NeXus Recapitulation and Developments

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- Decisions from NIAC 2010
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NeXus Mission

- 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
- Store a full beamline description (FBD)
- 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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Decisions from NIAC 2010

- NXsubentry
- NXcollection
- Support for CIF style coordinate systems
- Non C-storage order arrays: offset, stride attributes
- Python tree API becomes part of NAPI
- Look into NAPI thread safety and PHDF

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

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Developments since 2010

- HDRI Meeting Hamburg
- PanData floundered
- Code Camp 2011
- Collaboration with DECTRIS
- Code Camp 2012
- NAPI release 4.3, NXDL 3.2 == 1.0

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HDRI: High Data Rate Initiative

- German synchrotron and neutron sources
- Collaboration with little money
- Invented something NeXus alike
- Later convinced to go NeXus
- Additional and revised synchrotron base classes
  - NXcapillary
  - NXbending_magnet
  - NXinsertion_device
  - NXxray_lens
- Current state: Eugen?

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PanData

- European project to standardize logins, data catalogs and data
- NeXus at first well received
- Then plans to develop method specific formats between facilities
- Dormant ever since

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- At APS
- NX_UNLIMITED for all dimensions
- 64 bit dimensions
- HDF-5 1.8
- Documentation updates
- WWW-site from manual
- NXimpatient dodument: NeXus in 8 pages
- Test for python-API 30% complete
- Python Tree API cleaned up
- PHDF not useful
- New C++ Tree API (Eugen)

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Collaboration with DECTRIS

- Manufacturer of Pilatus and Eiger detectors
- Going for NeXus/HDF-5 for Eiger
- Detector Software writes NXdetector group
- More fields added to NXdetector to accomodate pixel detectors
- This is well on its way

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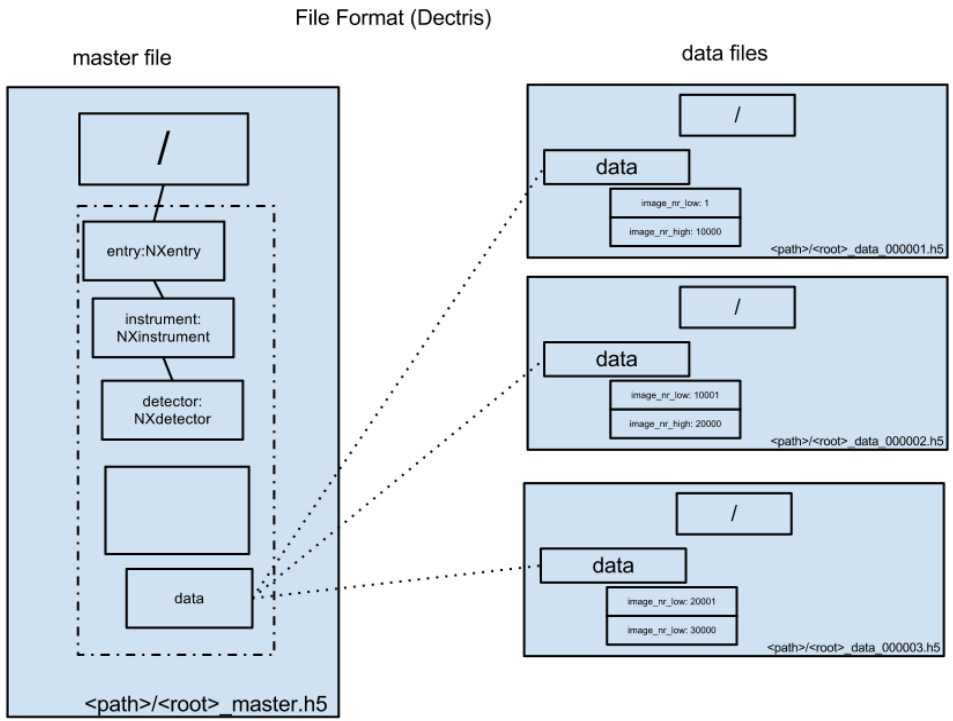
DECTRIS File Structure



Rationale

- DECTRIS has a problem:
  - Detector outputs 5-10 GB/sec
  - The deliver the detector and the computer going with it
  - They cannot ask their customers to provide the appropriate hardware for such a detector: parallel file system etc.
  - Must compress and write the file on one computer
  - Compression has to be parallel as CPU intensive
- File structure a workaround for HDF-5 not allowing sections of datsets in different files
- Sidenote: LZ4 or snappy compression; up to 450MB/sec on write

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Upcoming DECTRIS Meeting with Community

- DECTRIS aims at meeting customers in october
- How far can we compromise?
- Anyone from the NeXus community who wishes to join?
- Comment from code camp: ask for tool to convert to HDF-5 standard compression

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- May 2012
- Organised with DECTRIS to address performance issues
- HDF people gave overview of new developments in HDF-5
- DECTRIS (and DESY) pays for:
  - Writing pre compressed chunks
  - Dynamically loadable filters

