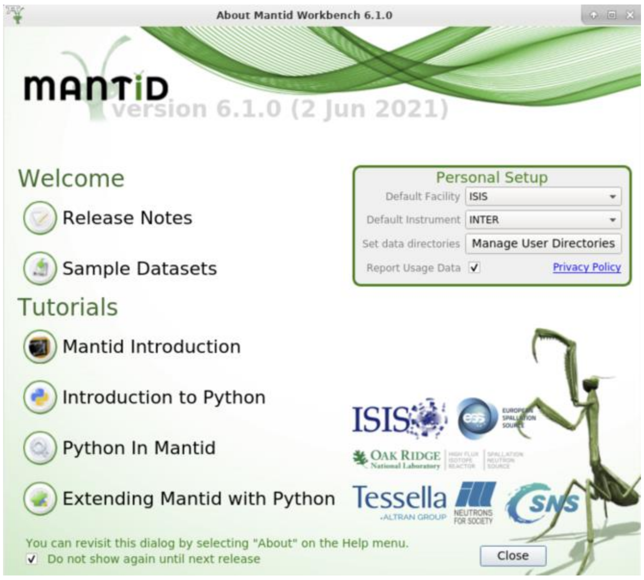
Data reduction with

MANTID

in 7 easy steps

Maximilian Skoda



About Mantid Workbench 6.1.0

MANTID version 6.1.0 (2 Jun 2021)

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Personal Setup

Default Facility: ISIS

Default Instrument: INTER

Set data directories: Manage User Directories

Report Usage Data ☑ Privacy Policy

You can revisit this dialog by selecting "About" on the Help menu.

☑ Do not show again until next release

Close

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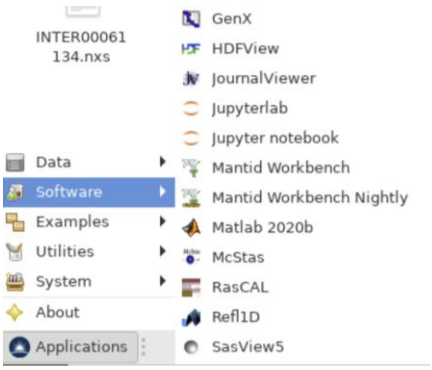
2 LAUNCHING MANTID AND LOADING FILES

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



Personal Setup

Default Facility: ISIS

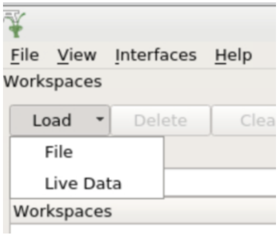
Default Instrument: INTER

Set data directories: Manage User Directories

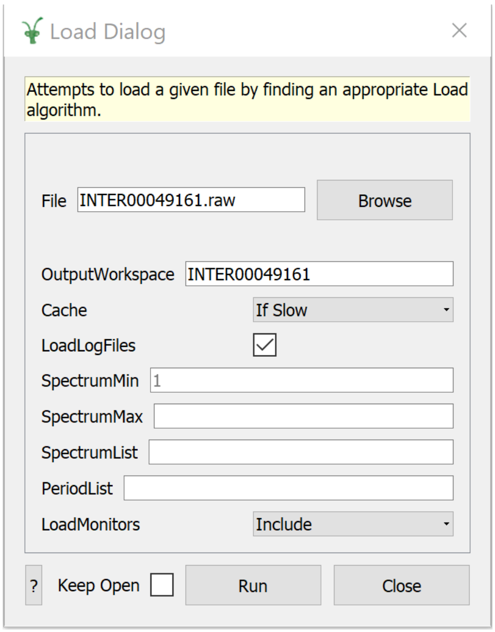
Report Usage Data: ☑ Privacy Policy

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 “Load->File”:



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



Load Dialog

Attempts to load a given file by finding an appropriate Load algorithm.

File: INTER00049161.raw

OutputWorkspace: INTER00049161

Cache: If Slow

LoadLogFiles: ☑

SpectrumMin: 1

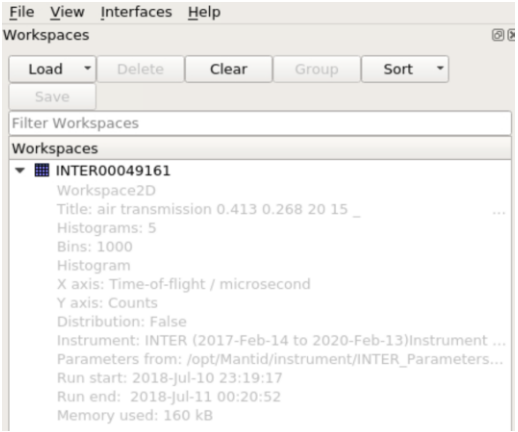
SpectrumMax:

SpectrumList:

PeriodList:

