Minutes of NeXus Committee (NIAC) meeting, ORNL, 7th and 8th October 2010-10-31

The meeting was preceded by a code camp on 5th and 6th October, also held at ORNL. There were 12 NIAC representatives present:

Freddie Akeroyd (ISIS neutron facility), Steve Cottrell (Muon community), Matthias Drochner (Forschungzentrum Jülich), Nick Hauser (ANSTO), Jens-Uwe Hoffmann (HZB), Pete Jemian (APS), Jiro Suzuki (J-PARC), Mark Koennecke (PSI), Peter Peterson (ORNL), Tobias Richter (Diamond Light Source), Armando Sole (ESRF), Benjamin Watts (Swiss Light Source)

After an introduction by Peter Peterson (current NIAC chairman), Mark Koennecke (technical committee chair) presented a review of NeXus developments since the last full NIAC meeting in 2008 and summarised items for discussion at the meeting. This talk is on the NIAC web pages (http://www.nexusformat.org/NIAC2010) and the main points covered were:

- New application/technique definitions produced since 2008

- New tools nxvalidate and nxplot developed since last NeXus code camp

- A list of definition related topics for later consideration at this NIAC e.g. NXsubentry, scaled data, event data

- Some of the work done at the recent code camp, such as adding thread safety to the NeXus API at the NXhandle level (HDF5 serialises all file access and so no increase in performance will probably be seen - for more performance we would need to look at parallel HDF5, but as this requires some API development work we need to ask community if the work is appropriate).

- Additions to the NeXus coordinate system to support imgCIF like axes

- The plan to ask for input from communities on application definitions

Other items raised for consideration at this meeting were:

- Steve Cottrell : ratification of updated muon nexus definition

- Ray Osborn: adding the python tree API to the distribution

- Nick Hauser asked if an NXDL tutorial could be given at the NIAC and how to do validation with the new NXvalidate program

- Ray Osborn asked whether the definitions and API releases should be linked together. At the moment they are kept separate as they develop at different rates, but with the NXvalidate program being part of the API tree they now have a dependency. This matter was discussed later.

ACTION: Freddie to look at merging svn definitions and code back together.

- Nick Hauser was interested in how many people were using the NeXus API or writing nexus compatible files using e.g. h5py

ACTION: do a poll at the NIAC (see Appendix A of these minutes)

ACTION: Improve documentation in the manual on how to write NeXus compatible files without using NeXus API

- Pete Jemian had been asked by his facility director how much file sharing was actually going on with NeXus.

ACTION: poll on where NeXus has enabled file exchange/sharing

- The question was raised about using a Wiki v Docbook for the documentation – this would be covered in a later discussion

- It was suggested that base classes might better be described as "component dictionaries" in the documentation

- Mark Koennecke reported that a NeXus for neutrons meeting would be held next year as part of PANDATA (http://www.pan-data.eu/) initiative – this would aim to obtain consensus on key neutron definitions

Committee Business

New facility members

- Vote for Ben Watts as new SLS representative – ALL in favour

Existing facility members who are about to expire

- Vote to renew Nick Hauser: ALL in favour

- Vote to renew Matthias Drochner: ALL in favour

- Vote to renew Peter Peterson: ALL in favour

New non-facility member

- Vote for Ray Osborn as a non-facility member on the NIAC: ALL in favour

Paul Kienzle, Emmanuel Farhi, Nick Maliszewskyj and Stephane Poirier were not present and will be contacted by the new NIAC secretary regarding their membership.

Nominations for committee posts

As full NIAC meetings only happen every 2 years, it was proposed to elect officers every 2 years at the time of full NIAC rather than yearly as now.

VOTE: to change term of office to 2 years for officers – ALL in favour

VOTE: constitution change to remove term limit for officers – 2 abstain, rest for ALL

The following nominations were received for committee posts:

- Chair: Mark Koennecke

- Secretary: Stuart Campbell

- Technical committee chair: Freddie Akeroyd

- Documentation release manager: Pete Jemian

VOTE: These were approved by the NIAC: 2 abstain, rest for

Discussions

Ray Osborn tabled the idea of independent funding for attending NIAC meetings as e.g. NIST representatives are often not able to come due to timing of meeting with different facility financial years. An issue with such schemes, however, is usually "who holds the money".

