OAK RIDGE National Laboratory

Mantid and data reduction tutorial

Single Crystal Workshop
ACNS Conference
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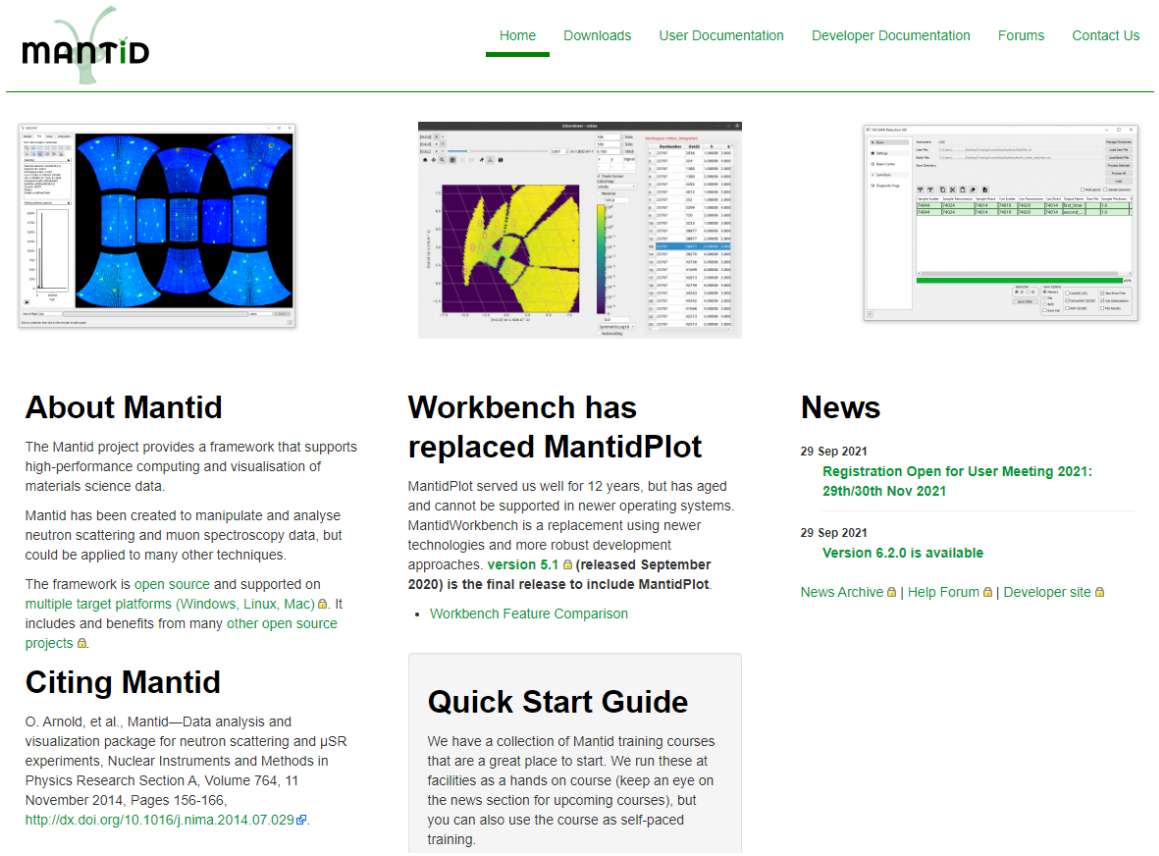
ORNL is managed by UT-Battelle LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

https://mantidproject.org/



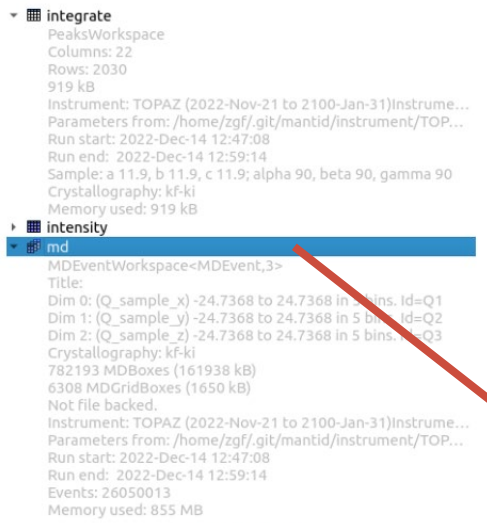
Mantid Workbench

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.