LoadMonitors: Include

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.:



```
INTER00049161
    Workspace2D
    Title: air transmission 0.413 0.268 20 15 _                    ...
    Histograms: 5
    Bins: 1000
    Histogram
    X axis: Time-of-flight / microsecond
    Y axis: Counts
    Distribution: False
    Instrument: INTER (2017-Feb-14 to 2020-Feb-13)Instrument ...
    Parameters from: /opt/Mantid/instrument/INTER_Parameters...
    Run start: 2018-Jul-10 23:19:17
    Run end:  2018-Jul-11 00:20:52
    Memory used: 160 kB
```

Run 49161 is the transmission run. By repeating the procedure, load "INTER00049162.raw". **Run 49162 is the sample run.**

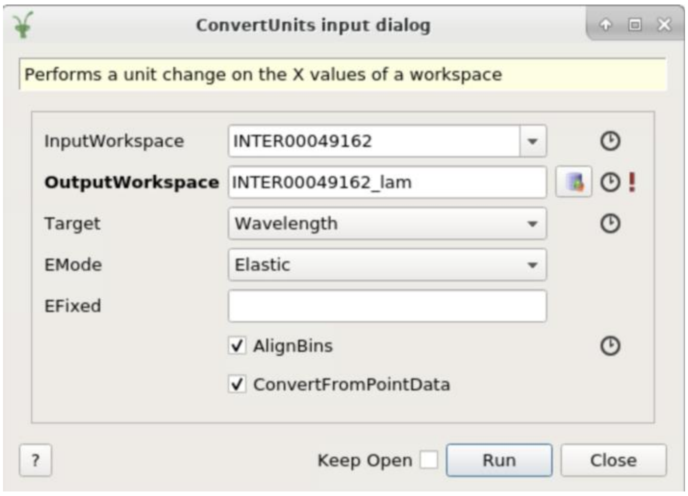
By right clicking on a workspace, you can plot the workspace histograms and view other properties.

3 STEP 1 – CONVERT TO WAVELENGTH

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

ConvertUnits

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



Performs a unit change on the X values of a workspace

InputWorkspace: INTER00049162

OutputWorkspace: INTER00049162_lam

Target: Wavelength

EMode: Elastic

EFixed:

☑ AlignBins

☑ ConvertFromPointData

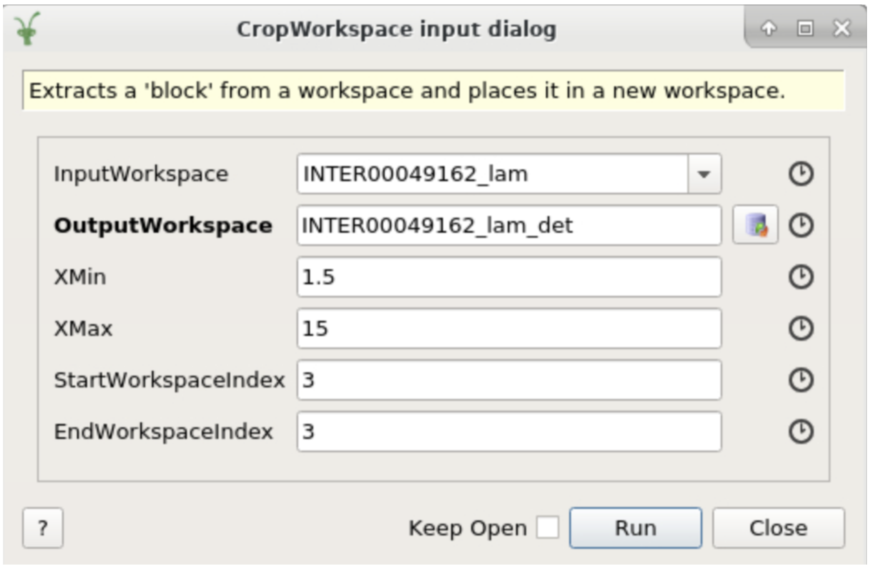
Do the same for the transmission workspace (INTER00049161).

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" worksapces 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:


CropWorkspace input dialog

Extracts a 'block' from a workspace and places it in a new workspace.

InputWorkspace: INTER00049162_lam

OutputWorkspace: INTER00049162_lam_det

XMin: 1.5

XMax: 15

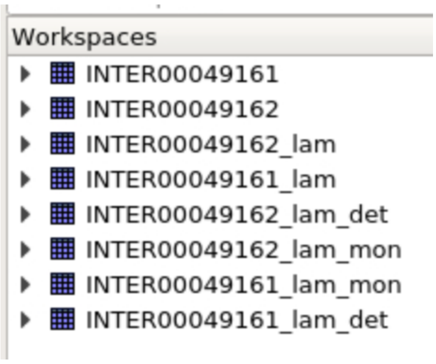
StartWorkspaceIndex: 3

EndWorkspaceIndex: 3

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:

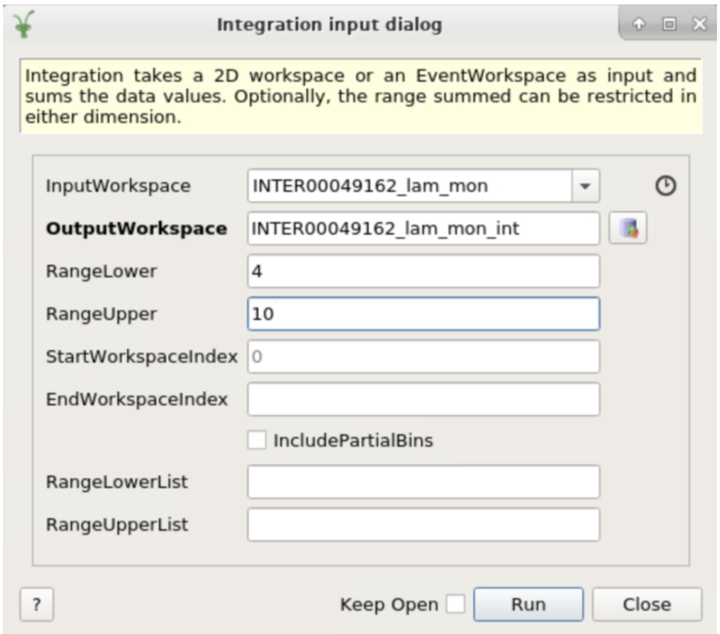

Workspaces

- INTER00049161
- INTER00049162
- INTER00049162_lam
- INTER00049161_lam
- INTER00049162_lam_det
- INTER00049162_lam_mon
- INTER00049161_lam_mon
- INTER00049161_lam_det

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:



Integration takes a 2D workspace or an EventWorkspace as input and sums the data values. Optionally, the range summed can be restricted in either dimension.

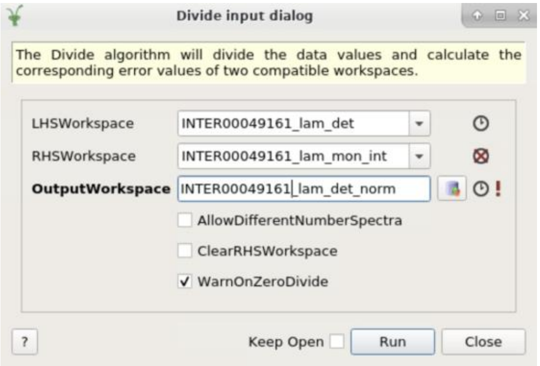
InputWorkspace	INTER00049162_lam_mon
OutputWorkspace	INTER00049162_lam_mon_int
RangeLower	4
RangeUpper	10
StartWorkspaceIndex	0
EndWorkspaceIndex	
	☐ IncludePartialBins
RangeLowerList	
RangeUpperList	

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:

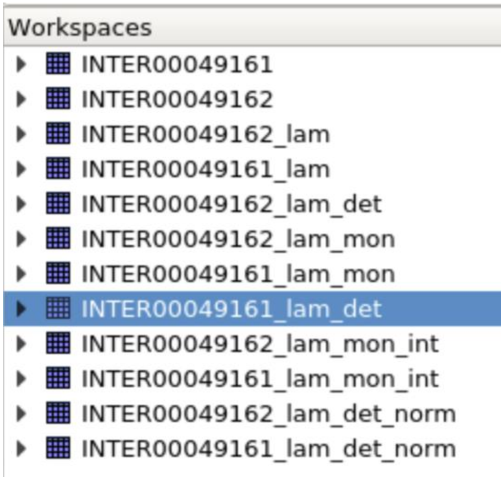


The Divide algorithm will divide the data values and calculate the corresponding error values of two compatible workspaces.

LHSWorkspace	INTER00049161_lam_det
RHSWorkspace	INTER00049161_lam_mon_int
OutputWorkspace	INTER00049161_lam_det_norm
	☐ AllowDifferentNumberSpectra
	☐ ClearRHSWorkspace
	☑ WarnOnZeroDivide

