Arthur
WILCKE

22/06/2015 –
21/08/2015

Comparison of MANTID and LAMP for TOF and SANS data

Institut Laue-Langevin

Computing for Science
Mark Johnson

Introduction

In order to prepare for the implementation of MANTID at the ILL, a comparison of the data-treatment methods of LAMP and MANTID was necessary. In this summary, we will look at two TOF data-sets from IN6, namely data-sets 164198-164200 and 161389-161400, as well as a SANS data-set from D33, namely 001420-001431.
For the TOF data, comparison was done on a step-by-step basis, comparing each part of the algorithms with the counterpart in the other program, looking at differences and similarities. When differences were found, we tried to remove the steps in the algorithms so that a direct comparison of later steps was still relevant. Modifications of several algorithm, both in LAMP and in MANTID were necessary.
As for the SANS data, as the treatment was done in a single step, we could only compare directly.

All comparisons were done in Mantid 3.2.1, which was the latest version readily available on the machine used.

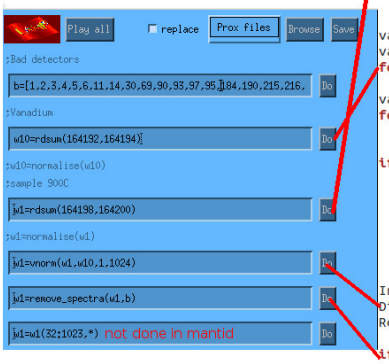
Table of Contents

TOF

Introduction

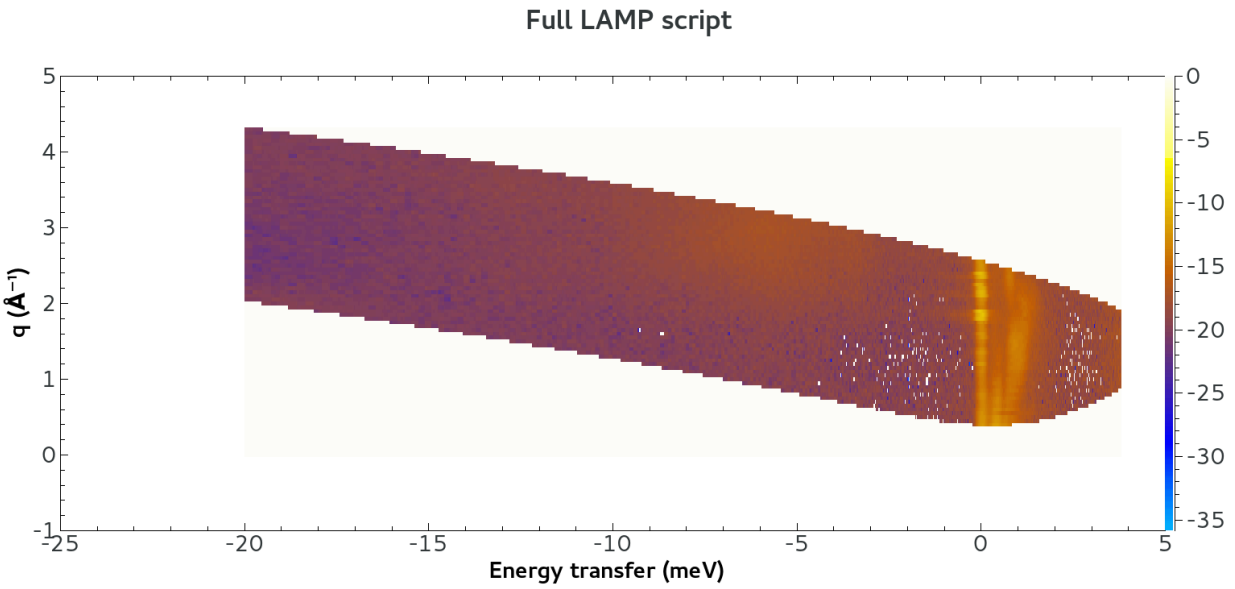
After looking at the LAMP .prox file we tried to recreate it in MANTID, to be as close as we could. The end result was the following script, and its equivalence to LAMP.