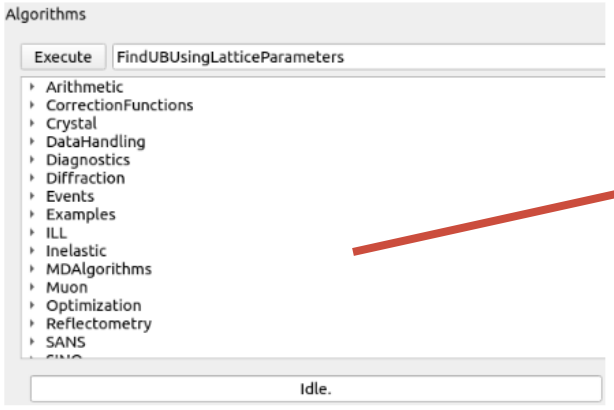
Selecting a default facility (SNS/HFIR) and instrument (TOPAZ/MANDI/CORELLI/SNAP/DEMAND/WAND²).

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



Workspaces. #

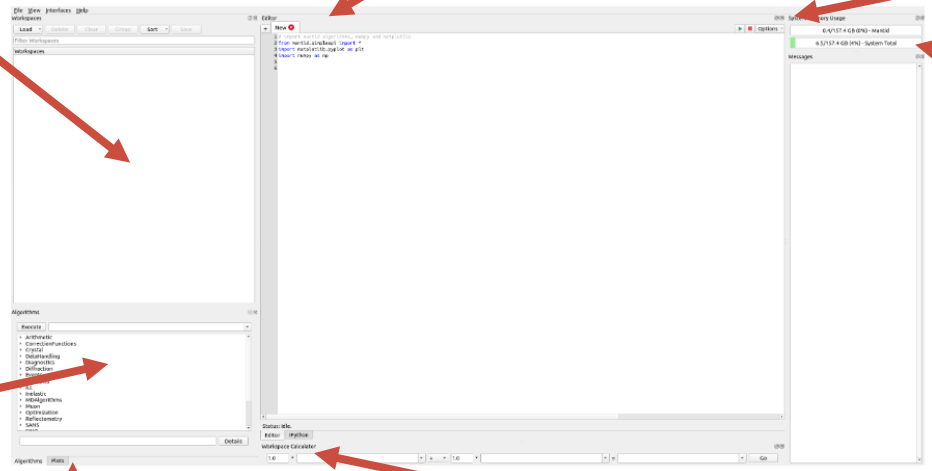


Algorithms.

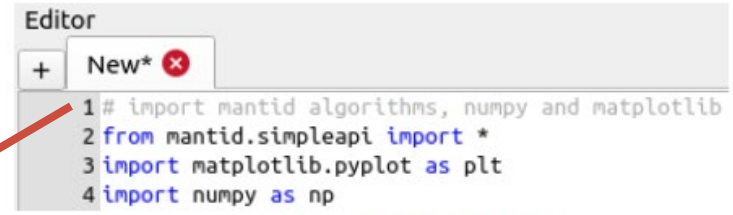
Main page

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

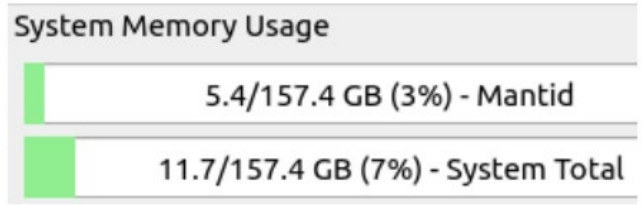


Mantid Workbench.

