NeXus Rules and Details

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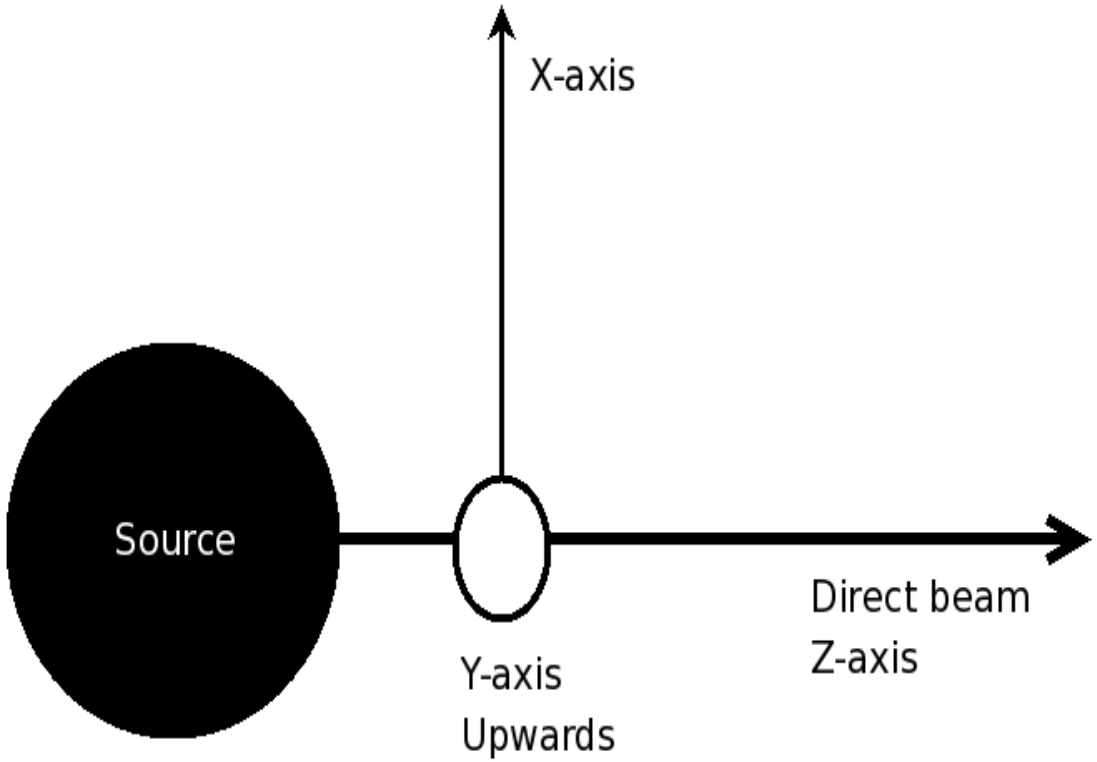
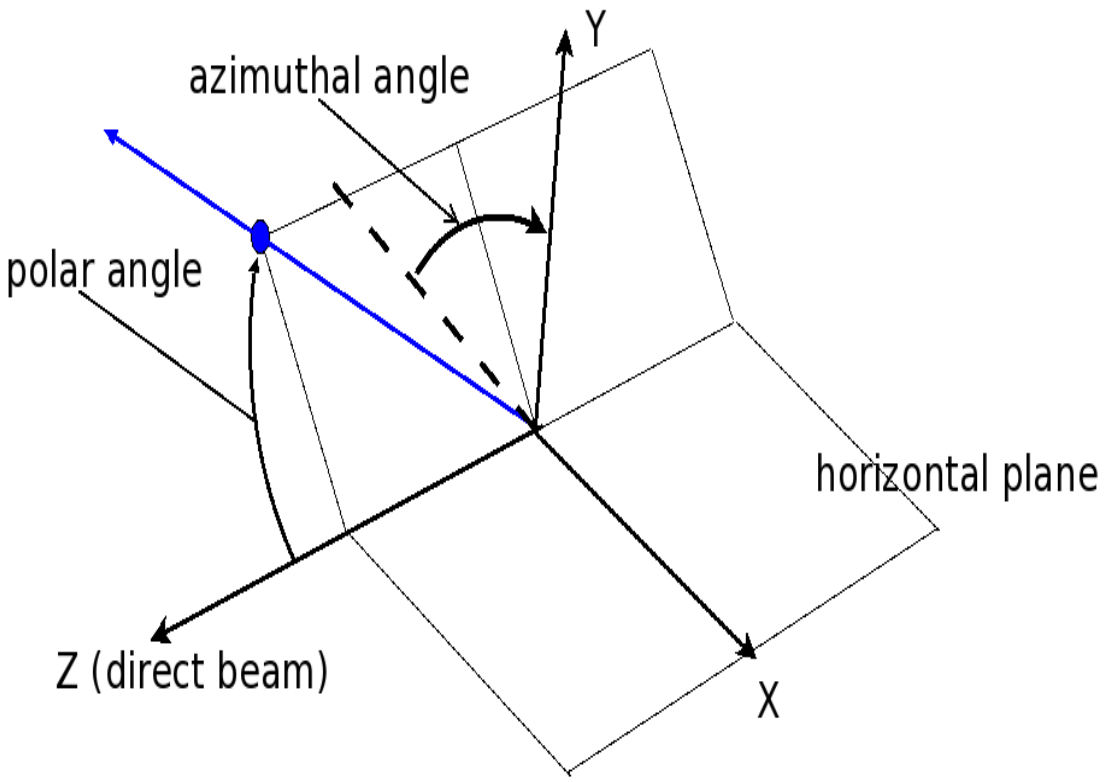
Overview