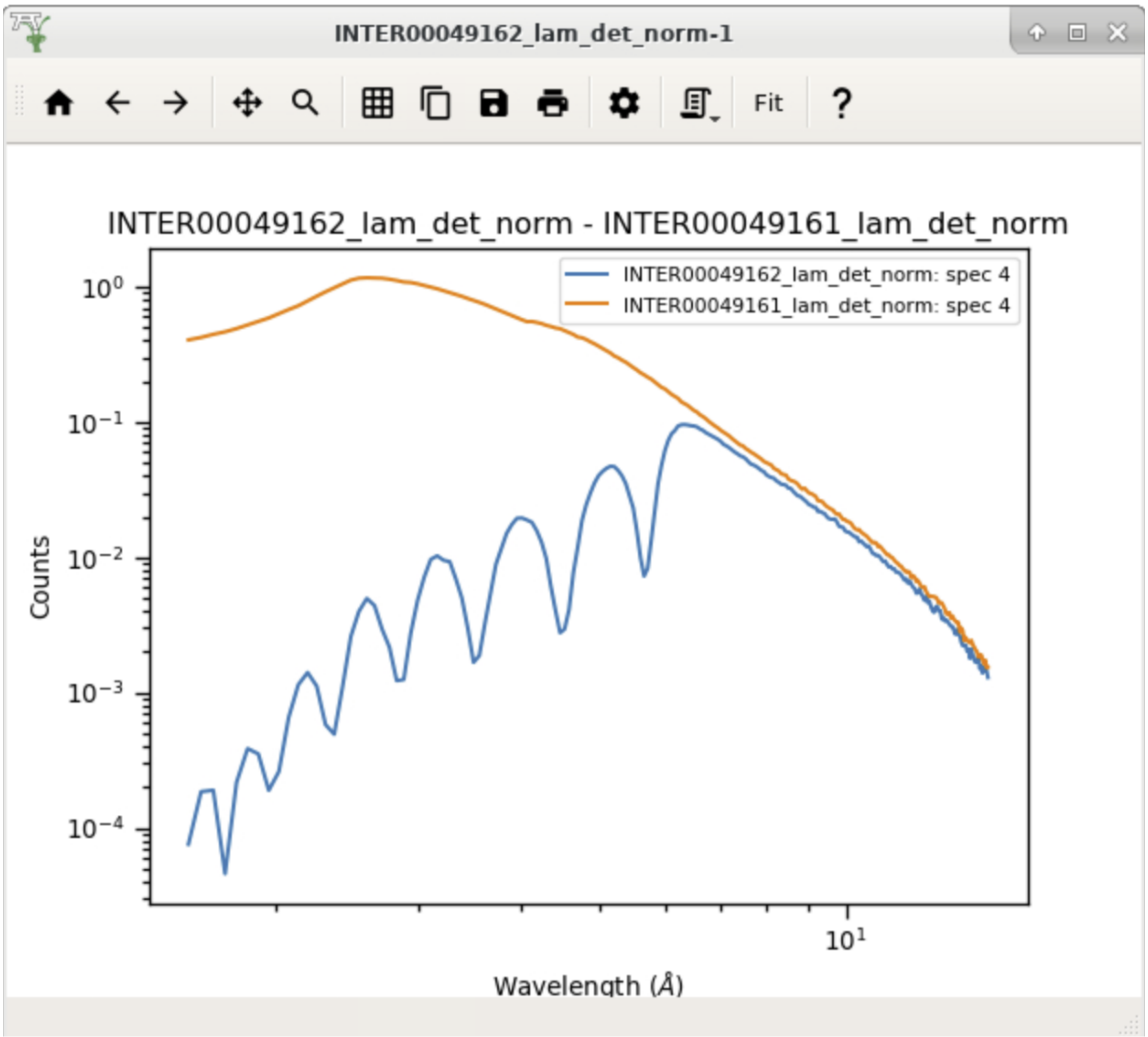
Repeat the division for the corresponding other workspaces.

The list should not contain the following workspaces:



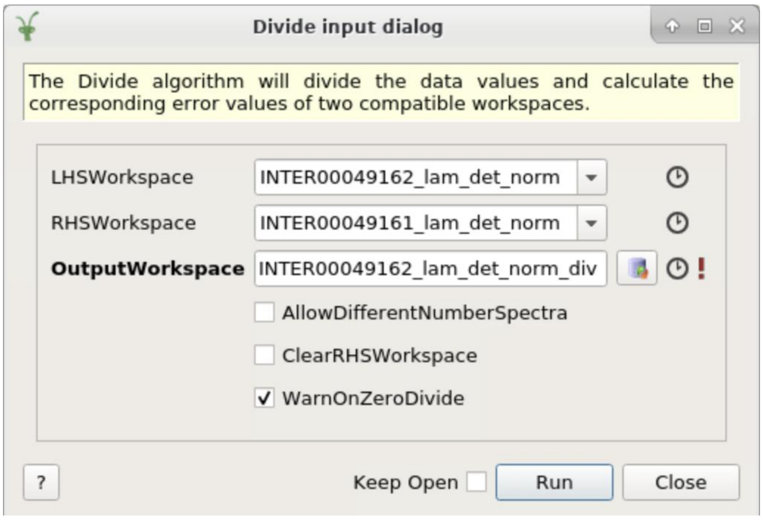
Workspaces
- INTER00049161
- INTER00049162
- INTER00049162_lam
- INTER00049161_lam
- INTER00049162_lam_det
- INTER00049162_lam_mon
- INTER00049161_lam_mon
- INTER00049161_lam_det
- INTER00049162_lam_mon_int
- INTER00049161_lam_mon_int
- INTER00049162_lam_det_norm
- INTER00049161_lam_det_norm

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:



Divide input dialog

The Divide algorithm will divide the data values and calculate the corresponding error values of two compatible workspaces.

