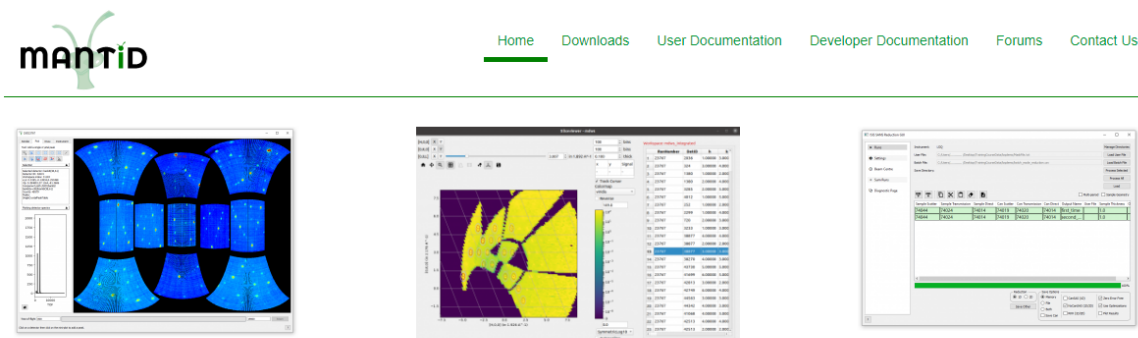


Mantid and data reduction tutorial

Single Crystal Workshop
ACNS Conference
June 20, 2024

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About Mantid

The Mantid project provides a framework that supports high-performance computing and visualisation of materials science data.

Mantid has been created to manipulate and analyse neutron scattering and muon spectroscopy data, but could be applied to many other techniques.

The framework is [open source](#) and supported on [multiple target platforms](#) (Windows, Linux, Mac) [📄](#). It includes and benefits from many [other open source projects](#) [📄](#).

Citing Mantid

O. Arnold, et al., Mantid—Data analysis and visualization package for neutron scattering and μ SR experiments, Nuclear Instruments and Methods in Physics Research Section A, Volume 764, 11 November 2014, Pages 156-166, <http://dx.doi.org/10.1016/j.nima.2014.07.029> [📄](#).

Workbench has replaced MantidPlot

MantidPlot served us well for 12 years, but has aged and cannot be supported in newer operating systems. MantidWorkbench is a replacement using newer technologies and more robust development approaches. **version 5.1** [📄](#) (released September 2020) is the final release to include MantidPlot.

- [Workbench Feature Comparison](#)

Quick Start Guide

We have a collection of Mantid training courses that are a great place to start. We run these at facilities as a hands on course (keep an eye on the news section for upcoming courses), but you can also use the course as self-paced training.

News

29 Sep 2021

[Registration Open for User Meeting 2021: 29th/30th Nov 2021](#)

29 Sep 2021

[Version 6.2.0 is available](#)

[News Archive](#) [📄](#) | [Help Forum](#) [📄](#) | [Developer site](#) [📄](#)

Mantid Workbench

Workbench is the graphical user interface for Mantid. Opening Workbench, the first page presented is a splash screen for selecting a facility and instrument. This step is optional, but it may be desirable as some shortcut presets are automatically filled in to reflect the chosen instrument.



Selecting a default facility (SNS/HFIR) and instrument (TOPAZ/MANDI/CORELLI/SNAP/DEMAND/WAND²).

There is a option to skip this splash screen the next time Workbench is opened. Click this before closing the screen in order to save as default.