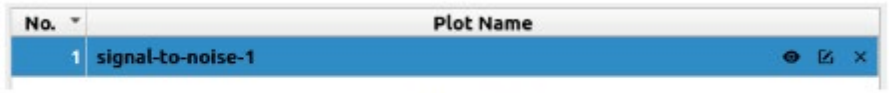


Mantid Workbench editor. #

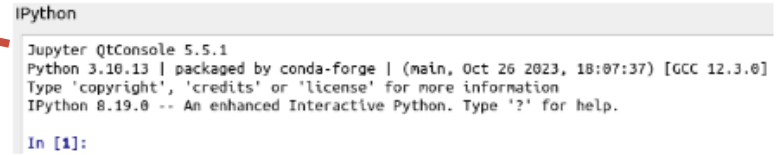
Script editor play/stop buttons.



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



Plots. #

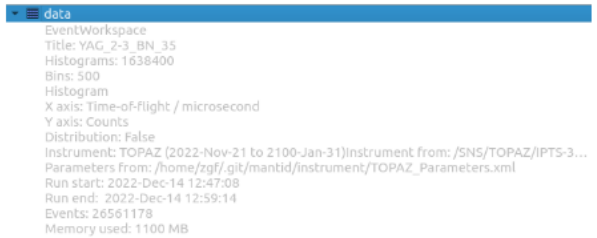


IPython console.

