

NIAC2012

From NeXus

Planning is currently underway for the NIAC / Code Camp meeting in 2012. This is being organised to take place at The Cosner's House, Abingdon, UK (<http://www.stfc.ac.uk/About+STFC/44.aspx>) and occur prior to the NOBUGS meeting (<http://www.nobugsconference.org/>) .

Dates are:

- NeXus code camp -> 18th / 19th September 2012
- NIAC Meeting -> 20th / 21th September 2012

- NoBugs meeting (<http://www.nobugsconference.org/Conferences>) -> 24th-26th September 2012

Contents

- 1 Location and Accommodation
- 2 Travel
- 3 Logistics
- 4 List of Attendees
- 5 Agenda
 - 5.1 NeXus Code Camp
 - 5.2 NIAC Meeting
- 6 Meeting Minutes

Location and Accommodation

The Cosner's House, Abingdon, UK (<http://www.stfc.ac.uk/About+STFC/44.aspx>)

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Science and Technology Facilities Council
The Cosener's House
Abbey Close
Abingdon
Oxfordshire
OX14 3JD
United Kingdom
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The fee of £200 per event covers two nights accommodation and all meals during the days - see Logistics below

Registration is via the NOBUGS conference website
(<http://www.nobugs2012.org/NOBUGS/registration/NeXus.html>)

Travel

If arriving at Heathrow, take the Oxford "airline" bus (http://www.oxfordbus.co.uk/main.php?page_id=24) , but get off at the penultimate stop St Aldates (<http://www.oxfordbus.co.uk/content/img/cms/wtboxfordmap2100512.jpg>) rather than Oxford bus station. Public transport to Abingdon leaves from St Aldates (<http://www.oxfordbus.co.uk/content/doc/cms/CityCentre%20120212.pdf>) either Oxford bus company buses 35 or X3 (http://www.oxfordbus.co.uk/main.php?page_id=21) or Thames travel bus X2 (<http://www.thames-travel.co.uk/timetables.htm>) get off at the Vineyard or Stratton Way and walk to Coseners house (<http://www.stfc.ac.uk/About+STFC/44.aspx>)

If you are arriving later and wish to take a taxi/minicab from Oxford to Coseners House, there is a taxi rank at the final Oxford "airline" stop (Gloucester Green coach station). More information about taxi/minicab services in Oxford are on this page (http://www.oxford.gov.uk/PageRender/decTS/Public_transport_occw.htm) .

Logistics

People arriving for the NIAC and staying on for NOBUGS conference the following week at RAL (<http://www.stfc.ac.uk/About+STFC/51.aspx%7C>) can keep their rooms in Cosner's. Daily transport will be available to and from the NOBUGS venue at the RAL site.

The meeting fee for NIAC/Nexus code camp is the Coseners house 24 hour delegate rate, which covers Dinner, B+B, plus lunch. So:

- the code camp fee will cover dinner on Monday and Tuesday evenings, 2 nights accommodation, breakfast+lunch on Tuesday and Wednesday.
- the NIAC fee will cover dinner on Wednesday and Thursday evenings, 2 night accommodation, breakfast+lunch on Thursday and Friday.

If you will be staying Friday evening (and onwards) you need to reserve and pay for this separately yourself with Coseners house (<http://www.nobugs2012.org/NOBUGS/accommodation.html>)

List of Attendees

Please add your name to this table after registering for the meetings via the NOBUGS site (<http://www.nobugs2012.org/NOBUGS/registration/NeXus.html>)

Name	Company/Institute	Code Camp (18/19)	NIAC (20/21)	NOBUGS (24-26)	Arrival date (accommodation needed from)	Departure date
Freddie Akeroyd	ISIS Facility, Rutherford Appleton Laboratory, UK	YES	YES	YES	Day attendee	Day attendee
Tobias Richter	Diamond Light Source, UK	YES	YES	YES	Day attendee	Day attendee
Steve Cottrell	ISIS Facility, Rutherford	NO	YES	YES	Day attendee	Day

