

NIAC meeting – HMI, Berlin (Germany)

24, 25, 26 September 2007

The NIAC meeting for 2007 was held at HMI (Berlin) in September 2007.

List of attendees

Gwenaëlle Abeille, Synchrotron Soleil, France

[Frederick Akeroyd](#), ISIS Facility, Rutherford Appleton Laboratory, UK

[Stuart Campbell](#), Diamond Light Source, UK

[Stephen Cottrell](#), ISIS Facility, Rutherford Appleton Laboratory,

[Matthias Drochner](#), Forschungszentrum Jülich, Germany

Stefan Flemming, The Open University, UK

[Andrew Gotz](#), European Synchrotron Radiation Facility, France

[Nick Hauser](#), Australian Nuclear Science and Technology Organisation, Australia

[Jens-Uwe Hoffmann](#), Hahn-Meitner-Institut Berlin, Germany

[Pete Jemian](#), Advanced Photon Source, USA

[Mark Koennecke](#), Paul Scherrer Institut

[Laurent Lerusse](#), Rutherford Appleton Laboratory , e-Science

[Ray Osborn](#), Argonne National Laboratory, USA

[Peter Peterson](#), Spallation Neutron Source, Oak Ridge National Laboratory, USA

Frédéric Picca, Synchrotron Soleil, France

[Stephane Poirier](#), Synchrotron Soleil, France

[Thomas Proffen](#), Lujan Neutron Scattering Center, Los Alamos National Laboratory, USA

Rainer Schneider, [STRAINET](#) c/o HMI Berlin, Germany

Jiro Suzuki, KEK, Japan

Welcome

Pete Peterson (president) gave a welcome talk. In this talk he proposed that

- the term of the current acting officers has come to an end and they should be re-elected or new officers elected

Nick proposed to talk about NexusBeans and object orientation.

Mark mentioned that he had prepared a talk on object orientation.

Someone mentioned that the NXGeometry supports boxes and cylinders.

Nexus paper :

Mark noted that there is a publication on Nexus which appeared as part of the ICNS proceedings :

- Physica B 385-386 (2006) 1343-1345

There was a short discussion on scans. What is the role ScanRaw, Nick wants to know if this is a Nexus scan object

Action : Nick to take over NXgenericScan

The outstanding action item to request NSF money was discussed :

- [Paul Kienzle](#), [Nick Hauser](#), and [Peter Peterson](#) - will look into making an NSF proposal to request for money

It was decided to leave this action item open.

Action : Pete + Nick to look into requesting money frm the NSF for Nexus

Nick and Peter Turner mentioned they have requested and obtained funds for doing something around NexusBeans.

The linking problem for when you need the source and target names to be different has been fixed by Mark. A new api call has been added :

NXMakeNamedLink()

The point was raised that there is no explanation on the wiki on how to change a Nexus class definition. A new action item was created :

- [Peter Peterson](#) - to explain how to change a definition

Action : Pete Peterson to explain how to change a definition

- [Frederick Akeroyd](#) - some definitions exist only on the WIKI, some are in source control (Subversion); they should all be moved into Subversion. **STATUS:** all base classes moved, input from other NIAC members required on naming of instrument definitions before moving them.

Open question how to name some definitions like TofRaw

Pete Jemian suggests differentating names between Instruments + Base classes

Action : ALL - check old <http://www.nexus.anl.gov> web site and report any content that has not been moved to new WIKI server

OK. Ray suggests leaving it there with its warning.

Vote to redirect site (pending moving logos) –

FOR = all , AGAINST = none

Action: redirect old site to new web site (Ray)

Action: move logos to new web site

From [2006 ILL Meeting](#)

- [Peter Peterson](#) - Write down the current responsibilities for the officers and circulate to the committee for approval
- [Andrew Götz](#) - Write a report on NeXus and submit to both the Neutron News and Synchrotron News

Not done. Mark has an article in ICNS 2005. Everyone is incited to cite this paper.

Action: Andy to publish the article, don't wait for comments, set a deadline

- Darren Kelly and [Raymond Osborn](#) - Existing definitions will be rendered in colored meta-DTD and table formats. Results will be added to website

Done by Freddie on the wiki

Closed

- Darren Kelly - Style sheets (XSLT) will be created to convert definitions into colorized meta-DTD and table formats
- Unassigned - Update website with constitution changes (some are even from the last meeting)

Action : Pete Peterson to update website with constitution changes

- Unassigned - Modify/add base class definitions in accordance with what was voted on in February.