- NeXus coordinate systems
- File structural rules
- Rules for storing data items
- Rules for special applications
- Special NeXus groups

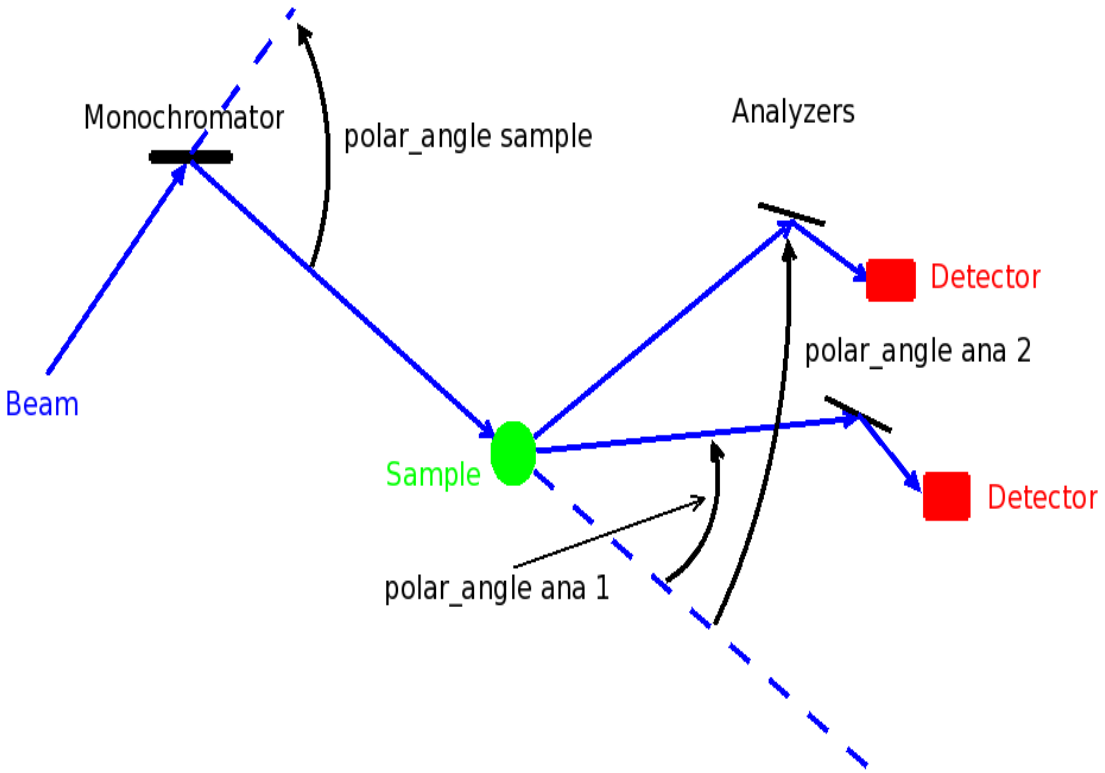
McStas Coordinate System



NeXus Simple Coordinate System



Polar angle is always relative to the previous component



CIF like Coordinates (Proposed)

