NeXus Recapitulation and Developments

Mark Könnecke

NeXus International Advisory Committee

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The Predicament of the Traveling Scientist

- A different data format wherever she goes

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- Spends lots of time converting formats or writing readers
- Waits even longer to load data from inefficient data formats
- DA requires N files in different formats, notes, local knowledge
- Cannot read her collaborators data
- Has to keep extra information in yet another form

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NeXus Design

- Complete data for typical use
- Extendable, add additional data as you please
- Self describing
- Easy automatic plotting
- Platform independent, public domain, efficient
- Suitable for a wild variety of applications

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NeXus Levels

1. Physical file format and API for accessing files
2. Rules for storing data in files
3. Component and application definitions
4. NeXus Utilities

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Physical File Format

- Portable, self describing, extendable, public domain
- Hierarchical data format, NCSA, HDF-4, later HDF-5
- HDF-5:
  - grouping support
  - on the fly compression
  - reading/writing subsets
  - first dimension appendable
  - Public domain C, F77 access library
  - Used by: NASA, Boing, the weathermen, ...
- XML for those who wish to edit their data

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NeXus API

- NeXus-API hides complex HDF API
- Transparent access to all three supported physical file formats
- ANSI-C implementation
- Bindings: F77, Java, SWIG
- January, 4, 2010: 1311217 files processed at PSI alone
- NEW: first class bindings to C++, python, IDL

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NeXus Objects

- Files
- Groups identified by name and a classname beginning with NX
- Scientific data sets
- Attributes
- Links

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entry:NXentry
- sample:NXsample
- instrument:NXinstrument
  - source:NXsource
  - velocity_selector:NXvelocity_selector
  - detector:NXdetector
    - data[xsize,ysize], signal=1 (1)
- control:NXmonitor
  - data
- data:NXdata
  - link to (1)

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Why the Hierarchy??

- Supports self description and allows short names in components

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- Name, classname pair allows for multiple components of the same type

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- NXdata supports automatic plotting

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Why the Hierarchy??

- Supports self description and allows short names in components
- Name, classname pair allows for multiple components of the same type
- NXentry allows for multiple datasets in the same file
- NXdata supports automatic plotting
- Take care once when writing, use n times

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- Come in all shapes and sizes
- Captured by rules:
  - Store all varied parameters as arrays of length NP at the appropriate place in the NeXus hierarchy
  - For multi detectors, NP, number of scan points is always the first dimension
  - In NXdata: create links to counts and varied variables

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Scan Example 1: rotating sample

entry:NXentry
- sample:NXsample
  - rotation_angle[NP], axis=1 (1)
- instrument:NXinstrument
  - detector:NXdetector
    - data[NP],signal=1 (2)
- control:NXmonitor
  - data[NP]
- data:NXdata
  - link to (1)
  - link to (2)

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Scan Example 2: complex scan in Q

entry:NXentry
- sample:NXsample
  - rotation_angle[NP], axis=1 (1)
  - phi[NP], axis=1 (2)
  - chi[NP], axis=1 (3)
  - h[NP], axis=1 (4), primary=1
  - k[NP], axis=1 (5)
  - l[NP], axis=1 (6)
- instrument:NXinstrument
  - detector:NXdetector
    - data[NP],signal=1 (7)
    - polar_angle[NP],signal=1 (8)
- data:NXdata
  - link to (1)
  - link to (2)
  - link to (...)
  - link to (8)

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Scan Example 3: sample rotation, area detector

entry:NXentry
- sample:NXsample
  - rotation_angle[NP], axis=1 (1)
- instrument:NXinstrument
  - detector:NXdetector
    - data[NP,xsize,ysize],signal=1 (2)
- control:NXmonitor
  - data[NP]
- data:NXdata
  - link to (1)
  - link to (2)

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Storing Single Data Items

- Units have to specified
- Locating axis, by example
- NEW: Taking care of scaled data

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Coordinate Systems

- McStas Coordinate System
- Angle based coordinates
- NXgeomtry for enginnering coordinates and describing shapes

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NeXus Component and Application Definitions