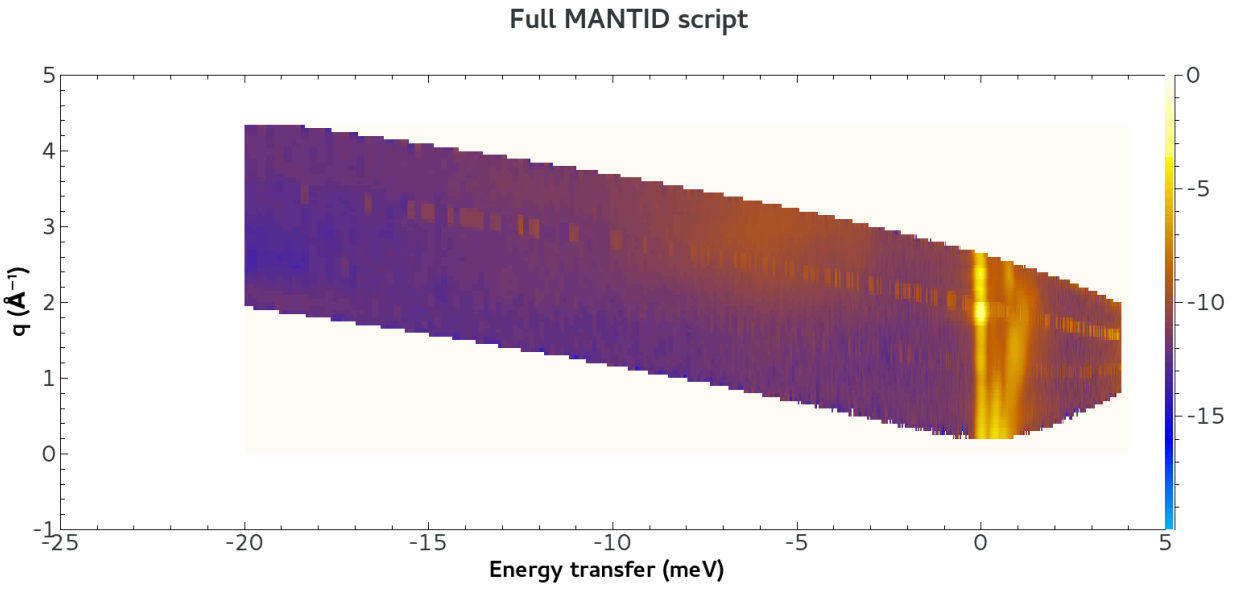
Equivalence of LAMP and MANTID scripts

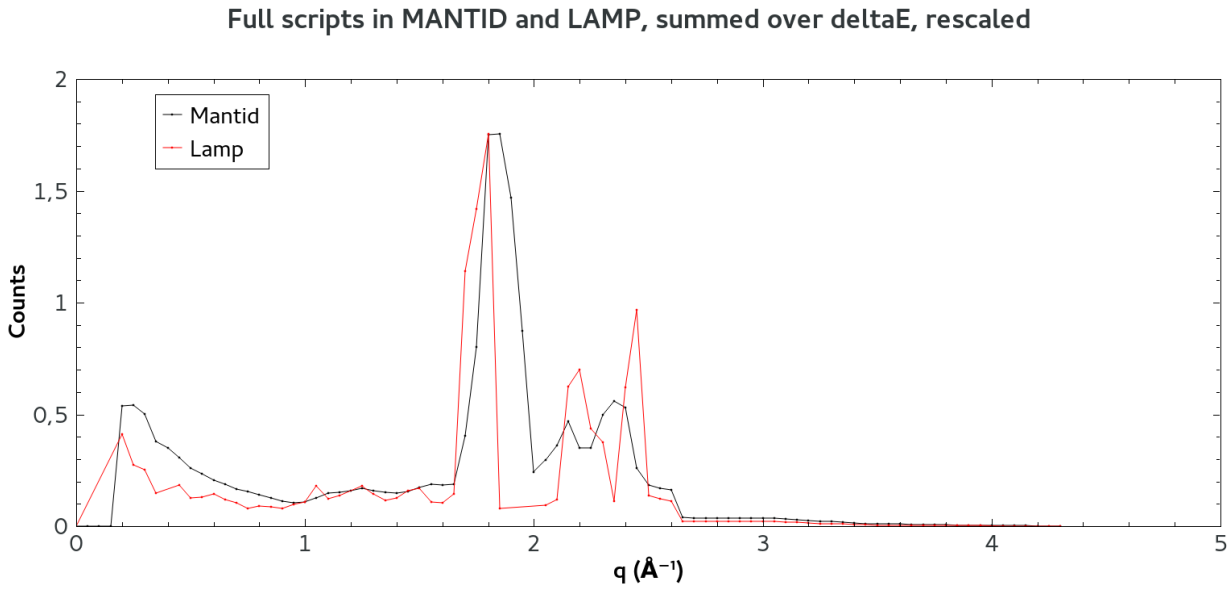


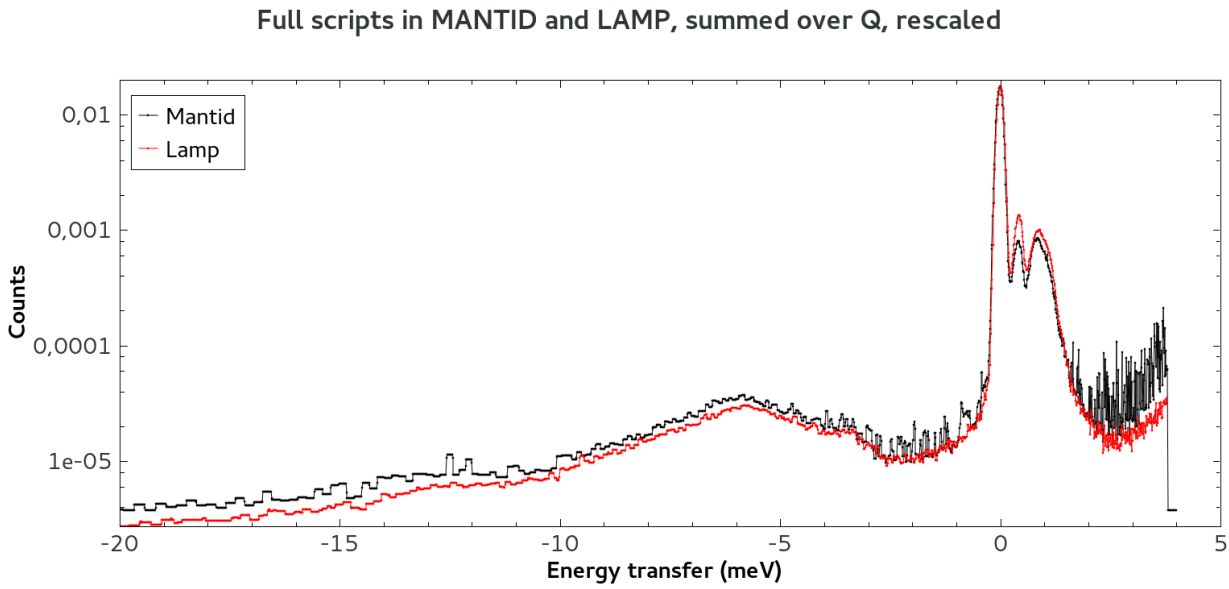

```
dataFolder = '/home/cs/wilckea/Downloads/SampleData-ILL/IN6'

rebiningInEnergy = '-20,0.01,4'
rebiningInQ = '0,0.05,4.35'
spectraListToMask = [1,2,3,4,5,6,11,14,30,69,90,93,97,95,184,190,215,216,217,251,252,253,335,337]


fileRange = [164198,164200]
dataFileNames = []
for i in range(fileRange[0], fileRange[1] +1):
      dataFileNames.append(str(i))
mergedWorkspaceName = 'data_merged'
for file in dataFileNames:
    fullPath = os.path.join(dataFolder,file+'.nxs')
    Load(Filename=fullPath,OutputWorkspace=file)
if len(dataFileNames) > 1 :
    fileNamesToMerge = ','.join(map(str,dataFileNames))
    MergeRuns(InputWorkspaces=fileNamesToMerge,OutputWorkspace=mergedWorkspaceName)

vanaRange = [164192,164194]
vanaFileNames = []
for i in range(vanaRange[0], vanaRange[1] +1):
      vanaFileNames.append(str(i))
vanaMergedWorkspaceName = 'vana_merged'
for file in vanaFileNames:
    fullPath = os.path.join(dataFolder,file+'.nxs')
    Load(Filename=fullPath,OutputWorkspace=file)
if len(vanaFileNames) > 1 :
    fileNamesToMerge = ','.join(map(str,vanaFileNames))
    MergeRuns(InputWorkspaces=fileNamesToMerge,OutputWorkspace=vanaMergedWorkspaceName)



Integration(InputWorkspace='vana_merged',OutputWorkspace='Vanadium_I')
Divide(LHSWorkspace='data_merged',RHSWorkspace='Vanadium_I',OutputWorkspace='Division',ClearRHSWorkspace='1')
ReplaceSpecialValues(InputWorkspace='Division',OutputWorkspace='Data_c',NaNValue='0',InfinityValue='0')

if spectraListToMask is not None:
    MaskDetectors(Workspace='Data_c',SpectraList=spectraListToMask)

ConvertUnits(InputWorkspace='Data_c',OutputWorkspace='deltaE',Target='DeltaE',EMode='Direct')
CorrectKiKf(InputWorkspace='deltaE',OutputWorkspace='deltaE_c')

DetectorEfficiencyCorUser(InputWorkspace='deltaE_c',OutputWorkspace='deltaE_effc')

Rebin(InputWorkspace='deltaE_effc',OutputWorkspace='deltaE_r',Params=rebiningInEnergy,PreserveEvents='0')

SofQW3(InputWorkspace='deltaE_r',OutputWorkspace='SofQW',QAxisBinning=rebiningInQ,EMode='Direct')
```

The first step was to run the whole scripts and compare the final results.





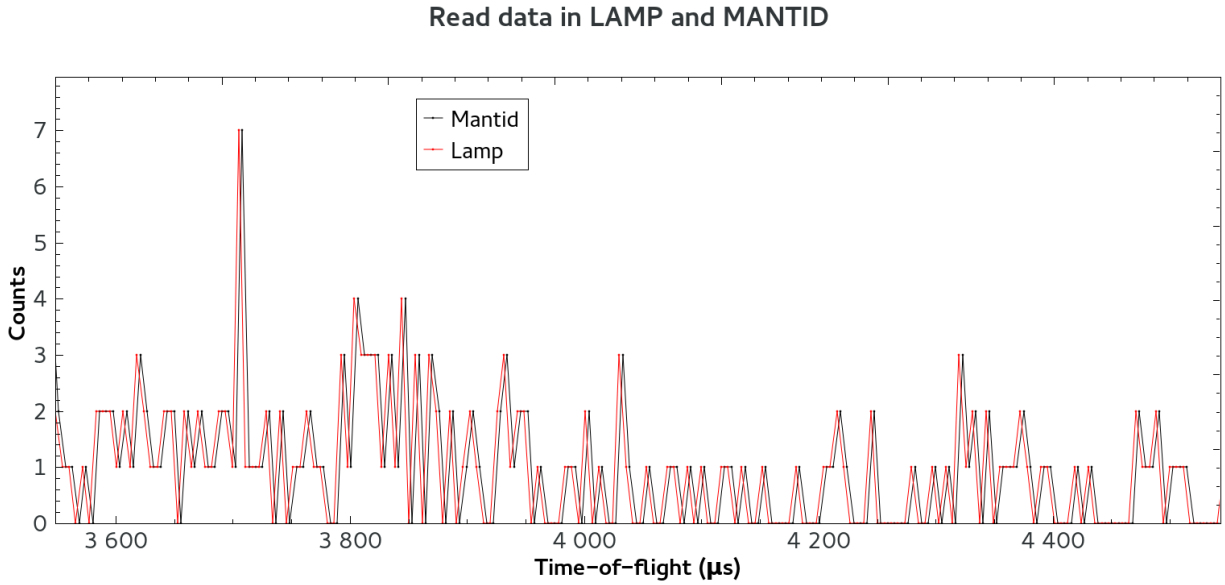




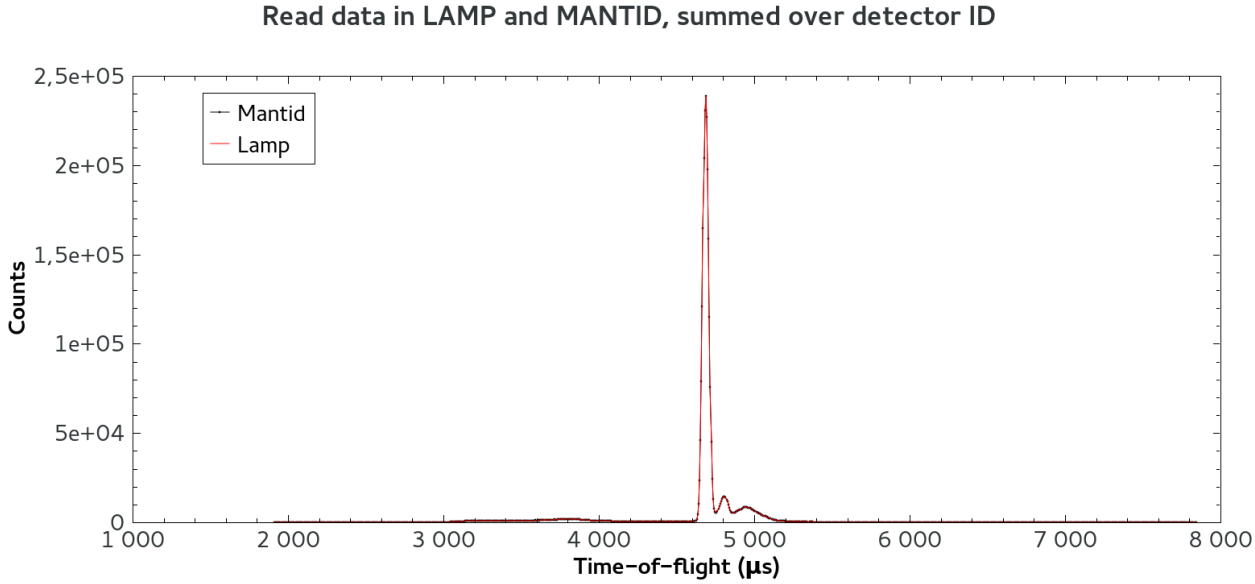
We saw that the final results were quite similar, but still significantly different. To try and identify where these differences were coming from, we then went on to do a step-by-step comparison.

