

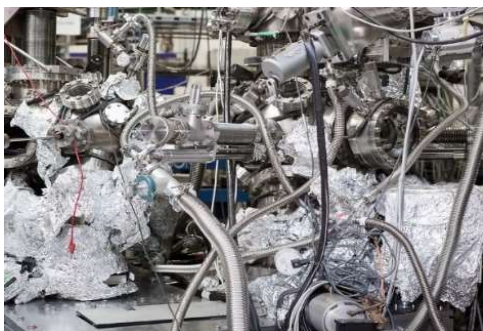
NeXus @ HZB: Instrumentation Metadata

Gerrit Günther

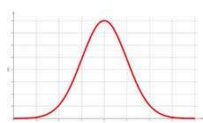
Helmholtz Metadata Collaboration (HMC)
Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)

www.helmholtz-metadata.de

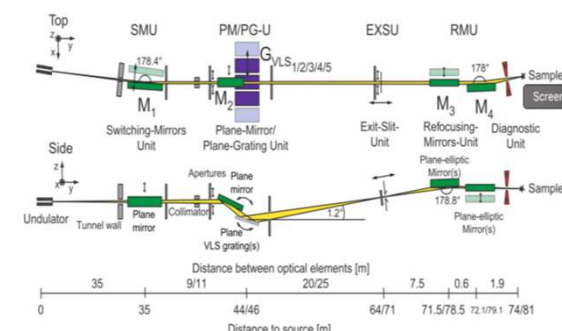
Instrument vs. Simulation



Beamline: Real World Object



Compare output (verification)



Simulation: Digital Object

Data curation

- instrument
- absorbed_beam
- beamline
 - Crystal
 - Crystal_1
 - Dipole
 - Slit
 - Slit_1
- incoming_beam
- monochromator
- name
- source



NeXus instrumentation



ICAT repository

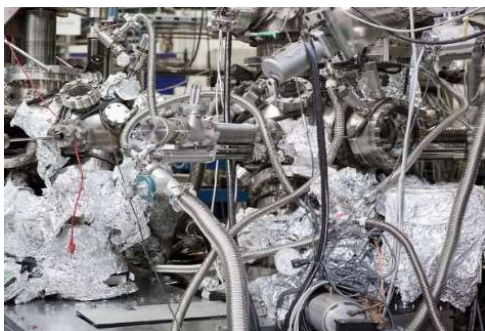
Simulation

```
<?xml version="1.0" encoding="UTF-8" ?>
<lab>
<version>1.0</version>
<beamline>

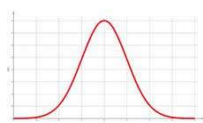
<object name="Dipole" type="Dipole">
  <param id="numberRays" enabled="T">50000</p>
  <param id="sourceWidth" enabled="T">0.065</p>
  <param id="sourceHeight" enabled="T">0.04</p>
</object>
</beamline>
</lab>
```

RayUI configuration file

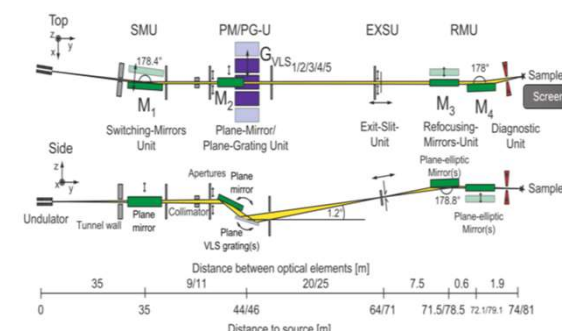
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NeXus instrumentation



ICAT repository

Get instrument information

Simulation

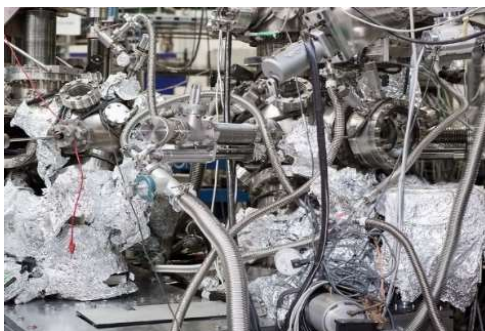
```
<?xml version="1.0" encoding="UTF-8" ?>
<lab>
<version>1.0</version>
<beamline>

<object name="Dipole" type="Dipole">
  <param id="numberRays" enabled="T">50000</p>
  <param id="sourceWidth" enabled="T">0.065</p>
  <param id="sourceHeight" enabled="T">0.04</p>

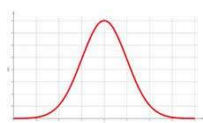
```

