Object Oriented NeXus Classes

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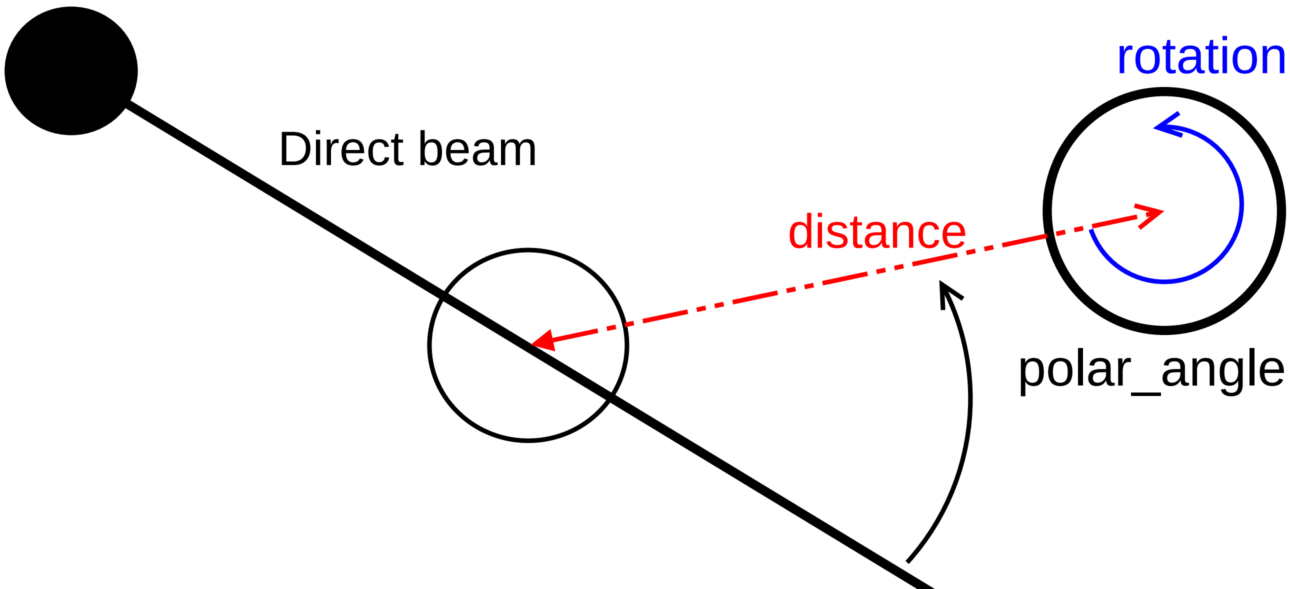
Simple Coordinate System

- The plane perpendicular to the main rotation axis of the sample table defines the scattering plane of the instrument.
- As components are commonly positioned using angles, a polar coordinate system is used.
- When distances are required then we assume that the sample is a zero. Distances towards the source are negative, distances behind the sample, towards the detector are positive.

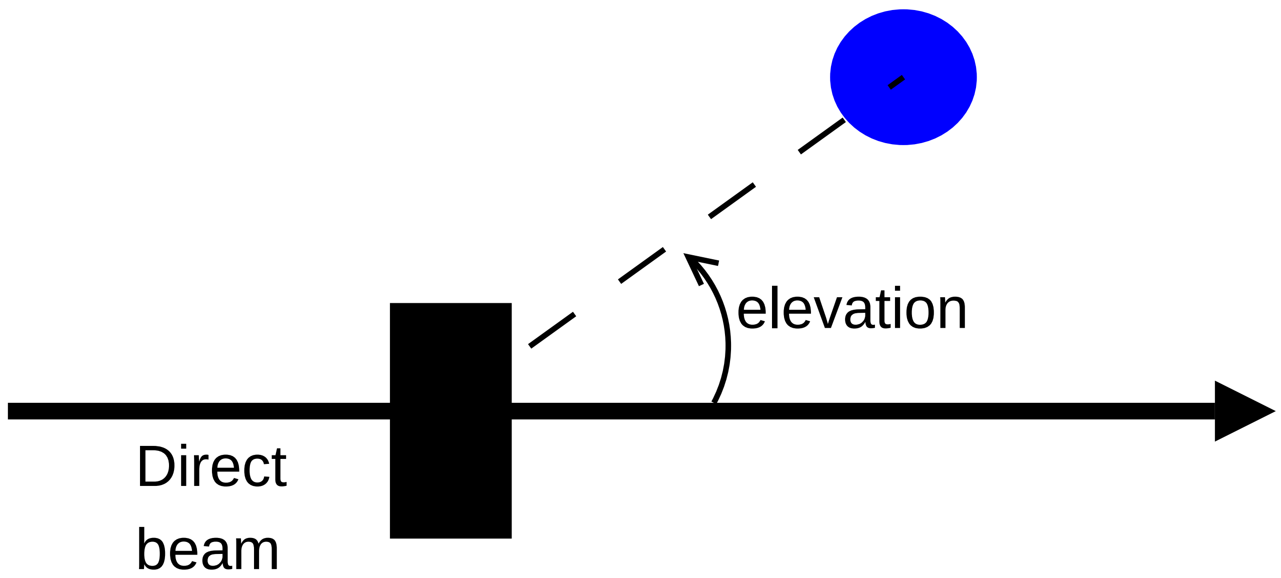
Polar Angle, Distance and Rotation

- The angle between the extension of the direct beam between a given component and its previous component and the projection of a third component onto the scattering plane is the polar_angle. This corresponds to longitude in a a geographical coordinate system. In scattering this is synonymous with two theta or gamma in normal beam geometry.
- Birds eye view on scattering plane:



Elevation

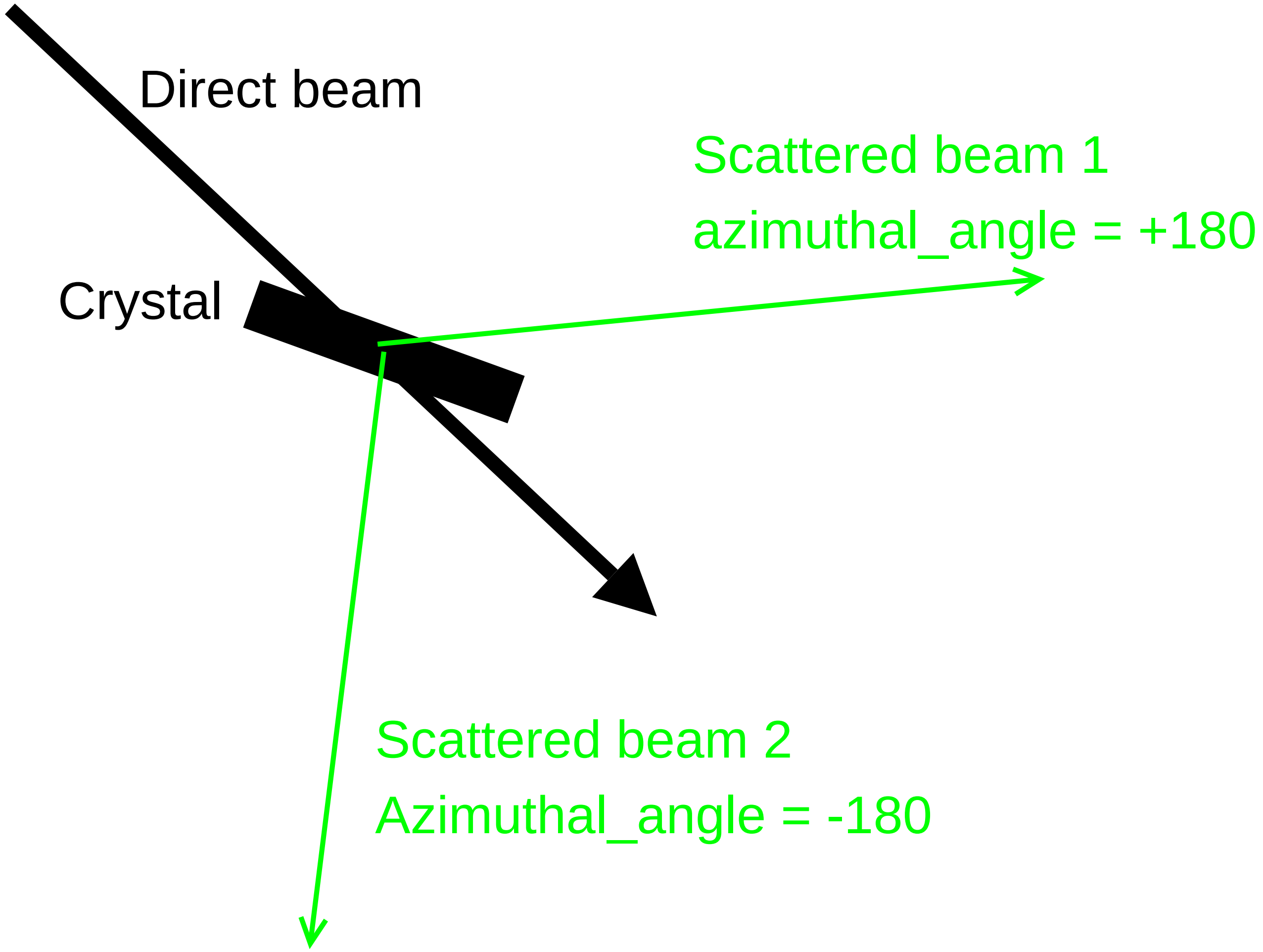
- Standing besides the instrument:



- Elevation corresponds to latitude in geography. In neutron scattering this is often the angle nu.

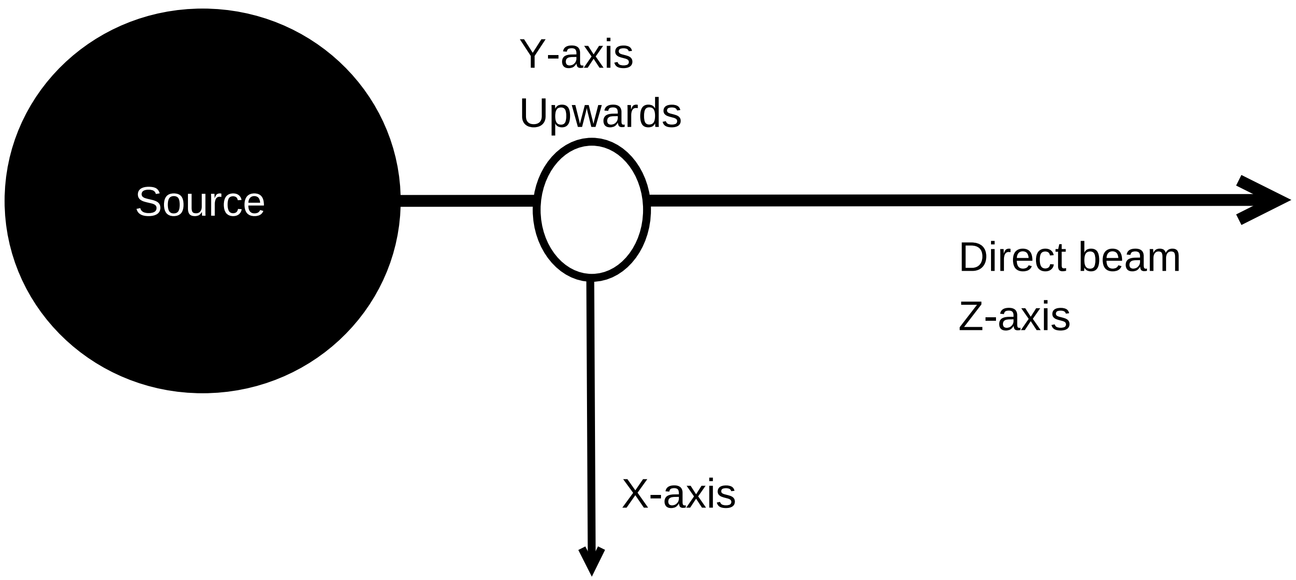
Azimuthal Angle

- Again birds eye view onto the scattering plane



McStas Coordinates

- Birds eye view again:



Miscellaneous Classes

NXreflection

+h:NX_FLOAT32:[1..n]
+k:NX_FLOAT32:[1..n]
+l:NX_FLOAT32:[1..n]

NXmirrormaterial

+substrate_material:String
+substrate_thickness:NX_FLOAT32
+substrate_roughness:NX_FLOAT32
+coating_material:String
+coating_thickness:NX_FLOAT32
+coating_roughness:NX_FLOAT32
+m_value:NX_FLOAT32

NXspectrum

+wavelength:NX_FLOAT32:[1..n]
+intensity:NX_FLOAT32:[1..n]

NXlog

+starttime:NXtime
+offset:NX_INT32:[1..n]
+value:NX_FLOAT32:[1..n]