ACTION: Ray to look into NeXus subscription / how to hold money

Peter Peterson mentioned the NeXus technical committee teleconferences that happen roughly every two weeks as well as the yearly technical committee meetings. Nick Hauser commented that due to time zone issue it had been hard for him to participate (America/Europe/Australia results in awkward hours for either America or Australia)

ACTION: need to record these meetings better, maybe a podcast?

Pete Jemian demonstrated the NXDL language for writing definitions and the new Docbook documentation. Freddie Akeroyd then demonstrated using NXvalidate. The points raised were:

- We should try and get docbook documentation integrated into the wiki so people can comment on it – maybe convert it to wiki syntax or render html in a wiki page? The wiki has a talk section on each page which is good for comments

- NXDL: should use <dimensions rank=...> rather than <dimensions size= ...>

- NXDL: Having a wildcard for the name <NXlog name="temp*"> and maybe also more specific multiplicity

- Licence for documentation: example code is under LGPL, do docs under GNU FDL.
  VOTE : 1 abstain, rest for

Mark gave a talk on the NXsubentry proposal. There was then a discussion about whether "subentry" was the best name and other suggestions were: NXapplication, NXsubentry, NXentry, NXchildentry, NXview, NXdefinition. Ben volunteered to collate opinions and after making a presentation NXsubentry was agreed.

An NXmeasurement working group was also set up (Ben, Armando, Stuart) and reported back.
VOTE: NXcollection name preferred over NXmeasurement 1 against, 1 abstain, rest for

Scaled data: it was agreed to use an offset/ stride mechanism rather than direction/precedence to indicate array reading order. For scaling data, there was much discussion of how the parameters p0 etc. be used and a request to be able to combine transforms? Armando formed a working group to consider options and the final proposal was:

VOTE: develop an NXformula class using e.g. muParser syntax to describe a data transform. Implementing an automatic converter in the NeXus API would be considered.   1 abstain, 10 for

VOTE: Proposed addition of tags of "scalar","image" for dataset: 1 against, 10 for

VOTE: Addition of a deprecated attribute to NXDL, contents of which will be message saying what to use instead/advisory message. Deprecated, if present, cannot be an empty string (new xsd rule) – unanimous

At the moment official NeXus classes have an NX prefix, but unofficial ones can have any prefix. Should we suggest NXU for non-standard classes?
ACTION: defer to tech subcommittee for consideration

Other NeXus related work

Tobias: working on getting nexus package into Debian, epel, fedora; also on splitting out packages

Steve Cottrell: written Origin importer for nexus

Pedro: "Hdf explorer"   www.space-research.org and also   nxtraverse (now in the NeXus repository)

 Ray gave a talk on NeXpy which provides a powerful interface based on the NeXus python tree API. (see http://www.nexusformat.org/NeXpy) The python tree API will become part of the standard NeXus API; Peter and Ben have volunteered to maintain it

New definitions

New Muon nexus format proposed by Steve Cottrell (see http://www.nexusformat.org/images/3/3e/Elements_for_Muons.pdf for the elements voted on)

1) OK, but also to add to "definition field". All for, 2 abstains

2) OK, follow conventions to label axes from NXdata if required. Multidimensional > 2 allowed. 1 abstain, rest for.

3) Runlog -> NXcollection

4) Selog -> NXcollection

5) NXperiod – defer for now

6) NXdae – use NXcollection

7) NXbeamline - more components agreed, but not NXbeamline itself - suggested using "beamline attribute"; Freddie to check. Names for magnets reserved, but need to make NXDL for these, put into contrib and send to NIAC for consideration. Many of the magnet definitions were similar so it was asked why a single NXmagnet would not suffice? Steve Cottrell replied that there would be other fields to add in future to allow for e.g. simulations and these would ultimately make the definitions different

Ray: proposal for handling nexus errors. An "uncertainties" attribute to any numeric array, can be scalar or array of same length.
VOTE: 1 abstrain,rest for.
In the future may need to define an attribute to say if errors are poisson, Gaussian etc

Interpretation attribute - **???**

Coordinates attribute: vote in three weeks - probably need a number_vertices="" attribute as well

TOF event data -looking at changing some of the field names to make it more applicable to other techniques e.g. muons. Technical committee will make a proposal.