Some of the TOF base class has not made it to SVN

Action : Freddie to add missing TOF base class to SVN

Completed Actions

From [2006 LBL Meeting](#)

- [Frederick Akeroyd](#) - to move NeXus code and definitions from CVS to Subversion
- [Frederick Akeroyd](#) - to move NeXus mailing lists from anl.gov to lists.nexusformat.org
- [Frederick Akeroyd](#) - to provide a Mediawiki extension for rendering definitions held in Subversion onto a Wiki page in a tabular format on the fly
- [Mark Könnecke](#) and [Raymond Osborn](#) - Shut down existing website and mirror, leaving a redirection page to new site. [The original website at <http://www.nexus.anl.gov/> contains a redirect message, but is still online so that NIAC members can check for content missing on the wiki.]
- [Peter Peterson](#) - to write up the versioning mechanism

From [2006 ILL Meeting](#)

- Unassigned - NXcharacterization needs to be formalized and ratified - this has been repeated in [#11](#)
- Unassigned - Synchronize the website definitions with those in cvs (the website are considered more correct) - this is formalized as an action item at the 2006 LBL meeting

THANKS : Freddie for setting up the wiki

THANKS : Jens for organising the meeting

Tags

Version 1.0 = prior to 2006-2

Version 2.0 = everything ratified at 2006-2

Version 3.0 = next version

Member Renewal

Matthias Drochner – to be renewed

Andy Gotz – to be renewed

Peter Link – expired (no news)

Nick Maliszewskyj – replaces Przemak for NIST

VOTE : to renew members

FOR = all ; AGAINST = none

ACTION : have meeting in October in the future, not in September at the end of the fiscal year

Officer Renewal

Andy gives up secretary

Freddie and Stuart ready to be secretary

Nick to stay technical chair if not Mark will take it

VOTE : for technical chair

FOR = all ; AGAINST = none

VOTE : for Freddie and Stuart as secretary

FOR = all ; AGAINST = none

VOTE : for Pete as president

FOR = 1 ; AGAINST = none

Nick Hauser raised the point how to speed up adopting proposals. Thomas mentioned there is a lack of manpower. Therefore we need a simple web interface. Freddie suggested adding an upload page. Mark said put new proposals on the wiki. Send an email to the niac.

Andy raised the point that we need a manual. The current documentation is very techie oriented. There is no introduction for beginners. Ray said the wiki is the documentation. Pete Jemian suggested making full use of the wiki and the discussion page on the wiki. Mark said the problem is the wiki is not kept updated.

Conclusion – breakout group on how to organise wiki for users

Pete Petersons' talk - Trees

Pete gave a fascinating talk about trees and Nexus. 42 is the answer. In his vision Nexus would be machine validated in future versions (V2.1), object oriented definitions (V3.0) i.e. get rid of meta-DTD

Nick's talk - Meta-DTD vs. Schema

Schema are machine readable XML. How to generate the schema ? A small group of specialists will do this. Use a graphical schema editor. Easy to generate meta-DTD from schema. Tools – emacs, Eclipse + WTP, Netbeans are all free. General interest in using Eclipse + WTP and providing it as a web start. Jens showed his C++ tool for defining instruments. Thomas was convinced.

Proposal : canonical Nexus definitions to be stored in schema

Meta-dtd can be generated from these

Thomas – 3 action types – move to schema, explain tools,

Vote : Nexus meta-DTD to be moved to schema

FOR : all ; AGAINST : none

Mark use schema for V3.0 and object oriented

Vote : Version 3.0 will be schema based

Nick happy to manage this move with help others

What other formats should we support e.g. html, tables, uml

Mark's talk – Primer on Nexus and object oriented

Mark presented uml diagrams for the different base classes. Thomas said an Instrument definition is actually an experiment definition i.e. analysis-driven. Thomas suggested having multiple instrument classes stored for the same instrument stored in the same file e.g. GSAS class and Instrument class..

Nick presented NexusBeans as a Java technology. Ray said there is general agreement that an object oriented type api is the way to go.

Pete Petersons's talk – on URL's

URI – version, implementation version e.g.