	Appleton Laboratory, UK					attendee
Ben Watts	Swiss Light Source, Paul Scherrer Institut, Switzerland	YES	YES	NO	18/09/2012	22/09/2012
Jiro Suzuki	J-PARC, KEK, Japan	NO	YES	YES	19/09/2012	
Joachim Wuttke	JCNS at FRM II	NO	YES	YES	19/09/2012	
Mark Koennecke	Paul Scherrer Institute, Switzerland	YES	YES	YES	17/09/2012	
Jens-Uwe Hoffmann	Helmholtz-Zentrum Berlin	YES	YES	YES	18/09/2012	
Eugen Wintersberger	DESY	YES	YES	YES	17/09/2012	
Herbert J Bernstein	Dowling College, USA	NO	YES	YES (24th)	19/09/2012	21/09/2012
Fajin Yuan	Diamond Light Source	YES	YES	YES	Day attendee	Day attendee
Graeme Winter	Diamond Light Source	YES (19th)	YES (20th)	NO	Day attendee	Day attendee
David Mannicke	ANSTO	YES	YES	YES	17/09/2012	27/09/2012
Peter Peterson	SNS, ORNL, USA	NO	YES	YES	19/09/2012	27/09/2012
Armando Sole	ESRF	NO	YES	NO	19/09/2012	22/09/2012
Pete Jemian	APS	Skype	Skype	NO	2012-09-18 (Skype only, no lodgingrequired)	2012-09-21



Pete Jemian's physical avatar at the meeting

Agenda

Both meetings are taking place in the Hamilton room at Coseners house, starting at 9am. Evening meal is scheduled for 7pm each day

NeXus Code Camp

The code camp allows existing NeXus developers to meet and work together on developing software or resolving particular NeXus design issues. A preliminary list of items is listed below, but the exact subset is decided on the first day of the meeting.

- Finish CIF coordinate issue
- PyTree API Tests
- Cleanup NeXus applications
- NXdict replacement design
- Automatisation and documentation of NeXus release process
 - Implement Continuous Integration
 - Write more unit tests
- Change documentation from DocBook to Restructured Text (Sphinx)
(<http://download.nexusformat.org/sphinx/>)
- Cleanup trac-tickets
- Discuss timed data
- Develop a materials definition to present to NIAC
- Do we switch to CMake for all builds?
- How to integrate sphinx documentation building into Cmake

NIAC Meeting

This is a meeting for members of the NeXus International Advisory committee and other interested persons. It generally discusses matters of policy and strategy, but can discuss specific NeXus instrument definitions if the relevant experts are in attendance.

- Report on the status of NeXus and Overview
- Voting officers
- Strategy discussion: Where do we go with NeXus?
- Develop and ratify material definition for samples and sensors
- Roadmap to OO-NeXus
- Review of DECTRIS additions to NXdetector
- Review of added synchrotron beamline base classes
- Will the tech committee be allowed decide on fields and base classes?

Meeting Minutes

Date: 20 Sept 2012

Attendees:

- Mark Koennecke, SING
- Fred Akeroyd, RAL
- Tobias Richter, Diamond
- Peter Peterson, SNS
- David Mannicke, ANSTO
- Armando Sole, ESRF
- Herbert Bernstein, imgCIF
- Jiro Suzuki, JPARC
- Joachim Wuttke, FRM and JCNS
- Ben Watts, SLS
- Eugen Wintersberger, DESY
- Jen-Uwe Hoffmann, HMI
- Steve Cottrell, Diamond
- Graeme Winter, Diamond
- Pete Jemian, APS (via Skype)

- introductions
- Recap NeXus and recent developments
 - Previous meeting
 - NXsubentry and NXcollection classes
 - Support for CIF style coordinates
 - Non C-storage order arrays: offset, stride attributes
 - Python Tree API part of API

- HDRI: High Data Rate Initiative making something NeXus-like
 - Asked to revise synchrotron base classes
 - Eugen: software to write files is nearly ready and implementation will be installed at as many beamlines as possible in the Dec shutdown
- PANDATA
 - NeXus at first well received
 - made plans for method-specific formats