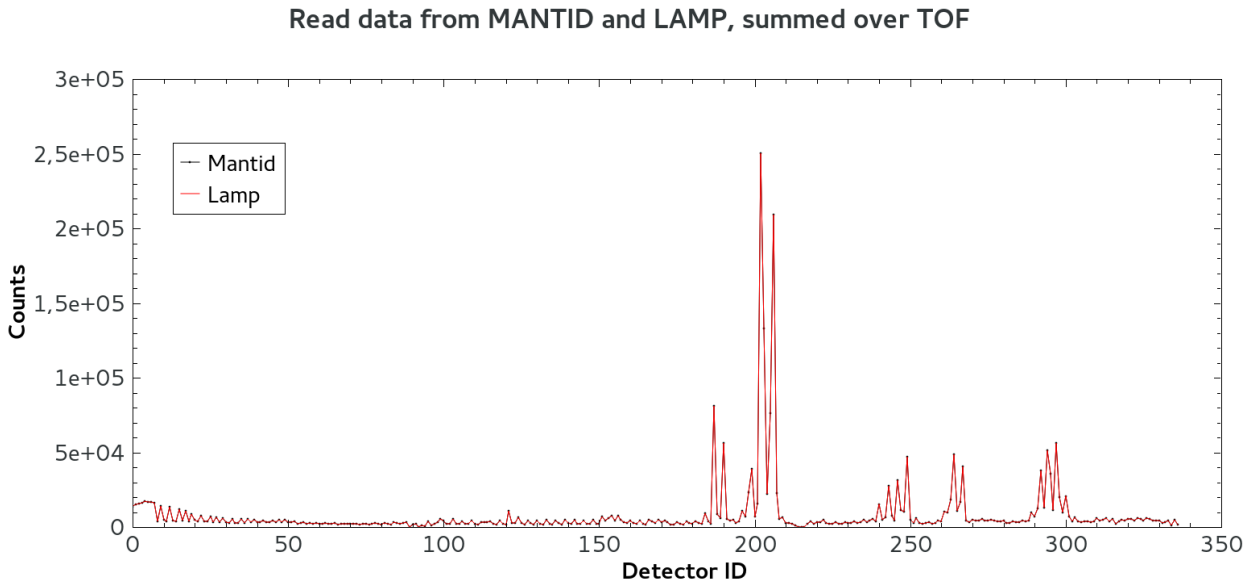
Reading the data

In both LAMP and MANTID, the data was imported and merged, no further modifications were made. Direct comparison was not meaningful, as LAMP imports the data as Count/Detector Number whereas MANTID imports it as Count/Time-of-Flight.
We created SetUnits to solve this issue. This algorithm enables us to give the units we want to a workspace, and, if we want, to replace the x-values of a workspace with those of another, without changing the y-values, so that a direct comparison is possible

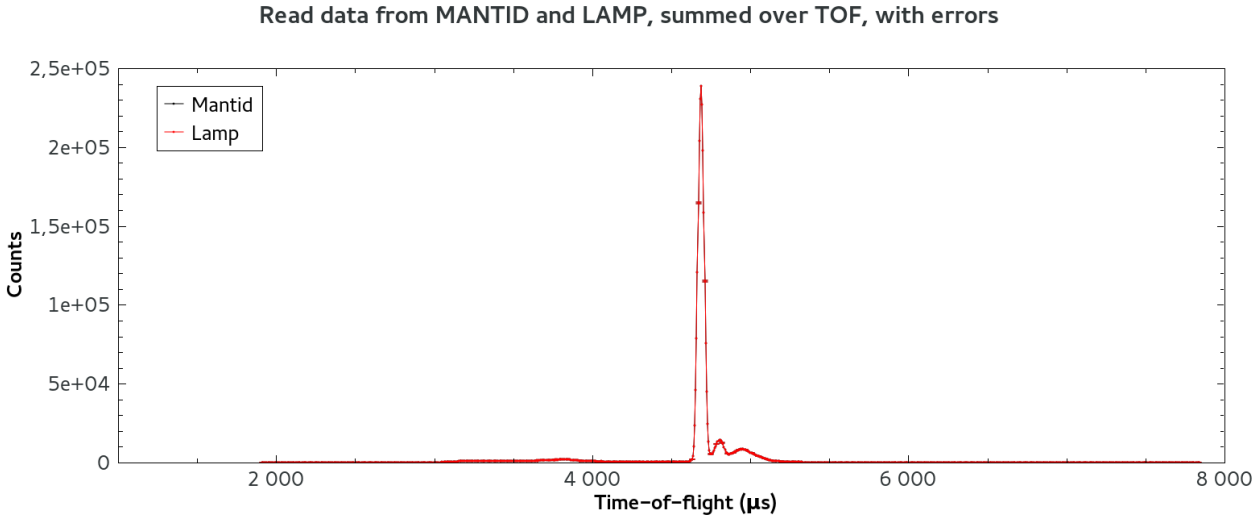


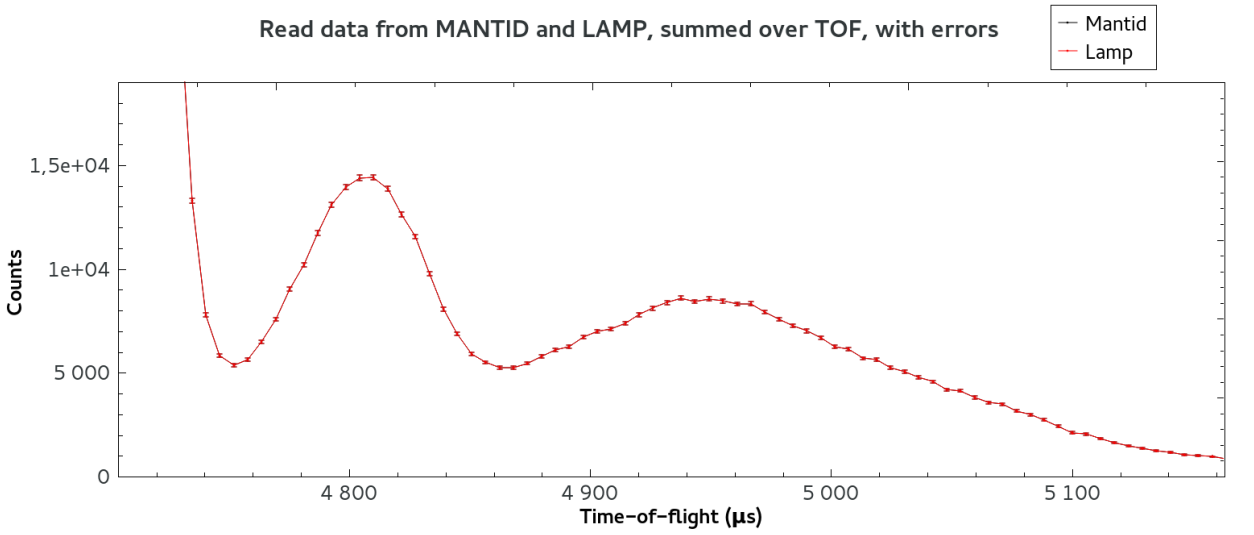
Even after correcting the units, there was a half-channel offset between the otherwise identical data-sets. We eventually understood that this offset was due to the differences in how LAMP and MANTID plot data. LAMP plots data using midpoints, whereas LAMP plots it using end-points, which means that MANTID has an extra X-value compared to LAMP, and when trying to plot LAMP data, would create this half-channel offset as it did not have the correct number of x-values.
We extended SetUnits to be able to calculate an extra x-value, so we could accurately plot LAMP data in MANTID.





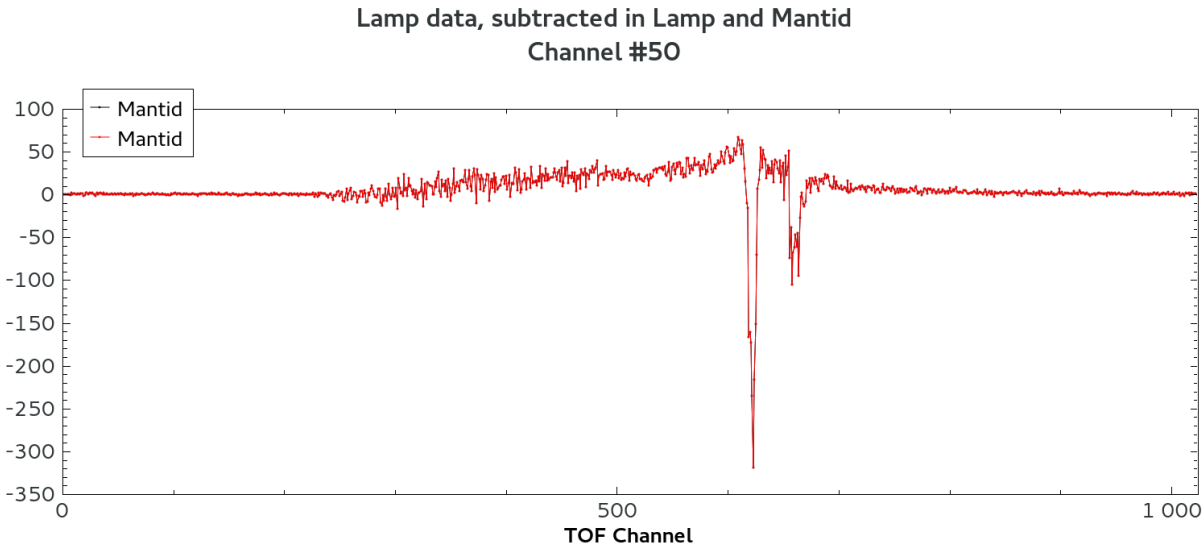
After correcting the offset and removing the monitor channels, that are not present in the LAMP data, we were able to see that the read data is exactly the same.
Concerning errors, they are also conserved.



