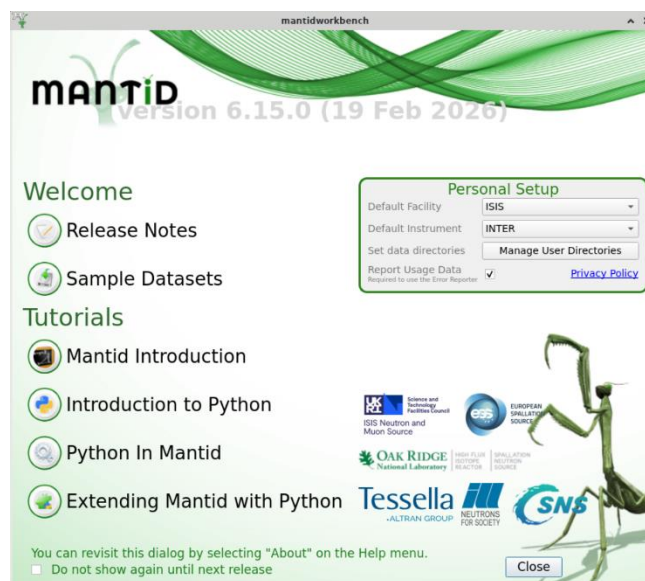


Data reduction with



in 7 easy steps

Maximilian Skoda

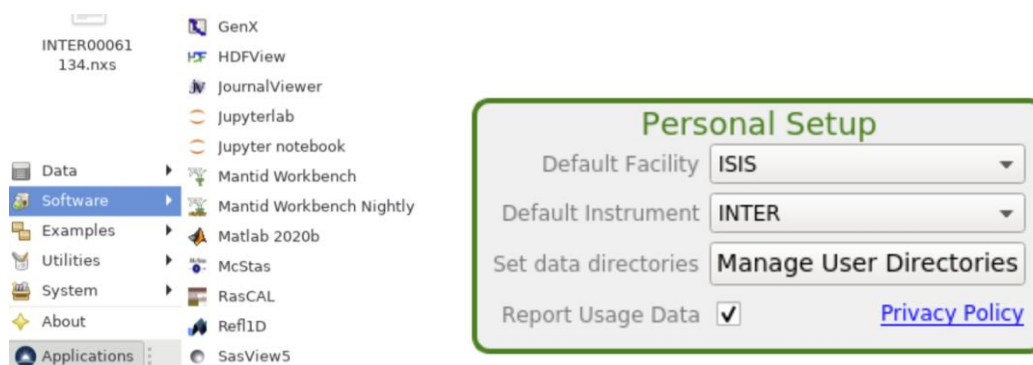


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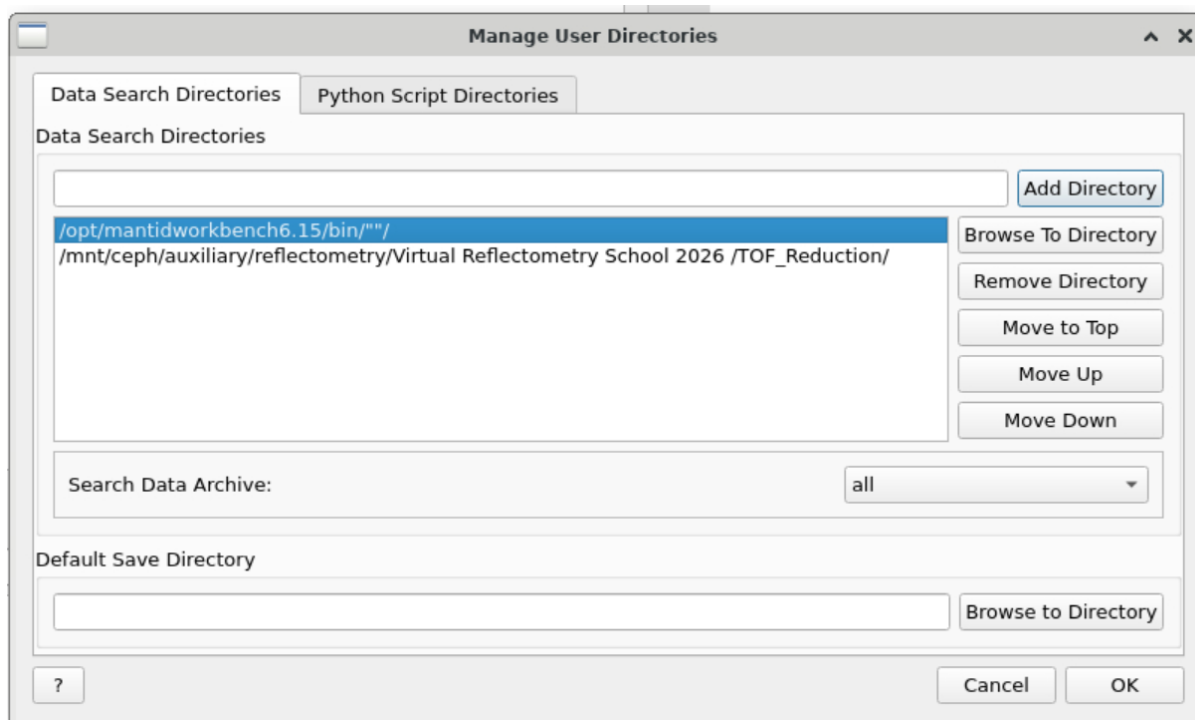
2 LAUNCHING MANTID AND LOADING FILES