- Dormant
- 2011 Code Camp in APS
 - NX_unlimited for all dimensions
 - 64 bit dimensions
 - update to HDF5-1.8
 - Doc updates. now reasonable up to date and understandable.
 - WWW-site from manual
 - tests for python API 30% complete
 - Python Tree API cleaned up
 - Parallel HDF deemed not useful for NeXus because performance limited systems don't want any extras
- DECTRIS collaboration (Pilatus and Eiger manufacturer)
 - NeXus/HDF5 for Eiger
 - Add extra fields for detector parameters
 - write sets of ~10,000 images into separate files (workaround for data rate issues and HDF5 doesn't allow sections of same data group in different files)
 - write with compression (5-10GB/s data rates!!!)
- How much can we compromise with DECTRIS
 - Tool to convert data to standard HDF5 (they are using non-standard compression)
- HDF5 workshop at PSI
 - DECTRIS (DESY) pays for writing pre-compressed chunks and compression plugins
- HDF5 new features
 - Asynchronous IO
 - Journaling
 - Single writer, multiple reader semantics
 - better fault tolerance
 - in-memory HDF5 files (very fast writing)
 - shared object headers
- HDF5 intended features
 - better multi-threading
 - virtual object layer, completely replaces storage layer
 - can use HDF5 data model without the file formats
 - allows more storage models
 - metadata server for better parallel support
 - mirroring, stacking
 - better parallel support
- NAPI release 4.3, Application defs 3.1
 - features from 2011 code camp
 - preparing packages in linux repos
- code camp 2012
 - move docs to sphinx
 - more wiki-like syntax - easier!
 - URL: ?? (bug in build process, so not quite ready yet)
 - cleaned up trac tickets
 - drop autoconf for CMake
 - Resolved CIF coordinate issue
 - good suggestion for handling axes of multidimensional data sets
 - cleanup of applications: nx2dtd, NXdump, ... dropped
- Topics for NIAC 2012
 - Quo vadis

- roadmap OO
- CIF coordinates
- process for changing base classes
- review synchrotron classes
- review addition to NXdetector
- Materials defs
- Multi-D array axes encoding
- what to do about expired NIAC members?
- Elect new officers
- Questions from code camp
 - anyone using NXcharacterisation?
 - who is using F77 API?
 - do we get into timed data?
- discuss priorities (reordered below in descending priority)
 - Elect new officers (defer by 1 day to allow newcomers to get to know others)
 - Quo vadis
 - CIF coordinates
 - roadmap OO
 - Multi-D array axes encoding
 - Materials defs
 - what to do about expired NIAC members?
 - questions from code camp
 - anyone using NXcharacterisation?
 - who is using F77 API?
 - do we get into timed data?
 - DECTRIS meeting
 - process for changing base classes
 - review synchrotron classes
 - review addition to NXdetector
- CIF revisit (MK presents CIF and options for adaptation to NeXus)
 - Options:
 - NXdependency group
 - depends_on attribute (tech committee preferred and recommended by HB)
 - make vector mandatory and add offset_unit
 - HB will push CIF to make gravity declaration mandatory to ensure mapping between CIF and NeXus coords is possible

Motion to accept CIF-style angle descriptions with discussed additions.
 Vote: for 9 against 0, abstain 4

Coffee break

- Quo Vadis
 - Intro by Mark
 - existence since 1996 and uptake is slow
 - Do we persist in the same manner or change our ways?
 - Others often reinvent NeXus
 - New instruments often implement NeXus

- results of survey are surprisingly positive with more NeXus implementations than expected
- New developments:
 - Dictionary Based Programming Techniques - Common Data Model (CDM)
 - Tree Based Programming
 - Requirements for data formats changing
 - disks are cheap
 - full logging becomes possible
 - data rates are very high in some cases
- Discussion

AS: ESRF advocate dictionary/HDF5 and just use the few parts of NeXus they want and ignore the rest (very pragmatic view).

TR: Need to take larger view and not get tied up in technical details. need to engage with facilities using NeXus (eg ALBA).

BW: Need to emphasise community involvement - dictating standards is historical problem of creating an example to start with.

JW: What is NeXus, is it something interchangeable? Have we been truthful about what it can achieve? I have no problem in maintaining tools to convert data to whatever format the users ask for.

