State Of The NeXus Data Format

Mark Könnecke

NeXus International Advisory Committee

September 26, 2012

NeXus Mission

- NeXus is a data format for X-ray and neutron scattering and muSR spectroscopy
- 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

- 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

NeXus Levels

- Physical file format and API for accessing files
  - HDF-5 for large binary data sets
  - XML for ASCII lovers
- NeXus Utilities
- Rules for storing data in files
- Dictionary of names and components to use in files (base classes)
- Validatable application specific standards as application definitions
- File hierarchies for raw and processed data

NeXus Raw Data File Structure

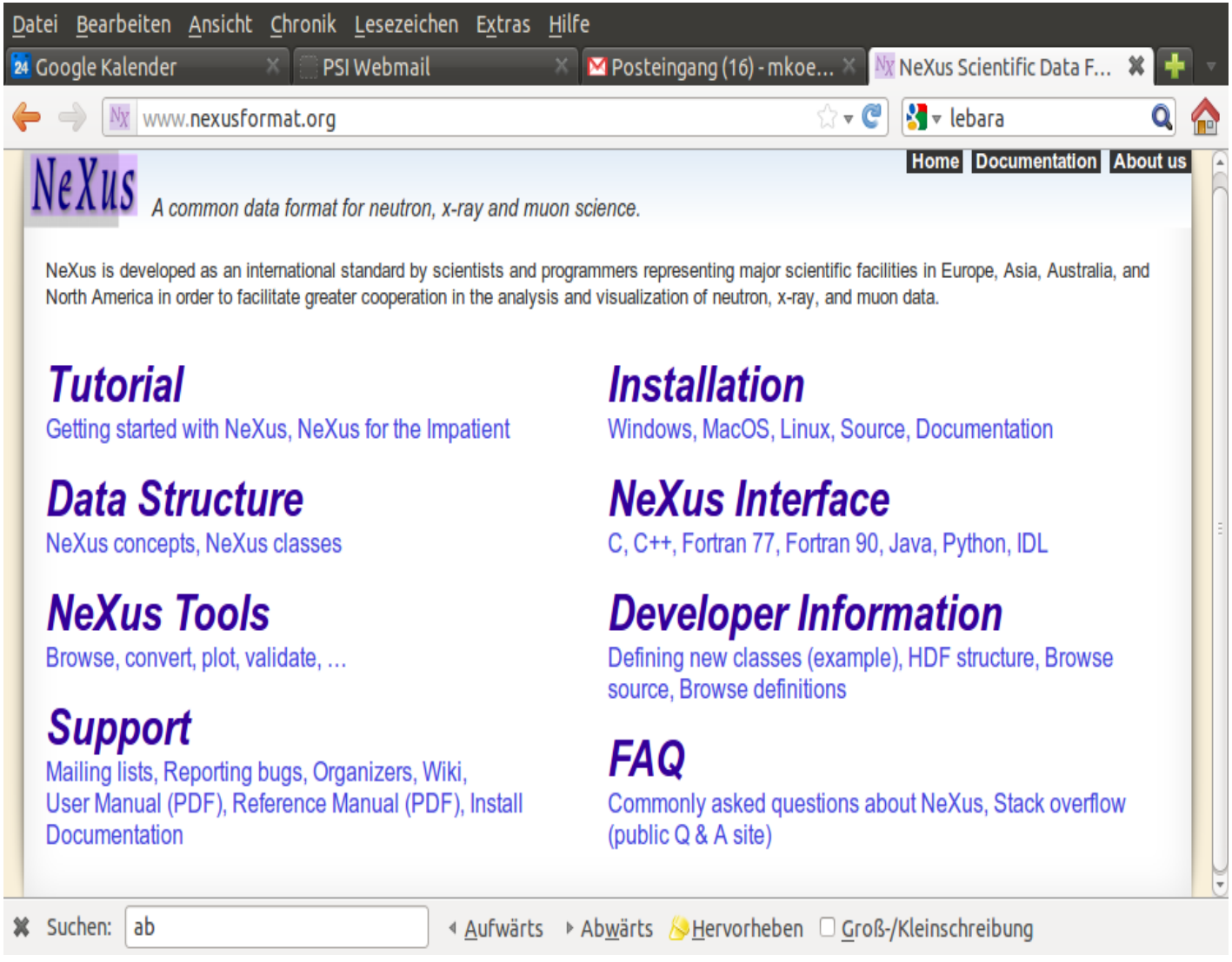
entry:NXentry
- sample:NXsample
- instrument:NXinstrument
  - source:NXsource
  - velocity_selector:NXvelocity_selector
  - detector:NXdetector
    - data[xsize,ysize], signal=1 (1)
- control:NXmonitor
  - data
- data:NXdata
  - link to (1)

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

- Documentation and WWW-site has been revised and updated
- NeXus for the Impatient document
- Documented process to write NeXus files with HDF-5 alone
- NAPI Release 4.3.0, NXDL 3.1.0
- Collaboration with DECTRIS
- Collaboration with HDRI: added synchrotron beamline components
- Finalized CIF support
- Review of NeXus