Mantid Workbench

integrate

- PeaksWorkspace
- Columns: 22
- Rows: 2030
- 919 kB
- Instrument: TOPAZ (2022-Nov-21 to 2100-Jan-31)Instrume...
- Parameters from: /home/zgjf/git/mantid/instrument/TOP...
- Run start: 2022-Dec-14 12:47:08
- Run end: 2022-Dec-14 12:59:14
- Sample: a 11.9, b 11.9, c 11.9; alpha 90, beta 90, gamma 90
- Crystallography: kf-ki
- Memory used: 919 kB

intensity

- md**
- MDEventWorkspace<MDEvent,3>
- Title:
- Dim 0: (Q_sample_x) -24.7368 to 24.7368 in 2 bins. Id=Q1
- Dim 1: (Q_sample_y) -24.7368 to 24.7368 in 5 bins. Id=Q2
- Dim 2: (Q_sample_z) -24.7368 to 24.7368 in 5 bins. Id=Q3
- Crystallography: kf-ki
- 782193 MDBoxes (161938 kB)
- 6308 MDGridBoxes (1650 kB)
- Not file backed.
- Instrument: TOPAZ (2022-Nov-21 to 2100-Jan-31)Instrume...
- Parameters from: /home/zgjf/git/mantid/instrument/TOP...
- Run start: 2022-Dec-14 12:47:08
- Run end: 2022-Dec-14 12:59:14
- Events: 26050013
- Memory used: 855 MB

Workspaces. #

Algorithms

Execute FindUBUsingLatticeParameters

- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Diagnostics
- Diffraction
- Events
- Examples
- ILL
- Inelastic
- MDAlgorithms
- Muon
- Optimization
- Reflectometry
- SANS
- SANS

Idle.

Algorithms.

Main page

The main page provides several areas to navigate. Among them are:

- Workspaces (upper left): viewing data
- Algorithms/Plots (lower left): running a data processing step or viewing a previous plot
- Editor/IPython (central): running a script or performing calculations
- Messages (right): console messages including errors, intermediate results, and status

Mantid Workbench.

The workspaces area contains a list of all workspaces currently in memory. The dropdown below each name contains information about the workspace including its type.

Editor

+ New* x

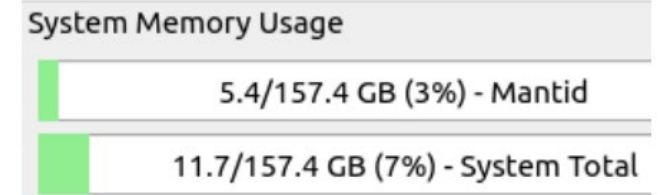
```

1 # import mantid algorithms, numpy and matplotlib
2 from mantid.simpleapi import *
3 import matplotlib.pyplot as plt
4 import numpy as np
    
```

Mantid Workbench editor. #



Script editor play/stop buttons.



IPython

```

Jupyter QtConsole 5.5.1
Python 3.10.13 | packaged by conda-forge | (main, Oct 26 2023, 18:07:37) [GCC 12.3.0]
Type 'copyright', 'credits' or 'license' for more information
IPython 8.19.0 -- An enhanced Interactive Python. Type '?' for help.

In [1]:
    
```

IPython console.