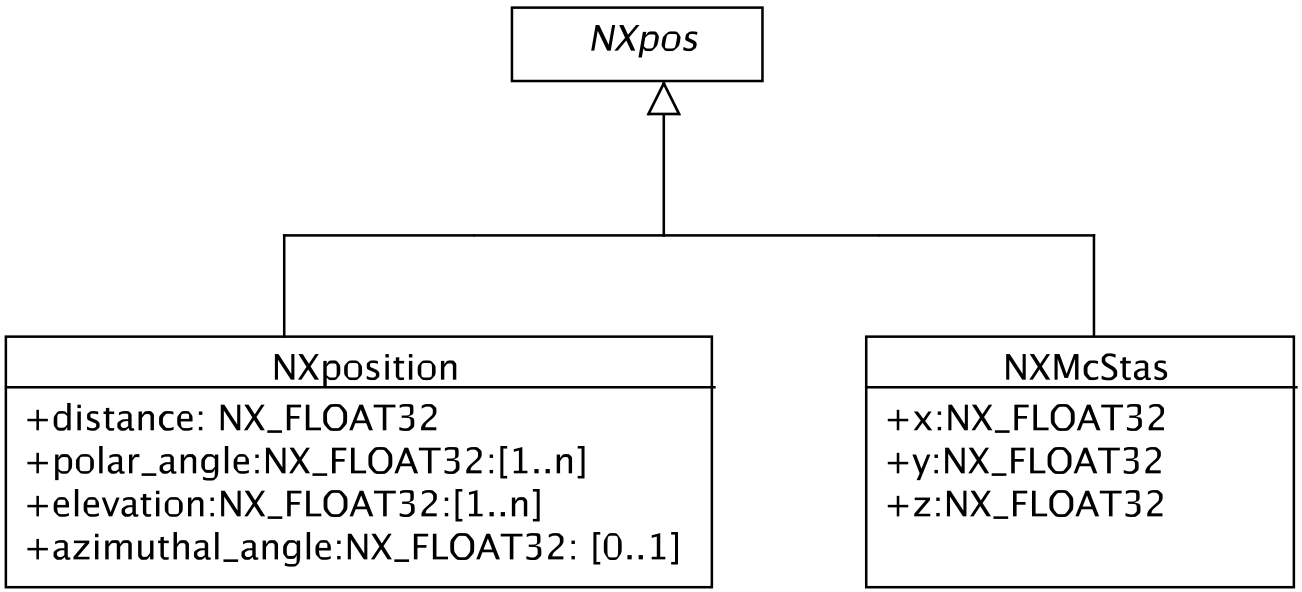
NXuser

+name:String
+affiliation:String
+address:String
+e-mail:String

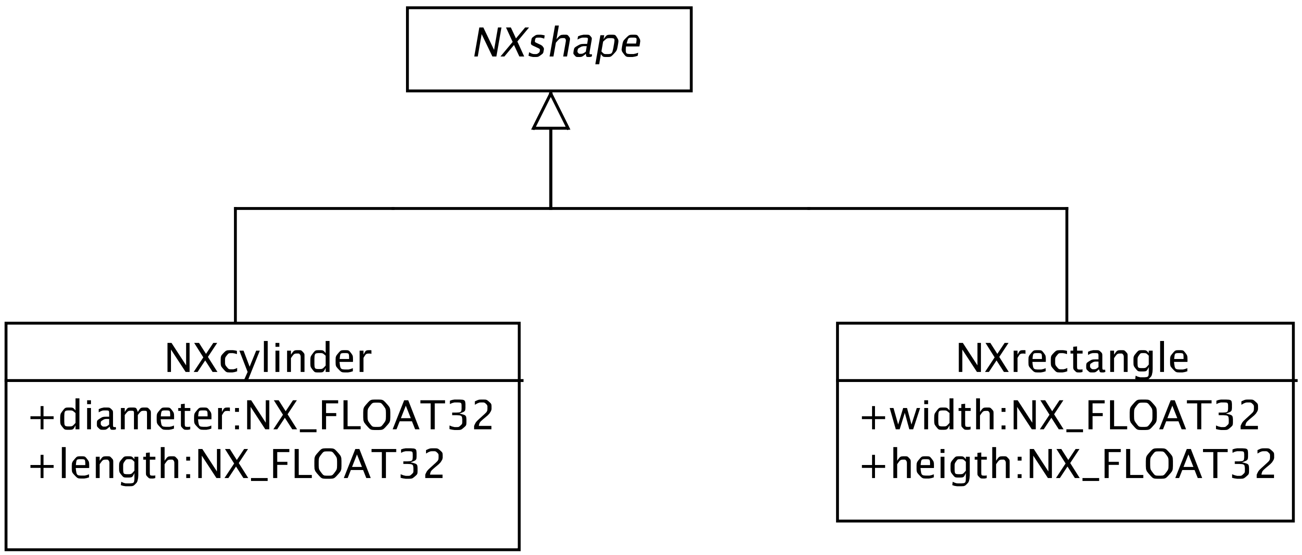
NXarchive

+user:NXuser
+instrument_reponsible:NXuser
+sample:String
+proposal_id: String
+experiment_stardate:NXtime
+title: String

