed. It is decided that holding the meeting during or adjacent to ICNS in Sydney is not desired. Instead it is agreed that the next meeting should be in Grenoble during January or February of 2006. Ron Ghosh will start working on the logistics.

Action Item: A whitepaper will be written to describe a mechanism for linking to external information. The group will be Freddie Akeroyd, Mark Koennecke, and Peter Peterson, chaired by Koennecke.

Action Item: A conventions for definition labeling (name, URI, and version number) will be determined. The group will be Freddie Akeroyd, Nick Maliszewskyj, and Peter Peterson, chaired by Akeroyd.