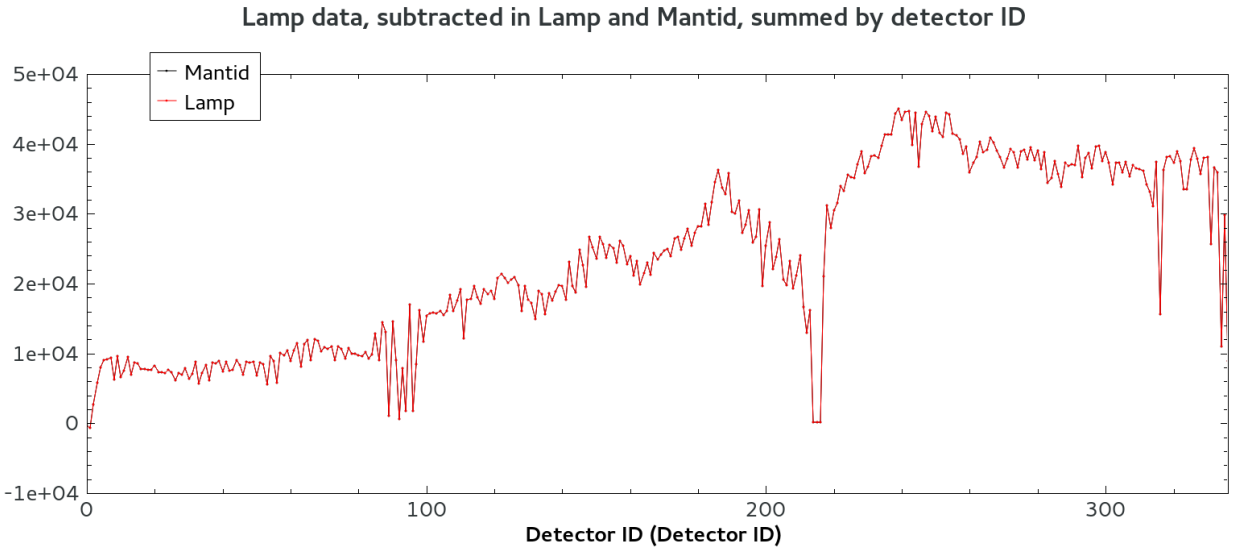


Empty Can Subtraction

Some treatments involve subtracting an empty can. To make sure that the subtraction is not different in LAMP and MANTID, we looked at both methods. Looking at a single channel, we see that the data is exactly the same.



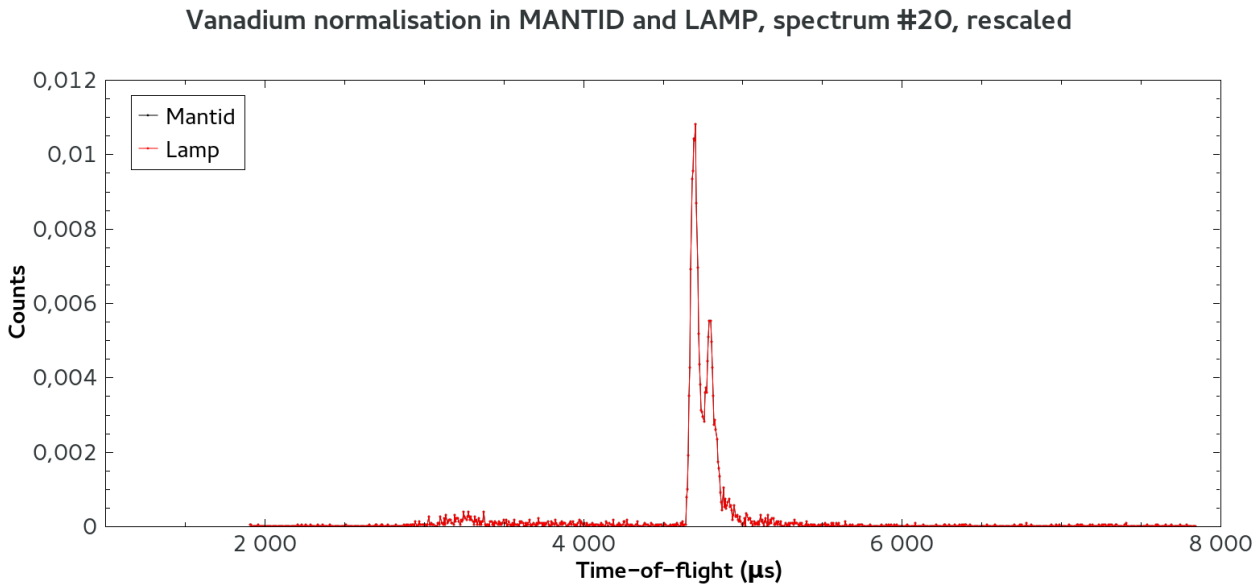
Summing by detector ID confirms this.



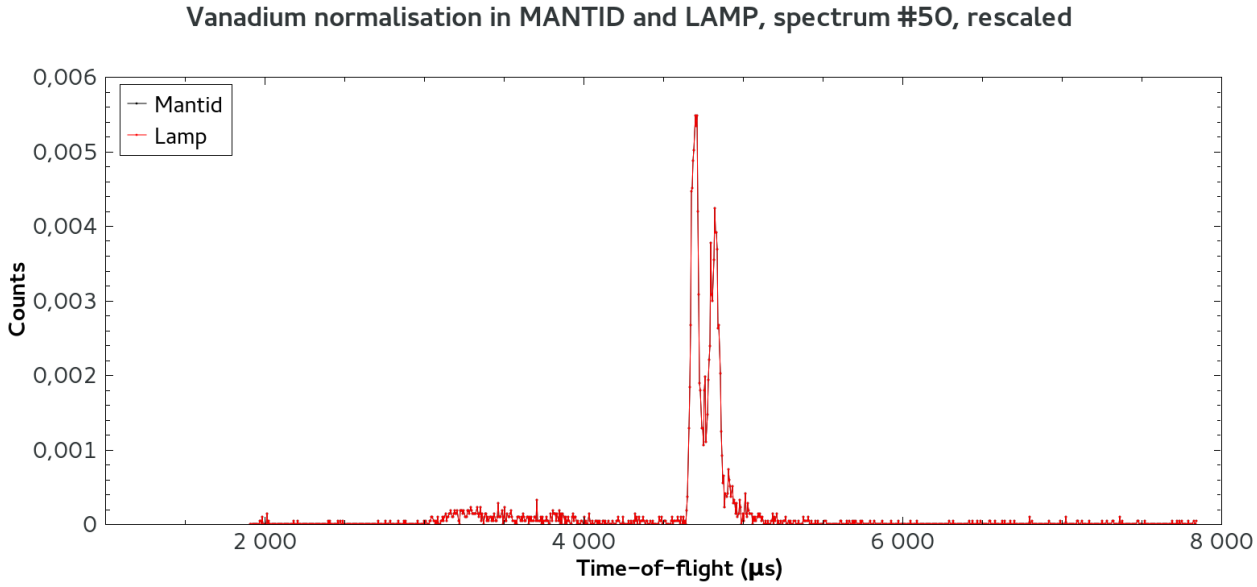
Thus the subtraction algorithms are identical.

Vanadium Normalisation

When comparing the vanadium normalisation, the data was read and normalised in both programs, then imported and histogrammed correctly to be comparable in MANTID.
When looking at an individual spectrum, the data overlays perfectly when rescaled.