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New Feautures for HDF-5 1.10

- Asynchronous I/O
- Journaling
- Single Writer, Multiple Reader semantics
- Better fault tolerance
- In memory HDF-5 files
- Shared object headers

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Other Things the HDF people work on

- Better multi threading support
- Virtual Object Layer, completely replace storage layer
  - Use HDF-5 data model but not file format
  - Opens path to more storage models
  - Metadata server for better parallel support
  - Mirroring, stacking
- Better parallel processing support: meta data server

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NAPI Release 4.3, Application Definitions 3.1

- 64 bit dimensions
- HDF-1.8
- NX_UNLIMITED everywhere
- Alpha python tree API included
- First release of applicaton definitions
- Updated manual

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- Moved documentation to sphinx
  - Wiki like syntax allows for easier editing then docbook
  - URL:
- Cleaned up trac tickets
- Decided to drop autoconf in favour of CMake
- Resolved CIF coordinate issue
- Devised a good suggestion for handling axes at multidimensional datasets
- Cleanup of NeXus applications: nx2dtd, NXDump, nxtraverse, NXformat_dfn dropped
- Got NAPI 4.3 release ready

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Topics for NIAC 2012

- Review of NeXus: where are we headed?
- Roadmap OO-NeXus
- CIF coordinates
- Process for changing base classes
- Review synchrotron beamline classes
- Review additions to NXdetector
- Materials definition
- Multi dimensional array axes encoding
- What to do about expired NIAC members?
- Electing new officers

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Questions from Code Camp

- Is anyone using NXcharacterization? Remove?
- Who is using F77 NAPI? How much effort to put into this?
- Do we go into timed data?

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CIF Revisited

- Finalize
- Hope for endorsement of CIF community
- AIM: provide data necessary to derive positions of components from transformation matrics

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$$T = \begin{pmatrix} 1 & 0 & 0 & x \\ 0 & 1 & 0 & y \\ 0 & 0 & 1 & z \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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$$T = \begin{pmatrix} 1 & 0 & 0 & x \\ 0 & 1 & 0 & y \\ 0 & 0 & 1 & z \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$R = \begin{pmatrix} r11 & r12 & r13 & 0 \\ r21 & r22 & r23 & 0 \\ r31 & r32 & r33 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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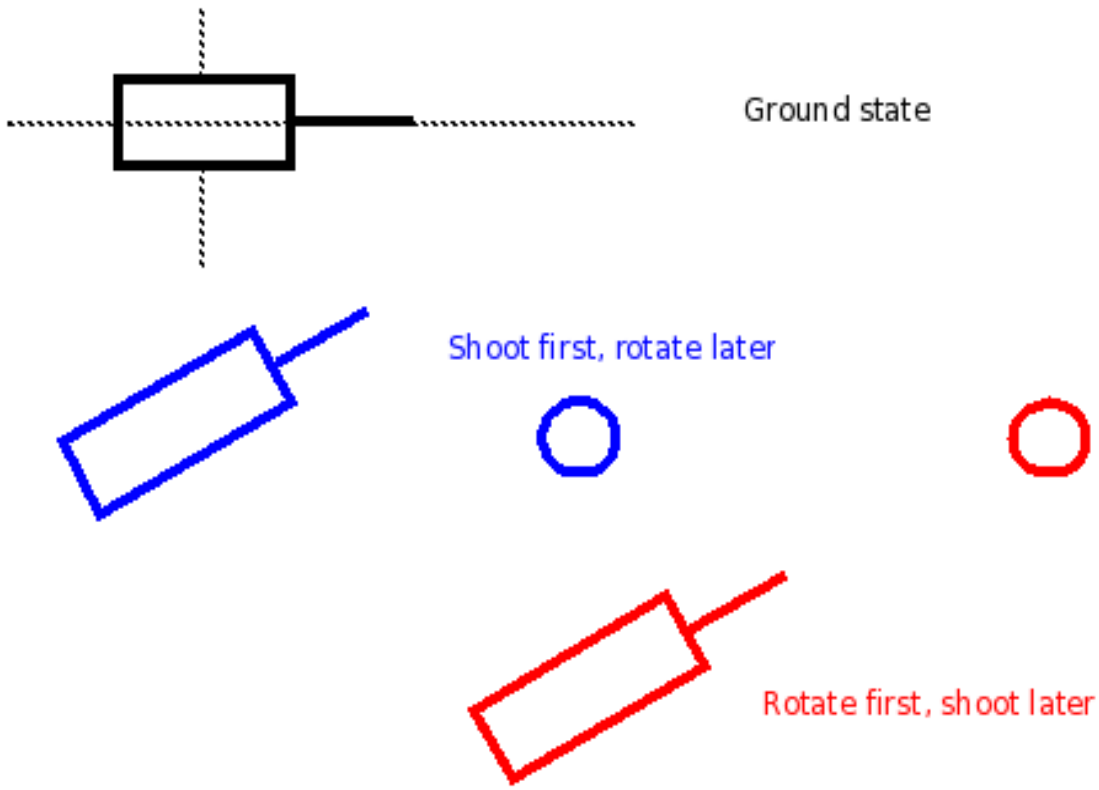
Combining Transformations



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Some Properties

- Transformations can be combined by matrix multiplications
- Individual matrices can be derived by looking at the situation when everything else is 0
- Absolute positions can be obtained by multiplying the resulting matrix with its transpose
- Defines new coordinate systems at components
- CIF contains a duplication: vector, offset scheme

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What Use Is This?