JH: Users want physical meaning for the data recorded, not just numbers whose meaning is obscured by instrument details. But to understand the instrument, also need more raw values.

MK: Different use cases; 1. understanding instrument (raw values), 2. exchange/data analysis (physical)

GW: Standard has value if I can read and understand a file without any further information. As soon as you move away from that, it becomes a huge problem to support the variants.

HB: Seen 2 issues; dictionary of names and format. People can use any format and you have no control anyway. The only thing you need is that every uses a common vocabulary. vocabularies tend to merge. separate vocab and application definitions.

FA: if we concentrate app defs and vocab, then we are working towards standards, tools are not required (there are plenty available). People are choosing HDF5, help them come together and talk.

GW: data rates are a problem - HDF5 are needed. Don't want to have facility-specific dialects of NeXus. Need consistence and completeness (single file).

AS: performance issues get in the way of a single file, multiple files must be acceptable.

GW: don't water it down - all or nothing!

EW: I tried to invent better than NeXus but failed. Users just want basic data, but beamline scientist want to record everything in order to know what the instrument is actually doing. Sometimes will need to correct for strange instrument behavior that requires info not normally needed by users. Making this general enough to use at more than one beamline quickly leads to something NeXus-like.

HB: Offer - if you can agree on your vocab, I'll give you an IUCr working group for adopting/working on

your dictionary. I.e. CIF and NeXus join forces!

JW: I support this. Clarity would help me. vocab is valuable to me, but formats are minor technical details.

EW: Important thing is to make entry to Nexus easy. Some instruments are unique and we don't have to worry about them. OO can help us define terms.

HB: we use "prefixes" for namespaces, but are considering using general XML. want to make sure terms don't conflict.

PJ: have image that NeXus legislates, but we should put out message that we want to collaborate to reduce conflicts.

MK: make an action that we concentrate on dictionaries and appl defs.

GW: ImageCIF has good library that does a lot of work for me. It would be easier to persuade people to use Nexus if we had the same kind of library - part of analysis work is done by the library.

HB: maintaining libraries will get done if there is adoption.

GW: If we can get Nexus routines included in CBFLib, then my work becomes much easier. analysis program writers will not resist.

Everyone agrees that moving CIF and NeXus closer would be great.

HB: CIF will make addition docs for IUCr people and will put a link to NeXus doc from the IUCr website.

MK and HB: lets arrange a meeting between NIAC and IUCr to discuss cooperation.

GW and SC: want to make sure that IUCr don't steamroll vocabularies of other communities

MK: Can we put NAPI into maintenance mode?

PP: what is status of validation tool?

FA: GUI tool works and I have used it, waiting for colleague to finish CLI tool

FA + HB: cooperation on validation tools could be useful. NeXus backend for CBFLib validation tool is possible.

MK: break for lunch and after lunch we will try to bring the discussion to a close.

Lunch break

- NeXus guiding statements:
 - The main focus of the NeXus community is to further develop the dictionaries, base classes and application definitions.
 - The NIAC is a forum for resolving issues.
 - The NIAC acts as a custodian for NeXus: definitions, examples, documentation, reference implementations.
 - NeXus can be mapped to different physical file formats:

- HDF5 is the preferred physical file format.
- NeXus-XML is the currently supported ASCII file format.

Motion to accept above statements.
 vote: for 8, against 1, abstain 0

- We should put together a wish-list of features to forward to the HDF group
- Statements/promises:
 - NAPI and applications are considered stable
 - The use of NAPI is not mandatory and examples using HDF5 APIs will be provided
 - The validation tool is actively developed

Motion to accept above statements.
 vote: for 12, against 0, abstain 1

- We seek cooperation with IUCr and CIF
 - Have a meeting with them to figure out what this means
 - Maybe have another NIAC next year to agree on this (in conjunction with ECM)
 - MK volunteers to take a lead
 - We encourage the inclusion of NeXus into CBFlib
- We invest into cleaning up NeXus, remove outdated, old or broken stuff
- We invest into documenting NeXus better through bringing inheritance or composition to NeXus base classes

Motion to support above commitments.
 vote for 14

Coffee break

- What do we do in terms of advocating NeXus?
 - Persue new facilities? existing instruments? Analysis/reduction software?
 - Support users and program writers on the mailing lists
 - NeXus-developers merged into NeXus mailing list
 - Approach facilities using NeXus but not represented in the NIAC and encourage them to nominate new NIAC candidates.