RayUI configuration file

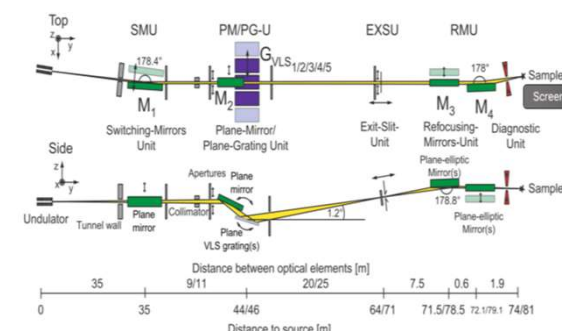
Instrument vs. Simulation



Beamline: Real World Object



Compare output (verification)



Simulation: Digital Object

Data curation

- instrument
- absorbed_beam
- beamline
 - Crystal
 - Crystal_1
 - Dipole
 - Slit
 - Slit_1
- incoming_beam
- monochromator
- name
- source



NeXus instrumentation



ICAT repository

Get instrument information

Create RayUI configuration file

Simulation

```
<?xml version="1.0" encoding="UTF-8" ?>
<lab>
<version>1.0</version>
<beamline>

<object name="Dipole" type="Dipole">
  <param id="numberRays" enabled="T">50000</p>
  <param id="sourceWidth" enabled="T">0.065</p>
  <param id="sourceHeight" enabled="T">0.04</p>
</object>
</beamline>
```

RayUI configuration file

Assign component's class: Ray type vs. NX_class

The screenshot shows a tree view on the left with the following structure:

- instrument
 - beamline
 - M4
 - M5
 - Premirror_M2
 - Slit_Horizontal
 - RayUI_parameters
 - alignmentError
 - azimuthalAngle
 - centralBeamstop
 - distancePreceding
 - geometricalShape
 - rotationXError
 - rotationYError
 - rotationZError
 - totalHeight
 - totalHeightStop
 - totalWidth
 - totalWidthStop
 - translationXError
 - translationYError
 - translationZError
 - worldPosition
 - worldXdirection
 - worldYdirection
 - worldZdirection
 - depends_on
 - transformations
 - x_gap
 - y_gap
 - Slit_Vertical
 - m1
 - pgm
 - u49_2
 - motors

The 'Object Attribute Info' window is open, showing the following table:

Name	Array Size	Value[50](...)
NX_class	Scalar	NXslit
Ray_preceding	Scalar	entry/instrument/beamline/pgm
Ray_type	Scalar	Slit
Ray_version	Scalar	1.1

A blue arrow points from the 'NXslit' value in the table to the 'NX_class' field in the JSON configuration file shown in the next block.

RayUI configuration file

```
<object name="Slit Horizontal" type="Slit">
  <param id="geometricalShape" comment="rectangle" enabled="T">0</param>
  <param id="totalWidth" enabled="T">3</param>
  <param id="totalHeight" enabled="T">20</param>
  <param id="centralBeamstop" comment="none" enabled="T">0</param>
  <param id="totalWidthStop" enabled="F">20</param>
  <param id="totalHeightStop" enabled="F">1</param>
  <param id="distancePreceding" enabled="T">2000</param>
  <param id="azimuthalAngle" enabled="T">0</param>
  <param id="alignmentError" comment="No" enabled="T">1</param>
  <param id="translationXError" enabled="F">0</param>
  <param id="translationYError" enabled="F">0</param>
  <param id="translationZError" enabled="F">0</param>
  <param id="rotationXError" enabled="F">0</param>
  <param id="rotationYError" enabled="F">0</param>
  <param id="rotationZError" enabled="F">0</param>
  <param id="worldPosition" enabled="F">
    <x>-718.279</x>
```

```
Slit.json
1 {
2   "NX_class": "NXslit",
3   "Ray_type": "Slit",
4   "data": {
5     "totalWidth": {
6       "value": {
7         "x_gap": "text"
8       }
9     },
10    "attributes": {
11      "units": "const:mm",
12      "enabled": "enabled"
13    }
14  },
15  "totalHeight": {
16    "value": {
17      "y_gap": "text"
```

