
# NIAC Meeting 2014

Review
&
Topics

# Not the Tech Committee

Have Been Busy

# What was done since 2012?

- MX application definition together with COMCIFS
  - actual application definition
  - NXtransformations
  - variants
  - To be ratified
- NXpinhole and NXslit

- Lots of work on the manual (thanks Joachim, Pete)
- Moved to github
- New NeXus publication (Journal for Applied Crystallography)
  - ACCEPTED as of yesterday!
- Code Camp 2014

# NXpinhole and NXslit

Because NXaperture is to complex

**NXpinhole:group**
- **depends_on**
- **diameter**

**NXslit:group**
- **depends_on**
- **x_gap**
- **y_gap**

Add fields to position

# Moved repository to github

- Git is the cool version control system of today
- Rely less on infrastructure at ISIS
- https://github.com/nexusformat/definitions
- https://github.com/nexusformat/code
- https://github.com/nexusformat/communications

# News from the Code Camp

- The NAPI configuration will be revised to drop most utilities and build for HDF-5 only by default
- New tool: nexpy based on h5py by Ray Osborn et al.
  - pip install nexpy
- The validation tool will be rebuilt.
  - In python, based or Ray Osborns nexpy
  - In ANSII-C
- We prepared many pending things for ratification

# Pending Ratifications

- NXmx + NXtransformations
- Associating axes with data
- Annotating errors
- NXformula
- Changes to NXfluo
- sequence_index in NXprocess, NXnote
- OS Thumbnail storage in special NXnote
- Finding default data
- NXstxm
- Reserve name „features“ for an experimental way of detailing groups
- Allow optional content in application definitions

# Further NIAC Topics

- Deprecate old positioning schemes
- Procedural questions
- Confirm new members
- Elect new officers
- Minor constitution change
  - change wording of "instrument and group class definitions" to contemporary terms (base classes and instrument definitions)

# MX Application Definition (1)

- Meeting with COMCIFS, august 2013
  - Data rates of modern detectors asks for a container format
  - Why not HDF5/NeXus?
  - Collaboration agreed upon
  - First MX, other application definitions may be later
- An application definition for MX was developed, mainly at Diamond
- CIF <—> NeXus works, DA too
- CBFlib support
- Thanks to: Jonathan Sloan, Graeme Winter, Tobias Richter, Herbert Bernstein
- Paper to be submitted soon

# MX Application Definition (2)

- Two new concepts:
  - variants
  - NXtransformations
- Some additional fields
- Rest is well known NeXus

# Variants

- The Problem: CIF had the capability to store variants of the same field.
  - Example: wavelength, refined_wavelength, guessed_wavelength
- Intense Discussion how to do this in NeXus
- Our Solution:
  - variants chain

```
distance
    @variant=distance_from_reading
distance_from_reading
    @variant=distance_as_guessed_by_cleaner
distance_as_guessed_by_cleaner
```

# NXtransformations

- NXtransformations stores
  - All axes needed to move a component into its place with the CIF coordinate style attributes
  - A depends_on field
- One stop group to locate all transformations necessary for a given component

- Rationale: the PX do not like to standardize on names; this solution is name independent
- This is a compromise to accomodate CIF
- But useful beyond NXmx

# NXtransformations example

```
sample:NXsample
    transform:NXtransformations
            rotation_angle
              @transformation_type=rotation
              @vector=0,1,0
              @offset=0,0,0,
            chi
              @transformation_type=rotation
              @vector=0,0,1
              @offset=0,0,0,
              @depends_on=rotation_angle
            phi
              @transformation_type=rotation
              @vector=0,1,0
              @offset=0,0,0,
              @depends_on=chi
            depends_on
              phi
```

http://download.nexusformat.org/doc/html/classes/contributed_definitions/NXtransformations.html