<http://www.nexusformat.org/instruments/NXmonotas>

Laurent suggested do not include the version in the uri. Freddie wanted to have a url and uri.

imgCIF

A discussion ensued on imgCIF and what is happening in this field. Nick read an email from Bernstein. Freddie mentioned the imgCIF meeting in Manchester. There it was decided that the first step is to do an imgCIF to NX and back converter, Freddie and Bernstein will handle this. Stuart is our official contact with imgCIF.

netCDF

Nick gave a talk about netCDF. netCDF has a number of advantages e.g. gives array manipulation in Java. Nick proposes to promote netCDF within the Nexus community as a tool for reading and writing HDF5 in Nexus. netCDF have added support for Nexus. Mark said there are a lot of issues to consider, array manipulation of netCDF is an advantage, we need to discuss with netCDF team to see how far they can go to support us. Pete P. said there is a discussion on an Nxutility api. Nick said netCDF provides a memory object. Pete P. discussion is about an in memory data format. Ray needs a white paper with more information. Pete P. create a separate api based on netCDF. Nick noted if the NIAC adopts netCDF for internal data representation then this opens the way to sharing more code. Andy suggested to start sharing netCDF between a few institutes to gain more experience and then report back to the committee before making a general decision on whether to support netCDF or not.

Conclusion – more people to try out netCDF and bring this up again at the meeting

Nexus top level entry

Ray relayed a request from microscopists to have a top level entry which identifies Nexus files e.g. /nexus. Mark said we should invite someone from this community to discuss with us. NXEntry is an attribute and not a namespace. This could be done automatically by the napi. Nick said there was a problem with conformity and validation.

Laser community want to use Nexus

Laurent mentioned the laser community would like to use Nexus. Laurent will be the representative

Argonne Scattering and Imaging Institute

Ray gave a talk on the ASI² proposal. If it gets funding then would be largest investment by the DOE in software. Other communities are solving problems which are of interest to us, idea is to get these people on board. How should this group interact with the Nexus group ? ASI² could replace IPNS as institute. Pete Jemian proposed next NIAC to be held at Argonne

Improving Scientific efficiency at APS

Pete Jemian gave a talk on Improving Scientific Efficiency at APS. He showed the canonical Scientific Workflow Diagram – feedback is open loop at the moment. There is a working group

headed by Ken Evans. APS has created a Scientific Software Section for solving local challenges as opposed to the ASI² which is for grand challenges. The group consists of one person at present, it will grow in time. There is a pilot visualisation application with 1-ID. There is resistance to Java + Eclipse - Python is the lingua franca of scientists. This group could look after a Nexus person. Nick said the NIAC should endorse this position. The group is interested in helping the community.

Ray said we need funding for Nexus meetings. Thomas suggested this should be contributed by each institute.

Action : Pete P to talk to SNS to setup a fund for NexusBeans

Action : everyone to talk to their management on how much they can contribute to the fund

Action : everyone to send their Berlin trip costs to the secretaries

Action : Thomas to look into how much it costs to finance half a person

Next meeting candidates are :

- Argonne
- Australia (NOBUGS)
- SNS

Conclusion

- next NIAC meeting at NOBUGS
- 6 month meeting possibility at Argonne if ASI² is funded

25 September

There was a long discussion about breakout groups.

Nexus API OO

Mark gave a talk about the Nexus OO API. He made the following proposals :

- maintain file structure as a tree in memory
- larger data sets are left on file and retrieved or written on demand

- Nxclose, Nxflush serialise all changes to disk
- how to link items together ?
- what shall the shape of the Iterator class be ?
- how much leeway are implementors allowed ?

There was a counter proposal by Pete Peterson. A python api which uses the Nxfile as an object. Ray said this is not object oriented. Ray wants to add to NXData together. Pete is against building a Nexus scripting framework like Ray wants it. Pete P. said for python drop swig and write python binding by hand, return NumPy objects. Pete proposes to write zeroth level python binding – strings are python strings, scalars are python basic types (he has already done most of the work)

ACTION : Pete to do Python binding to NumPy

Ray will play with the Python binding to generate a library for manipulating Nexus data

ACTION : Ray to play with Python binding and make a proposal for manipulating Nexus data

Pete proposed code for C++ binding, supports void and std::vector put_slab()

Pete – current Java binding returns an object which has to be cast to the right type, Pete proposes to extend the api to return a typed type

ACTION : Freddie to add Pete's C++ binding to be added to Nexus source code distribution

Mark would like templates to be an option in the C++ binding

Pete would like to have doxygen comments in the C napi,

ACTION : Mark will add doxygen comments to napi.h

Mark proposed an IDL binding

ACTION : Freddie to add Mark's IDL binding to Nexus repository

TRAC items

Went through open items and closed those that could be.

Discussion on memory allocation in the NXU utility library

ACTION : Freddie to add a somebody user to TRAC backend

Could we add an external link to a non-Nexus file

Pete – should we write native bindings for Matlab, IDL, etc

Mark – no, NAPI is 3 to 4000 lines

Nxtranslate

Pete P. gave a talk on Nxtranslate, a plugin based system. All plugins are statically linked. Walked through test_simple.nxs example. SNS uses Nxtranslate. Freddie has developed a dynamic retriever which uses dynamic shared libraries.