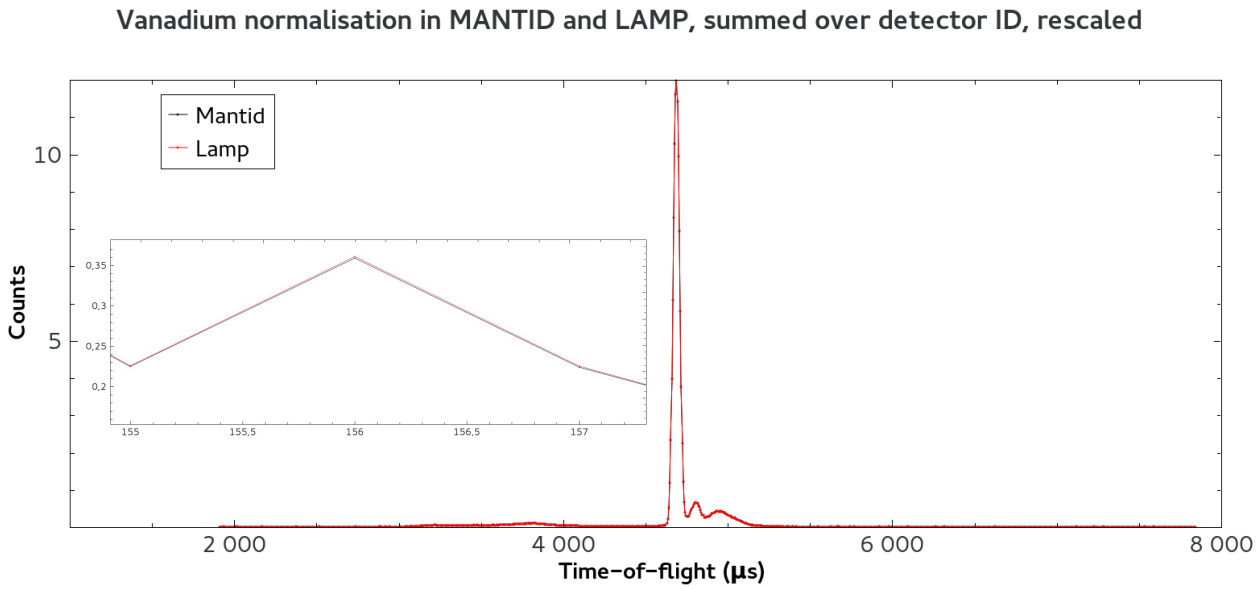


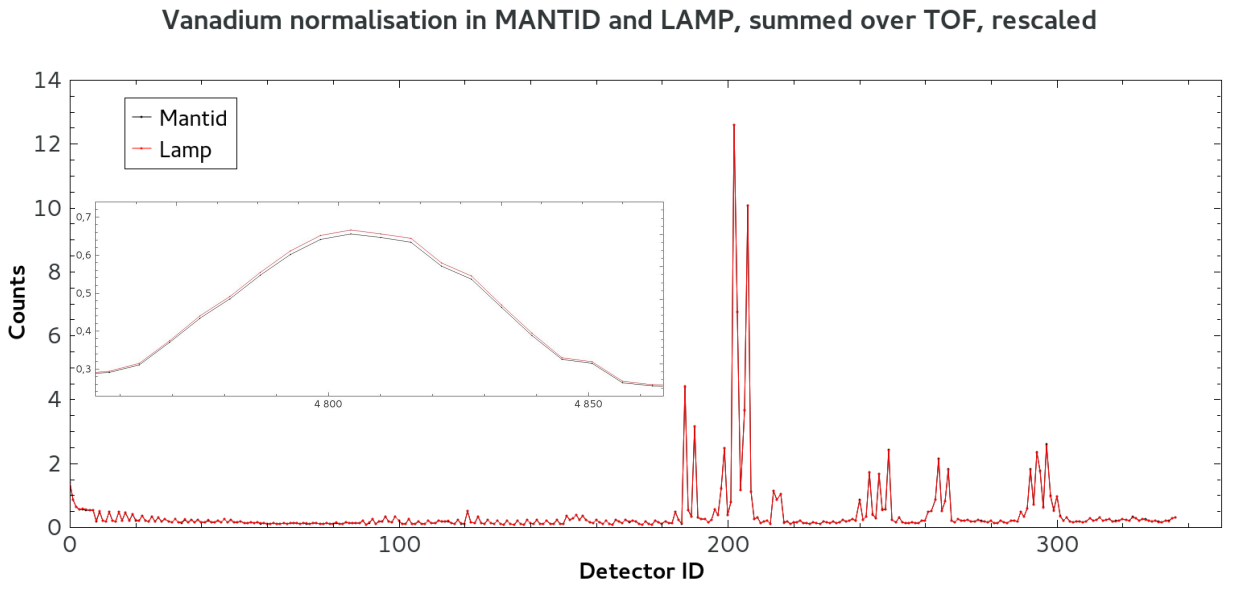
However, the rescaling factor is not constant for all spectra. For example, spectrum 20 has a scaling factor of 428.740305598.



Whereas spectrum 50 has a scaling factor of 429.512705318. The normalisation algorithms are thus similar, but one of them rescales the data.

As the rescaling factor is not constant, when looking at the sums over the whole data-set, we see small differences.





In order to make sure the rescaling factor did not affect later treatment, the vanadium normalisation was removed from the process.

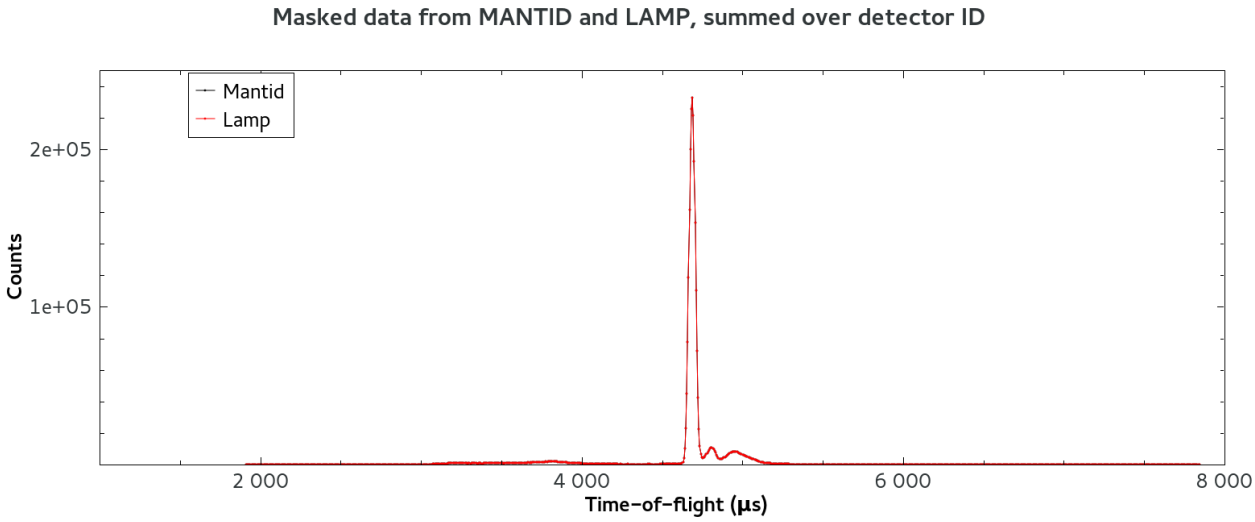
Masking unwanted spectra

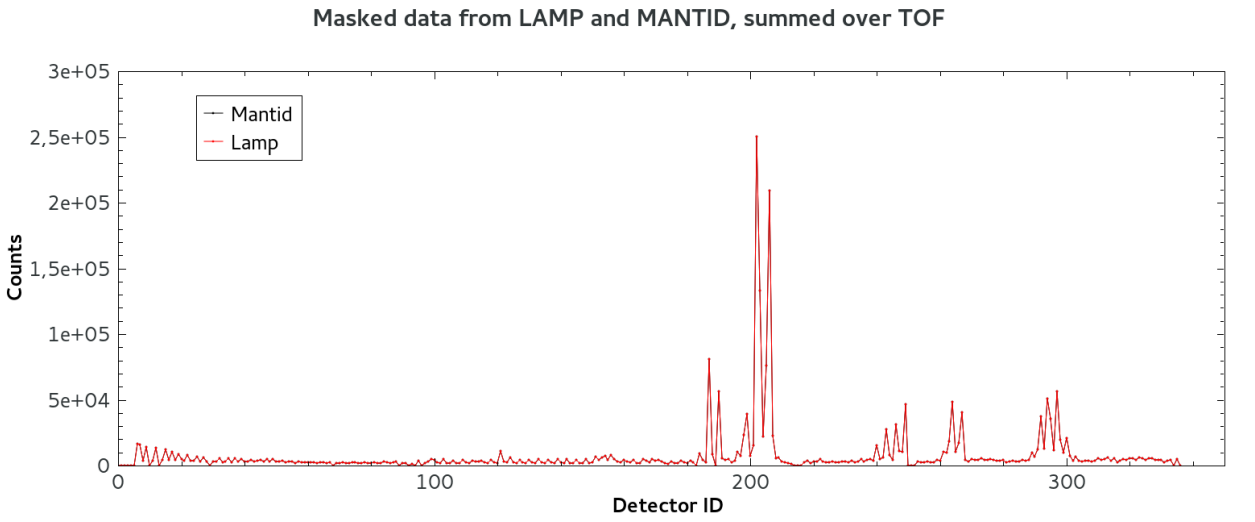
Masking is handled in a different way by both programs. LAMP completely deletes the selected spectra, reducing the dimension of the data, whereas MANTID keeps the same dimension, it just sets the Y-values of the selected spectra to 0.
Another complication arises from the 3 monitor detectors that are in the MANTID data, which creates an offset in spectrum number that must be taken into account.

Therefore, to have a meaningful comparison, you must:

1. Add the number of monitors (here, 3) to each spectrum in the spectraListToMask
2. Add blank rows where they have been deleted in LAMP so that you have data with the same dimensions

Now the data is in comparable format. For this comparison, data was read into each program and masked, with no vanadium normalisation.





The data is exactly the same, which means that the masking, although done differently, has the same effect.
To be sure that the different masking techniques did not alter further results, masking was not included in later steps of the comparison.

Conversion to deltaE

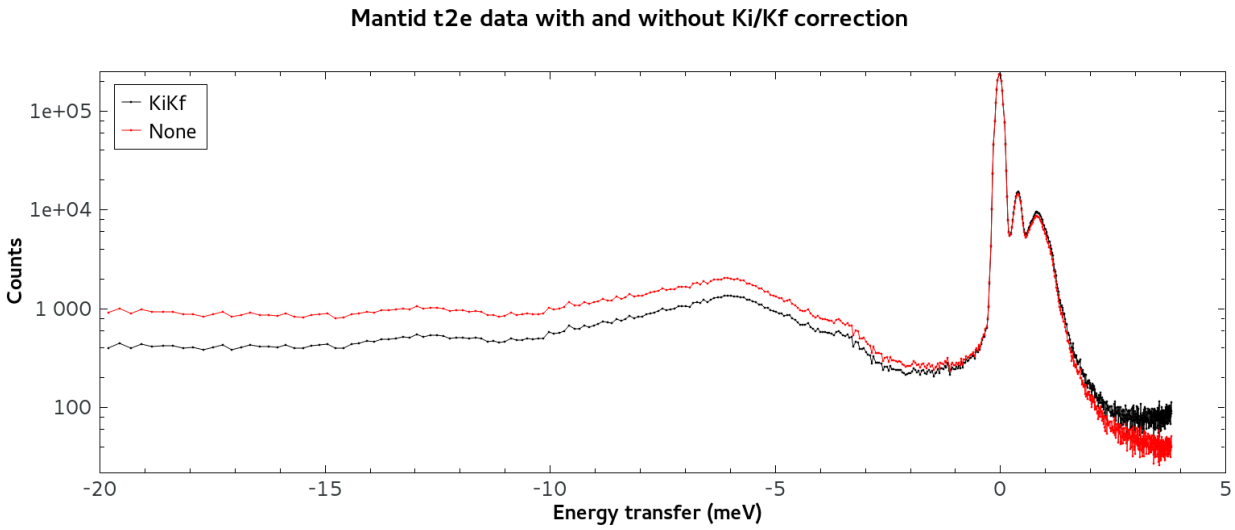
The TOF-to-deltaE (or t2e) conversion in LAMP and MANTID is handled differently. In LAMP, everything is handled by a single command : t2e, which does everything, whereas in MANTID there are 2 different algorithms.

