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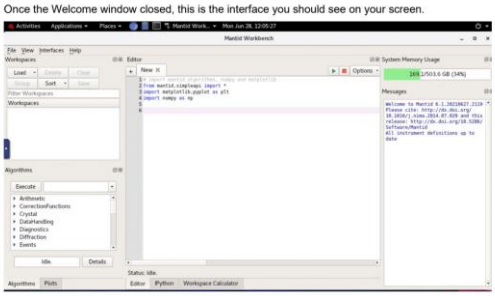
DEMAND user data accessing and processing basics

There are two ways one can access the data after login with the ORNL PAS account:

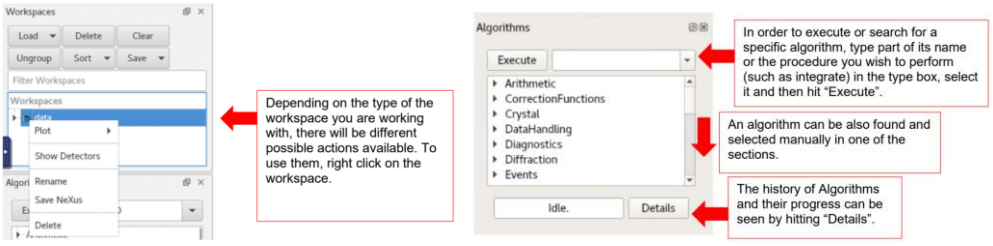
1. The data can be accessed from DEMAND at oncat.ornl.gov within the IPTS folder directory. One can use  to save CSV for summary of the experiment scans results or thumbnails to help. The data are listed with the time the scans were performed, the commands that were using, title, scan number…. You can download the data with the help of FTP tools and process them with data processing software you are used to.
2. The data can also be accessed on analysis.sns.gov server. Data processing software like Mantid, MATLAB are also installed under the education directory on the server. Go through home/data/HFIR/HB3A you can see your ipts and one can access the data.

There are different data types saved in DEMAND. With the exp folder, you can find all sorts of experiment information including reduced .nxs data under your ipts folder, UB information in the exp**/UbConf folder and data in exp**/Datafiles/. With our area detector, each point in scans is an image as the .xml file, we pick a ROI area(only the detector ROI is initially setting correctly in default) on the detector to extract the intensity of each point, then gives the data in .dat file or later script processing. The .dat files are the ascii format line plots saved during measurement(For users who were used to Graffiti, these data can still be viewed and plotted with it when saved to local PC.). The .xml files are directly detector pixel frame data records that data in each step of the scans, you can also find binary data in the binary folder. Detector images for each step are saved in the image folder.

The IPTS/shared/autoreduced folder contains the .nxs files that are compatible with Python based data process software Mantidworkbench that's installed in the analysis.sns.gov server. You can find it from the front page: 

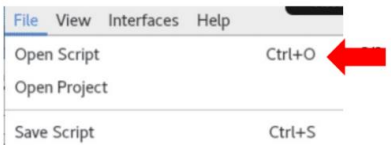


There are a few things to know in Mantid.

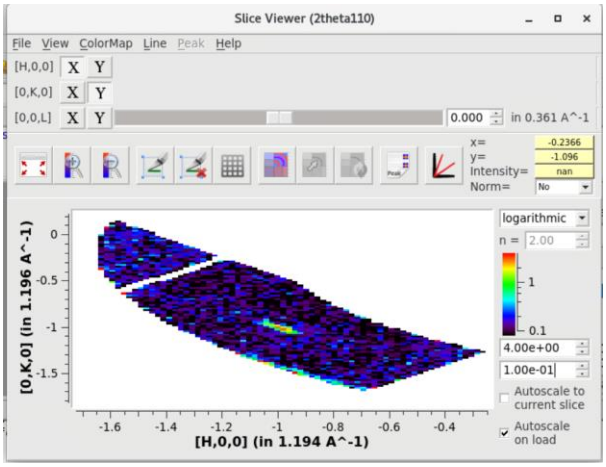


If you use Mantid to process the data, you can run our precomposed scripts or a combination of individual algorithms. Those could be found on analysis server under HFIR/HB3A/shared/Scripts. To start, all scripts are a combination of the algorithms in sequence with some environmental settings. If you need to run any individual steps in it, you can check the script for the algorithms needed.

