# **Minutes of the NeXus International Advisory Committee** Meeting in Pasadena, CA Sept. 8-10, 2003

## In attendance:

Michael Aivazis (Cal Tech, USA) aivazis@caltech.edu Frederick Akeroyd (ISIS, UK) freddie.akeroyd@rl.ac.uk Joern Beckmann (FRM-II, Germany) ioern.beckmann@frm2.tum.de

Stephen Cottrell (ISIS, UK) s.p.cottrell@rl.ac.uk Mathieu Doucet (NCNR, USA) doucet@nist.gov Ron Ghosh (ILL, France) ron@ill.fr

Nick Hauser (ANSTO, Australia) nha@ansto.gov.au Jason Hodges (SNS, USA) hodges@anl.gov Tim Kelly (Cal Tech, USA) tkellev@caltech.edu Paul Kienzle (NCNR, USA) pkienzle@nist.gov przemek@nist.gov Przemek Klosowski (NCNR, USA) Mark Koennecke (PSI, Switzerland) mark.koennecke@psi.ch

Nicholas Maliszewskyj (NCNR, USA) nickm@nist.gov

Michael McKerns (Cal Tech, USA) mmckerns@caltech.edu

Ray Osborn (IPNS, USA) rosborn@anl.gov Toshiya Otomo (KENS, Japan) toshiya.otomoto@kek.jp petersonpf@ornl.gov Peter Peterson (SNS, USA) tproffen@lanl.gov Thomas Proffen (MLNSC, USA)

# Members of the NeXus International Advisory Committee (NIAC):

Frederick Akeroyd Joern Beckmann Stephen Cottrell Ron Ghosh Nick Hauser Jason Hodges Przemek Klosowski Mark Koennecke Ray Osborn (Chair) Toshiva Otomo Peter Peterson (Executive Secretary) Thomas Proffen

# Members of the Technical Special Interest Group:

Frederick Akerovd (ISIS, UK) Joern Beckmann (FRM-II, Germany) Uwe Filges (PSI, Switzerland) Przemek Klosowski (NCNR, USA) Mark Koennecke (PSI, Switzerland)

Kevin Knowles (ISIS, UK)

Jens Krueger (FRM-II, Germany) Nick Maliszewskyj (NCNR, USA) Christopher Moreton-Smith (ISIS, UK) Ray Osborn (IPNS, USA)

Peter Peterson (SNS, USA) John Tischler (APS, USA)

# Monday, September 8, 2003

## Action Items:

- 1. Write a summary report to send to facility directors
- 2. Compile biographies of existing members to publish on NeXus website

## Resolved Items:

- 1. Ratified terms of reference
- 2. Approved method for ratifying new NeXus classes

## Tuesday, September 9, 2003

## Action Items:

- 1. Write a white-paper on using XML Schema (XSD) as archival form of instrument definitions and class templates. (Oct 10: F. Akeroyd and P. Peterson)
- 2. Report on more complex mark up for XML format (Sep 25: N. Maliszewskyj)
- 3. A series of HOWTOs and FAQs will be compiled. Topics to be covered will be
  - a. Compiling, linking against, and installing
  - b. Reading and writing a file
  - c. Writing an instrument definition
  - d. Identifying plottable data
  - (P. Klosowski)
- 4. Formal proposal of Nxposition, which incorporates Nxgeometry and Nxtranslation. (Sep 25: F. Akeroyd)
- 5. Formal detector geometry proposal. (Nov 15: J. Hodges, P. Peterson, F. Akeroyd, M. Koennecke)
- 6. Formal proposal of API implementation of "link" attribute. (M. Koennecke)

#### Official Recommendations:

1. Preferred file extension is ".nxs", but use of ".hdf", ".h5", ".xml" and other extensions are permitted.

## Resolved Items:

- 1. Instrument definitions and class templates will be stored in metaDTD format until more appropriate final storage can be determined. (J. Beckmann against)
- 2. Instrument definitions and class templates will be fully self describing.
- 3. Archival form of instrument definitions and class templates will reside in a CVS repository.
- 4. Class templates will exist for base classes which can be put together to create an instrument definition which is used for validation.

- 5. <analysis> item within an Nxentry will be replaced with an item <definition version="">{URL}</definition>.
- 6. A right-handed coordinate system is defined with the positive z-axis along the beam when facing downstream.
- 7. Instrument definitions, or class templates, will not be subclassed.
- 8. If a simplified position is needed the entries will be distance, polar\_angle, azimuthal angle.
- 9. When NXdetector is included in a file, there will be a one-to-one correspondence between NXdata and NXdetector.
- 10. Units will be specified in the singular.
- 11. Axes in NXdata will described in one of two ways:

```
counts type="NX_FLOAT[i,j]"
    axes="[time_of_flight,polar_angle]"/>
    <time_of_flight units="micro*second" type="NX_FLOAT[i]"/>
    <polar_angle units="degree" type="NX_FLOAT[j]"/>
    <counts type="NX_FLOAT[i,j]"/>
    <time_of_flight units="micro*second" type="NX_FLOAT[i]"
        axis="1" primary="1"/>
    <polar_angle units="degree" type="NX_FLOAT[j]" axis="2"
        primary="1"/>
    <wavelength units="10^8 meter" type="NX_FLOAT[i] axis="1"
        primary="2"/>
```