In IDAaaS, from the Applications menu, open ‘Mantid Workbench’:



Once Mantid has started, on the start screen, select “ISIS” as facility and “INTER” as instrument. From File->Manage User Directories select for “Search Data Archive” “default facility only – ISIS”.

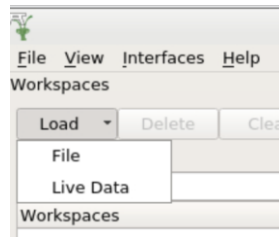
Click on “Manage User Directories”:



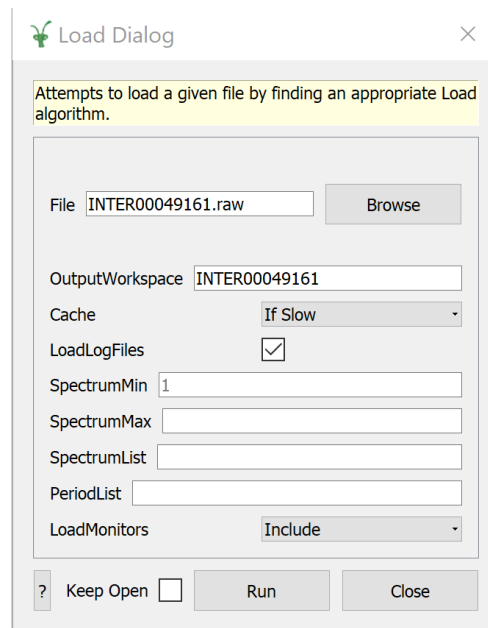
Click on “Browse To Directory” and navigate to “/mnt/ceph/auxiliary/reflectometry/Virtual Reflectometry School 2026/TOF_Reduction/” and click “Open” in the top right corner.

Mantid is now instructed to look for data in the above directory.

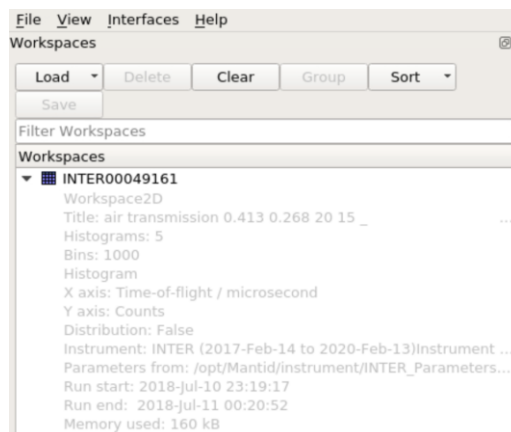
Click “Load->File”:



In the “Load Dialog” type: INTER00049161.raw”, then “Run”:



A workspace with the same name should appear on the left, in the box for the list of workspaces. By clicking the small arrow, you can inspect Workspace properties, such as title, number of histograms etc.:



Run 49161 is the transmission run. By repeating the procedure, load “INTER00049162.raw”.

Run 49162 is the sample run.

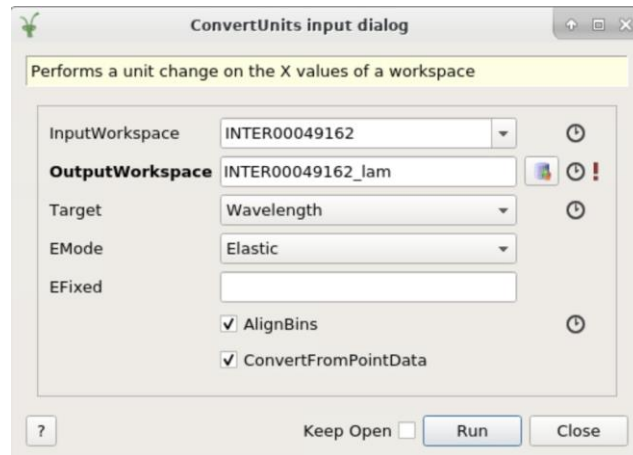
By right clicking on a workspace, you can plot the workspace histograms and view other properties.