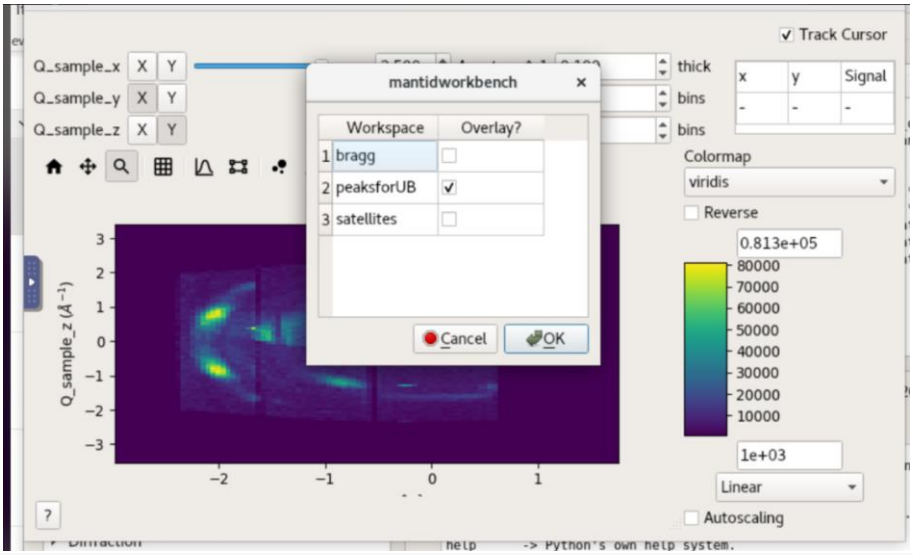
3) ***Editor*** – part of the software that uses scripts. A specific script can be open by following going to **File** the left upper corner and hit "**Open Script**" or **Ctrl+O.**



1. To view a single scan in HKL space or Q, you can check the result of Two_axis_peak_integration.py. You can always use an individual algorithm listed in the script. The script contains algorithms to convert the detector space data to Q space or HKl space. All DEMAND scans can be viewed this way. Below is showing an example of a rocking curve scan "scanrel omega -3 3 0.3" plotting in hkl space.



2. To view a single scan in detector space, one can load the .nxs data in an earlier version of Mantidplot(61) from your ipts/exp/shared/autoreduce. Right click on the data workspace select slice viewer to check on the data. The vanadium file saved in shared folder can be used as normalization file. One can determine the ROI by checking this way. Load can be used for loading single scans or multiple scans.
3. The rocking curve peaks integrated intensity can be processed with the Python script four_circle_peak_integration.py saved in the HB3A shared folder when using MantidworkbenchQa. The scripts is a pile of the Mantid algorithms listed in a general way of data process sequence. Modify the script to input your IPTS, expno, scan list and ROI(region of interest, pixel range of the peak on detector). The vanadium file needed for normalization is also saved in the share folder, you may change the van_file_name to a newer file(as you can see in the share folder with cycle no.). Outputs are fullprof input files format hkl intensity list with header .int file and a pdf format graph summary for the fitting result. For magnetic peaks with non-integer wavevectors, use the four_circle_satellitepeak_integration.py for the right format for magnetic peak inputs.
4. Integrated intensity for peaks within 2-axis mesh scans(or 4 circle mode mesh scans) can be processed with Two_axis_peak_integration.py also can be found in the HB3A shared folder. There are more details regard of the crystal structure information needed to change in the code including sample structure information and often need some works of refining the UB matrix to increase the accuracy of get the right peaks. This is a good way to check for peaks in all modes as it merges all the input scans and displays them in Q and HKL space(with the right UB matrix of course) as well as processing integrated intensities of the peaks(HB3Aintegratedpeak).
5. If you need to recalculated the UB matrix, you can first run findpeakMD with input merged, get a peak table, then sliceviewer on merged, overlay the find peaks table like below:



Then go through the peak workspace table to sort it out, adding or removing peaks on the graph with clicking the cross to make sure all the peaks in the table are right peaks not background. Then do algorithm findUBwith (), usually we do FFT but it didn't work for me this time, so I choose with lattice parameters. You can indexpeaks of the peak table, the peak table contains the UB matrix now. Then saveISAWUB with the input of the peak table and load ISAWUB to a data workspace and use it for UB when converting to HKL elsewhere(convertQtoHKLhisto works for converting the merged to hkl in the version of Mantidworkbench). You can view the data slices with plotting the HKL or merged workspace with slice viewer. For getting the integrated intensity of the newly found peaks with new UB indexs and save it in the Fullprof format as the script output, one can run algorithm HB3Aintegratedpeak as in the script for the new peak workspace to get the integrated intensity and savereflections to save the data.

6. To plot out an order parameter or rocking curve, one can directly use table data analysis software to plot out the .dat line plot with the right choice of ROI or write programs in Mantid or with other programming software to process the .xml or .nxs data with the user defined new ROI. Peak 2theta cuts can also be obtained as the peak distribution on the x-pixel of the detector is also 2theta distributions.