Minutes of the NeXus International Advisory Committee Meeting
Paul Scherrer Institut, Villigen, Switzerland
October 21-22, 2004

In attendance:

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Members of the NeXus International Advisory Committee (NIAC):

Frederick Akeroyd	ISIS Pulsed Neutron Facility, UK
Stephen Cottrell	ISIS Pulsed Muon Facility, UK
Matthias Drochner	Forschungzentrum Juelich, Germany
Ron Ghosh	Institut Laue Langevin, France
Andy Goetz	European Synchrotron Radiation Facility, France
Nick Hauser	Bragg Institute, Australia
Przemek Klosowski	NIST Center for Neutron Research, USA
Mark Koennecke	SINQ, Switzerland
Hartmut Gilde[1]	FRM2, Germany
Nick Maliszewskyj[2]	NIST Center for Neutron Research, USA (Technical Committee Chair)
Ray Osborn	Intense Pulsed Neutron Source, USA (Chair)
Jiro Suzuki[3]	J-PARC, Japan
Peter Peterson	Spallation Neutron Source, USA (Executive Secretary)
Thomas Proffen	Lujan Neutron Scattering Center, USA

[1] substituting for Peter Link
[2] non-voting member
[3] substituting for Toshiya Otomo

Thursday, October 21, 2004

Welcome and Introductions

The NIAC recorded its thanks to Mark Koennecke for making arrangements for this meeting, and to Peter Peterson for keeping the committee on task throughout the past year.

VOTE: To add Peter Peterson as the SNS representative to the committee in place of Jason Hodges [12 for, 1 abstain]

Review of NIAC'2003 Minutes

VOTE: To confirm that both class and instrument definitions will continue to use the NeXus meta-DTD format, rather than XML schema [13 for].

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

ACTION ITEM: Mark Koennecke will add support for the `NX_BOOLEAN` and `NX_BINARY` datatypes to the NeXus API.

VOTE: To approve the minutes from the previous meeting [10 for, 3 abstain]

Organizational Issues

AMENDMENT: The Chair and the Executive Secretary will be reelected by the NIAC at the beginning of each annual meeting, effective at the end of that meeting.

ACTION ITEM: Nick Hauser will look into holding the next annual NIAC meeting at or near ANSTO around the time of International Conference on Neutron Scattering, being held in Sydney at the end of November, 2005.

ACTION ITEM: All committee members will look into alternative locations and dates

AMENDMENT: To create the new post of Chair of the Technical Committee with responsibility to oversee the NeXus API. The tasks of the chair are to coordinate tests, manage and announce releases, and promote code from the contributed directory to the regular release build. The position is renewable at the same time as the NIAC Chair and Executive Secretary. The person that holds the position does not need to be an existing member of the NIAC, and does not vote unless he/she is a regular member. [13 for]

VOTE: To appoint Nick Maliszewskyj as the first Chair of the Technical Committee [13 for]

ACTION ITEM: If the number of facilities requesting voting members on the NIAC exceeds twenty, plans to reorganize the committee will be considered. One proposal is to split the committee into two groups, a larger group for discussion and a smaller group (elected from the larger one) that is eligible to vote on policy decisions.

ACTION ITEM: Anyone adding a page to the NeXus Swiki should ensure that it contains a list of "interested parties" supervising discussions on that page.

Presentation of Related Projects

Elena Pourmal gave a presentation of recent developments in both HDF4 and HDF5, including the development of a Java viewer common to both formats and the addition of dimension scales to HDF5. There are also plans to port HDF5 to VMS with sponsorship from Boeing. The new ability in HDF5 to list groups according to creation order, rather than alphabetical order, will be used to provide consistency with the HDF4 version of the NeXus API.

Freddie Akeroyd gave a presentation of NXnet, a proposal to use the San Diego Supercomputer Center Storage Resource Broker (SRB) API to provide common access to neutron and other scientific data. This is being developed as part of the UK e-Science Programme, but the Spallation Neutron Source has expressed interest in the project so it may become an international standard. There was some discussion about ensuring that the most reliable metadata are stored in any archived NeXus file, but there was no consensus about whether NIAC should seek to influence facility management on this issue.