Motion to elect HB into NIAC as the CIF representative.
 vote for 14, against 0

- AS: proposes flattening the heirarchy in NeXus files.
 - What he really means is that the NXxas application appears to require links to specific locations and he wants the application definition to be simpler.

Motion to allow application definitions to be flat and simple (not implement the full instrument
 vote: for 12, against 2, abstain 1.

- ■ We recommend to use the NeXus heirarchy in application definitions, but we do accept application definitions with a flattened hierarchy.
- heading on web page is wrong: "NeXus Application Classes" --> "NeXus Application Definitions" in <http://download.nexusformat.org/doc/html/ClassDefinitions.html>
- Who is using NXcharacterisation?
 - PP added it but isn't using it because icat is better.
 - We deprecate it
- continue support for the F77 API?
 - don't expend effort on it, but don't throw it away either.
- Examined NXarpes application definition
 - suggest talking to someone using a toroidal analyser
 - minor corrections pointed out.
- ■ ■ END DAY ***

21 Sept 2012

- Elect new officers

Motion to elect MK as Chairman
 vote - for for 13, against 0, abstain 1

Motion to elect TR as Executive Secretary
 vote - for for 13, against 0, abstain 1

Motion to elect FA as Technical Chair
 vote - for 13, against 0, abstain 1

Motion to elect PJ as Documentation Chair (PJ notes that his travel will be very limited)
 vote - for for 14, against 0, abstain 0

- PJ presents the new sphinx-generated documentation, using the draft currently available at: <http://download.nexusformat.org/sphinx/>
 - Looks nicer
 - not everything works currently, but can be fixed - no apparent show-stoppers.
 - cannot easily have automatic numbering of figures is biggest disadvantage
 - MK, FA: that's OK, we can drop it.
- Roadmap to object oriented (OO) NeXus
 - base classes would be OO with some kind of inheritance
 - this would make the base classes clearer to users

Motion to investigate possible technical implementations of NeXus with object oriented base classes
 vote: for 12, against 1, abstain 0

- Multidimensional axes proposal from TR
 - use of @signal=I is easily confused with signal=1 (position is different though).
 - suggest changing name
 - How many multiple competing versions do we want to encourage/support/allow?
 - How many plots should be put into each NXdata?

Motion to move signal and axes attributes into NXdata group attributes.
 vote - for 12, against 0, abstain 2

Motion to accept as a possible solution and invite TR to present sample implementations.
 vote - for 12, against 1, abstain 1

Coffee Break

- DECTRIS
 - HDF5 doesn't support parallel writing with compression - need a workaround!
 - write a master file (with metadata) with links to separate files for data (with ~10,000 images in each).
 - want to use non-standard compression (not distributed with mainline HDF5 libraries)
 - comment from code camp: ask for tool to convert to HDF5 standard compression.
 - Meeting with DECTRIS and customers in October - who wants to attend? MK

FA: maybe use detector bank approach?

EW: split file drive approach would work better.

HB & MK: this is a bug in HDF5, but DECTRIS can't wait for it to be fixed (years)

EW: are they using the most recent version; performance problems before 1.8.6

HB: they are and plan to ship with 1.8.10

Motion to work as closely as possible with this community to get this under NeXus.
 vote - for all.

- BW presents mechanism for verifying communities and resolving conflicts
 - good idea and will keep in mind but do not want to consider implementing until a real need arises.
- Process for ratifying changes to NeXus classes.
 - waiting for the NIAC to meet makes changes slow.
 - minor changes can waste time at NIAC meetings.
 - allow non-breaking changes to base classes, etc to be ratified via mailing lists?

Motion: Changes to base classes must be ratified tech committee and put on the nexus mailing list
vote - for 12

- Do we investigate better ways to record "timed data"
 - NXlog mostly works, but probably not optimal
 - HB: Verner Banger is collaborating with the HDF group on this topic - should look at his work

BW: It would be nice if we could have option items in application definitions

PP: Already can! you just set the "minimum required" attribute to zero.