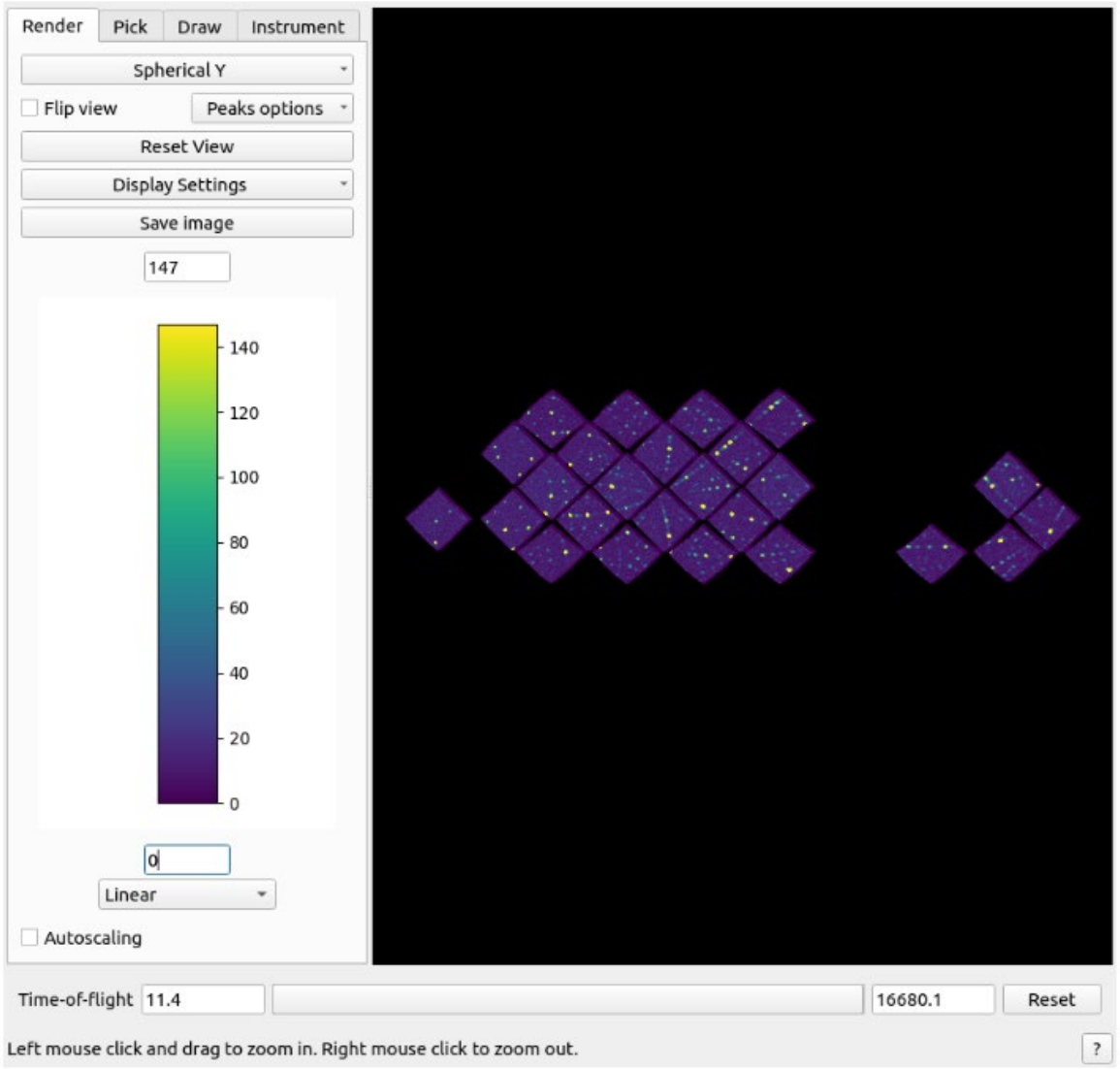
Instrument viewer

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*



Event data workspace.

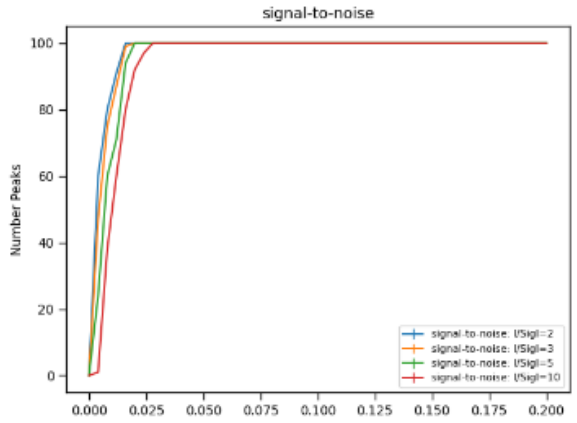


Plotting

Plot viewer

Certain workspaces can be viewed as a plot.

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



Plot.

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.

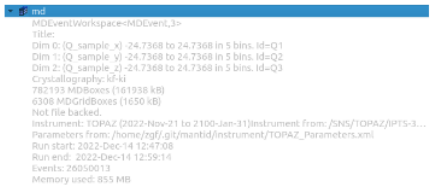
Plot tool bar.

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:

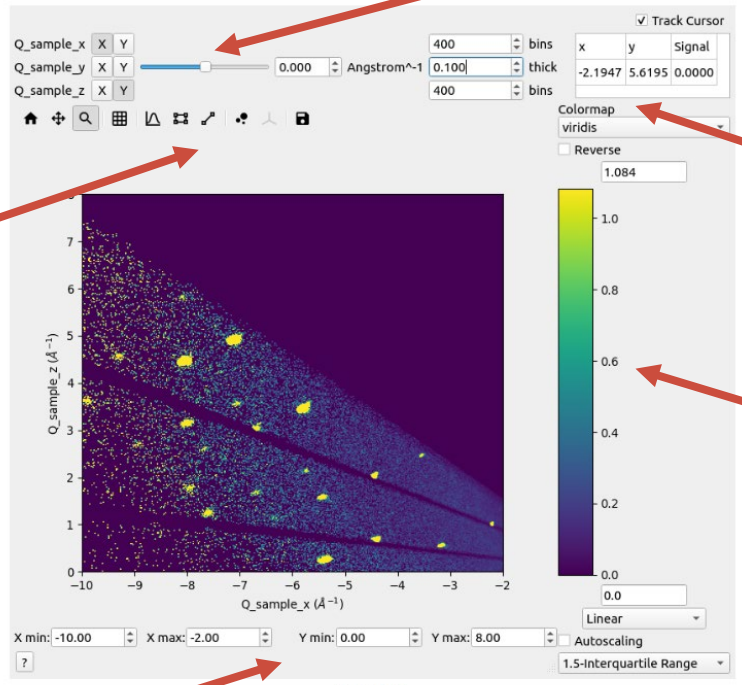
- Right-click *md*
- Left-click *Show Slice Viewer*



Event data workspace. #

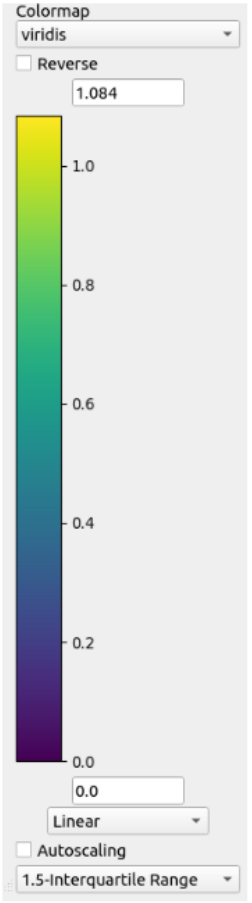
Display axis and slider value shown of a typical *x0z*-slice for Q-sample data. #

Tool bar options.