NeXus Position

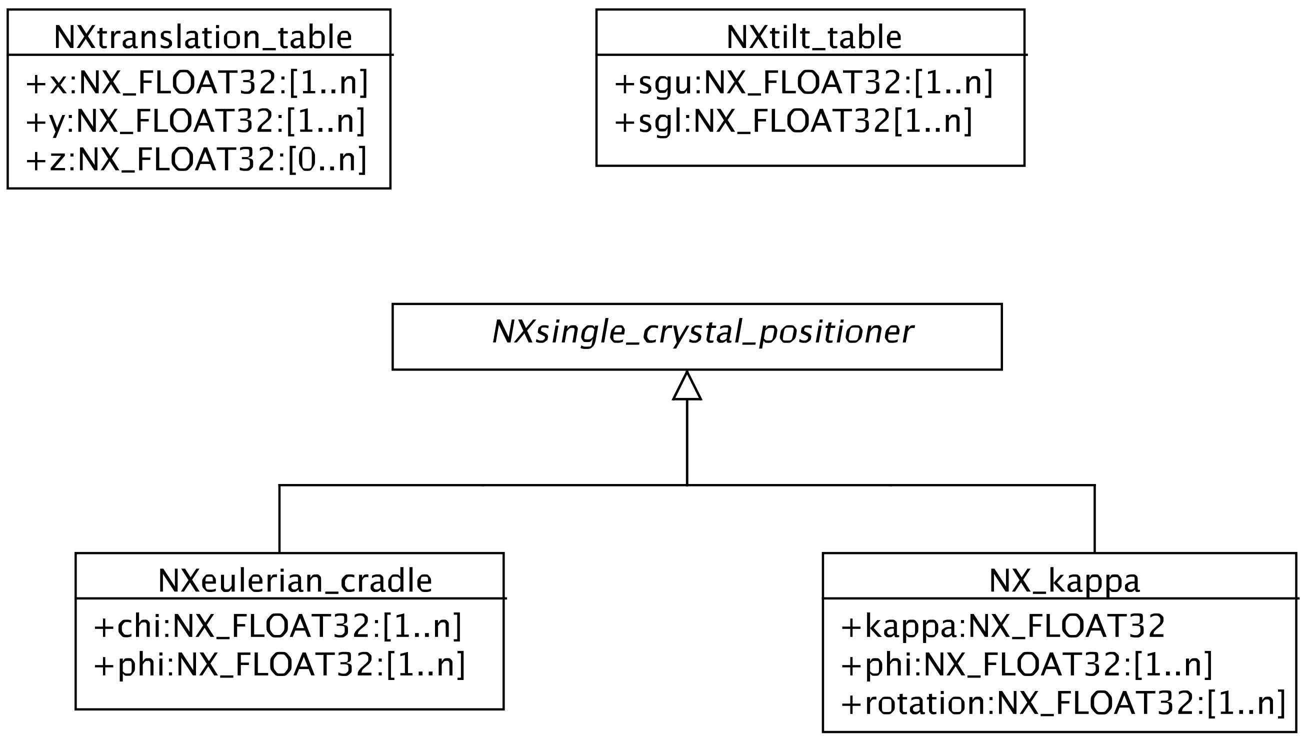


NeXus Shape

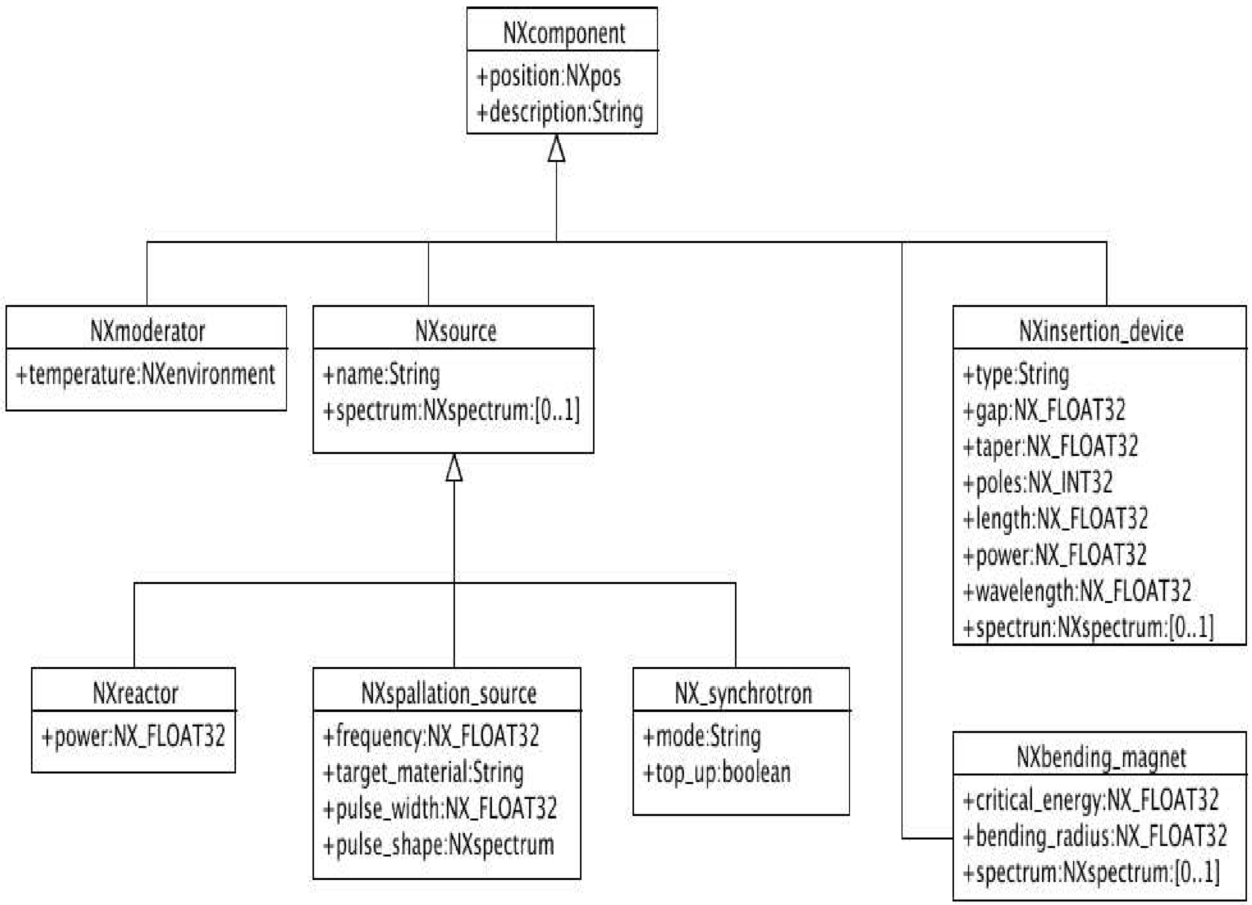


NXshape
NXcylinder
+diameter:NX_FLOAT32
+length:NX_FLOAT32
NXrectangle
+width:NX_FLOAT32
+heigth:NX_FLOAT32