Image CIF axes extensions: proposal for meridional_angle and other items from Mark
VOTE: Abstain 2 rest for.
Using a transform field looked the most popular way of chaining translations/rotations

ACTION: tech committee to make a proposal discussing the options of NXdependency V transform field

Project plan:

- API release 4.3 with nxvalidate to go with NXDL 1.0 (base+app defs, xsd for nxdl) definitions

- Move to Cmake/cpack to ease cross platform build and installation

- Performance + thread optimisation of API

- Try and find somebody to travel around facilities talking to experts to get input on definitions and also raise awareness of nexus

- Manual and web site need to be closer and allow people to comment – see php.net help for example of user comments. Add blog box to pages? Maybe use a CMS? Joomla drupal

- Look at getting more money for NeXus

- Need to keep definable things list small to allow it to be achieved

Closing

Thank you to Stuart Campbell and Peter Peterson for hosting the meeting and to Peter Peterson for his work as chairman over the last few years

Appendix A: NeXus census on what is happening at facilities

At the NIAC meeting a poll was carried out on the current use of NeXus. Eight facilities were present, all using API 4.2 or better to some degree. However some were also producing nexus via other routes:

- SNS: writing nexus Xml from java

- ESRF: Hdf5 written using hypy and native hdf5 libraries

- APS: Native hdf5 used in image server program

- HZB: hdf4 libraries used directly in a department

Nexus reading

- The HDFview software is used by all

- IDL is used at SNS

- Peter Jemian reported that Raw hdf libraries in c++ are used at APS

- ISIS uses matlab for reading HDF5

- Armando reported that ESRF use h5py for reading NeXus files

- What programs can read other facility data? 7 facilities (sns, isis, esrf, diamond, aps, ansto,)

  - Mantid: (sns, isis)

  - Dave: (program written at nist, reads sns nexus)

  - Pymca: (esrf hdf5, diamond, soleil)

  - Edna : esrf(hdf5)

  - ISAW: (lujan nx, sns nx)

  - Open GENIE: (isis neutron + muon, sns, …)

  - IGOR PRO from nist : reads ansto nexus, nist ascii

  - LAMP: HZB nexus, ANSTO nexus

  - IDL, MATLAB – can read any HDF5 nexus file, but needs local interpretation of contents

  - GDA/SDA – reads diamond nexus, soleil nexus

  - Gumtree – reads ansto nexus, SINQ nexus

  - TVNeXus/Bean – read hzb nexus

- NeXpy: sns arcs nexus, isis neutron nexus

ACTION: People to upload example files from their facilities

ACTION: provide a NeXus -> NXDL converter to create a first-pass NXDL definition; this will provide a starting point for people already generating NeXus files.

Language binding usage for nexus:

- SNS using c, c++, java, python

- ISIS muons – fortran ,c

- J-PARC – nexus c api

- Diamond gda java, python

- SINQ C, c++, java, idl, python, tcl

- SLS: not at moment, but will use python

- HZB: c api

- ISIS neutron: C, c++, fortran

- Juelich: python

- ANSTO: netcdf, c napi

Operating systems

- SNS: rhel5, ubuntu, snow leopard, windows 7 64bit

- APS: Windows xp, windows 7, rhel5,solaris10

- ISIS: Open vms, linux, windows xp, windows 7, vista

- Diamond: redhat 32+64, windows xp, ubuntu

- J-PARC: ubuntu, redhat

- SLS: sl5, windows xp

- SINQ: macos10

- HZB: windows 2003 64 bit, vista, suse 32+64 bit

- Juelich: Fedora, ubuntu, netbsd

- ESRF rhel4 32bit, rhel5 64bit, ubuntu 10.04

- ANSTO suse 9.,10.x ubuntu 32bit 9.x 10.x windows xp