LHSWorkspace INTER00049162_lam_det_norm

RHSWorkspace INTER00049161_lam_det_norm

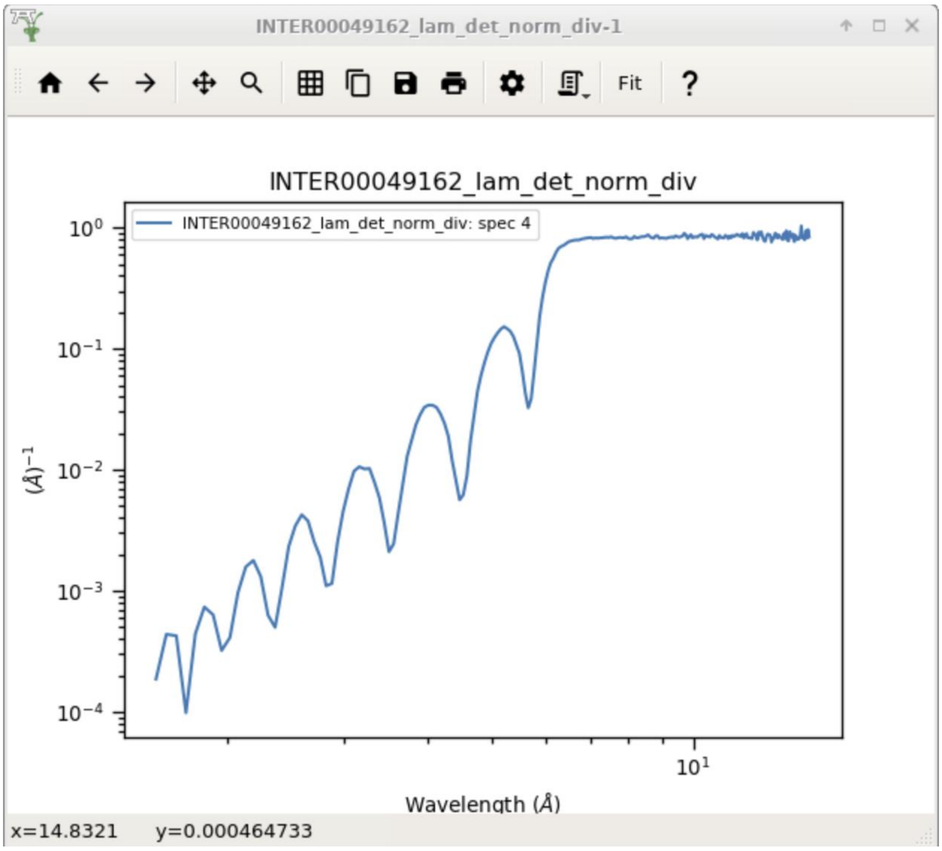
OutputWorkspace INTER00049162_lam_det_norm_div

☐ AllowDifferentNumberSpectra

☐ ClearRHSWorkspace

☑ WarnOnZeroDivide

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



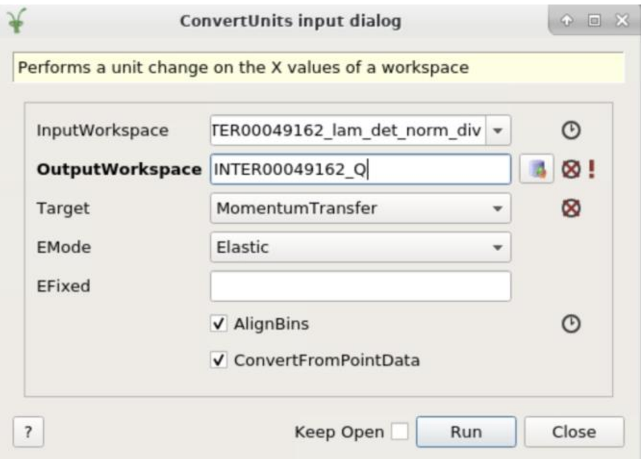
x=14.8321 y=0.000464733

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:

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

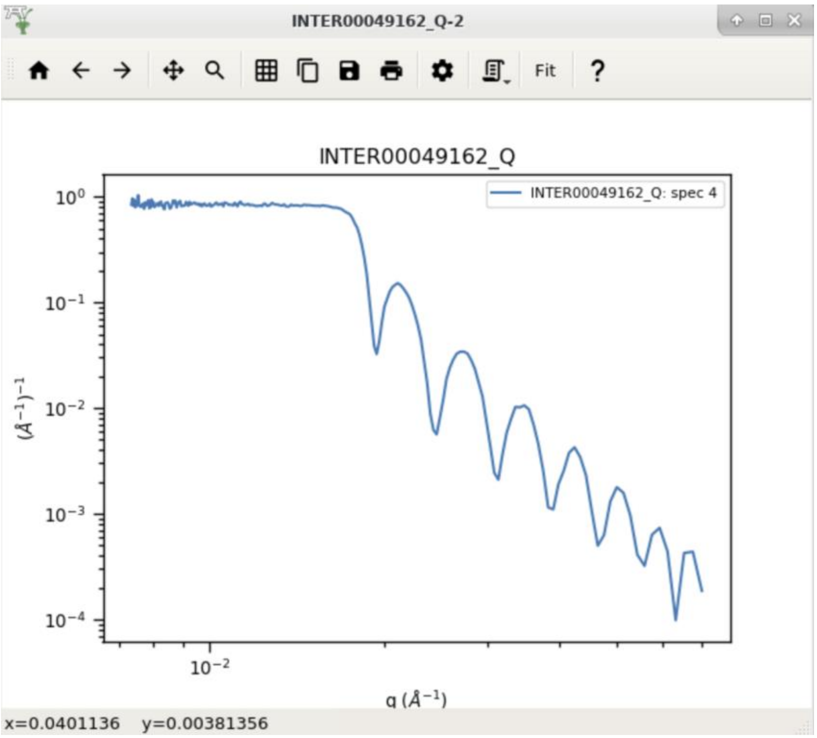
Where Q is the momentum transfer, λ is the wavelength and θ is the measurement angle of the sample run. This formula, as well as the measurement angle are stored in the run file (workspace) as metadata, such that simply running “**ConvertUnits**” yields the correct axis conversion:



Performs a unit change on the X values of a workspace

InputWorkspace: TER00049162_lam_det_norm_div
OutputWorkspace: INTER00049162_Q
Target: MomentumTransfer
EMode: Elastic
EFixed:
☑ AlignBins
☑ ConvertFromPointData

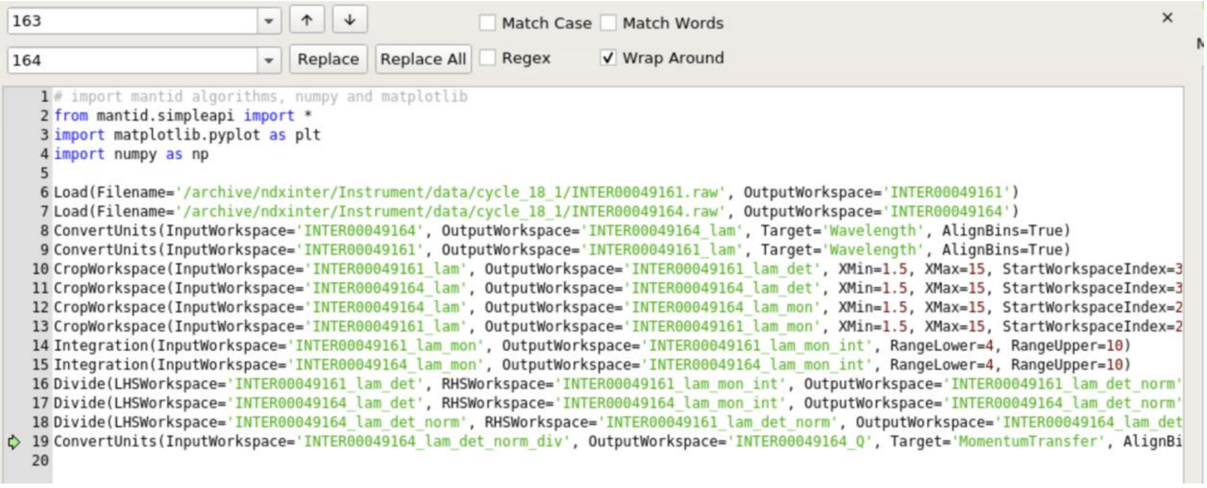
Rename the **OutputWorkspace** to a sensible name (e.g. INTER00049162_Q). The final plot should look like this (on a log-log scale):



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’.