Stephen Cottrell gave an overview of the status of NeXus at muon science facilities. The International Society of μSR Spectroscopy, whose members represent all the major muon facilities, has officially approved his membership on NIAC. Three of the four facilities will be producing NeXus files within the next year.

Review of Base Classes

VOTE: To make it a violation of the NeXus standard to name an item or give it a class name that starts with "NX" unless approved by the NIAC. [13 for]

VOTE: To add a "NIAC version number" in the header of the base classes, which should be kept synchronized with the classes' CVS tag. [13 for]

VOTE: If an item is to be linked outside its parent group, a "source" attribute should be specified with the absolute address of the source item. [13 for]

ACTION ITEM: Mark Koennecke will add a new function to the NeXus API called `NXopengroup(path)`, which opens the group above the path specified.

VOTE: To allow the use of polar and cylindrical coordinates, in addition to Cartesian coordinates, within NXtranslation groups. [13 for]

VOTE: To allow dimension scales within a NXdata group to have arbitrary rank in order to cope with non-linear coordinate schemes. [12 for, 1 against]

VOTE: For the data errors to be specified, the data errors will be named `<datasetname_errors>`, or the dataset will have an attribute, `error_formula`, specifying how the errors are calculated. [13 for]

Friday, October 22, 2004

The NIAC thanked Mark Koennecke and Heinz Heer for arranging an excellent dinner the previous night.

Review of Base Classes (contd)

VOTE: To remove NXcharacterizations from the NXentry definition. [13 for]

ACTION ITEM: Thomas Proffen will consider improvements to the Nxcharacterizations base class before it is ratified.

ACTION ITEM: Thomas Proffen will propose a new version of NXprocess to supercede the existing ratified version.

ACTION ITEM: Peter Peterson will propose a new version of NXuser that is consistent with the Dublin Core Metadata Initiative.

ACTION ITEM: Ron Ghosh will create a clearer definition for the orientation (UB) matrix that exists inside the NXsample class.

ACTION ITEM: Peter Peterson will propose a change to the chemical formula to allow for isotopes.

ACTION ITEM: Ray Osborn will merge the NXdisk_chopper and NXfermi_chopper classes into a unified NXchopper class.

ACTION ITEM: Andy Goetz will propose changes to the NXsource class to make it applicable to x-ray synchrotron facilities.

ACTION ITEM: Andy Goetz will propose a NXinsertion_device class to add to the NXinstrument class, to use in synchrotron data files.

ACTION ITEM: Nick Maliszewskyj will propose changes to NXcrystal to account for the scattering sense of triple axis measurements.

ACTION ITEM: Peter Peterson will propose improved documentation for the NXguide class.

VOTE: To require that every instrument component should contain an item named `distance` and a group of class `NXgeometry.` [13 for]

ACTION ITEM: Ray Osborn will edit all of the base classes to insure that they have both `distance` and `NXgeometry` groups defined.

ACTION ITEM: Nick Maliszewskyj will propose a NXpolarizer class.

ACTION ITEM: Mark Koennecke will propose changes to NXbeam_stop to make it more consistent with usage in small angle scattering instruments.

ACTION ITEM: Nick Maliszewskyj will propose a change to the NXmonitor class to make it more consistent with instruments that scan for fixed statistics rather than fixed time.

VOTE: To specify that the end–of–line terminator in the NXnote class is a single linefeed character, "\n". [12 for, 1 against]

ACTION ITEM: Ron Ghosh will propose a change to NXbeam to make it consistent with usage in McStas.

Instrument Definitions

There are 13 instrument definitions, eleven of which are unique. There was discussion concerning the scope of the instrument definitions, whether they should they be the minimum required to perform a basic analysis or the maximum to allow more sophisticated data treatments. There was concern that these definition files should not become prohibitively complicated. This discussion was resumed later in the day (see below).