3 STEP 1 – CONVERT TO WAVELENGTH

Select the sample workspace (INTER00049162) and type “**ConvertUnits**” into the “Algorithms” box:



Choose the following selections and rename the **OutputWorkspace**:



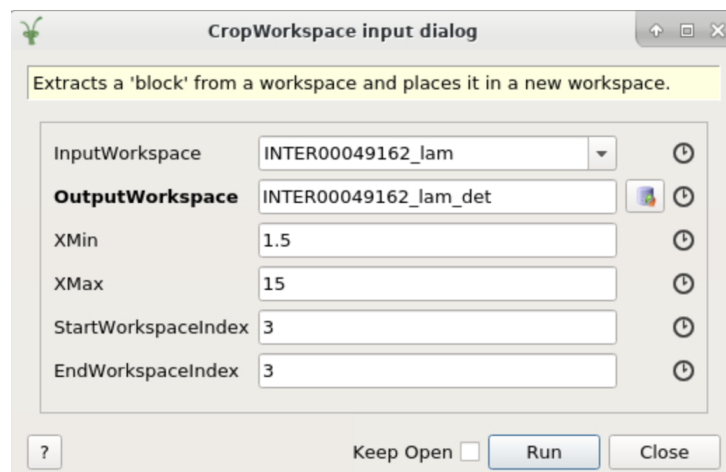
Do the same for the transmission workspace (INTER00049161).

There should now be 4 workspaces in the list (INTER00049161, INTER00049162, INTER00049161_lam and INTER00049162_lam).

4 STEP 2 – SEPARATE DETECTOR AND MONITOR SPECTRUM

The “_lam” workspaces still contain both monitor and detector spectra. In order to proceed, the detector spectrum (WorkspaceIndex=3) needs to be separated from the monitor spectrum, which will be used for normalisation (WorkspaceIndex=2 in this case).

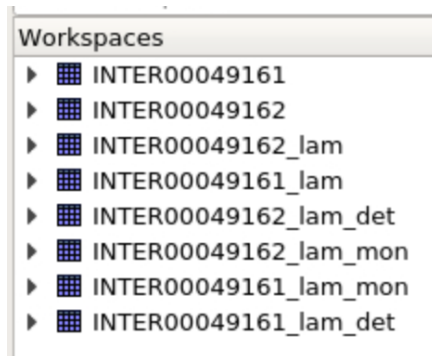
Type “**CropWorkspace**” into the “Algorithms” box:



Do this again on INTER00049162_lam, but name the OutputWorkspace “_lam_mon” and select Start- and EndWorkspaceIndex=2.

Repeat both steps for the other workspace (INTER00049161).

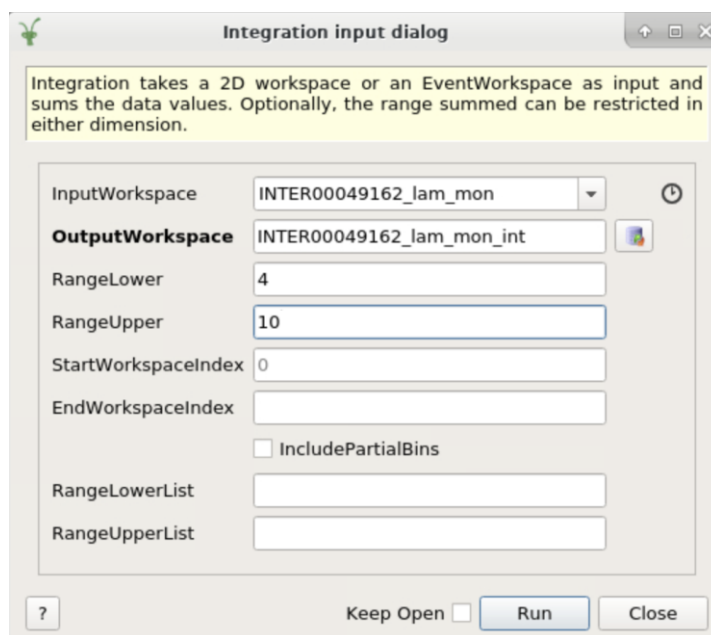
The list should contain:



5 STEP 3 – INTEGRATION OF MONITOR SPECTRA

The pre-sample monitors record a fraction of the neutrons in the beam, which is proportional to the total number of neutrons incident on the sample. The **monitor spectrum** can be used to normalise all sample and transmission runs. This is necessary in order to bring runs of different durations, angles etc to the same scale. There are several ways to apply normalisations. In this case, the monitor spectrum of each sample and transmission run is integrated between two (arbitrary, but identical) wavelengths, in this case between 4 and 10 Ångström (RangeLower and RangeUpper).