- Allows to calculate absolute positions of components in the laboratory coordinate systems
- Can directly convert from a detector coordinate system to vectors in Lab coordinate system
- Calculate things like impact of primary beam on detector, SAS
- Allows arbitray axis to be expressed
- Intuitively describe an instrument with angles and translations and still be able to recover absolute coordinates

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NeXus Axis Mapped

- rotation_angle, polar_angle, rotate 0 1 0
- azimuthal_angle, rotate 0 0 1
- distance, translate 0 0 1
- chi, rotate 0 0 1
- phi rotate, 0 1 0
- NeXus polar coordinate system: rotate azimuthal_angle, rotate polar_angle, translate by distance

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CIF Dependency Table

axis-id	type	equipment	dependson	vector	offset
gonio_phi	rotation	goniometer	.	1,0,0,	...
det_z	translation	detector	.	0,0,-1	0 0 0
det_y	translation	detector	det_z	0,1,0	0,0,0
det_x	translation	detector	det_y	1,0,0	0,0,0

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Expressing Axis Dependency in NeXus

- Implied: use existing NeXus coordinate system
- dependson attribute pointing to depending axis
- transform field in base classes which becomes a comma separated list of the path to the transformations required to position this component
- Create a special container to hold axis dependencies, NXdependency, to collect the dependencies in one place for easy access. This is what CIF does

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Dependons Option

sample,NXsample
    rotation_angle
    chi (dependson rotation_angle)
    phi (dependson phi)

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Transform Option

```
sample,NXsample
        rotation_angle
        chi
        phi
        transform = rotation_angle,chi,phi
```

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Separate Group Option

```
sample,NXsample
        rotation_angle
        chi
        phi
dependency,NXdependency
        sample/chi =
                sample/rotation_angle
        sample/phi =
                sample/chi
        instrument/detector/x_translation =
                instrument/detector/distance
        instrument/detector/distance =
                instrument/detector/polar_angle
```

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```
sample,NXsample
        rotation_angle (vector 0,1,0)
        chi (depends_on rotation_angle, vector 0,0,1)
        phi (depends_on chi, vector 0,1,0)
        depends_on
                phi
```

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Tech Committe Recommendation Continued

- Add offset attribute to fully cover CIF. This is an extra translation
- offset_unit to give units for offset
- The vector attribute becomes mandatory
- This gives us CIF endorsement!

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Process for Adding Fields and Classes

- Passing them through NIAC is slow (2 years!)
- Must be documented well enough, no duplicates
- Suggestion: leave to technical group
- Suggestion2: technical group publishes changes to NIAC for intervention

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Review of Synchrotron Beamline Components

- NXcapillary
- NXbending_magnet
- NXinsertion_device
- NXxraylens

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NXdetector Additions for DECTRIS

```
acquisition_mode:NX_CHAR
angular_calibration:NX_FLOAT[i,j]
angular_calibration_applied:NX_BOOLEAN
bit_depth_readout:NX_INT
countrate_correction__applied:NX_BOOLEAN
countrate_correction:NX_FLOAT[i,j]
detector_readout_time:NX_FLOAT
exposure_time_time:NX_FLOAT
flatfield:NX_FLOAT[i,j]
flatfield_applied:NX_BOOLEAN
flatfield_error:NX_FLOAT[i,j]
frame_start_number:NX_INT
frame_time:NX_FLOAT[NP]
```

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NXdetector Additions for DECTRIS 2

```
gain_setting:NX_CHAR
pixel_mask:NX_FLOAT[i,j]
pixel_mask_applied:NX_BOOLEAN
saturation_value:NX_INT
sensor_material:NX_CHAR
sensor_thickness:NX_FLOAT
threshold_energy:NX_FLOAT
trigger_dead_time:NX_FLOAT
trigger_delay_time:NX_FLOAT
```

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Materials Definition Recommendation

- This is about defining materials: samples, filters, multi layers etc.
- Bag of worms
- Recommendation
  - Use textual description
  - When decisive for DA: community should suggest enums

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Time Based Data

- Neutron event data to be correlated with other time based data
- Dynamic scans collecting detector frames and other data with possibly different sampling rates
- FELS will collect data only dynamically
- We have NXlog
- Questions to the NIAC:
  - Shall NeXus expand into this market?
  - Is the tech committee to be tasked to develop a recommendation how to store this better?

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