HDF4

HDF4 to be marked as deprecated. New users should use only HDF5.

VOTE : all in favour of deprecating HDF4 i.e. do not add new features to NAPI for HDF4

FOR = all-2 ; AGAINST = 2 (Freddie + Steve)

ACTION : Freddie to put a How To on the wiki for Nxtranslate and other programs with links to the pdf and doxygen documentation

ACTION : Pete to propose an outline for a Nexus manual in docbook

ACTION : Freddie to look how to integrate this into the wiki

Long discussion about how to integrate the docbook into the wiki and include user comments. Frederic Picca suggested taking a look at asciidoc. Pete P comments should go on the wiki, changes on subversion.

NXGeometry

Mark presents simple coordinate system + polar coordinate system. Ray corrected Mark's notion of polar angle, Ray says polar angle should be defined wrt to beam direction (Z). Pete P. said do not call it theta or whatever, it should be called polar angle.

ACTION : Pete to dig out jpeg demonstrating NXGeometry

ACTION : document the McStas convention for coordinate transformation i.e. translate then rotate or vice versa – pick one

Jens wants to store only the information about the physical information concerning the detector. Pete P. said do consumer's need to calculate how to convert your Nxpositioners to scientific units e.g. HKL. Ray wants to add cylindrical coordinates.

VOTE : accept NXcone definition

FOR = all ; AGAINST = none

Nxarchive + Nxingest

Laurent Lerusse gave a talk on NXarchive and Nxingest. Some points he raised :

- do not archive multiple Nxentry, only archive metadata in first Nxentry
- this caused discussion about not enforcing one Nxentry per file, ICAT should be changed
- this is a limitation of ICAT
- Nxarchive is simply a definition i.e. what ICAT expects, and does not exist per se in the Nexus file

Event data in Nexus

Pete Peterson gave a talk on event data in Nexus and how SNS event data are being stored in Nexus

ACTION : Pete P to look at Root to see how they handle events

Nxextract – extracting data from Nexus at Soleil

Stephan Poirier gave a talk on a tool he has developed (Nxextract) which allows data to be extracted from Nexus files into almost any format. Some points raised :

- tool is called Nxextract
- allows data to be extracted from a Nexus file using a proprietary extraction language
- Pete P – would like a feature to do maths on extracted data
- why not use an existing scripting language

ACTION : Stephane to upload Nxextract to Nexus applications

- binding Nxextract to a scripting language is a new project

Flat Cone diffractometer

Jens gave a talk on Nexus and the Flat Cone diffractometer.

- Tvtueb a platform for analysing data from powder + flat cone diffractometer written in VC++ and MFC
- TVNexus is the new program for doing Reciprocal Space Explorer of Nexus files (similar to HDFView currently)
- TVNexus uses Win64 to be able to display large data sets > 4GB

NAPI is thread safe if you read/write to different files, but not if sharing the same Nxhandle in the different threads

Laurent – multiple Nxentry issue for archiving

- extended to support multiple Nxentries for indexing
- tools used to index data will not archive data if necessary items are not found
- killed run_number , replaced with entry_identifier as string

VOTE replace run_number with entry_identifier

FOR = ALL-1 ; AGAINST = 1 (Andy) ; ABSTAINED = 1 (Nick)

VOTE on NXarchive proposal

FOR = all ; AGAINST = none

ACTION : Laurent to get NXarchive information back to base class

ACTION : Nick to check the result with the schema

All changes must be reflected in the base class

Rainer Schneider's talk – STRAINET

- will make a proposal for STRAINET scanning Nexus format
- NIAC – would like to work with STRAINET and help them
- will start with powder definitions and then add missing tags needed by scanners

Breakout groups for Ccd's + Documentation

CCD

The breakout group for CCD's proposed adding the following to Nxdetector to accommodate CCD

- extended type to include “ccd, pixel, image plate, cmos”
- data_file
- flood
- flood_file
- dark
- dark_file
- spatial_distortion
- spatial_distortion_file

Discussion on whether Nxcharacterization would be more suitable. The flood, dark and spatial_distortion would be added as extra types of NXcharacterization. There can be multiple NXcharacterization entries with the NXdetector class. These would link to either another NXentry or external file. The data_file is added to NXdetector as an Nxnote. NXcharacterizations to be renamed to NXcharacterisation.