| No. | Plot Name |
|-----|-------------------|
| 1 | signal-to-noise-1 |

Plots. #

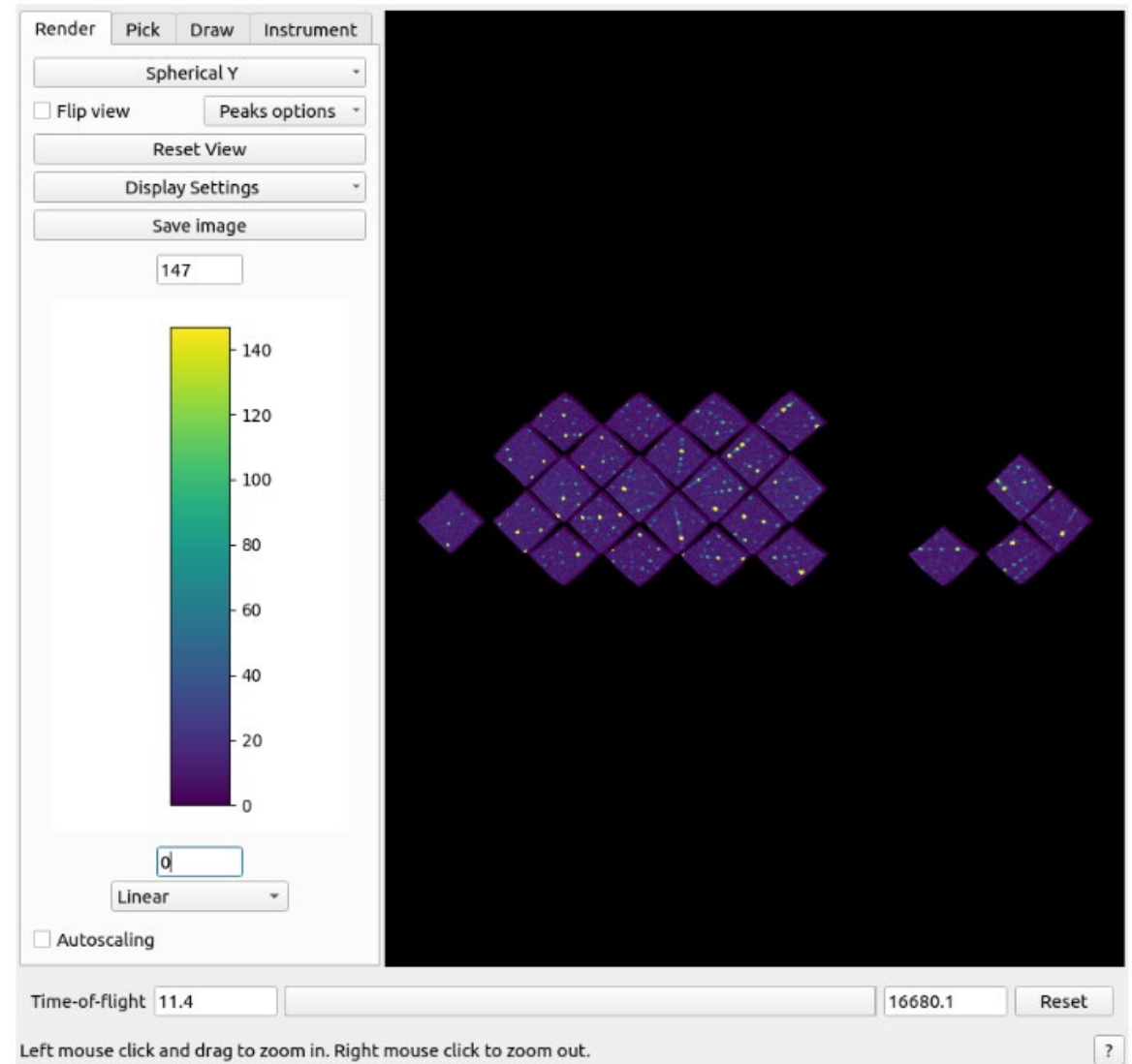
Instrument viewer

For event data, an instrument view is available for investigating the data in detector-space. This is done by navigating to the workspace area:

- Right-click *data*
- Left-click *Show Instrument*

```
data
├── EventWorkspace
│   ├── Title: YAG_2-3_BN_35
│   ├── Histograms: 1638400
│   ├── Bins: 500
│   └── Histogram
│       ├── X axis: Time-of-flight / microsecond
│       ├── Y axis: Counts
│       └── Distribution: False
│           ├── Instrument: TOPAZ (2022-Nov-21 to 2100-Jan-31)Instrument from: /SNS/TOPAZ/IPTS-3...
│           ├── Parameters from: /home/zgf/git/mantid/instrument/TOPAZ_Parameters.xml
│           ├── Run start: 2022-Dec-14 12:47:08
│           ├── Run end: 2022-Dec-14 12:59:14
│           ├── Events: 26561178
│           └── Memory used: 1100 MB
```

Event data workspace.