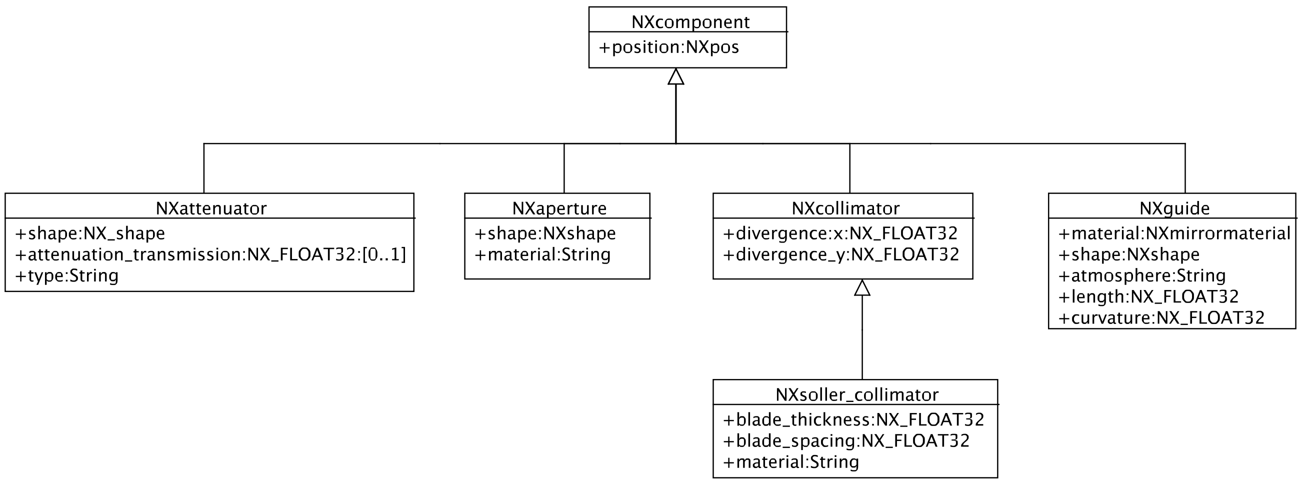
NeXus Stages



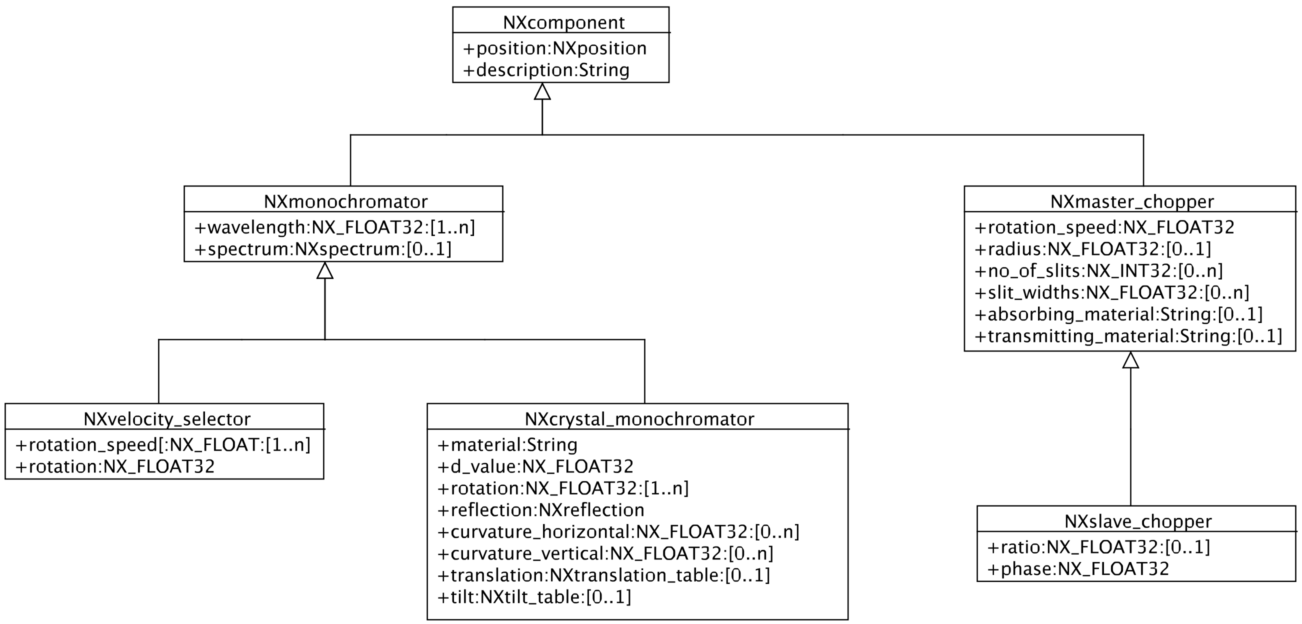
Source Components



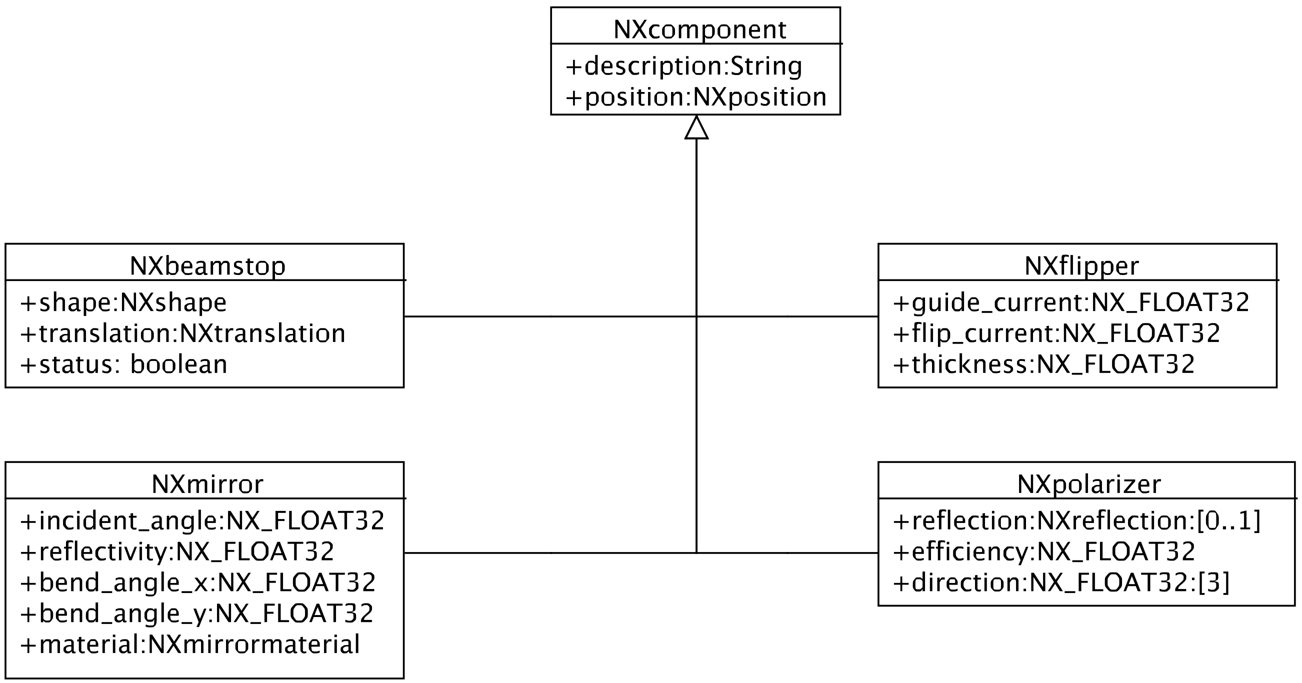
Passive Beam Line Components



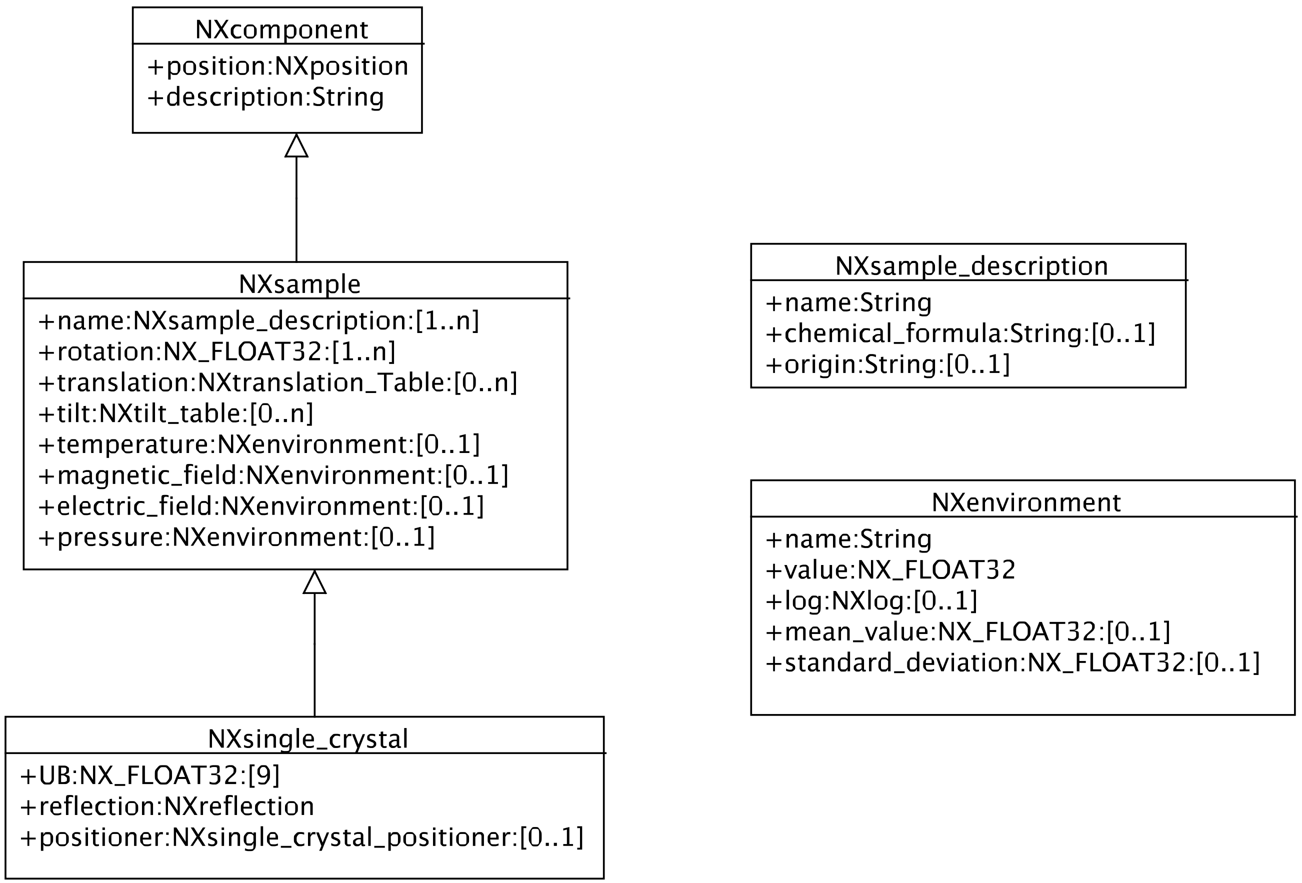
Active Beam Line Components



More Beamline Components



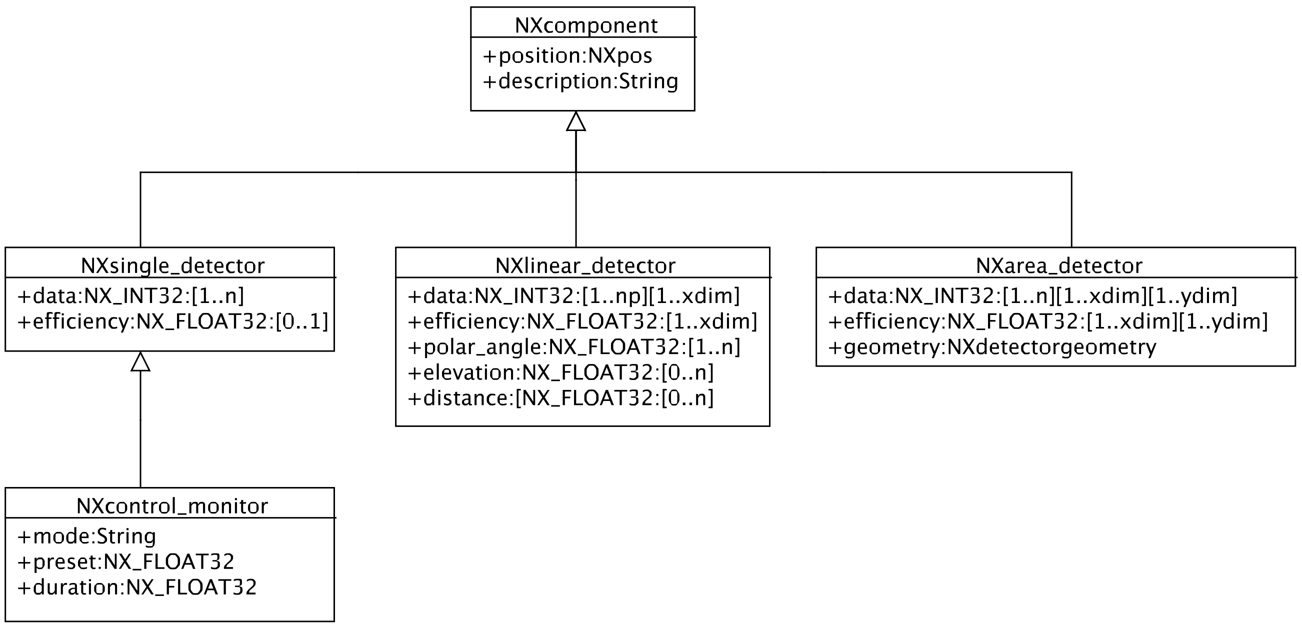
Samples


NXcomponent
+position:NXposition
+description:String
NXsample
+name:NXsample_description:[1..n]
+rotation:NX_FLOAT32:[1..n]
+translation:NXtranslation_Table:[0..n]
+tilt:NXtilt_table:[0..n]
+temperature:NXenvironment:[0..1]
+magnetic_field:NXenvironment:[0..1]
+electric_field:NXenvironment:[0..1]
+pressure:NXenvironment:[0..1]
NXsingle_crystal
+UB:NX_FLOAT32:[9]
+reflection:NXreflection
+positioner:NXsingle_crystal_positioner:[0..1]
NXsample_description
+name:String
+chemical_formula:String:[0..1]
+origin:String:[0..1]
NXenvironment
+name:String
+value:NX_FLOAT32
+log:NXlog:[0..1]
+mean_value:NX_FLOAT32:[0..1]
+standard_deviation:NX_FLOAT32:[0..1]