- Component definitions: dictionaries of allowed field names for the various NeXus groups
- Application Definitions
  - Define what has to be in a NeXus file for a certain application
  - Defines standards
  - Another view: Contract between file producers and users about what has to be in a NeXus file for a well defined purpose
  - Validation by NXvalidate
- Written in NeXus Definition Language, NXDL

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NEW: Available NeXus Application Definitions

- NXarchive
- NXreftof
- NXtas
- NXtomophase
- NXxnb
- NXtomoproc
- NXindirectof
- NXsastof
- NXtofsingle
- NXmonopd
- NXsas
- NXtofraw
- NXxeuler
- NXxrot
- NXtofsingle
- NXiqproc
- NXsqom
- NXxas
- NXrefscan
- NXscan
- NXtomo
- NXxkappa
- NXiqproc
- NXdirectof
- NXlauetof
- NXtofraw
- NXxasproc

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NeXus Tools

nxbrowse	CLI NeXus browser
nxtree	prints NeXus tree
NXmeta	dumps all NeXus meta data
nxtranslate	transforms into NeXus
nxvalidate	NEW: validates NeXus files
nxextract	converts from neXus to ASCII and binary
nxplot	NEW: plots any NeXus file

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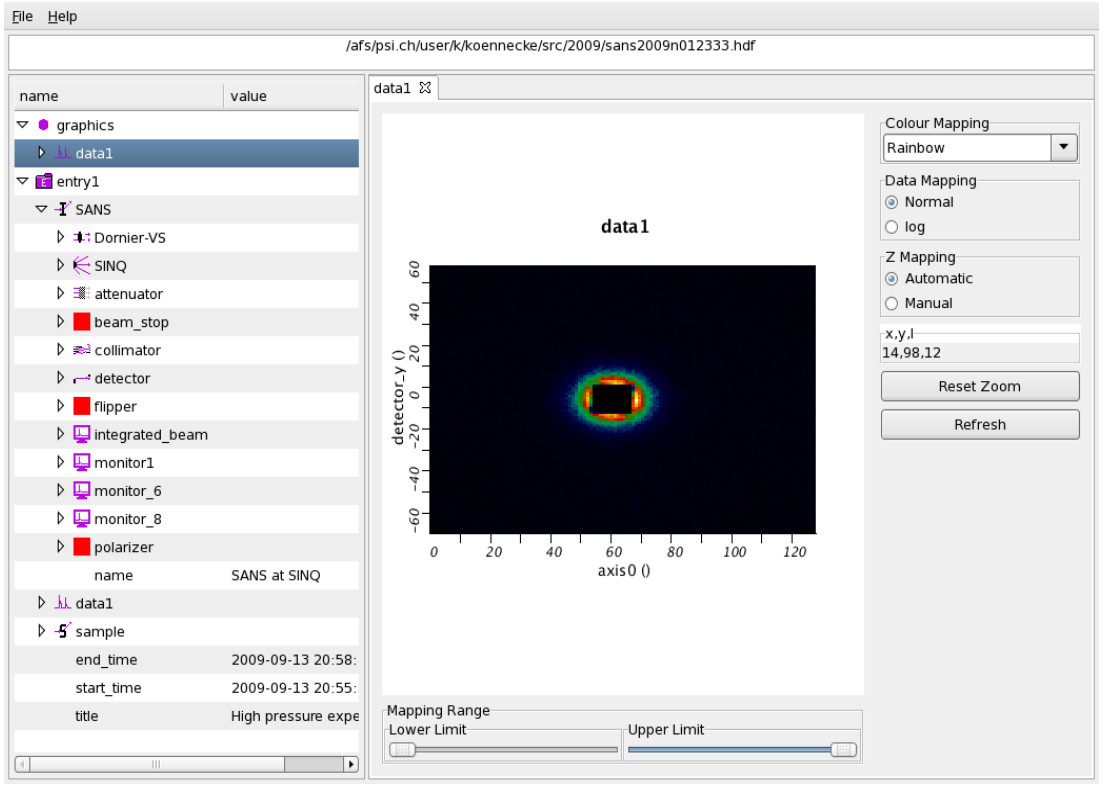
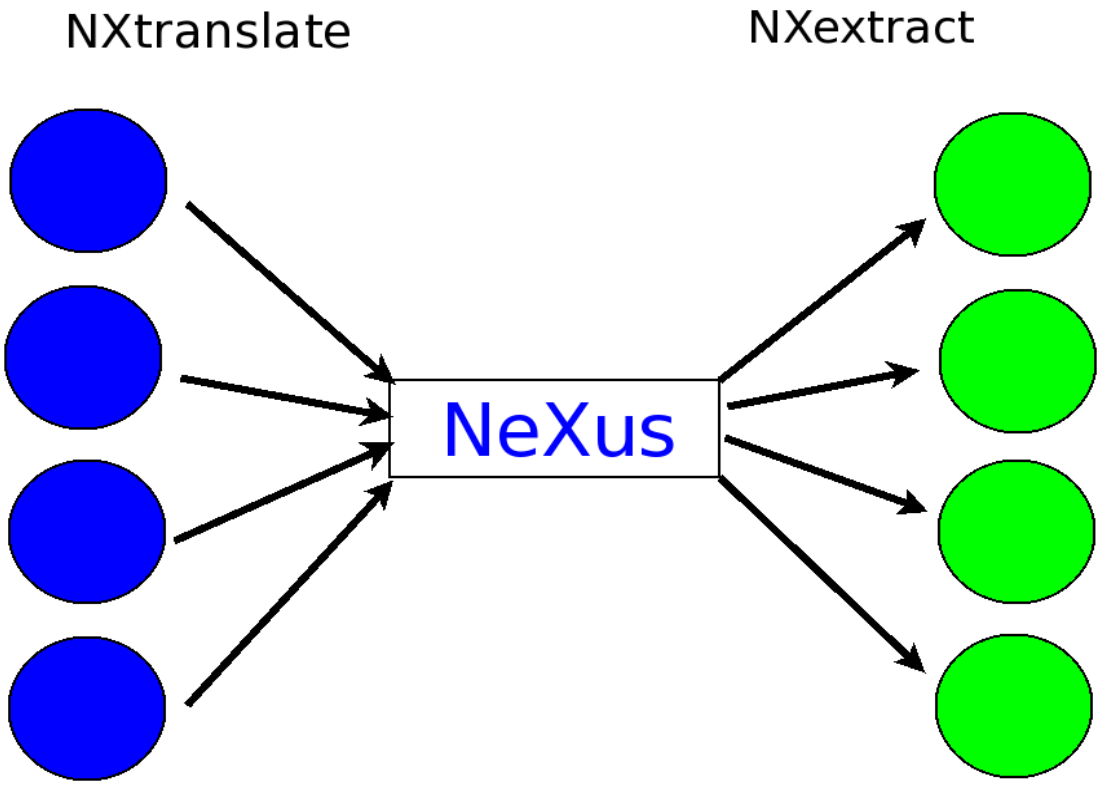
NXplot


File Help
/afs/psi.ch/user/k/koennecke/src/2009/sans2009n012333.hdf
name
value
graphics
data1
entry1
SANS
Dornier-VS
SINQ
attenuator
beam_stop
collimator
detector
flipper
integrated_beam
monitor1
monitor_6
monitor_8
polarizer
name
SANS at SINQ
data1
sample
end_time
2009-09-13 20:58:
start_time
2009-09-13 20:55:
title
High pressure expe
data1
data1
detector_y ()
axis0 ()
Colour Mapping
Rainbow
Data Mapping
Normal
log
Z Mapping
Automatic
Manual
x,y,I
14,98,12
Reset Zoom
Refresh
Mapping Range
Lower Limit
Upper Limit

NeXus Conversions



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Other Systems Using NeXus

- DANSE
- DAVE
- FABLE (ESRF)
- ISAW
- LAMP
- openGenie
- ICAT
- Mantid
- openGDA
- All HDF tools

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Who commits to NeXus?

Challenge 1 in science you are supposed to do new, non standard, things. These of course cannot be easily cast into a standard.