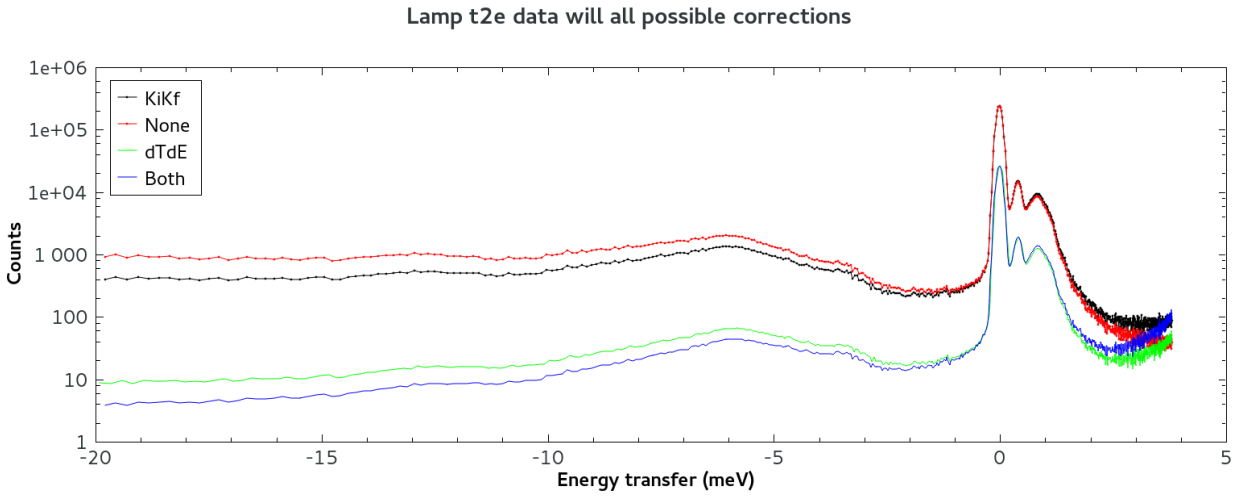
The steps of the conversion are :

1. Conversion to deltaE (ConvertUnits)
2. Ki/Kf correction (CorrectKiKf)
3. dT/dE correction (LAMP)

While both LAMP and MANTID do the Ki/Kf correction, the dT/dE correction is not present in MANTID.

In order to have a relevant step-by-step comparison, we created lamp commands without the ki/kf and dt/de correction.

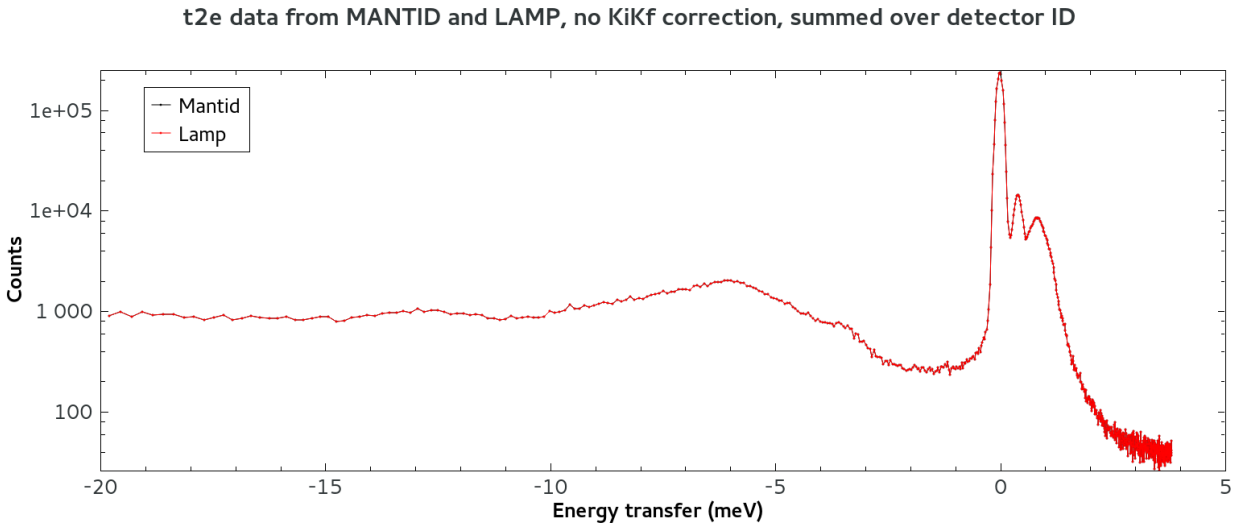


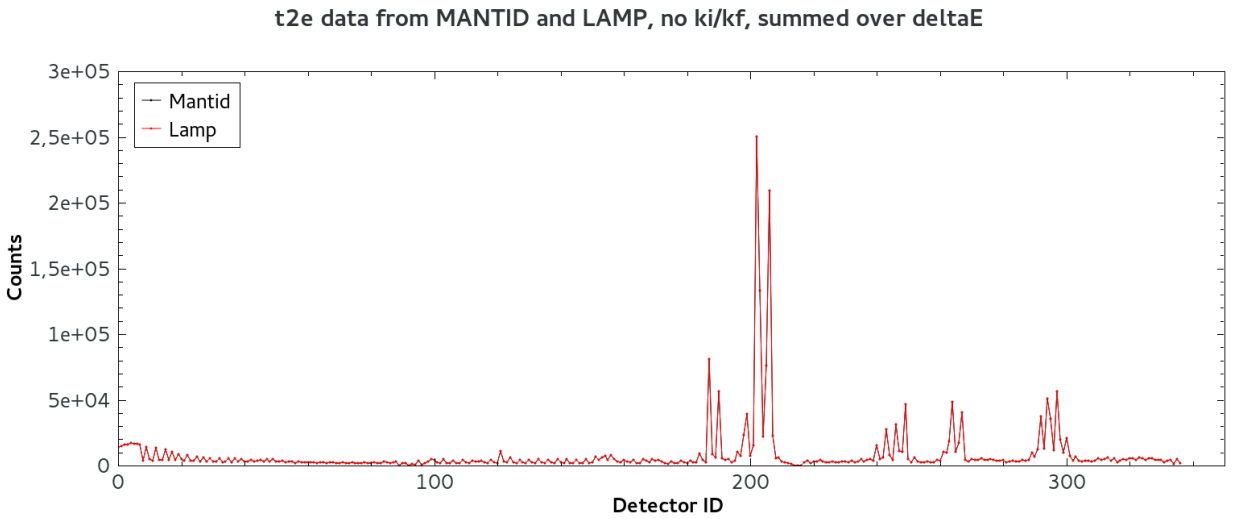


We see straight away that the both LAMP datasets with dTdE correction have a significantly different shape from all MANTID curves, and the two other LAMP curves, which indicates that the

dT/dE correction is not present in MANTID.

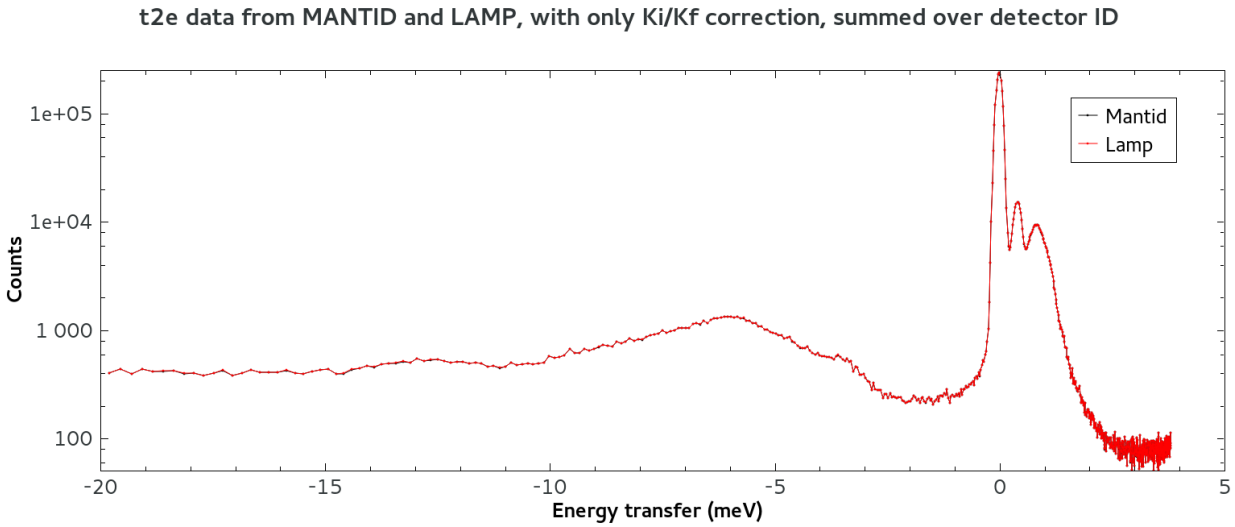
We then compared LAMP and MANTID data-sets one to one. At first we compared the data from LAMP and MANTID with no correction whatsoever.