A blue arrow points from the 'NXslit' value in the table to the 'NX_class' field in the JSON configuration file. Another blue arrow points from the 'Slit' value in the table to the 'Ray_type' field in the JSON configuration file.

json mapping

Assign NeXus term: Ray parameter vs. NeXus field

The screenshot shows a tree view on the left with the following structure:

- instrument
 - beamline
 - M4
 - M5
 - Premirror_M2
 - Slit_Horizontal
 - RayUI_parameters
 - alignmentError
 - azimuthalAngle
 - centralBeamstop
 - distancePreceding
 - geometricalShape
 - rotationXError
 - rotationYError
 - rotationZError
 - totalHeight
 - totalHeightStop
 - totalWidth
 - totalWidthStop
 - translationXError
 - translationYError
 - translationZError
 - worldPosition
 - worldXdirection
 - worldYdirection
 - worldZdirection
 - depends_on
 - transformations
 - x_gap
 - y_gap
 - Slit_Vertical
 - m1
 - pgm
 - u49_2
 - motors

The 'Object Attribute Info' window shows the following table:

Name	Array Size	Value[50](...)
NX_class	Scalar	NXslit
Ray_preceding	Scalar	entry/instrument/beamline/pgm
Ray_type	Scalar	Slit
Ray_version	Scalar	1.1

A small window titled 'x_gap at /entry/instru...' shows a '0-based' input field with the value '0' and a display field showing '1.91018...'.

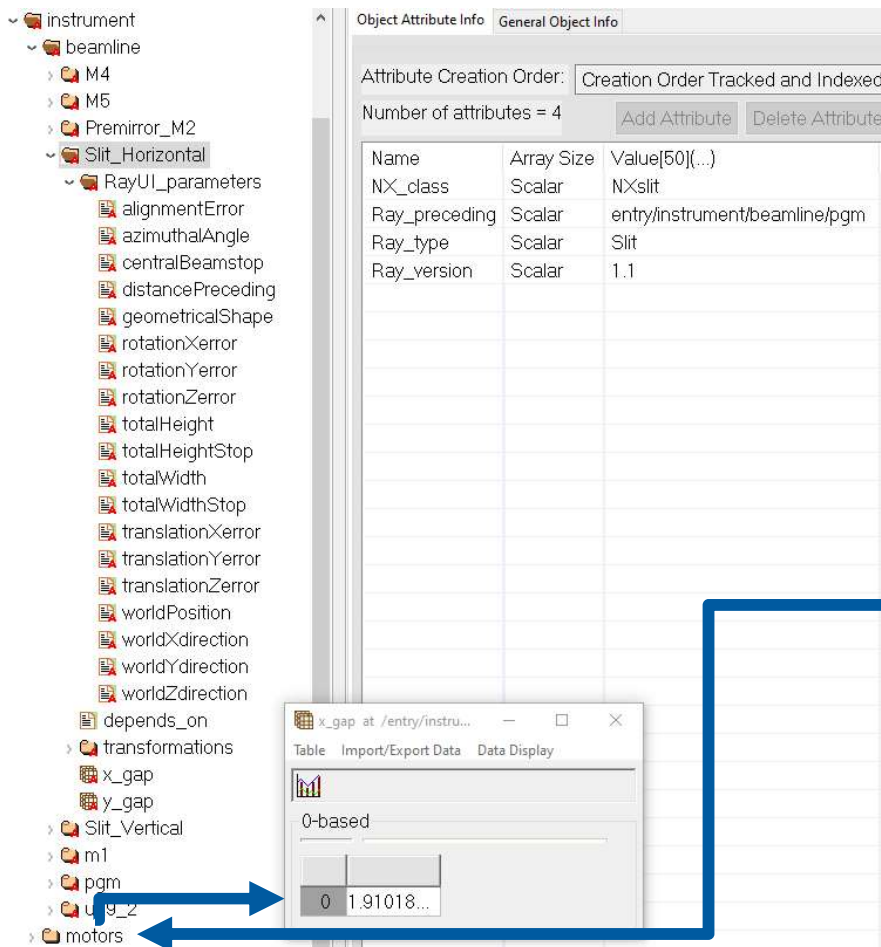
RayUI configuration file

```
<object name="Slit Horizontal" type="Slit">
  <param id="geometricalShape" comment="rectangle" enabled="T">0</param>
  <param id="totalWidth" enabled="T">3</param>
  <param id="totalHeight" enabled="T">20</param>
  <param id="centralBeamstop" comment="none" enabled="T">0</param>
  <param id="totalWidthStop" enabled="F">20</param>
  <param id="totalHeightStop" enabled="F">1</param>
  <param id="distancePreceding" enabled="T">2000</param>
  <param id="azimuthalAngle" enabled="T">0</param>
  <param id="alignmentError" comment="No" enabled="T">1</param>
  <param id="translationXError" enabled="F">0</param>
  <param id="translationYError" enabled="F">0</param>
  <param id="translationZError" enabled="F">0</param>
  <param id="rotationXError" enabled="F">0</param>
  <param id="rotationYError" enabled="F">0</param>
  <param id="rotationZError" enabled="F">0</param>
  <param id="worldPosition" enabled="F">
    <x>-718.279</x>
  </param>
</object>
```

```
Slit.json
1 {
2   "NX_class": "NXslit",
3   "Ray_type": "Slit",
4   "data": {
5     "totalWidth": {
6       "value": {
7         "x_gap": "text"
8       }
9     },
10    "attributes": {
11      "units": "const:mm",
12      "enabled": "enabled"
13    }
14  },
15  "totalHeight": {
16    "value": {
17      "y_gap": "text"
18    }
19  }
20 }
```