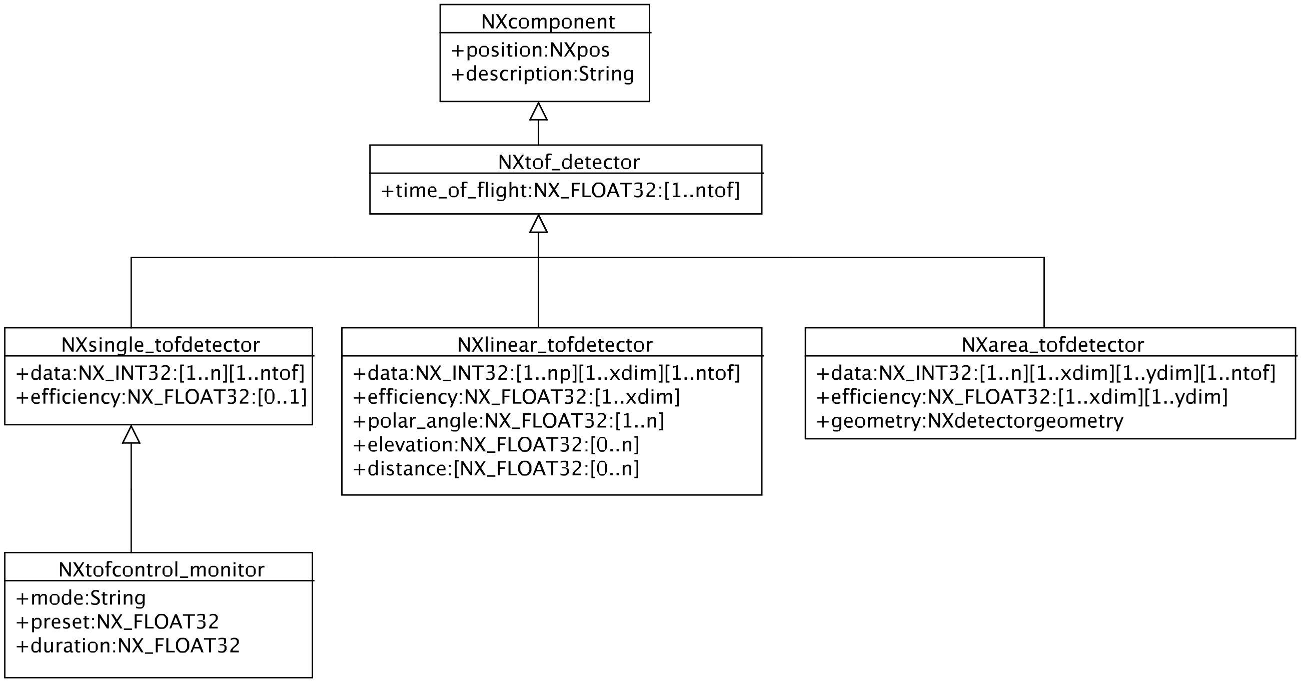
Detectors

- Concerning data handling there are the following types of detectors:
  - single detectors
  - linear detectors
  - area detectors
  - ID detectors
- Detectors have different geometries:
  - Detectors can have regular shapes: rectangles, lines etc which are best described as such
  - Some detectors (especially @ ISIS) are highly irregular: Then we need to describe each pixel.
- For each detector pixel we need to be able to deduce:
  - The scattering angle towards the previous component
  - The elevation out of the scattering plane
  - The distance to the previous component