Slice viewer.

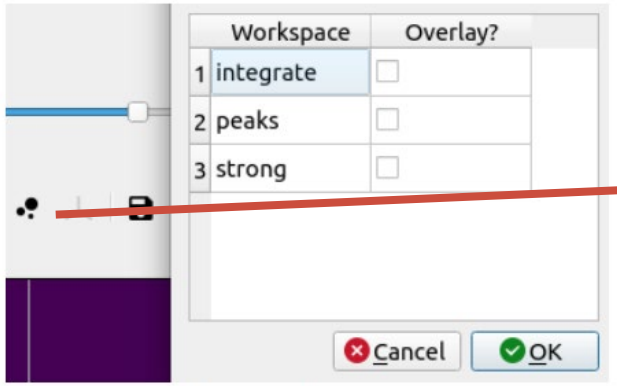
Cursor position and value.



Colorbar parameters. #

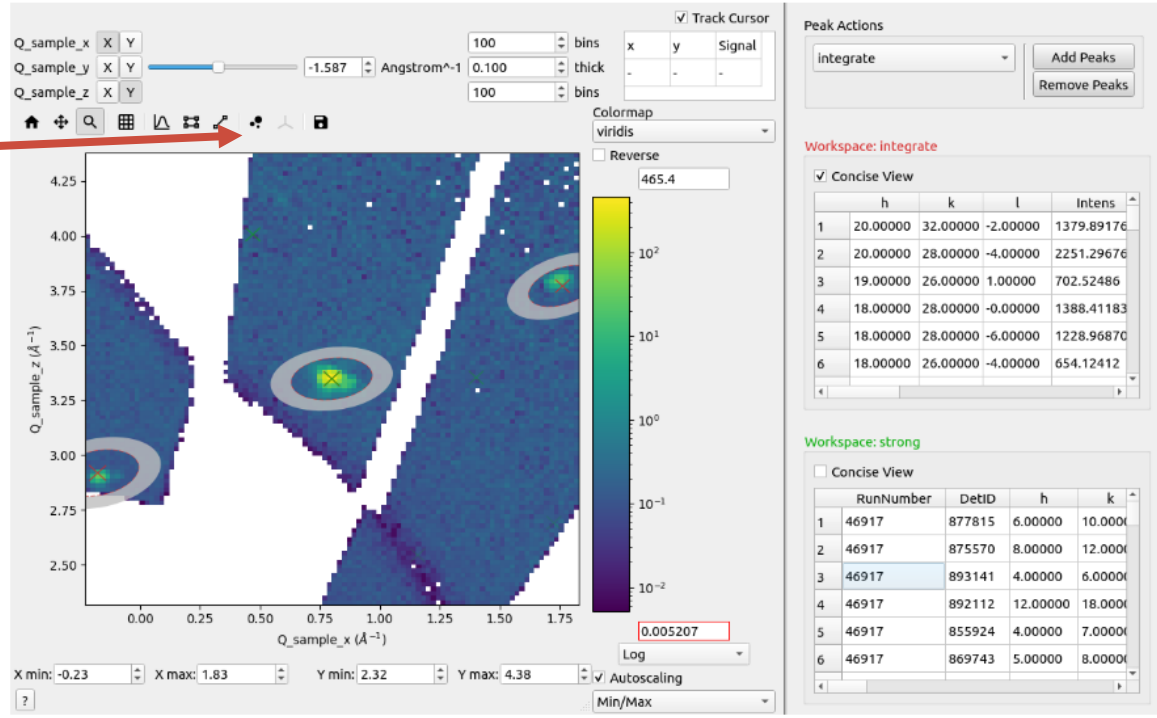
Display axis zoom limits.