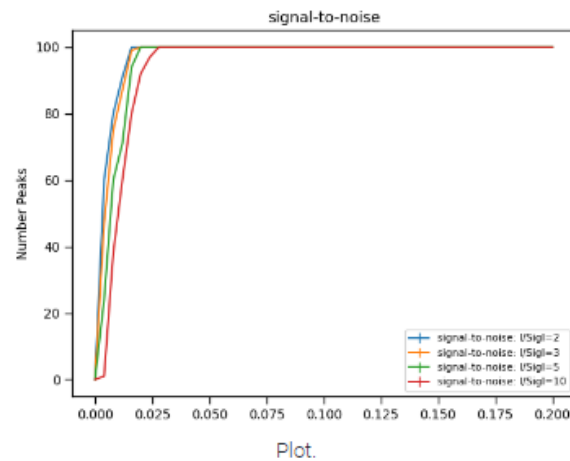


Plotting

Plot viewer

Certain workspaces can be viewed as a plot.

- Right-click *signal-to-noise*
- Right-click *Plot* > `Spectrum`
- Right-click *Plot All*



It is possible to change the look of the plot and save it to a file. Other options include the capability to fit the data or generate a script to generate the plot through the editor.



Plot tool bar.

Slice viewer

Slice viewer allows data to be displayed in various ways. For 3d data, the display axes X (horizontal) and Y (vertical) directions can be chosen. The remaining axis can be sliced where its level is chosen from the slider.

The slice viewer is a valuable tool for investigating three-dimensional data like reciprocal space data. This includes rebinnable 3d-event workspaces and 3d-histogram workspaces. Slice viewer for a workspace can be opened from the workspace area:

- Right-click *md*
- Left-click *Show Slice Viewer*

Q_sample_x X Y 400 bins

Q_sample_y X Y 0.000 Angstrom^-1 0.100 thick

Q_sample_z X Y 400 bins

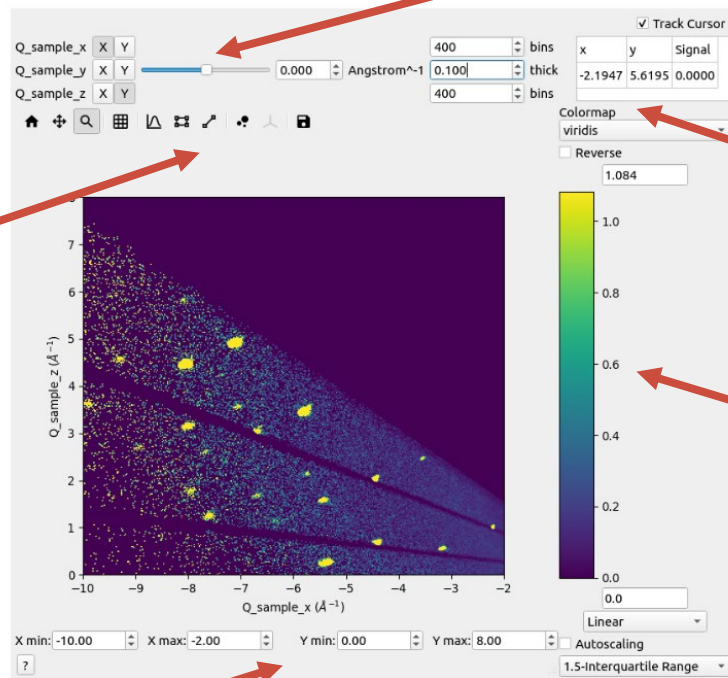
Display axis and slider value shown of a typical x0z-slice for Q-sample data. #

```
md
MDEventWorkspace=MDEvent_3-
Title:
Dim 0: (Q_sample_x) -24.7368 to 24.7368 in 5 bins. Id=Q1
Dim 1: (Q_sample_y) -24.7368 to 24.7368 in 5 bins. Id=Q2
Dim 2: (Q_sample_z) -24.7368 to 24.7368 in 5 bins. Id=Q3
Crystallography: kf-kf
782193 MDBoxes (161938 kb)
6308 MDGridBoxes (1650 kb)
Not file backed.
Instrument: TOPAZ (2022-Nov-21 to 2100-Jan-31) Instrument from: /SNS/10PAZ/PTS-3...
Parameters from: /home/jeff.gilman/inst/instrument/TOPAZ_Parameters.xml
Run start: 2022-Dec-14 12:47:08
Run end: 2022-Dec-14 12:59:14
Events: 26050613
Memory used: 855 MB
```

Event data workspace. #



Tool bar options.