json mapping

Include current instrument state: Ray parameter vs. motor value



The screenshot shows a tree view on the left with the following structure:

- instrument
 - beamline
 - M4
 - M5
 - Premirror_M2
 - Slit_Horizontal
 - RayUI_parameters
 - alignmentError
 - azimuthalAngle
 - centralBeamstop
 - distancePreceding
 - geometricalShape
 - rotationXError
 - rotationYError
 - rotationZError
 - totalHeight
 - totalHeightStop
 - totalWidth
 - totalWidthStop
 - translationXError
 - translationYError
 - translationZError
 - worldPosition
 - worldXdirection
 - worldYdirection
 - worldZdirection
 - depends_on
 - transformations
 - x_gap
 - y_gap
 - Slit_Vertical
 - m1
 - pgm
 - u_g_2
 - motors

The 'Object Attribute Info' window shows the following table:

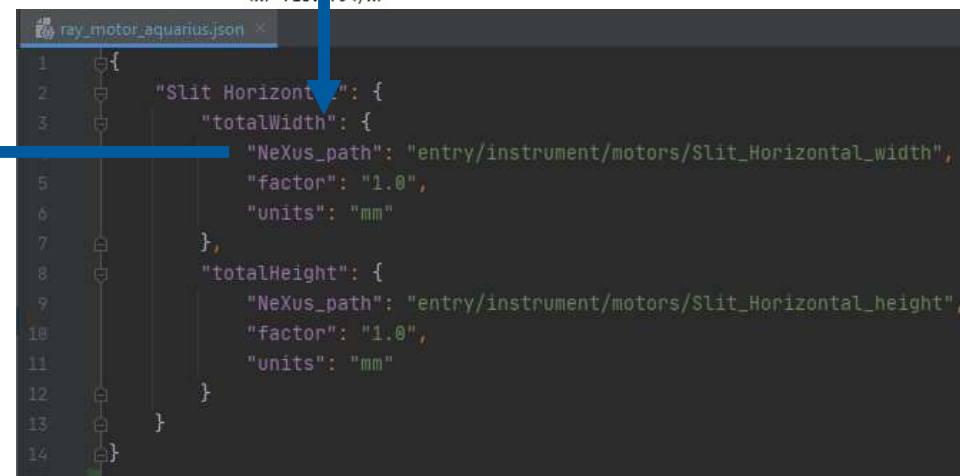
Name	Array Size	Value[50](...)
NX_class	Scalar	NXslit
Ray_preceding	Scalar	entry/instrument/beamline/pgm
Ray_type	Scalar	Slit
Ray_version	Scalar	1.1

A 'Data Display' window shows a table with the following data:

0-based	
0	1.91018...