New WWW-site


Datei Bearbeiten Ansicht Chronik Lesezeichen Extras Hilfe
Google Kalender
PSI Webmail
Posteingang (16) - mkoe...
NeXus Scientific Data F...
www.nexusformat.org
lebara
Home
Documentation
About us
NeXus
A common data format for neutron, x-ray and muon science.
NeXus is developed as an international standard by scientists and programmers representing major scientific facilities in Europe, Asia, Australia, and North America in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data.
Tutorial
Getting started with NeXus, NeXus for the Impatient
Installation
Windows, MacOS, Linux, Source, Documentation
Data Structure
NeXus concepts, NeXus classes
NeXus Interface
C, C++, Fortran 77, Fortran 90, Java, Python, IDL
NeXus Tools
Browse, convert, plot, validate, ...
Developer Information
Defining new classes (example), HDF structure, Browse source, Browse definitions
Support
Mailing lists, Reporting bugs, Organizers, Wiki, User Manual (PDF), Reference Manual (PDF), Install Documentation
FAQ
Commonly asked questions about NeXus, Stack overflow (public Q & A site)
Suchen: ab
Aufwärts
Abwärts
Hervorheben
Groß-/Kleinschreibung

NAPI 4.3.0

- Essentially a bug fix release
- Unlimited dimensions for all dimensions in HDF-5
- 64 bit dimensions for really large data
- Now requires HDF-5 1.8+
- Includes alpha version of python tree API
- Much better package management support
- Now thread safe
- To be released soon after NOBUGS

NeXus

NXDL Release 3.1.0

- First release of suggested application definitions
- See as a foundation for community discussions
- File validation tool
- Contains the updated NeXus reference manual
- Available at:
  http://download.nexusformat.org/kits/definitions/

Collaboration with DECTRIS

- Manufactures the Pilatus and upcoming EIGER detectors for X-rays
- Expected EIGER data rates of 5-10GB/sec blow lid of old data formats
- Working towards NeXus/HDF-5
- Programming model:
  - Detector SW writes what it knows into NXentry/NXdetector structures
  - Local DAQ system adds meta data
- NXdetector base class extended to cover pixel detectors
- DECTRIS is paying HDF group to develop:
  - Dynamically loadable filters
  - Storing precompressed data blocks
- The NIAC is committed to make this fly

Finalized CIF-NeXus Mapping Support

- Added features to NeXus to allow full mapping between CIF and NeXus
- Consequences:
  - There will be negotiations with the IUCR about a possible merger between NeXus and CIF
  - Herbert Bernstein promised to add NeXus/HDF-5 support to CBFlib
- The NIAC is in support of both moves

- NeXus around for 16 years
- Apparently slow uptake
- However: people starting on their own gravitate to something which looks like NeXus in the long run
- The NIAC reviewed NeXus on the basis of a questionaire sent out before the last NIAC Meeting

NeXus Usage

- Soleil: 20 out of 26 instruments do NeXus, 2 mill files
- PSI-SINQ: 11 from 16 instrument on NeXus, 1.4 Mill files
- Lujan/LANL: 11 instruments, no change, 1 million files
- ANSTO: 7 going to 10
- KEK: 10, 6 planned
- SNS: 14,3 in the pipeline
- DESY: 0, 11 in 2 Jahren
- Diamond: 7 NeXus only, 17 writing, moving to 18 as primary format
- ISIS: 8 using, 20 writing, planned: 20 using
- Less intense users:
- PSI-SLS: 2 planned,
- ESRF: 2 beamlines, limited to NXentry, NXcollection, NXdata, moving to 4
- HZB: 3 Neutron, 1 synchrotron, 3 planned
- Muons: 4 instruments

Focus for NeXus

- Base classes, dictionary, application definitions most important
- NIAC is a forum to resolve issues around these
- NIAC acts a custodian
- Validation is important and will continue to be developed

Consequences of the Refocussing

- NAPI: stable and in maintenance mode
- We encourage people to write NeXus files with HDF-5 tools
- Pedro Vincente contributed a minimal helper tool on top of H5L for this
- We accept application definitions with a flatter hierarchy from the community

Dispelling NeXus Myths

- NeXus has matured considerably over the course of time
- Everything in NeXus is there for a reason, often compiled from differing and conflicting requirements
- NeXus in inclusive
- NeXus is used
- NeXus does not require you to store lots of useless information
- NeXus allows to define and validate real standards
- NeXus is not restricted to binary formats

NeXus Conclusion And Outlook

- NeXus is used a lot
- NeXus adds meaning to HDF-5
- Planned:
  - Collaboration with DECTRIS
  - Collaboration with IUCR
  - Review of NeXus base classes and introduction of OO concepts
  - Look into how to store generalized time stamped data
- Please join or interact with the NIAC when trying to define a standard
- Get yourself heard: there are still facilities with no representative in the NIAC
- More information: www.nexusformat.org