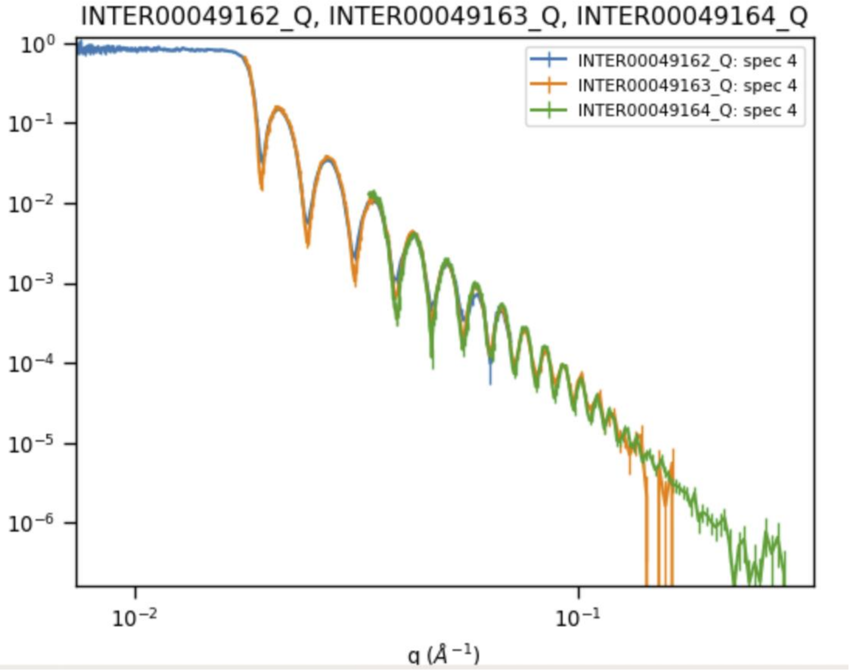
In order to obtain the other two reduced runs (49163 and 49164), the 6 reduction steps above, have to be repeated. There is however a shortcut for doing this: by selecting and right-clicking the final workspace (INTER00049162_Q), the reduction history can be displayed (“Show history”). This history can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



```python
# import mantid algorithms, numpy and matplotlib
from mantid.simpleapi import *
import matplotlib.pyplot as plt
import numpy as np

Load(Filename='/archive/ndxinter/Instrument/data/cycle_18_1/INTER00049161.raw', OutputWorkspace='INTER00049161')
Load(Filename='/archive/ndxinter/Instrument/data/cycle_18_1/INTER00049164.raw', OutputWorkspace='INTER00049164')
ConvertUnits(InputWorkspace='INTER00049164', OutputWorkspace='INTER00049164_lam', Target='Wavelength', AlignBins=True)
ConvertUnits(InputWorkspace='INTER00049161', OutputWorkspace='INTER00049161_lam', Target='Wavelength', AlignBins=True)
CropWorkspace(InputWorkspace='INTER00049161_lam', OutputWorkspace='INTER00049161_lam_det', XMin=1.5, XMax=15, StartWorkspaceIndex=3
CropWorkspace(InputWorkspace='INTER00049164_lam', OutputWorkspace='INTER00049164_lam_det', XMin=1.5, XMax=15, StartWorkspaceIndex=3
CropWorkspace(InputWorkspace='INTER00049164_lam', OutputWorkspace='INTER00049164_lam_mon', XMin=1.5, XMax=15, StartWorkspaceIndex=2
CropWorkspace(InputWorkspace='INTER00049161_lam', OutputWorkspace='INTER00049161_lam_mon', XMin=1.5, XMax=15, StartWorkspaceIndex=2
Integration(InputWorkspace='INTER00049161_lam_mon', OutputWorkspace='INTER00049161_lam_mon_int', RangeLower=4, RangeUpper=10)
Integration(InputWorkspace='INTER00049164_lam_mon', OutputWorkspace='INTER00049164_lam_mon_int', RangeLower=4, RangeUpper=10)
Divide(LHSWorkspace='INTER00049161_lam_det', RHSWorkspace='INTER00049161_lam_mon_int', OutputWorkspace='INTER00049161_lam_det_norm'
Divide(LHSWorkspace='INTER00049164_lam_det', RHSWorkspace='INTER00049164_lam_mon_int', OutputWorkspace='INTER00049164_lam_det_norm'
Divide(LHSWorkspace='INTER00049164_lam_det_norm', RHSWorkspace='INTER00049161_lam_det_norm', OutputWorkspace='INTER00049164_lam_det
ConvertUnits(InputWorkspace='INTER00049164_lam_det_norm_div', OutputWorkspace='INTER00049164_Q', Target='MomentumTransfer', AlignBi
```

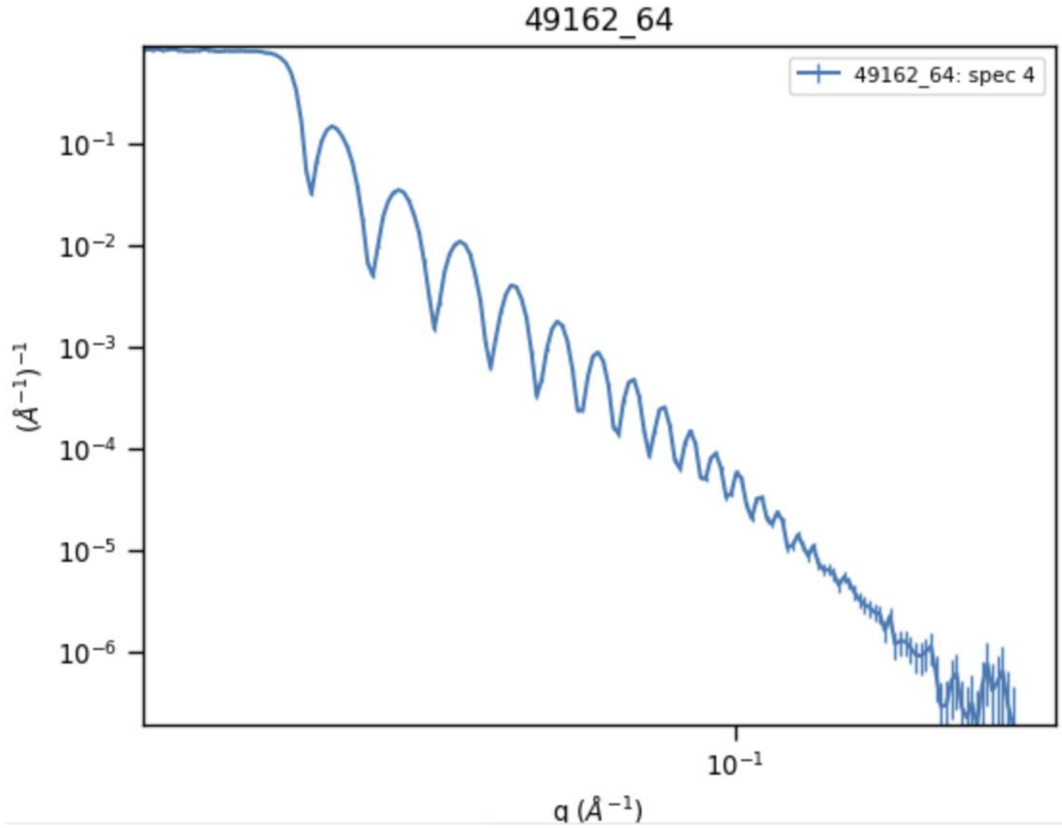
With Ctrl+f, the find/replace menu can be called and all run number entries for the sample run (162) can be replaced by the next run (163) and the script executed by pressing the green play button at the top right. The replace operation can be repeated for the third and final run (ending 164). The three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