VOTE on CCD proposal

FOR = all ; AGAINST = none

Documentation

The breakout group on documentation reported the following :

- Use Docbook for user manuals, including
 1. introduction
 2. FAQ
 3. HowTo
 4. JPEGs of UML schema
- Doxygen for source code and API
- Schema in UML
- HTML version of docbook for wiki

Have a section for active discussions and an archive for closed discussions (which should be marked closed). Create a “DISCUSSION” namespace to restrict editing of these pages to NIAC members only. The “discussion” tab would be open for everyone to edit for all pages.

ACTION: Freddie Akeroyd to add voting to the wiki.

Creation of a document editorial review committee (with initial members Freddie Akeroyd, Peter Peterson, Ray Osborn, Nick Hauser, Laurent L, Stuart Campbell)

ACTION: Ray Osborn to provide the skeleton structure for the document editorial review committee.

VOTE to create a Definition Release Manager role.

(VOTE): YES:ALL (12) -

This required a 2/3 majority of all committee members as it is creating a new officer's post: as 12 of the 17 committee members were present and the vote was unanimous, this was achieved.

VOTE Nick Hauser to take this role.

(VOTE): YES:ALL (12)

A proposal for a definition change should be discussed on the wiki for a period of time (6 weeks to 6 months). After this a vote would be held to ratify the changes. These would then be committed to the trunk. Then it would be at the Definition Release Manager's discretion to create a release.

Meeting Closed.

APPENDIX 1 – Herbert Bernstein's email

----- Forwarded message -----

Date: Fri, 21 Sep 2007 01:37:27 -0400

From: Herbert J. Bernstein <yaya@bernstein-plus-sons.com>

To: Peter Turner <turner_p@chem.usyd.edu.au>

Cc: p.turner@chem.usyd.edu.au, message@arcib.org,

"Akeroyd, FA (Freddie)" <F.A.Akeroyd@rl.ac.uk>

Subject: Re: NIAC meeting (fwd)

Dear Peter,

Here is the current status.

cif2nx: I have been working on a conversion utility from CIF or CBF to a NeXus file, but with additional groups so all the CIF tags can have a home without colliding with the existing NeXus tags. The idea will be to then complete the cross-mapping of the CIF table-oriented structure to the NeXus tree structure using the NeXus API and then to prune out the duplications. So far I have the complete parse of the CIF data and the loading of the CIF dictionaries and am working on the following initial mapping:

Each CIF data block maps to group NXentry, with the name of the datablock prefixed by "NXcif_"

Each CIF category within a CIF data block maps to a new group NXcifcat (as a subgroup of NXentry) with the name of the CIF category prefixed by "NXcif_"

Each column within a CIF category maps in one of two ways depending on whether it contains any binary sections. If there are no binary sections, the entire column maps as a rank 2 data array with a column of the CIF data values as strings and a column of the CIF data types as strings. In this case the entire column is one NeXus data set with the name of the CIF column prefixed by "NXcif_". If there are binary sections, then instead of using one data set, a column is mapped to a new group NXcifcol that contains multiple arrays of whatever ranks fit the binary sections, and the data sets are given names consisting of the row number converted to a string and prefixed by NXcif_. (This is a rework of the approach to the handling of columns that I had been following in which each data item in a column was a separate data set to allow for the handling of binary section. I think this new mixed approach will provide a reasonable balance between performance and flexibility.)

Each CIF save frame within a CIF data block maps to a new group NXcifs (as a subgroup of NXentry). Each CIF category within a CIF save frame maps to the group NXcifcat (as a subgroup of NXcifs in this case) and then the columns are handled as above.

It would be nice if we could add the packed and byte offset compressions to the current list of NeXus compressions, but this is not critical.

I hope to have this first cut done and tested in a few more days, and then I will try to upload this phase to the NeXus repository under contrib. Freddie offered to handle the NeXus side of the code, but I seem to be getting along well with the API, so I will try to go a little further first.

Once that is done, the next step is to do the denormalization of the CIF categories, using the dictionary information that has been loaded to identify the cases in which tables in subcategories should be broken up

and moved under the parent items in the supercategories.

Finally, the last step will be to translate those CIF tags that match NeXus tags into the equivalent NeXus tags. Those that don't match would stay as CIF tags.

nx2cif: If the cif2nx works out the other direction should be a lot easier, since there are fewer NeXus tags than CIF tags. The biggest problem will be preserving the finer type details from NeXus on the CIF side.

binutf: G. Darakev is working on integrating binutf into the NeXus API. This will allow fairly efficient handling of NeXus binaries in XML.

Regards,
Herbert