RayUI configuration file

```
<object name="Slit Horizontal" type="Slit">
  <param id="geometricalShape" comment="rectangle" enabled="T">0</param>
  <param id="totalWidth" enabled="T">3</param>
  <param id="totalHeight" enabled="T">20</param>
  <param id="centralBeamstop" comment="none" enabled="T">0</param>
  <param id="totalWidthStop" enabled="F">20</param>
  <param id="totalHeightStop" enabled="F">1</param>
  <param id="distancePreceding" enabled="T">2000</param>
  <param id="azimuthalAngle" enabled="T">0</param>
  <param id="alignmentError" comment="No" enabled="T">1</param>
  <param id="translationXError" enabled="F">0</param>
  <param id="translationYError" enabled="F">0</param>
  <param id="translationZError" enabled="F">0</param>
  <param id="rotationXError" enabled="F">0</param>
  <param id="rotationYError" enabled="F">0</param>
  <param id="rotationZError" enabled="F">0</param>
  <param id="worldPosition" enabled="F">
    <x>-718.79</x>
```



```
ray_motor_aquarius.json
1 {
2   "Slit Horizontal": {
3     "totalWidth": {
4       "NXus_path": "entry/instrument/motors/Slit_Horizontal_width",
5       "factor": "1.0",
6       "units": "mm"
7     },
8     "totalHeight": {
9       "NXus_path": "entry/instrument/motors/Slit_Horizontal_height",
10      "factor": "1.0",
11      "units": "mm"
12    }
13  }
14 }
```

Include instrument geometry (...and shape)

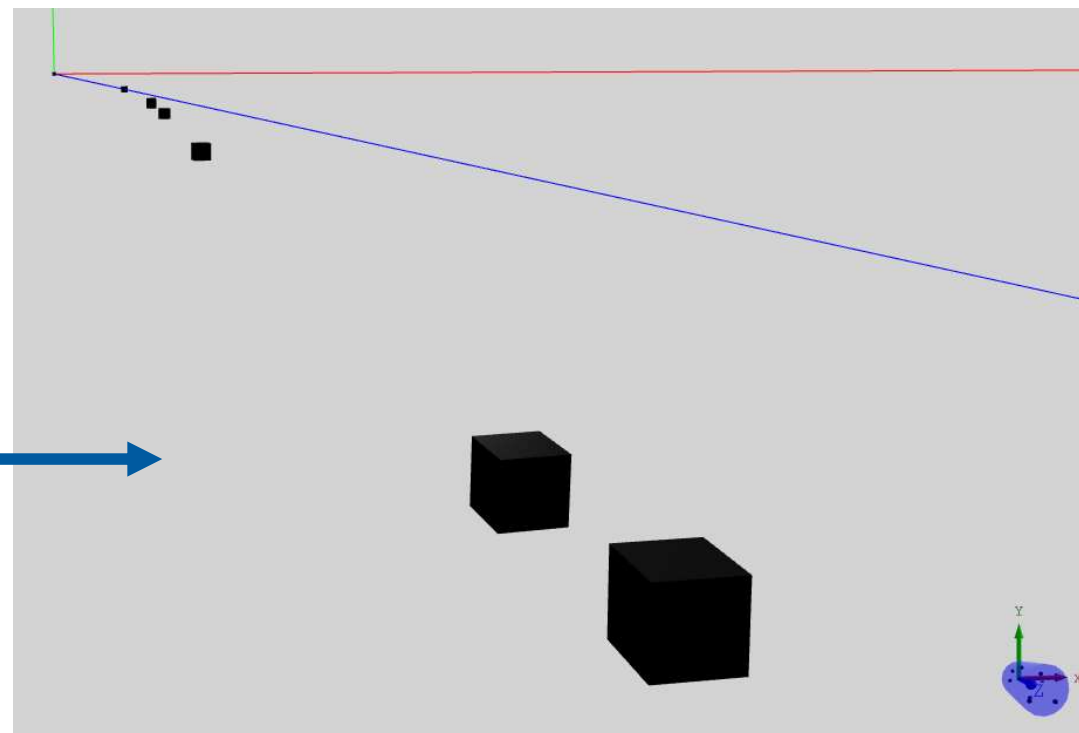
The screenshot shows the NeXus Constructor interface. On the left is a tree view of the instrument structure:

- instrument
 - beamline
 - M4
 - M5
 - Premirror_M2
 - Slit_Horizontal
 - RayUI_parameters
 - alignmentError
 - azimuthalAngle
 - centralBeamstop
 - distancePreceding
 - geometricalShape
 - rotationXerror
 - rotationYerror
 - rotationZerror
 - totalHeight
 - totalHeightStop
 - totalWidth
 - totalWidthStop
 - translationXerror
 - translationYerror
 - translationZerror
 - worldPosition
 - worldXdirection
 - worldYdirection
 - worldZdirection
 - depends_on
 - transformations
 - x_gap
 - y_gap
 - Slit_Vertical
 - m1
 - pgm
 - u49_2
 - motors