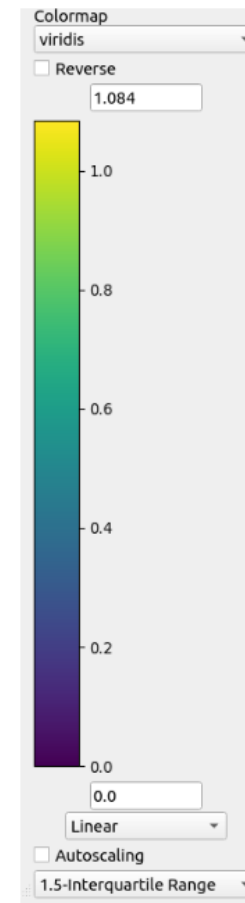


Slice viewer.

Track Cursor

| x | y | Signal |
|---------|--------|---------|
| -5.8068 | 3.4516 | 99.9456 |

Cursor position and value.



X min: -10.00 X max: -2.00 Y min: 0.00 Y max: 8.00

Display axis zoom limits.

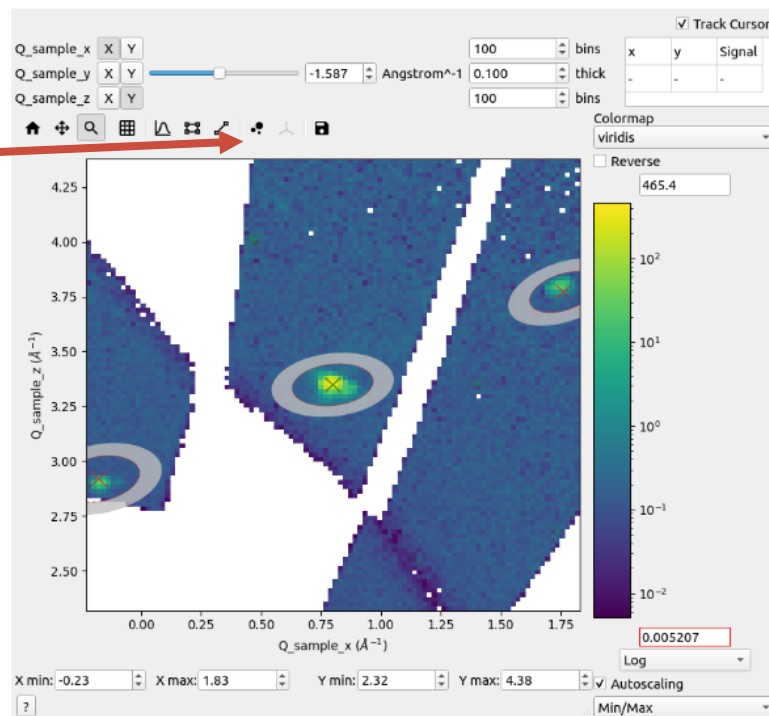
Slice viewer

| Workspace | Overlay? |
|-------------|--------------------------|
| 1 integrate | <input type="checkbox"/> |
| 2 peaks | <input type="checkbox"/> |
| 3 strong | <input type="checkbox"/> |

Cancel OK

Choose peaks to overlay.

Click on a row to highlight a peak and automatically zoom to the region near the peak.



Peaks in reciprocal space.