Type “**Integration**” into the “Algorithms” box:

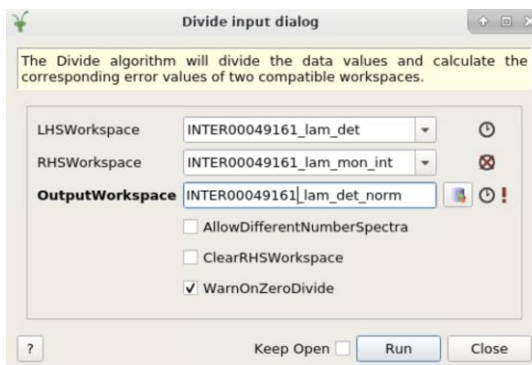


The integration has to be repeated for the other monitor “_lam_mon” workspace, with the same range (4 to 10 Ångström). The OutputWorkspace must be renamed accordingly.

6 STEP 4 – NORMALISATION BY MONITOR INTEGRAL

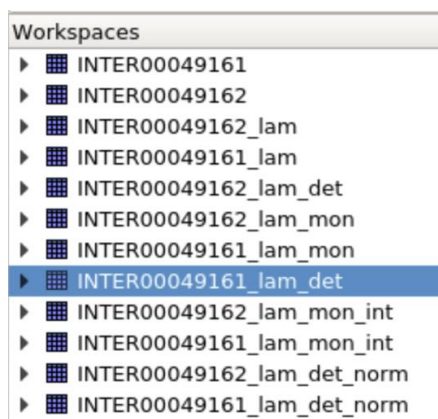
The monitor integrals (“_mon_int” workspaces) can be used to normalise the detector spectra for the sample and transmission runs (49162 and 49161).

Type “Divide” into the “Algorithms” box:

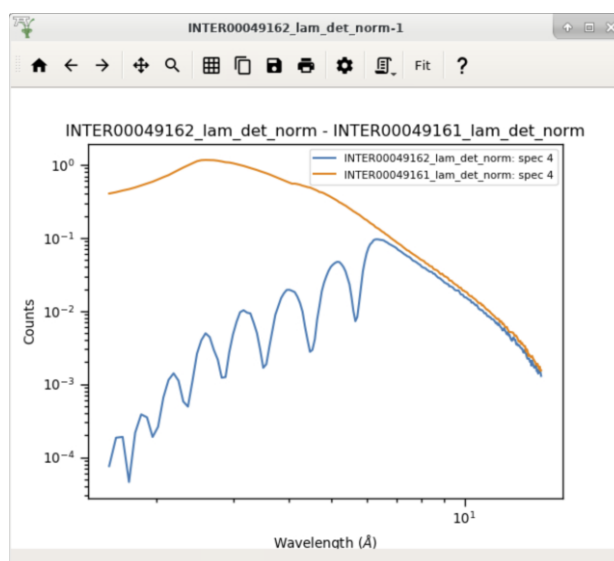


Repeat the division for the corresponding other workspaces.

The list should not contain the following workspaces:

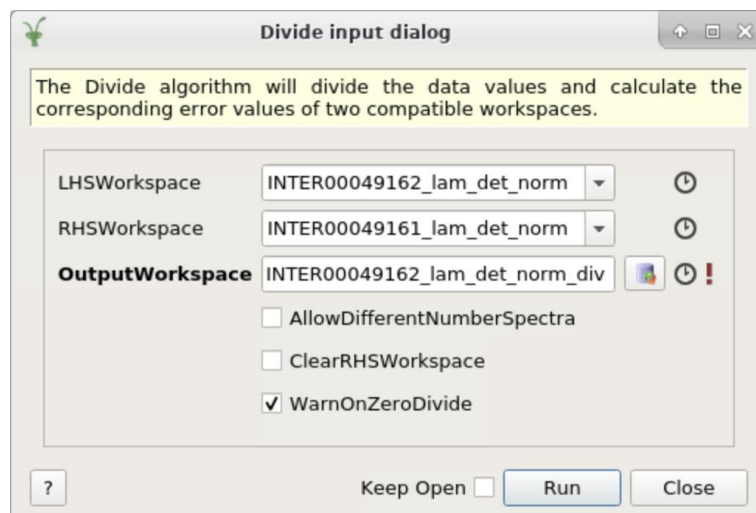


A plot of the normalised workspaces should look like this (it may differ initially due to axis scaling – the figure below is log-log). The axis scaling can be changed via right-click on the figure:

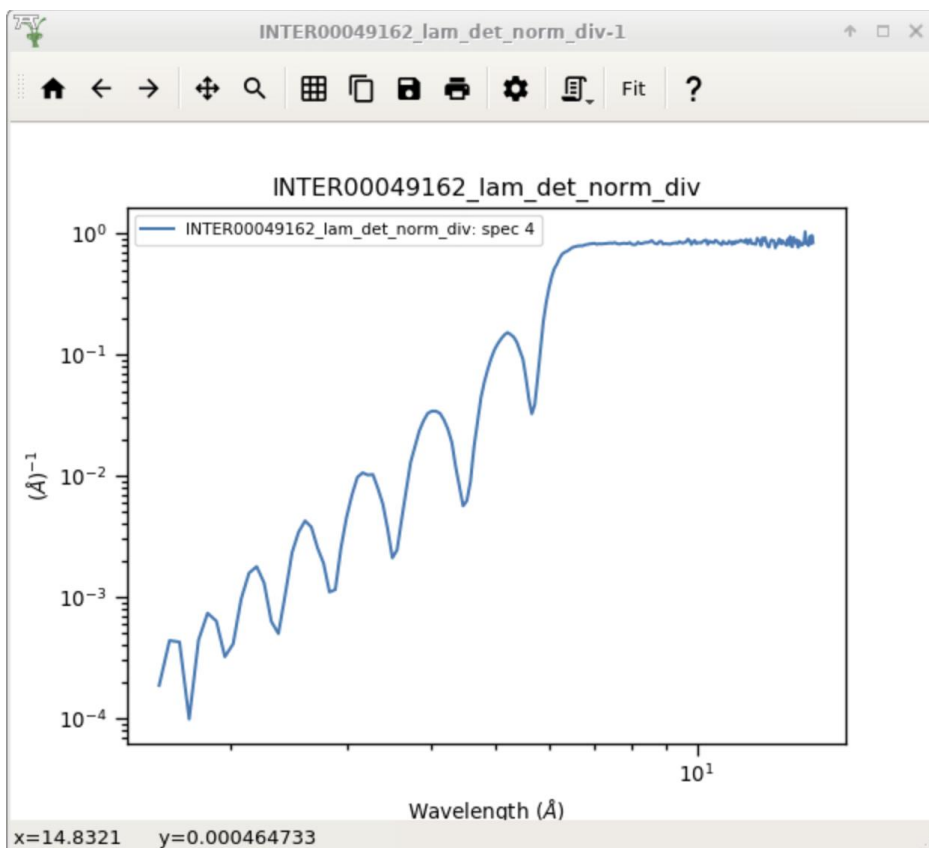


7 STEP 5 – DIVISION OF SAMPLE RUN BY TRANSMISSION RUN (TRANSMISSION CORRECTION)

Again using the “**Divide**” algorithm, the normalised (by monitor integral) sample run will be divided by the also normalised transmission run:



The **OutputWorkspace** can be named “INTER00049162_lam_det_norm_div” (see above). The resulting should look like this (again depending on axis scaling):