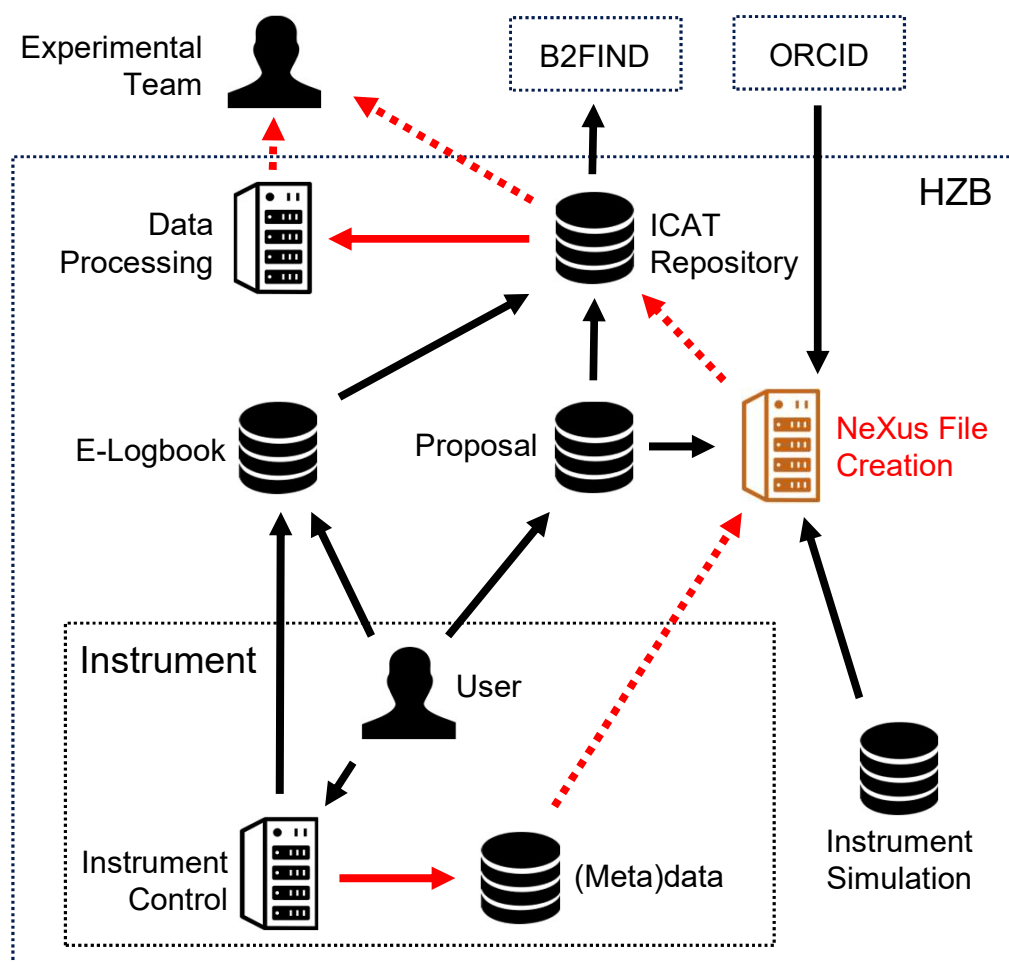
The 'Object Attribute Info' window is open, showing the following table:

Name	Array Size	Value[50](...)
NX_class	Scalar	NXslit
Ray_preceding	Scalar	entry/instrument/beamline/pgm
Ray_type	Scalar	Slit
Ray_version	Scalar	1.1

A blue arrow points from the 'x_gap' attribute in the tree view to the 'x_gap at /entry/instru...' window, which shows a value of 1.91018...



NeXus Constructor (<https://github.com/ess-dmsc/nexus-creator>)



NeXus File Pipeline Prototype:

- NeXus file creation based on h5py
- Heterogenous software landscape: external service
 - Independent of instrument operation
 - Regular updates
- Connection to additional sources, e.g.
 - Proposal system
 - ORCID

Current Work (...):

- Connection of instrument to NeXus file creation
- ICAT repository ingestion
- Keycloak for non-HZB user access
- Instrumentation from simulation configuration files