- Additional fields in base classes: transform, x_translation, y_translation, z_translation, aequatorial_angle
- $Pcurrent = op1 * op2 * op3 * ... * P0$
- transform is a komma separated list of axis to apply to the component to get into position.
- Additional data attributes:
  - type: translation or rotation
  - vector: rotation or translation axis
  - offset: offset to center of component
- Use this for documentation or arbitrary axis specifications

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NeXus Default Coordinates (CIF like)

- polar_angle: type= rotation, vector= 0,1,0, offset= 0, 0, -distance
- azimuthal_angle: type=rotation, vector 0,0,1
- transform: azimuthal_angle, polar_angle

- Special group structure which can be added to any base class

geometry:NXgeometry
translation:NXtranslation
translation[3]
shape:NXshape
shape: nxbox|nxcylinder|nxsphere,
orientation:NXorientation
vector[3]

NeXus General Rules

- NeXus reserves the prefix NX for group names.
- Store as much as possible
- A NeXus file has one to many NXentry groups
- There are two types of entries: raw data and processed data
- Multiple different techniques in one file go into separate entries
- If there is only one entry, the preferred name is entry, else entry1, entry2... entryn
- If an entry conforms to an application definition, the application definitions must be stated in the entries definition field.

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

Rules for Storing Data Items

- Store physical values
- Use NeXus components and dictionary names
- Missing names will be quickly accepted by the NIAC
- Names: full words separated by _
- Specify units in same format as used by UDunits
- Application definitions may restrict units

Scaled Data (Proposed)

- NeXus *STRONGLY* prefers plain data in C storage order
- Additional attributes: linearity, offset, scaling, direction, precedence
- Same meaning as in imageCIF
- linearity:
  - offset: Vtrue = Vraw + offset
  - scaling: Vtrue = Vraw * scaling
  - scaling_offset: Vtrue (Vraw/scaling) + offset
  - sqrt_scaled: $Vtrue = (Vraw/scaling)^2$
  - logarithmic_scaled: $Vtrue = 10^(Vraw/scaling)$
- direction allows to select between increasing and decreasing indices
- precedence determines storage order

Associating Axis and Data

- Data and axis live in the same NXgroup

entry:NXentry
    data:NXdata
        data[nx,ny,nz], signal=1
        x_axis[nx], axis=1
        y_axis[ny], axis=2
        z_axis[nz], axis=3

Multiple Axis

entry:NXentry
- data:NXdata
  - data[nx,ny,nz], signal=1
  - x_axis[nx], axis=1, primary=1
  - alternate_x_axis[nx], axis=1
  - y_axis[ny], axis=2
  - z_axis[nz], axis=3

Associating Axis and Data, Method 2

entry:NXentry
- data:NXdata
  - data[nx,ny,nz], signal=1, axes=x_axis,y_axis,z_axis
  - x_axis[nx]
  - y_axis[ny]
  - z_axis[nz]

- Preserve original dimensionality of detector, if possible
- Time-of-flight becomes last dimension
- Highly irregular detectors:

entry:NXentry
  instrument:NXinstrument
    detector:NXdetector
      data[ndet], signal=1
      polar_angle[ndet], axis=1
      azimuthal_angle[ndet]
      distance[ndet]

Scans

- 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

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)

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)

- This is rastering a sample at different wavelengths, positions etc.
- Same treatment as scans, NP replaced by NR number of raster points
- For the common case of rastering on a 2D grid one can store [nx,ny,detdim]. Be aware, though, that this causes problems if the rasterisation is aborted in mid operation.

name_of_logged_value:NXlog
- time[], start
- value[]
- description
- minimum_value
- maximum_value
- average_value

note:NXlog
- author
- type
- date
- description
- file_name
- data, NX_BINARY

All Base Classes

NXaperture
NXattenuator
NXbeam_stop
NXbeam
NXbending_magnet
NXcharacterization
NXcollimator
NXcrystal
NXdata
NXdetector
NXdisk_chopper
NXentry
NXenvironment
NXevent_data
NXfermi_chopper
NXfilter
NXflipper
NXgeometry
NXguide
NXinsertion_device
NXinstrument
NXlog
NXmirror
NXmoderator
NXmonitor
NXmonochromator
NXnote
NXorientation
NXparameters
NXpolarizer
NXprocess
NXsample
NXsensor
NXshape
NXsource
NXtranslation
NXuser
NXvelocity_selector