Peak Actions
Integrate Add Peaks Remove Peaks

Workspace: integrate

Concise View

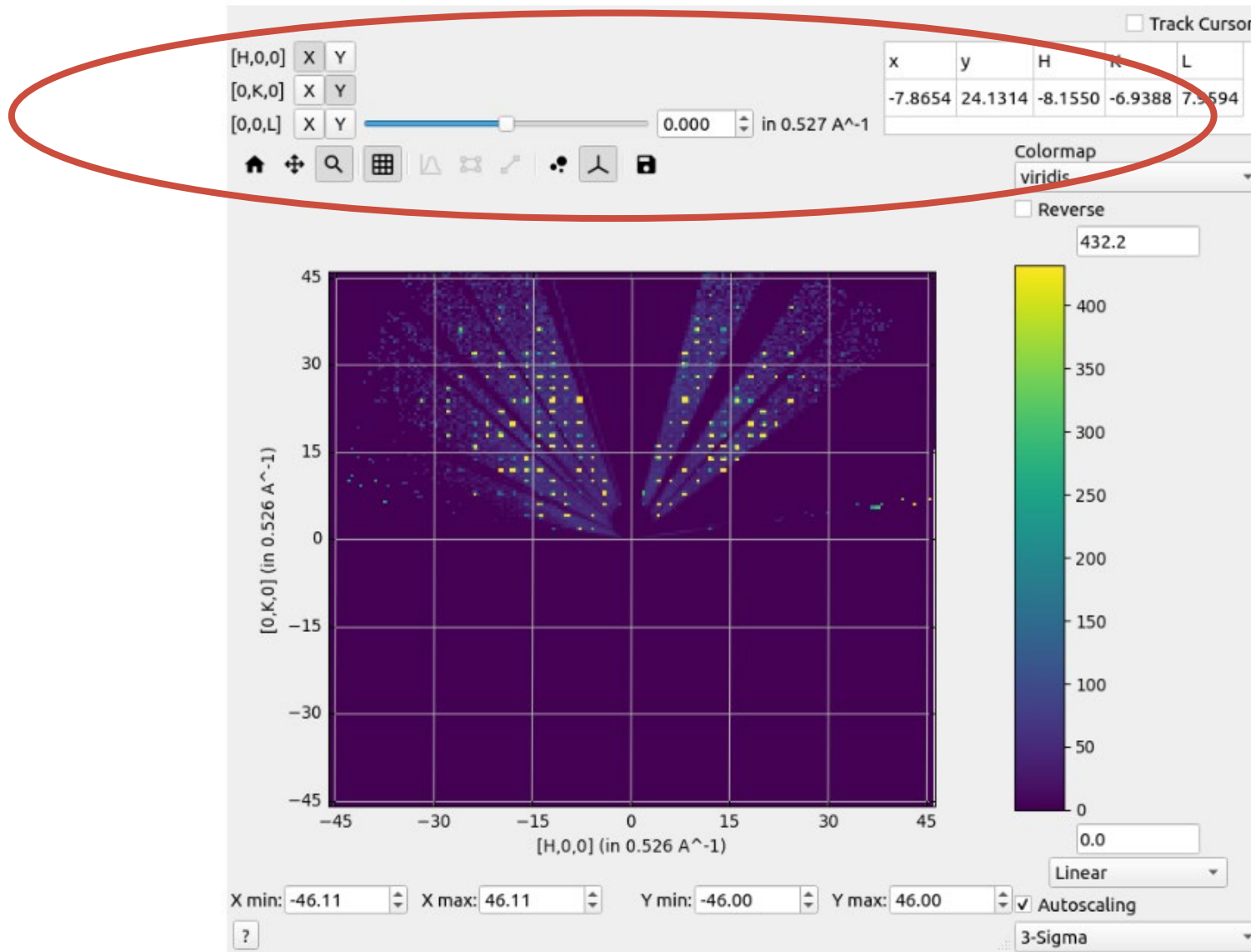
| | h | k | l | Intens |
|---|----------|----------|----------|------------|
| 1 | 20.00000 | 32.00000 | -2.00000 | 1379.89176 |
| 2 | 20.00000 | 28.00000 | -4.00000 | 2251.29676 |
| 3 | 19.00000 | 26.00000 | 1.00000 | 702.52486 |
| 4 | 18.00000 | 28.00000 | -0.00000 | 1388.41183 |
| 5 | 18.00000 | 28.00000 | -6.00000 | 1228.96870 |
| 6 | 18.00000 | 26.00000 | -4.00000 | 654.12412 |