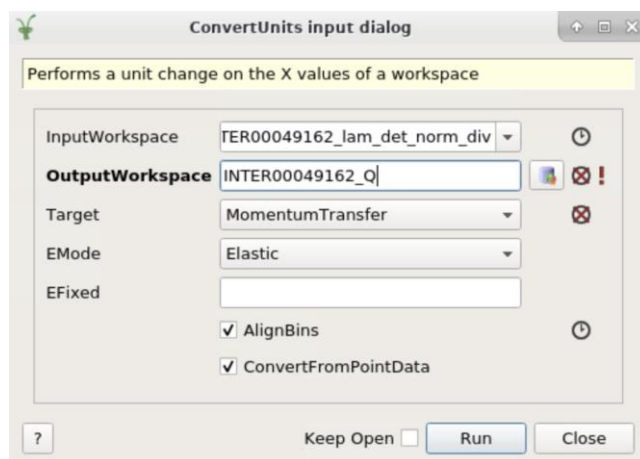


8 STEP 6 – CONVERSION TO MOMENTUM TRANSFER

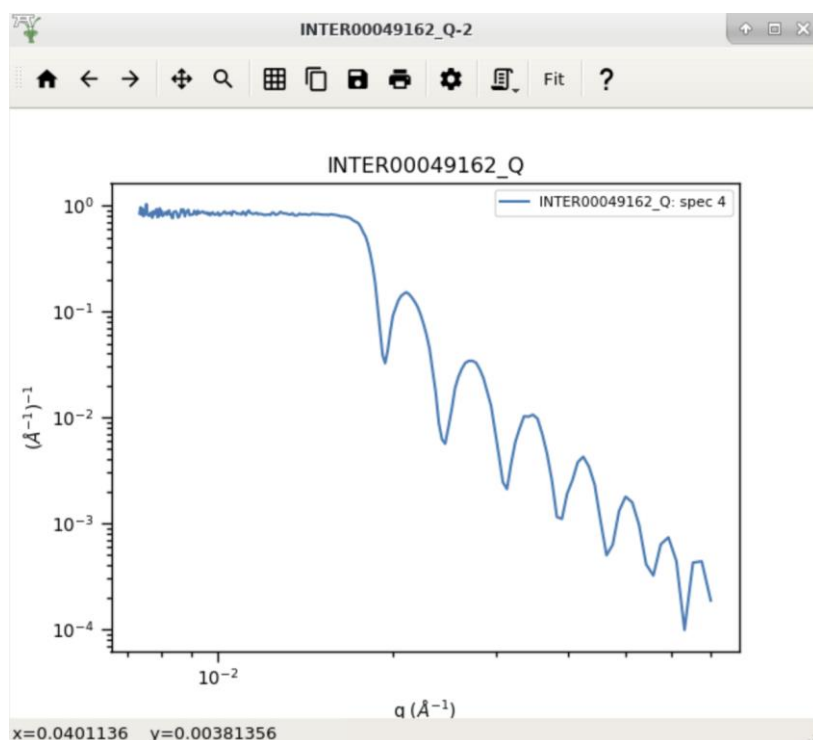
Having obtained a normalised (true reflectivity) sample run as function of wavelength, the final conversion is a second unit conversion from wavelength to momentum transfer according to:

$$Q = \frac{4\pi}{\lambda} \sin \theta,$$

Where Q is the momentum transfer, λ is the wavelength and θ is the measurement angle of the sample run. This formula, as well as the measurement angle are stored in the run file (workspace) as metadata, such that simply running “**ConvertUnits**” yields the correct axis conversion:



Rename the **OutputWorkspace** to a sensible name (e.g. INTER00049162_Q). The final plot should look like this (on a log-log scale):



9 STEP 7 - DATA 'STITCHING'

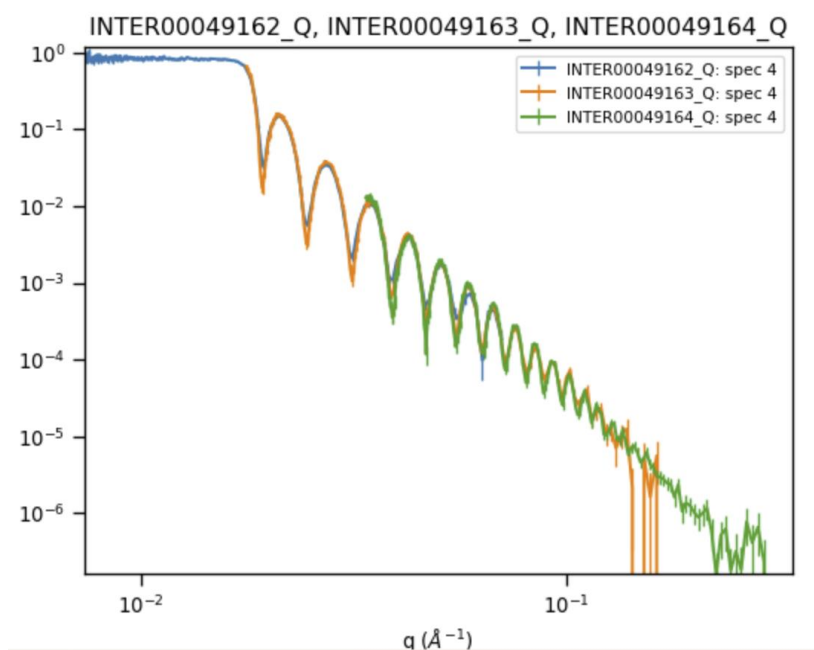
Since a typical complete reflectivity measurement will consist of a series of 'runs' taken at different sample angles (at ISIS usually 2 or 3 angles), a final step in the data reduction can be the combining of those angle runs, also called 'stitching'.