Slice viewer



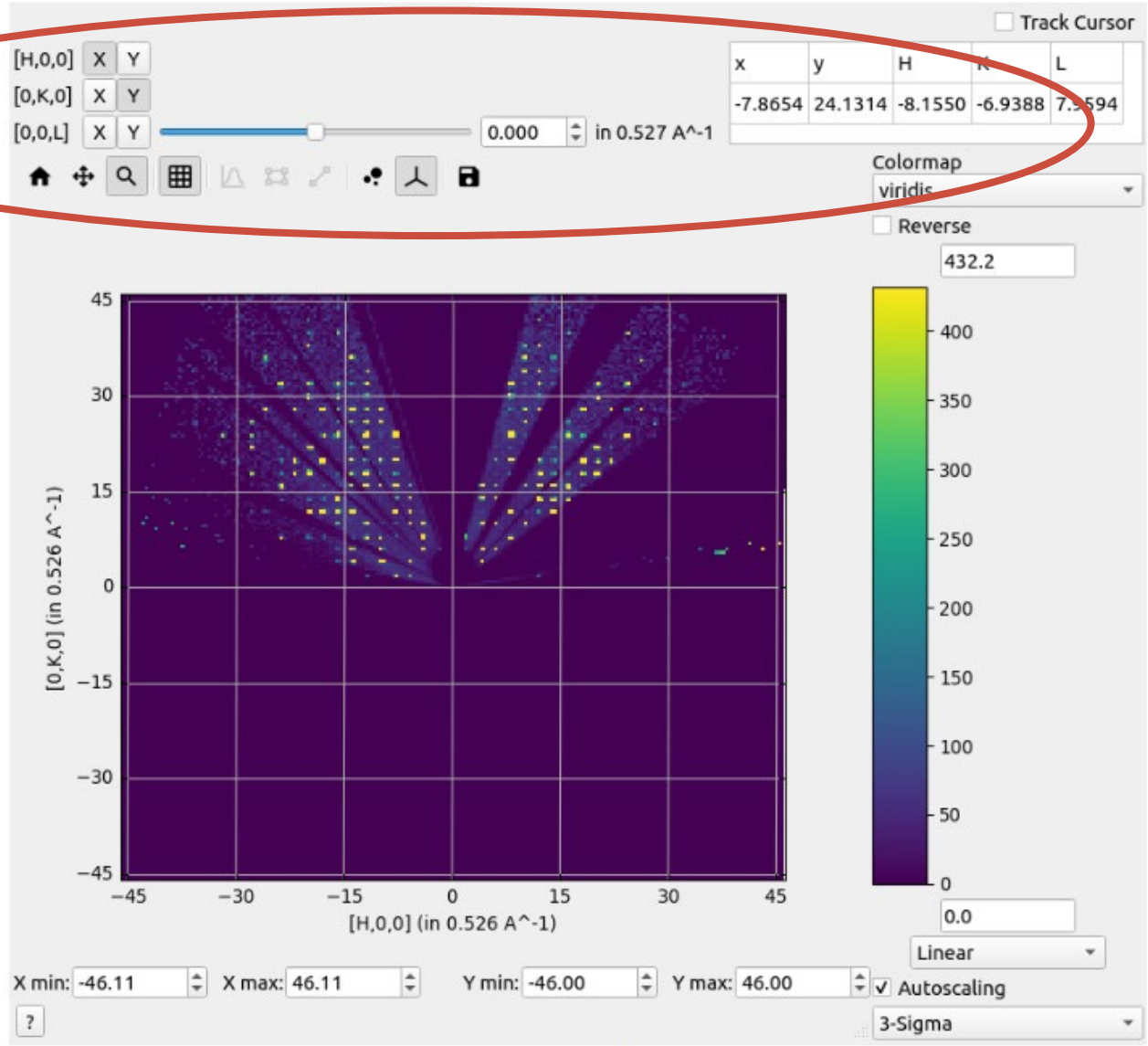
Choose peaks to overlay.

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



Peaks in reciprocal space.

Slice viewer



Reciprocal space *hkl*-map.

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 raio
- *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.

https://single-crystal.ornl.gov/home/index.html

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