Workspace: strong

Concise View

| RunNumber | DetID | h | k |
|-----------|-------|--------|----------|
| 1 | 46917 | 877815 | 6.00000 |
| 2 | 46917 | 875570 | 8.00000 |
| 3 | 46917 | 893141 | 4.00000 |
| 4 | 46917 | 892112 | 12.00000 |
| 5 | 46917 | 855924 | 4.00000 |
| 6 | 46917 | 869743 | 5.00000 |

Slice viewer



Peaks workspace

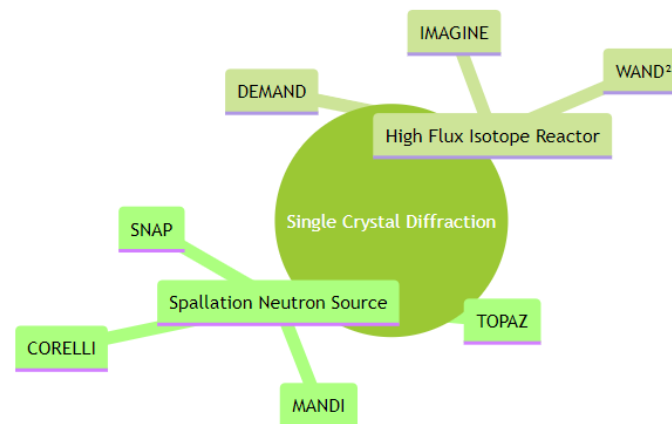
- *RunNumber*: Run number
- *DetID*: Detector (pixel) ID
- *h*: h-index
- *k*: k-index
- *l*: l-index
- *Wavelength*: Wavelength
- *Energy*: Energy
- *TOF*: Time-of-flight
- *DSpacing*: d-spacing
- *Intens*: Integrated intensity
- *SigInt*: Integrated intensity uncertainty
- *Intens/SigInt*: Signal-to-noise ratio
- *BinCount*: Bin count
- *BankName*: Bank name
- *Row*: Pixel row
- *Col*: Pixel column
- *QLab*: Q-laboratory vector
- *QSample*: Q-sample vector
- *PeakNumber*: Peak number
- *TBar*: Absorption weighted path length
- *IntHKL*: Integer hkl vector
- *IntMNP*: Integer mnp vector

