State Of The NeXus Data Format

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NeXus International Advisory Committee

October 12, 2010

NeXus Mission

- Solve the predicament of the travelling scientists
- Definition of a standard data format
  - Rules
  - Validation tools
- Promotion of NeXus
  - Documentation
  - NeXus API
  - Outreach to the scientific community

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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: HDF-4, HDF-5, XML
2. Rules for storing data in files
3. Component and application definitions
4. NeXus Utilities

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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
- NEW: first class bindings to C++, python, IDL
- NEW: experimental python tree API added

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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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NEW: NeXus Processed Data File Structure

entry:NXentry
- sample:NXsample
- processing_name:NXprocess
  - program
  - version
  - parameters:NXparameter
    - raw_file
- data:NXdata
  - data[nx,ny,nz], signal=1

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NEW: NXsubentry

entry:NXentry
- sample:NXsample
- instrument:NXinstrument
- .....
- 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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NEW: NXcollection

entry,NXentry
- measurement:NXcollection
  - positions:NXcollection
    - om
    - two_theta
  - scalars:NXcollection
    - title
    - wavelength
  - data:NXdata
    - detector1
    - mca5

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- 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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Storing Single Data Items

- Units have to specified
- Locating axis
- Store data as physical value and in C storage order
- NEW: Taking care of scaled data and other storage orders

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- McStas Coordinate System
- Angle based polar coordinate system
- NEW: full mapping imageCIF - NeXus now possible
- NEW: General axis and transformations

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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
nxextract	converts from NeXus to ASCII and binary
nxvalidate	NEW: validates NeXus files
nxplot	NEW: plots any NeXus file

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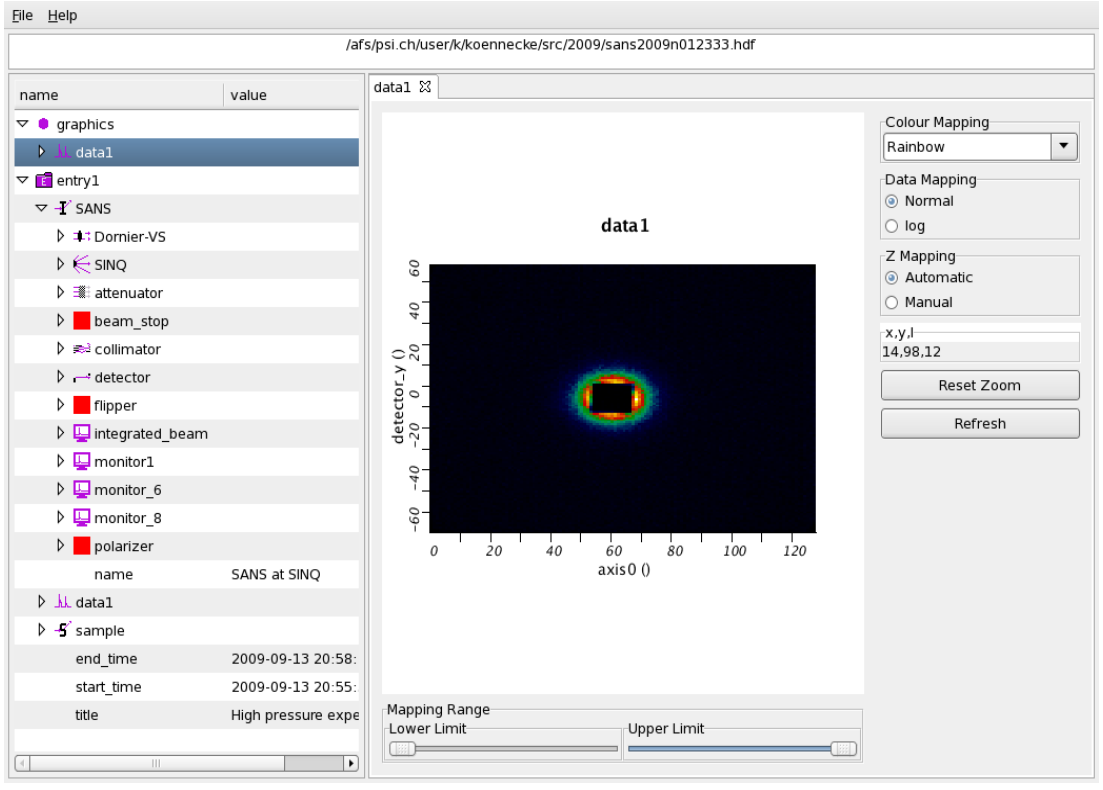
NXplot


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 Political

- PanData: european initiative for SSO, shared data catalogs and some.
  - Works with NeXus to make the shared data catalog fly
- Synchrotrons hitting the wall with current data formats
  - Two workshops in europe addressing this, at ESRF and PSI
  - Another one upcoming

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Benefit 6 Application Definitions

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NeXus Conclusion And Outlook

- NeXus is already in use at quite a number of facilities and is understood by a long list of applications
- New systems tend to use NeXus
- No competitor for a general purpose data format
- Planned:
  - Refine application definitions together with communities
  - Release application definitions and NXvalidate
  - Update manuals and the NeXus WWW-site
  - www.nexusformat.org, embarrasingly outdated, download manual

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