- 12. Histograms can be specified either by having an extra element in the axis array or with an attribute histogram\_offset in the axis.
- 13. Preferred method for connecting NXdata to NXdetector is by using a link attribute in an axis.
- 14. Physical units will be specified in accordance with the Unidata udunits utility, with restrictions to be proposed by M. Aivazis. Dates and times will be specified in accordance with the ISO8601 format.
- 15. Positions will be stored as the physical (effective) position. This includes, not exclusively, motor and detector positions. Motor offsets will be stored as attributes on the appropriate data.
- 16. Nxroot will be defined as

```
<NXroot file_name="{File name of original NeXus file}"
  file_time="{Date and time of file creation}"
  file_update_time="{Date and time of last file change at close}"
  NeXus_version="{Version of NeXus API used in writing the file}"
  HDF_version="?"
  HDF5_version="?"
  creator="{facility or program where file originated}?">
  <NXentry name="{entry name}">+</NXentry>
  </NXroot>
```

- 17. Templates will not specify bit length for primitives. e.g. NX\_UINT, NX\_INT, and NX FLOAT are all that are allowed for numerical items.
- 18. The template for Nxentry is

```
<NXentry name="{Entry Name}">
    <title>{Extended title for entry}</title>
    <definition version="{DTD version number}" URL="{URL of DTD
        file}">{Name of entry DTD}</definition>
```

```
<start_time type="ISO8601">{Starting time of
     measurement}</start time>
  <end time type="ISO8601">{Ending time of
     measurement}</end time>
  <duration type="NX INT" units="seconds">{Duration of
     measurement}</duration>
  <experiment identifier
     type="NX CHAR[]">{}</experiment identifier>
  <run number type="NX INT">{Number of run or scan stored in
     this entry}</run number>
  <run cycle type="NX CHAR[]">{}</run cycle>
  of
     program used to generate this file}</program name>
  <command line>{Name of command line used to generate this
     file}</command line>
  <notes>{Notes describing entry}</notes>
  <NXuser name="{user}"></NXuser>
  <NXsample name="{sample}"></NXsample>
  <NXinstrument name="{Name of instrument}"></NXinstrument>
  <NXmonitor name="{Name of monitor}"></NXmonitor>
  <NXdata name="{Name of data block}"></NXdata>
</NXentry>
```

## Wednesday, September 10, 2003

## Action Items:

- 1. Review the implications associated with Unicode in files (Technical Committee)
- 2. Review of the distribution attribute for specifying how histogrammed data is specified, such as integral value or density. (R. Osborn and F. Akeroyd)
- 3. XML based NEXUS API whitepaper (M. Koennecke, N. Maliszewskyj, P. Klosowski, and P. Peterson)
- 4. Methods for producing binary distributions will be established by N. Maliszewskyj (RPM), M. Aivazis (DEB), F. Akeroyd (Install Shield), and J. Beckmann (Digital Unix)
- 5. A working group will decide how the CVS directories will be reorganized (Oct 15: R. Osborn, J. Beckmann, M. Aivazis)
- 6. All known Python ports of the NeXus API will be resolved into a single version to be released to the public. Afterwards, an object oriented layer on top of the core NeXus API will be explored in Python. (M. Aivazis)
- 7. Voting on class templates will commence on November 1, 2003.
- 8. A whitepaper for converting existing NeXus files into files conpliant with the new standard will be written (M. Koennecke and P. Peterson)
- 9. Members of the NIAC will nominate instrument editors by October 1, 2003
- 10. The current templates with formatting changes and the ISIS NeXus document will be combined before debate will commence. (P. Peterson)
- 11. Definition of how to store sparse data, e.g. event data. (P. Peterson)

#### Official Recommendations:

- 1. Inside character array containing history logs, and outside of a Nxlog, a date or time should have "TIMESTAMP:" preceding the ISO8601 time to make parsing easier.
- 2. Before starting a new project focus on NeXus, such as porting the API to a new language or writing a NeXus-enabled application, an announcement should be made to the NeXus mailing list and a site should be put up for comments on the new project, *e.g.* on the NeXus Swiki.

#### Resolved Items:

- 1. New type NX\_BINARY (unsigned 8 bit integer) with an attribute mime\_type for storing a variety of binary data.
- 2. New type NX\_BOOLEAN with value zero (false) or one (true). Implementation of type to be determined later.
- 3. NX CHAR array should use end of line character "\n" in the text.
- 4. The NXcounter group will incorporated into the NXmonitor group.
- 5. Nxinstrument template consists of at least the following groups

```
<NXinstrument>
   <name short name="{abbreviated name of instrument}">{name
      of instrument}</name>
   <NXsource/>
   <NXcrystal/>
   <NXdisk chopper/>
   <NXfermi_chopper/>
   <NXvelocity selector/>
   <NXquide/>
   <NXcollimator/>
   <NXaperture/>
   <NXfilter/>
   <NXattenuator/>
   <NXpolarizer/>
   <NXflipper/>
   <NXmirror/>
   <NXdetector/>
   <NXbeam stop/>
</NXinstrument>
```

- 6. Each NXlog will contain information for one variable.
- 7. The definition of a NXlog is

8. File directories with a NeXus section will have "nexus" in lowercase.

- 9. An version of the NeXus API to read and write NeXus files in XML format will be created.
- 10. Current members of the NeXus developers mailing list are the members of the NeXus technical special interest group.