# NXmx definition

NXentry
- title
- definition
- NXinstrument
  - NXattenuator
    - attenuator_transmission
  - NXdetector
    - depends_on
    - NXtransformations
    - NXcollection
    - data[np,i,j]
- NXsample
  - name
  - NXbeam
    - incident_wavelength
  - NXtransformations
- NXdata

http://download.nexusformat.org/doc/html/classes/contributed_definitions/NXmx.html

# Deprecate Old Positioning

- Deprecate old coordinate system stuff
- Currently valid NeXus positioning schemes
  - CIF style
  - NXgeometry
  - polar coordinate system : polar_angle, azimuthal_angle

# Errors and Axes

- As of now we have error fields in some base classes
  - A more general scheme is required
- Associating axes with data
  - axes attribute on data
  - axis attribute on axis data
  - Falls over in some use cases
- Proposal derived from canSAS discussions
- http://wiki.nexusformat.org/2014_axes_and_uncertainties

# More Ratifications

- Ratification of classes
  - NXfluo: http://download.nexusformat.org/doc/html/classes/applications/NXfluo.html
  - NXarpes: http://download.nexusformat.org/doc/html/classes/contributed_definitions/NXarpes.html
  - NXstxm:
  - Review beam line stuff in contributed definitions

# NXformula

- Describe relationships in data files
- Last state from Telcos, based on Bens suggestion:
- NXformula
  - formula = A = B*c
  - A = link to some data item
  - B = link to some data item
  - c = 27.8
- Use muParser syntax
- Documentation only, implementation is not our business

# Sequence_numbers & optional content

- Optional fields in application definitions
  - Now: application definitions: required fields only
  - overwhelming community demand: optional fields
- Sequence_numbers
  - Processed data: the order of processing steps matters
  - NOW: only by naming scheme
  - Proposal: add sequence_index field to NXprocess and NXnote

# Finding Default Data to Plot

- Now: search NXdata, attribute signal=1
- Proposed:
  - add default attribute pointing to the NXentry at file level
  - add default attribute at NXentry level pointing to the good NXdata
  - use signal attribute to NXdata(agreed)

# Thumbnail

- Requirement: store a thumbnail and provenance data in some defined field for the OS to display

- NXnote does what we need

- Proposal: a NXnote named thumbnail at NXroot level.

# Feature Proposal

- Tobias

# NeXus Interfaces

- Motivation
  - Taming the NXdetector monster of ~60 defined fields
  - Remove repetition of often used fields in base class, for example positioning fields
- Why not OO?
  - NeXus not really OO: no associated methods
  - Inheritance not easily encodable in NeXus files
    - Base class explosion: NXarea_detector, NXsingle_detector, ……
- Use composition: implement interfaces
- Change  NXdetector and other base classes to implement one or more Interfaces:
  - NXIFbeamline_component, NXIFarea_detector, NXIFarea_tof_detector, …
- Tech Committee: experimental section in manual to try this out

# NIAC Process

- NeXus Processes
  - How do we assign priorities?
  - How do we deal with companies?
  - How do we remove NeXus ballast?
  - How to organize proposals and discussions?
  - NeXus as ISO standard?
  - Funding

# Code Camp Procedures Discussion

- Priorities:
  - Roberts's Rule
  - Chairman decides Agenda
    - Agenda can be challenged
- External companies
  - Invite as observers

# NeXus Funding

- Possible sources:
  - Facility contributions
  - Detector vendors
  - Foundation
  - Research Data Alliance
  - IUCR
  - A sponsor

# NeXus Business Plan

- Purpose: Develop the NeXus standard
  - Tutorial and dissemination activites
  - If we get a person:
    - Maintain NeXus
    - Develop tools
    - Go out and help facilities and DA SW writers with implementing NeXus
- NIAC Meetings

# More Procedures

- Better oversight
  - Invite users
  - Invite DA SW writers
- Do better work: wherever we meet, develop an application definition with an interested scientist
- More frequent NIAC meetings by Telco
- Do we want to become an ISO standard?