API Developments

Mark Koennecke presented the new version of the NeXus API that reads and writes NeXus files directly in XML.
- The API uses the Document Object Model (DOM) rather than the Simple API for XML (SAX) using the library mxml (http://www.easysw.com/~mike/mxml/), with modifications to treat numerical data efficiently. Version 2.1 of mxml will incorporate these changes, so it should be easy to install. This library was preferred to libxml2 because it is more compact.
- The new API can run the standard API read/write tests.
- Unlimited dimensions will not be implemented unless a user specifically requests that the technical committee do so.
- The NeXus API method to set the compression type is ignored by the XML API.
- Following discussion at the meeting, Mark Koennecke will amend the XML API to change the name of the NXlink object to something that cannot clash with a future NeXus class, *e.g.,* NAPIlink
- The data type of attributes will be encoded in the attribute itself, with the type NX_CHAR being implicit. For example, the integer attribute `signal` might be listed as `signal="NX_INT:1"`.

Peter Peterson presented NXtranslate, which reads a modified NeXus file, written in XML, with extra attributes `source`, `mime-type`, and `location`, to define how to include external data in a particular tag. It currently works for translating NeXus files from one definition to another, and it has been demonstrated that a plug-in architecture can be used to perform translations from other file formats, although the details are not finalized. In the future, it is possible that the NeXus API will be modified so that data can be transparently read from an external source, *e.g.* from electronic memory, without modifications to the NeXus application.

ACTION ITEM: Nick Maliszewskyj will consult with a NIST expert on plug-in architectures to recommend its implementation in NXtranslate.

ACTION ITEM: Freddie Akeroyd will produce method signatures for a C version of the NeXus Utility API that duplicates the functionality of the existing Fortran 90 Utility API.

Instrument Definitions (contd)

VOTE: To send out a call to the instrument editors to assist in writing instrument and other specialized NeXus file definitions by following these steps:

a. Draw a schematic diagram of the instrument (line art, not a CAD style drawing).
b. Write a brief document outlining the purpose of the instrument. In the summary, list existing packages that perform data reduction and/or analysis for this type of data. Also list the information that will (and will not) exist in the file including, but not limited to, characterization measurements used for subtracting a background or normalizing to an incident spectrum.
c. Ask the people that maintain the packages listed in step b to provide a list of essential variables that the data file should contain.
d. Send the document and the diagram to the NIAC who will nominate someone to construct a XML definition.
e. The NIAC will construct the XML definition.
f. Write a sample NeXus file conforming to the instrument definition (for example, using NXtranslate).
g. Test the file, repeating steps e and f as appropriate.
h. Request ratification once the testing phase is complete.

[10 for, 3 abstain]

VOTE: To recommend the appointment of editors to define the type of processed data required by a particular type of data analysis. Examples include Rietveld analysis, single crystal refinements, phonon density-of-states calculations, and total scattering measurements. Generic processed data should be stored as one or more NXdata groups within a distinct NXentry group that typically will contain the original NXsample group. [10 for, 3 abstain]

ACTION ITEM: Peter Peterson will propose a method for subclassing instrument definitions.

ACTION ITEM: Ray Osborn will identify common attributes. The list of common attributes will be compiled and stored separate from any individual base class.

ACTION ITEM: Mark Koennecke will produce a document describing "translation tables." A short description is that translation tables will work similar to NXtranslate, except the plugin architecture will exist within an extended NeXus API.

Closing Business

It was informally agreed that the next annual meeting should take place at or near ANSTO, near Sydney, Austalia, close to the ICNS meeting in November, 2005, subject to confirmation from Nick Hauser.

There was general agreement that it would be useful to meet again in six months for longer than two days, probably in late April or early May to coordinate with the ICANS meeting in Los Alamos. The meeting will be located somewhere in the USA, to be determined following suggestions by NIAC members.