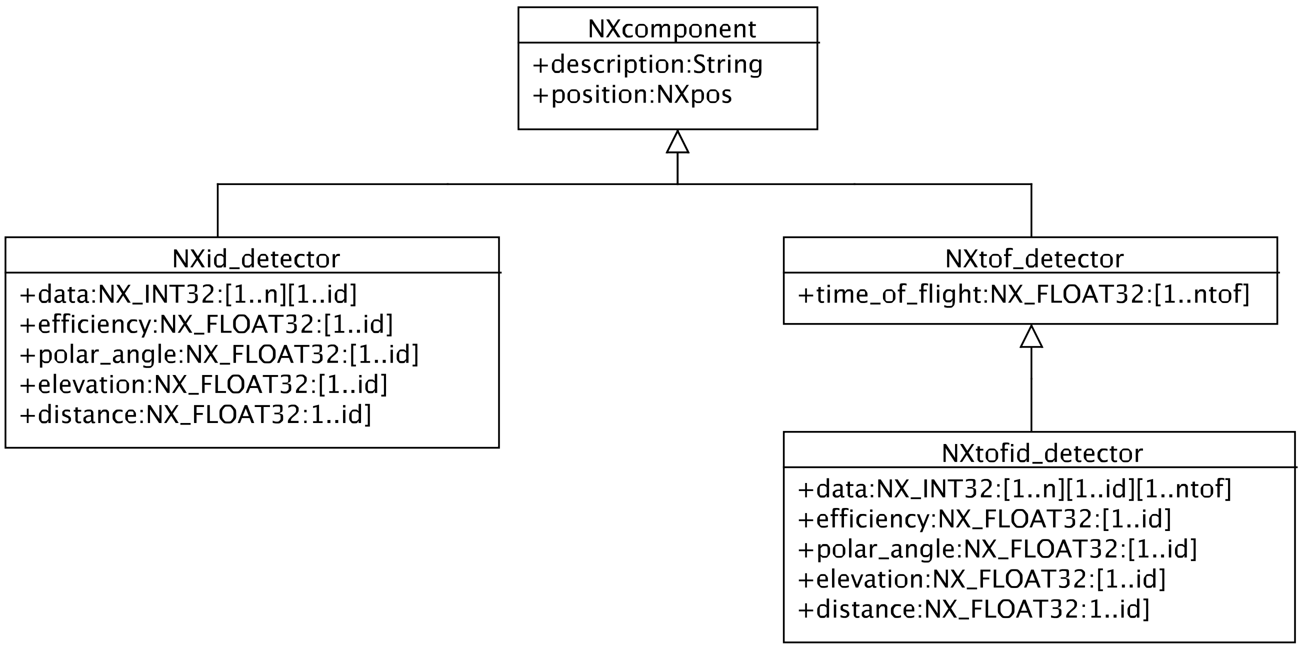
Non-TOF Detectors



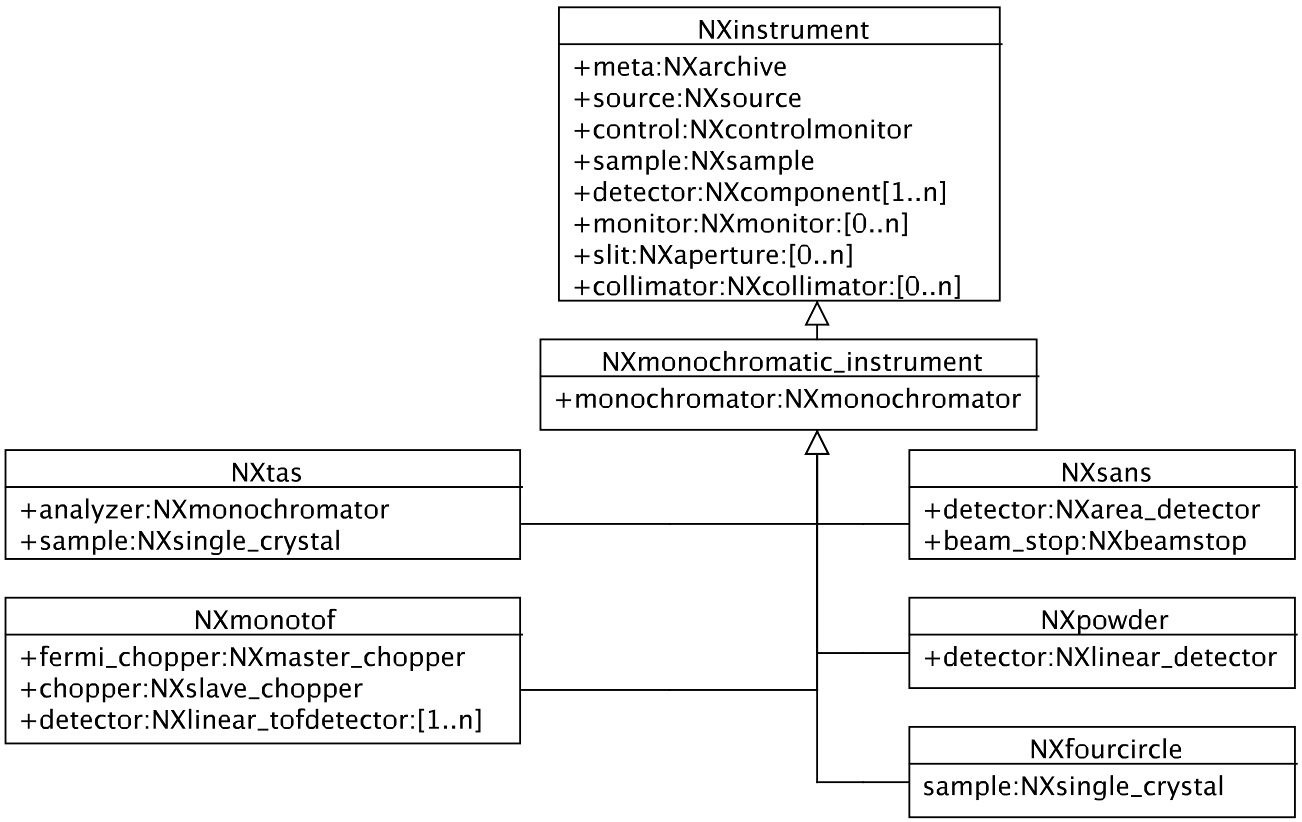
TOF-Detectors



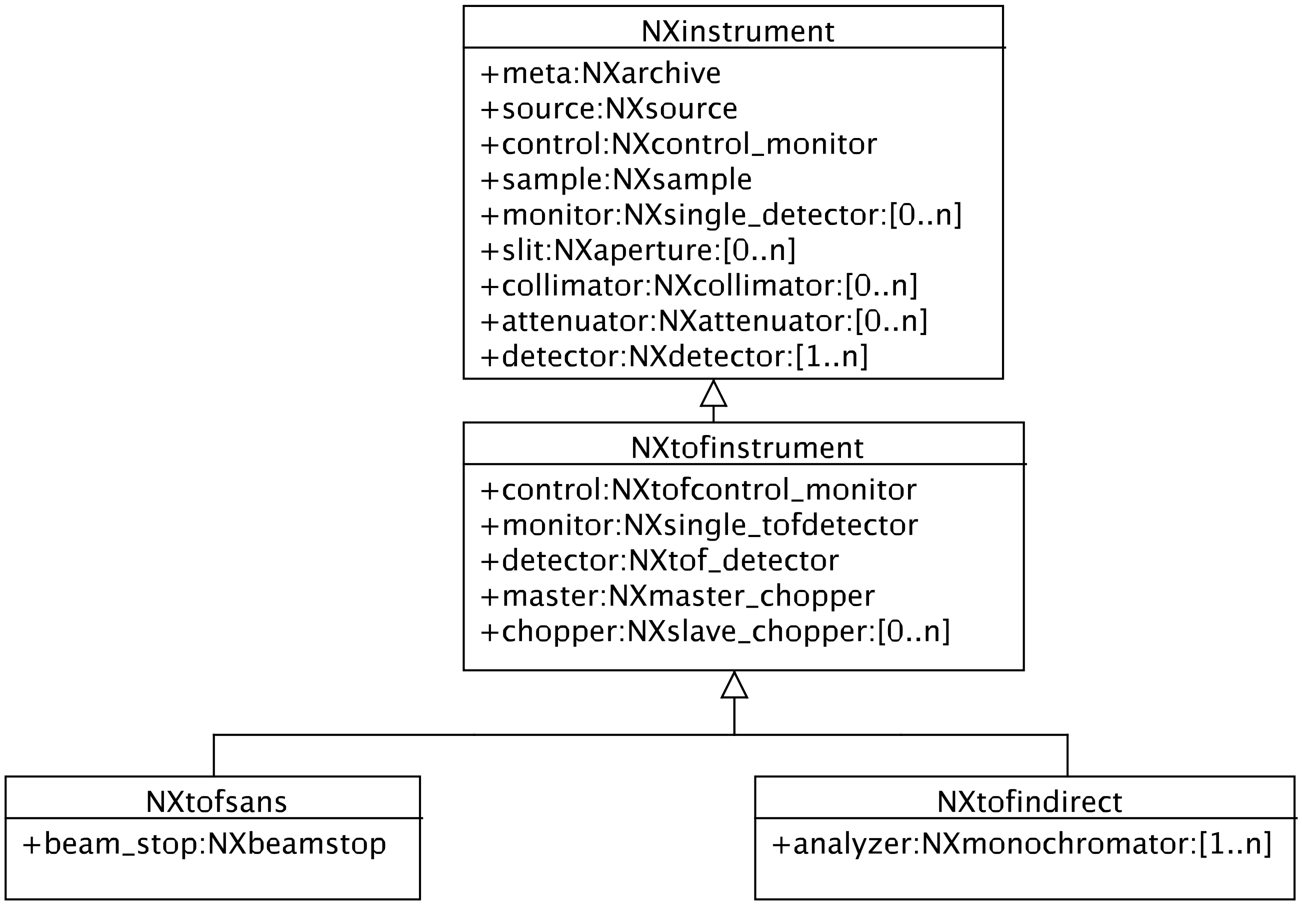
More Detectors



Monochromatic Instruments



TOF Instruments



Conclusion

- The current NeXus classes are messy due to lack of specialization
- More classes improve clarity
- Inheritance brings better maintainability: for instance adding NXellipitcal as a NXshape does not require changes downstream
- Caveats:
  - backwards compatability difficult
  - description in XML problematic