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

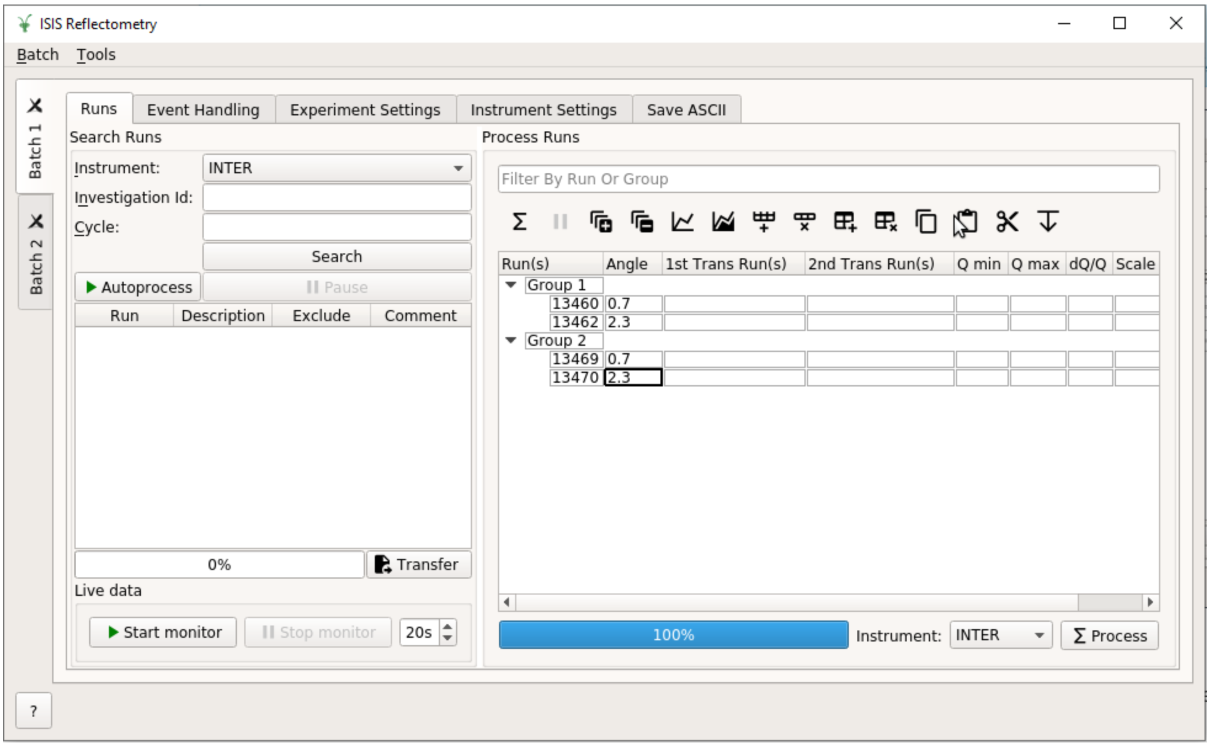
```
Stitch1DMany(['INTER00049162_Q', 'INTER00049163_Q', 'INTER00049164_Q'], Params='0.01,-
0.02,0.33', OutputWorkspace="49162_64")
```

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 of 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:



Instrument: INTER

Investigation Id:

Cycle:

0%

20s

Run(s)	Angle	1st Trans Run(s)	2nd Trans Run(s)	Q min	Q max	dQ/Q	Scale
Group 1							
13460	0.7						
13462	2.3						
Group 2							
13469	0.7						
13470	2.3						

100%

Instrument: INTER

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

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