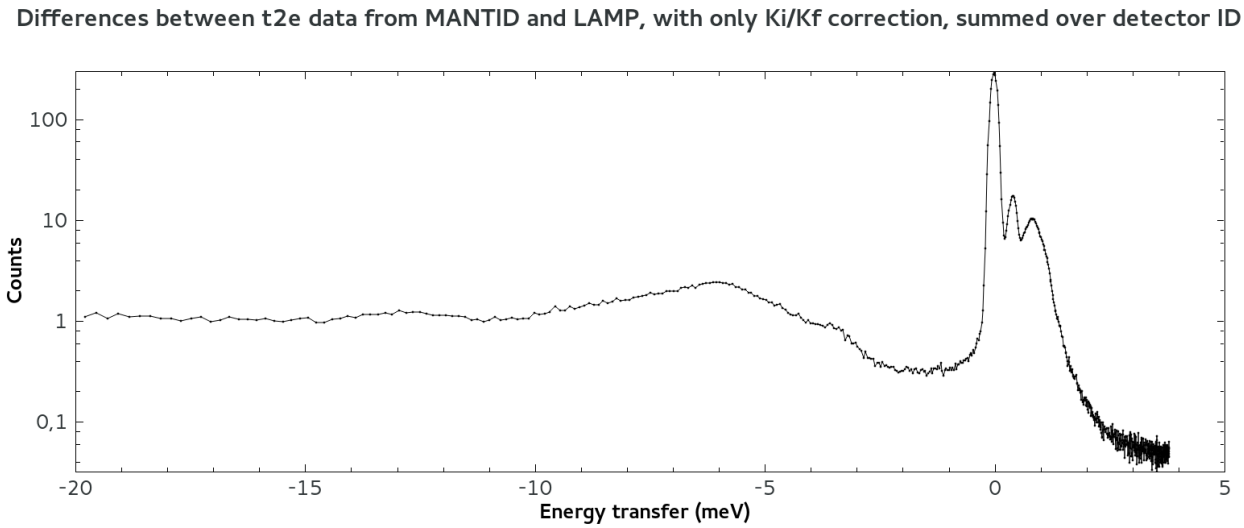


When summing over detector ID and deltaE we see that both data-sets are exactly identical, thus the basic t2e algorithms are the same. We see that the data is exactly identical, thus the basic t2e conversions are the same.

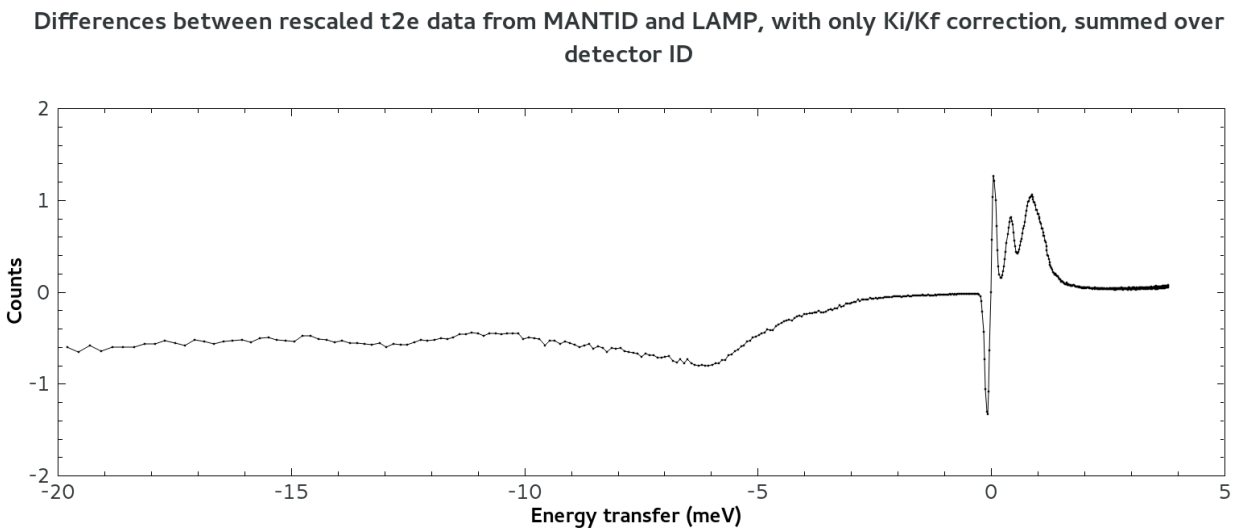
We then looked at the Ki/Kf correction, but without the dT/dE correction, as it is not present in MANTID.



There seems to be no difference. To confirm this theory, we calculated the differences between both data-sets, summed over deltaE.

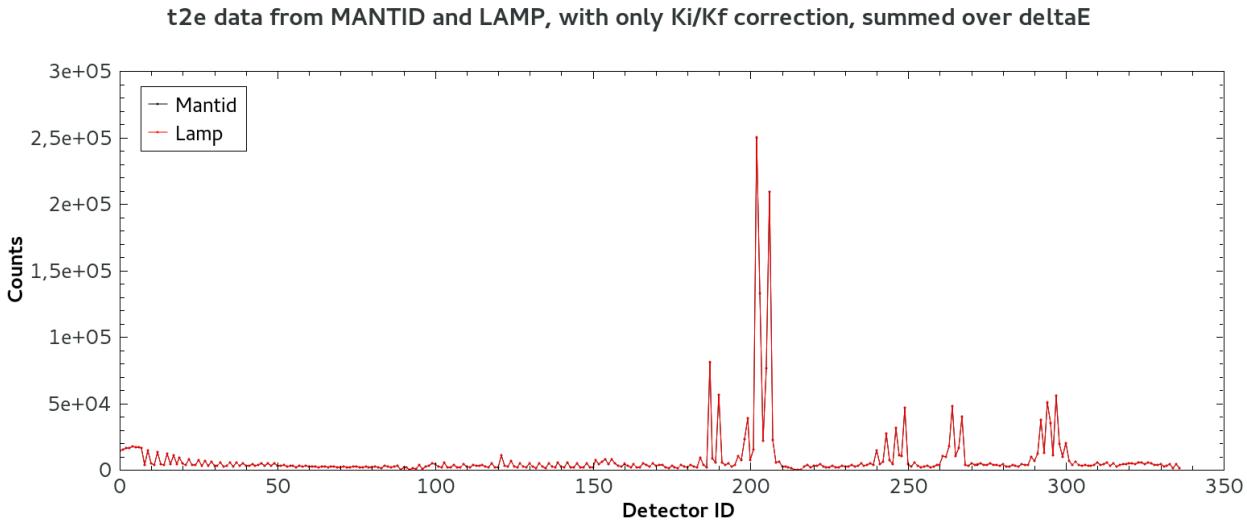


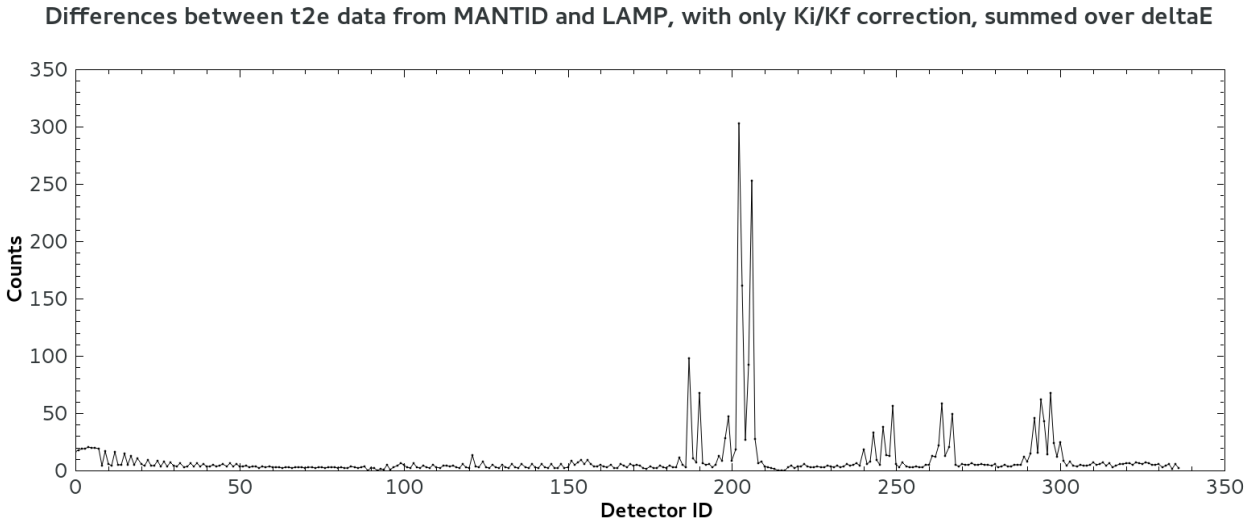
The differences have the exact same shape as the data itself, which would indicate a simple scaling difference. Thus, we scaled the data to have the same maximum point and did the same calculation again.