In order to obtain the other two reduced runs (49163 and 49164), the 6 reduction steps above, have to be repeated. There is however a shortcut for doing this: by selecting and right-clicking the final workspace (INTER00049162_Q), the reduction history can be displayed ("Show history"). This history can be copied to clipboard and pasted in the central script window:

```
163
164
 Match Case  Match Words
   Regex  Wrap Around

1 # import mantid algorithms, numpy and matplotlib
2 from mantid.simpleapi import *
3 import matplotlib.pyplot as plt
4 import numpy as np
5
6 Load(Filename='/archive/ndxinter/Instrument/data/cycle_18_1/INTER00049161.raw', OutputWorkspace='INTER00049161')
7 Load(Filename='/archive/ndxinter/Instrument/data/cycle_18_1/INTER00049164.raw', OutputWorkspace='INTER00049164')
8 ConvertUnits(InputWorkspace='INTER00049164', OutputWorkspace='INTER00049164_lam', Target='Wavelength', AlignBins=True)
9 ConvertUnits(InputWorkspace='INTER00049161', OutputWorkspace='INTER00049161_lam', Target='Wavelength', AlignBins=True)
10 CropWorkspace(InputWorkspace='INTER00049161_lam', OutputWorkspace='INTER00049161_lam_det', XMin=1.5, XMax=15, StartWorkspaceIndex=3)
11 CropWorkspace(InputWorkspace='INTER00049164_lam', OutputWorkspace='INTER00049164_lam_det', XMin=1.5, XMax=15, StartWorkspaceIndex=3)
12 CropWorkspace(InputWorkspace='INTER00049164_lam', OutputWorkspace='INTER00049164_lam_mon', XMin=1.5, XMax=15, StartWorkspaceIndex=2)
13 CropWorkspace(InputWorkspace='INTER00049161_lam', OutputWorkspace='INTER00049161_lam_mon', XMin=1.5, XMax=15, StartWorkspaceIndex=2)
14 Integration(InputWorkspace='INTER00049161_lam_mon', OutputWorkspace='INTER00049161_lam_mon_int', RangeLower=4, RangeUpper=10)
15 Integration(InputWorkspace='INTER00049164_lam_mon', OutputWorkspace='INTER00049164_lam_mon_int', RangeLower=4, RangeUpper=10)
16 Divide(LHSWorkspace='INTER00049161_lam_det', RHSWorkspace='INTER00049161_lam_mon_int', OutputWorkspace='INTER00049161_lam_det_norm')
17 Divide(LHSWorkspace='INTER00049164_lam_det', RHSWorkspace='INTER00049164_lam_mon_int', OutputWorkspace='INTER00049164_lam_det_norm')
18 Divide(LHSWorkspace='INTER00049164_lam_det_norm', RHSWorkspace='INTER00049161_lam_det_norm', OutputWorkspace='INTER00049164_lam_det')
19 ConvertUnits(InputWorkspace='INTER00049164_lam_det_norm_div', OutputWorkspace='INTER00049164_Q', Target='MomentumTransfer', AlignBi
20
```