Data Format Challenges

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Challenge 2 in order to establish a standard a lot of people need to agree

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Challenge 2 in order to establish a standard a lot of people need to agree

Challenge 3 a standard requires scarce scientific programming resources for adoption

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Data Format Chances

Chance 1 By using a discoverable data format like NeXus, XML, HDF-5, people can at least figure out what is in the data file.

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Chance 6 In many experiments not the technique but the sample is important: then an application definition simplifies life.

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- PanData
- Workshop: HDF5 as hyperspectral data format, January, ESRF
- NeXus workshop at PSI, May
- Upcoming: Data formats for HDR, DESY, end of october

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- European initiative for SSO, a shared data file catalog, DA etc
- PanData needs a shared data format in order to make the catalog fly
- Works with NeXus
- Prompted us to have a project plan which we actually executed by now!
- 5.5MM money

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HDF5 as hyperspectral data format

- NeXus well received
- Some confusion over a HDF-5 bug in 1.8
- Herbert Berstein conceded that imageCIF is mostly dead
- Demand: make it possible to fully map imageCIF to NeXus
- Missing in NeXus to do full CIF mapping:
  - Scaled data
  - CIF axis specification more accurate

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- Workshop at PSI
- NeXus seen as HDF-5 with NeXus structures, no interest in API
- Requests:
  - NXsubentry
  - Scaled data
  - Simplified hierarchy for experts
  - Indicate image dimensions
  - Higher level API

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Topics for this NIAC Meeting

1. Constitution change: NIAC – Tech
2. NXsubentry
3. Scaled data
4. Coordinate systems
5. Next project plan
6. Simplified hierarchy, NXmeasurement

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- Observation: the NIAC in its current form is inefficient, most of the time most people do not understand or are interested int the ongoing discussion
- Suggestion: Divide into two entities:
  - Full NIAC: votes officers, ratifies project plans, decides general directions
  - Technical subcommittee: decides technical and implementation details. Members selected on merit (contributed work) and approved by full NIAC

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entry:NXentry
    sas,NXsubentry
        sample:NXsample

        instrument:NXinstrument
            source:NXsource
            velocity_selector:NXvelocity_selector
            detector:NXdetector
                data[xsize,ysize], signal=1 (1)
        control:NXmonitor
            data
        data:NXdata
            link to (1)

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NXsubentry Rationale

- Multi-method instrument
  - Especially synchrotrons have instruments which combine multiple techniques in one experiment
  - Current NeXus would require seprate NXentries for each technique
  - This becomes unnatural with the additional requirement to store multiple experiments in the same file
  - Combining multiple application definitions in one NXentry would cause name collisions
  - The synchrotron people are aware that NXsubentry requires a lot of links but are willing to do the work
- Add application definition NXsubentries to existing files

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Scaled Data

- NeXus stronly suggests storing physical values
- But allow scaled data for performance or other reasons
- Implement through additional data attributes

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Scaled Data Attributes

- transform: This is the indicator that a transformation of the Vraw data is necessary. Transform can have one the following values:
  - offset: Vtrue = Vraw + offset
  - scaling: Vtrue = Vraw * scaling
  - scaling_offset: both an offset and scaling is applied. Vtrue = Vraw*scaling + offset
  - sqrt_scaled: Vtrue = (Vraw/scaling)*(Vraw/scaling)
  - logarithmic_scaled: Vtrue = (Vraw/scaling)**10
  - polynomial: Vtrue = p1 + p2*Vraw + p3*Vraw*Vraw + p4*Vraw*Vraw*Vraw ....
- direction: a komma separated list of length ndim which specifies for each dimension if it is increasing or decreasing
- precedence: a komma separated list of length ndim which gives the rank order in which array indexes change with respect to other indexes.
- coefficients, offset, scaling: parameters for calculating Vtrue

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entry,NXentry
- measurement,NXmeasurement
  - positions:NXpositioner
    - om
    - two_theta
  - scalars:NXscalar
    - title
    - wavelength
  - images:NXimagedata
    - detector1
    - mca5

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Ideas for Project Plan 2012

- Refinement of application definitions with communities
- OO base classes?
- Higher level NeXus-APIs?

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