Lunch Break

- Materials definition (samples, filters, multilayers)
 - Tech committee suggest just using a descriptive string
 - HB: look at protein data base and see what they are doing. follow community standards where they exist
 - EW: infinite levels of detail makes it impossible to standardise. Maybe use application definitions for community specific materials descriptions.
 - NXsample already has "chemical formula" (using CIF conventions), "description"
 - we would be open to suggestions from the community
- Time based data
 - event streams need to be time-stamped and correlated

EW: NXlog is fine if you have single values with time stamps. how to handle detectors?

MK: You need to have a sufficiently precise timing system that all the computers have access to.

AS: Market is maturing, let's wait and see what works in the community

PP: why not just let time be an independent variable?

MK: people will want to know which things need to be correlated.

Motion to ask tech committee to investigate possible solutions to recommend to users.
vote - for 12, against 0, abstain 1

- Interaction with HDF group?
 - we should try, but we don't know if we have leverage to motivate them to pay attention

EW: spoke to Heiner Billich: facilities should get together to make requests and pool funding - but should NeXus be part of this effort?

MK: NIAC might not be a good representative for that activity, this is beyond the scope of NIAC.

HB: Should make polite contact and say that we want HDF5 to work well - what can we do to help? What does the HDF group want the interaction with NIAC to be? NeXus should encourage the discussion.

Motion to support AS to open discussion with the HDF group on behalf of the NIAC.
 vote - for 12, against 0, abstain 1

- Examples of NeXus data files following application definitions.

PP: we wrote application definitions to match our files, so I have some.

JW: is it working? why are there so few compliant examples?

MK: It has taken some time to solidify a base to begin testing compliance

HB: we have driving force from facilities

BW: A code camp activity could be to generate example files for a new instrument.

Promises to supply valid example files:

- MK: 6-10
- PP, FA: 3
- SC: 1
- TR: 2

- Advocacy?
 - Not yet ready - need to examine files currently being generated for consistency. Need to clarify what we recommend.
 - We invite the community to write application definitions as a way of planning towards a standard, even if they don't intend to switch yet.
- Optional fields in application definitions?
 - while it is already possible, we clarify that we want it.

Motion to confirm that the feature allowing optional fields in application definitions is endorsed
 vote - for all

FA: is there a way to have the presence of one tag be dependent on the presence of another? TR thinks so.

Coffee break

- NXdetector additions for DECTRIS
 - "exposure_time" seems unlikely to be correct. "acquisition_time" is probably better. NXdetector already has "count_time".
 - typos
 - BW volunteers to discuss the subtleties of the words they want to use for the attributes
 - threshold_energy should be type NX_ENERGY
 - _time attributes should be type NX_TIME

Motion to encourage use of these attributes, with the corrections discussed.
 vote - for 12, against 0, abstain 1

- NXbending_magnet
 - Gerd Wellenreuther proposed attribute names. BW should discuss with him and sort out issues (specifically source_distance_x and __y)
 - BW to better document accepted_photon_beam_divergence (does it overlap with the divergence_x_minus etc?)
 - divergence attributes overlap - slight preference for a single array over multiple scalar attributes.
- NXcapillary
 - needs "material" attribute
 - need better documentation of "gain" and "transmission"
 - model should be included in the "manufacturer" string - add doc to explain
- NXinsertion_device
 - should "taper" be an NX_LENGTH or an NX_ANGLE
 - can we change "k" to "k_parameter" in order to avoid single-character names?
 - add "period" attribute, or rename "magnetic_wavelength"
 - verify with Gerd Wellenreuther
- NXxraylens
 - rename as "NXxray_refractive_lens" for descriptiveness and consistency
 - "aperture" doc to specify diameter only
 - correct lens_geometry options
 - Put to an expert because we don't have time/expertise
- Term limits of Chairman and Secretary
 - currently limited to 3 years
 - problem if terms end between major meetings
 - want to make it more likely that term limits occur at full NIAC meetings

Motion to set the term length to 2 years and the limit for executive officers as two terms.
vote for 11, against 0, abstain 0

Meeting End

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