| | RunNumber | DetID | h | k | l | Wavelength | Energy | TOF | DSpacing | Intens | SigInt | Intens/SigInt | BinCount | BankName | Row | Col | QLab | QSample | PeakNumber | TBar | IntHKL | IntMNP |
|----|-----------|--------|----|----|----|------------|---------|---------|----------|---------|---------|---------------|----------|----------|-----|-----|-----------------------------|----------------------------|------------|------|------------|---------|
| 1 | 46917 | 874923 | 20 | 32 | -2 | 0.515825 | 307.447 | 2411.16 | 0.316004 | 1379.89 | 120.456 | 11.4556 | 0 | bank13 | 171 | 89 | [9.62084,-6.27949,-16.2281] | [3.24701,-7.53468,18.1116] | 35 | 0 | [20,32,-2] | [0,0,0] |
| 2 | 46917 | 886324 | 20 | 28 | -4 | 0.527363 | 294.142 | 2465.18 | 0.344584 | 2251.3 | 135.923 | 16.563 | 0 | bank13 | 52 | 134 | [9.53856,-6.84189,-13.9531] | [3.68779,-5.52872,16.9799] | 52 | 0 | [20,28,-4] | [0,0,0] |
| 3 | 46917 | 908752 | 19 | 26 | 1 | 0.590219 | 234.828 | 2759.79 | 0.370523 | 702.525 | 66.0328 | 10.639 | 0 | bank13 | 208 | 221 | [9.45073,-3.97831,-13.5062] | [4.31124,-7.23369,14.719] | 89 | 0 | [19,26,1] | [0,0,0] |
| 4 | 46917 | 885727 | 18 | 28 | 0 | 0.590109 | 234.915 | 2758.82 | 0.358622 | 1388.41 | 93.0814 | 14.9161 | 0 | bank13 | 223 | 131 | [8.80682,-4.64941,-14.4148] | [3.31785,-7.36375,15.5476] | 112 | 0 | [18,28,-0] | [0,0,0] |
| 5 | 46917 | 865547 | 18 | 28 | -6 | 0.543711 | 276.719 | 2542.27 | 0.352963 | 1228.97 | 99.1645 | 12.3932 | 0 | bank13 | 11 | 53 | [8.34784,-7.69512,-13.7107] | [2.46387,-4.68828,16.9951] | 115 | 0 | [18,28,-6] | [0,0,0] |
| 6 | 46917 | 880947 | 18 | 26 | -4 | 0.576828 | 245.857 | 2696.4 | 0.374554 | 654.124 | 63.254 | 10.3412 | 0 | bank13 | 51 | 113 | [8.54152,-6.44931,-12.9172] | [3.11934,-5.0206,15.6993] | 122 | 0 | [18,26,-4] | [0,0,0] |
| 7 | 46917 | 891663 | 18 | 24 | -4 | 0.58896 | 235.833 | 2753.59 | 0.39438 | 1729.78 | 96.6106 | 17.9047 | 0 | bank13 | 15 | 155 | [8.57962,-6.22049,-11.8961] | [3.48535,-4.46479,14.891] | 128 | 0 | [18,24,-4] | [0,0,0] |
| 8 | 46917 | 909164 | 18 | 23 | -1 | 0.623078 | 210.713 | 2912.98 | 0.408559 | 586.951 | 50.3469 | 11.6581 | 0 | bank13 | 108 | 223 | [8.83025,-4.58444,-11.7269] | [4.10006,-5.5163,13.7576] | 129 | 0 | [18,23,-1] | [0,0,0] |
| 9 | 46917 | 883892 | 17 | 26 | -1 | 0.623053 | 210.73 | 2912.38 | 0.384123 | 737.87 | 60.216 | 12.2537 | 0 | bank13 | 180 | 124 | [8.25594,-4.83901,-13.2658] | [3.08143,-6.38914,14.7392] | 146 | 0 | [17,26,-1] | [0,0,0] |
| 10 | 46917 | 896348 | 17 | 23 | -2 | 0.640763 | 199.242 | 2995.18 | 0.416292 | 1150.11 | 66.2794 | 17.3524 | 0 | bank13 | 92 | 173 | [8.23201,-5.01112,-11.6158] | [3.48257,-5.10301,13.7708] | 157 | 0 | [17,23,-2] | [0,0,0] |

Peaks table viewer.

Single Crystal Diffraction

The [Neutron Diffraction Suite](#) at Oak Ridge National Laboratory includes dedicated single crystal diffraction beamlines both at the [High Flux Isotope Reactor](#) and [Spallation Neutron Source](#).



Capabilities

Single crystal diffraction is a powerful technique used in the study and exploration of material structure and phenomena. This technique spans diverse fields of materials science study including:

- Macromolecular and protein crystallography
- Chemical and mineral crystallography
- Condensed matter physics and quantum materials

<https://single-crystal.ornl.gov/guide/mantid/index.html>

Mantid

Mantid (<https://mantidproject.org/>) serves as one of the main tools for reducing and interacting with single crystal diffraction data.