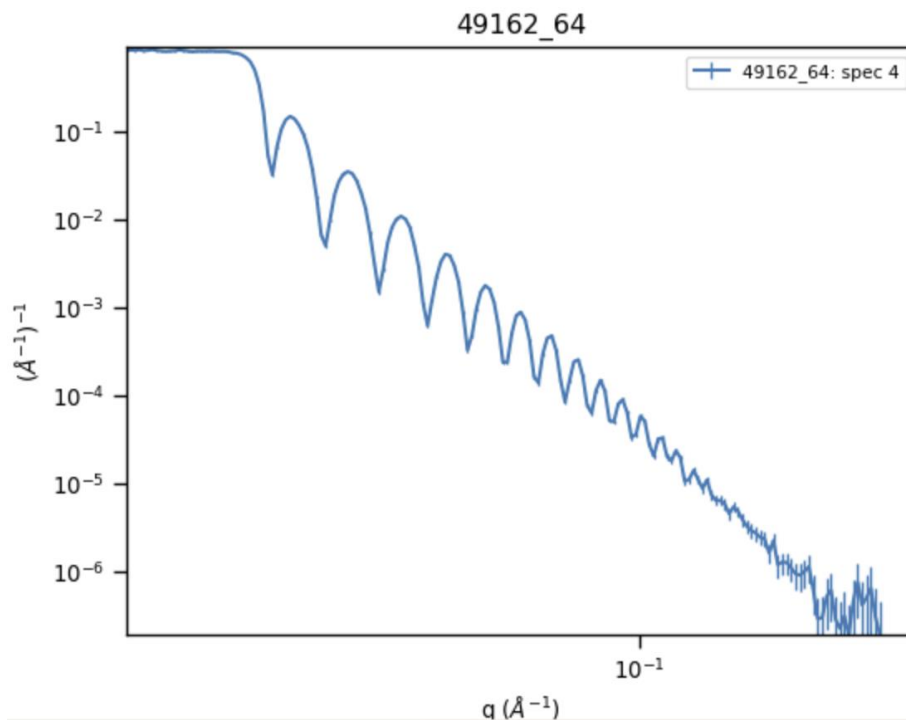
With Ctrl+f, the find/replace menu can be called and all run number entries for the sample run (162) can be replaced by the next run (163) and the script executed by pressing the green play button at the top right. The replace operation can be repeated for the third and final run (ending 164). The three reduced runs should look like this:



These three workspaces can then be combined (or stitched) by typing and executing:

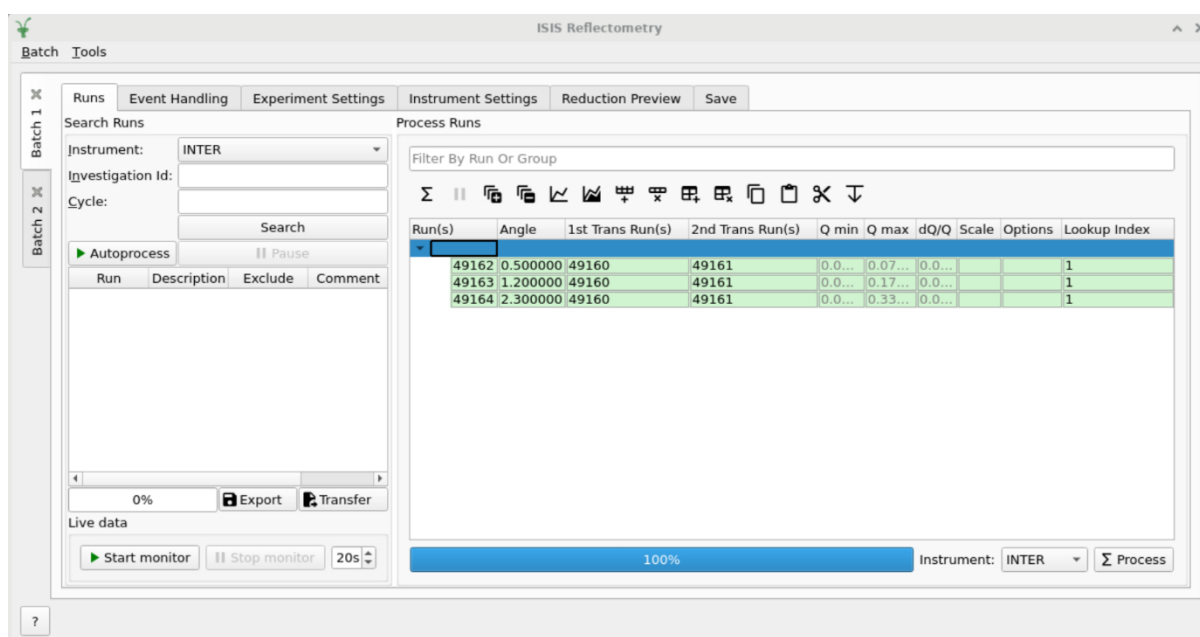
```
Stitch1DMany(['INTER00049162_Q', 'INTER00049163_Q', 'INTER00049164_Q'], Params='0.01,-0.02,0.33', OutputWorkspace="49162_64")
```

in the script window. The stitched workspace should look like this:



10 REFLECTOMETRY INTERFACE

There are many other options that can be applied to the data reduction, depending on the type of sample, the type of detector and the type of measurement (e.g. kinetics). But usually, all these options/settings are identical for all measurements in the same kind of experiment; they need to be applied repeatedly to all sample runs. Because of this, the whole data reduction process can be largely automated. In a normal experiment, the reflectometry interface would be used:



More information about how to use this interface can be found here:

<https://docs.mantidproject.org/nightly/interfaces/reflectometry/ISIS%20Reflectometry.html>