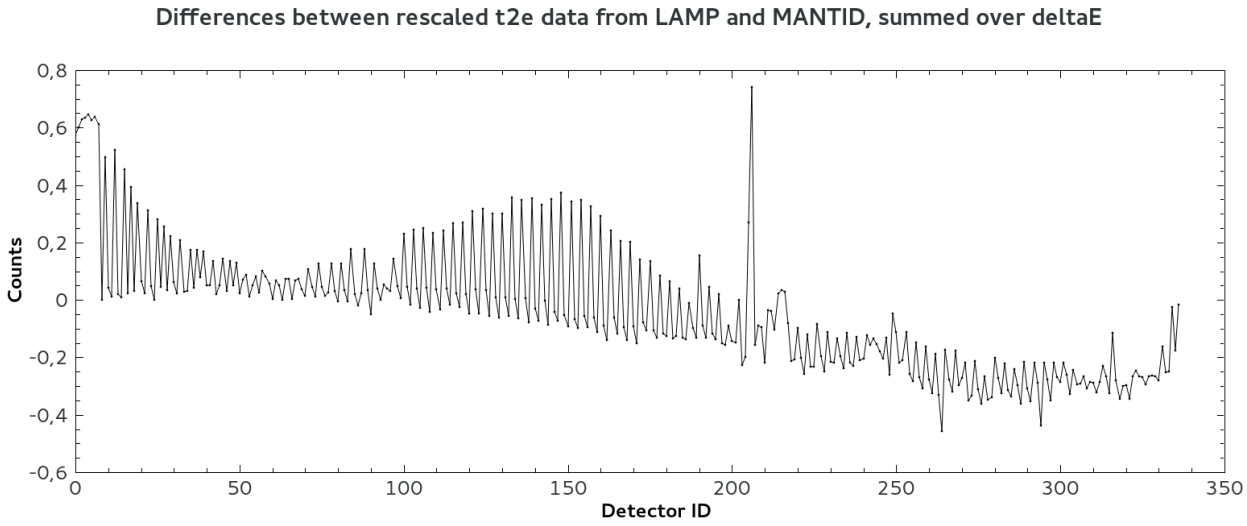


Even though the differences are very small, the Ki/Kf algorithms are not strictly identical.

The exact same differences were present when summing over deltaE.







Thus the closest we could get to the LAMP t2e with Ki/Kf correction was using ConvertUnits and CorrectKiKf in Mantid, which produced similar, but not quite identical, results.
No correction in MANTID enabled us to get a similar shape to LAMP when using dT/dE correction.

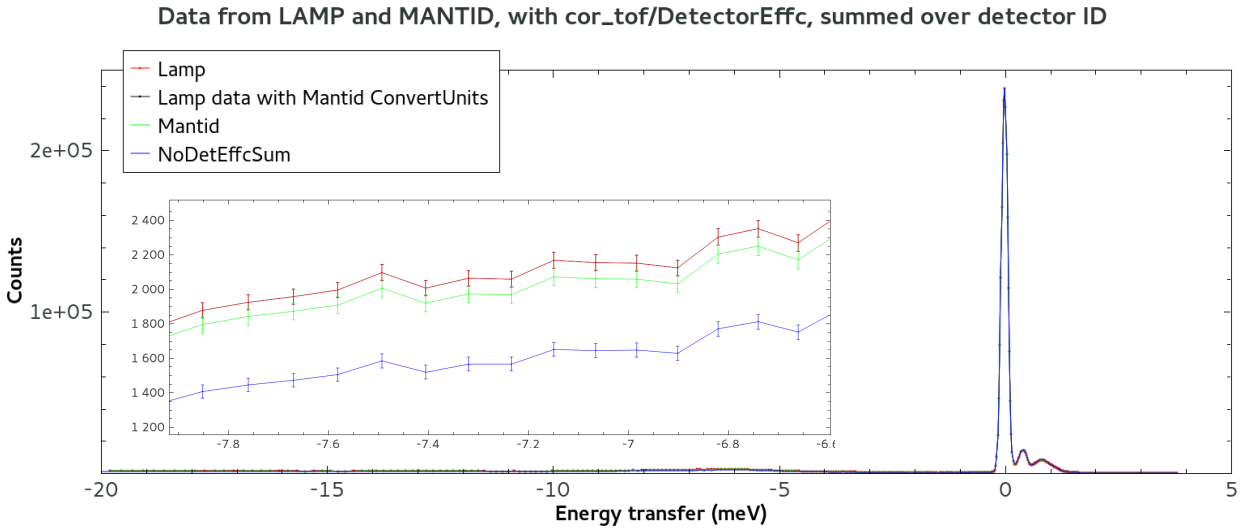
For a strictly identical comparison, no Ki/Kf correction was used in the later steps of the comparison.

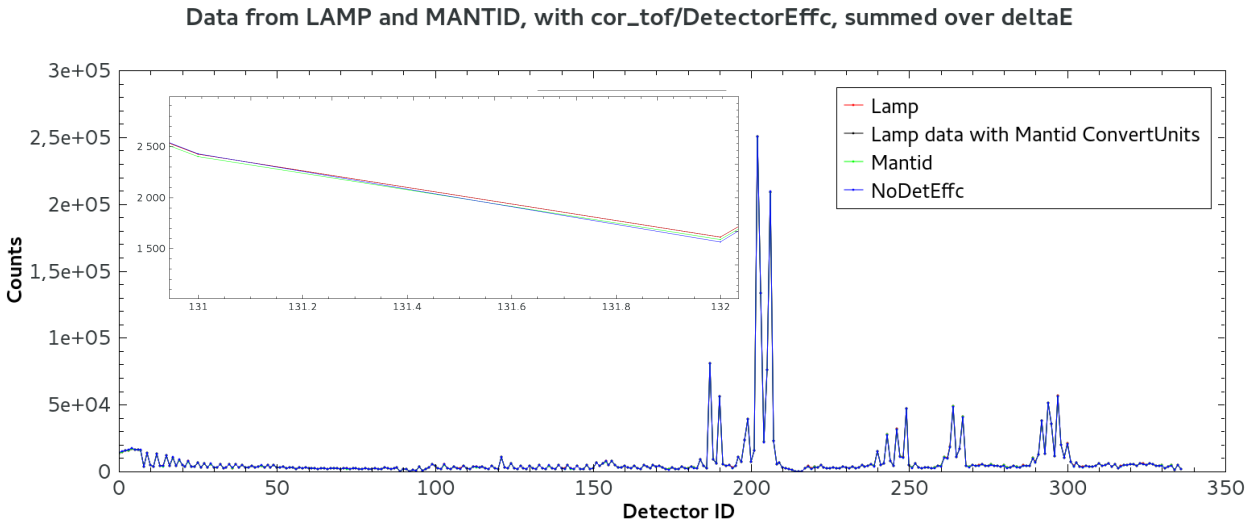
Detector Efficiency

Another correction is the Detector Efficiency correction, which is done before the conversion to energy in LAMP, and after in MANTID.
The LAMP command is cor_tof(/det_eff) and the MANTID algorithm is DetectorEfficiencyCorUser.

In order to compare the correction, we compared 4 data-sets:

1. LAMP
2. LAMP data, corrected in LAMP and converted to deltaE in MANTID
3. MANTID
4. Standard t2e data, with no Efficiency correction

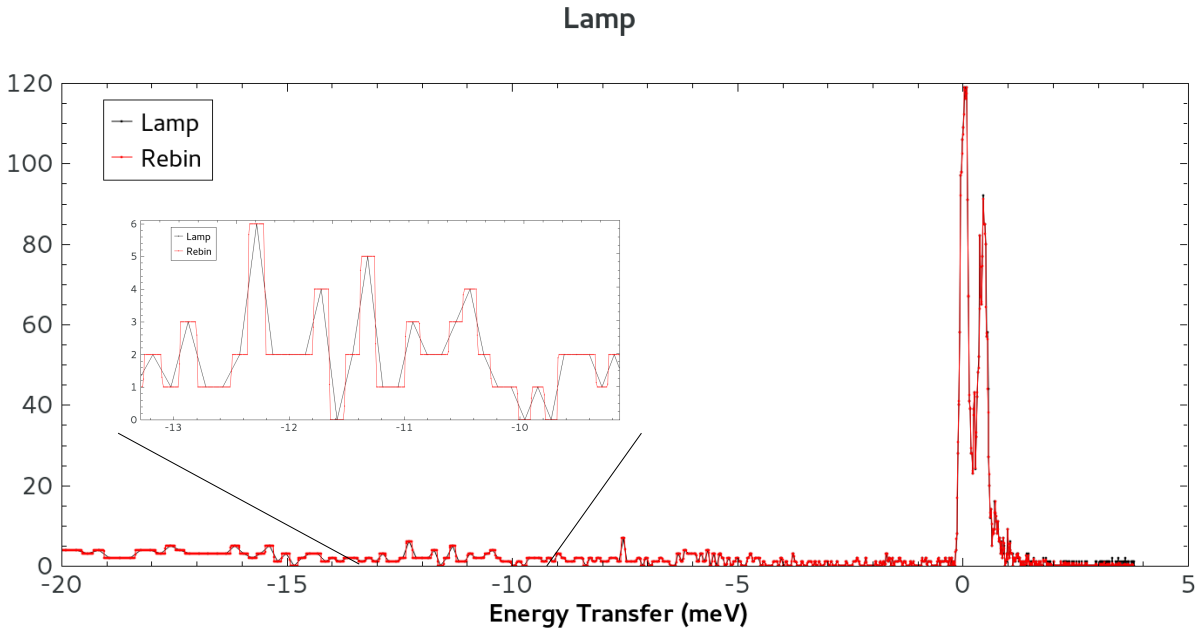


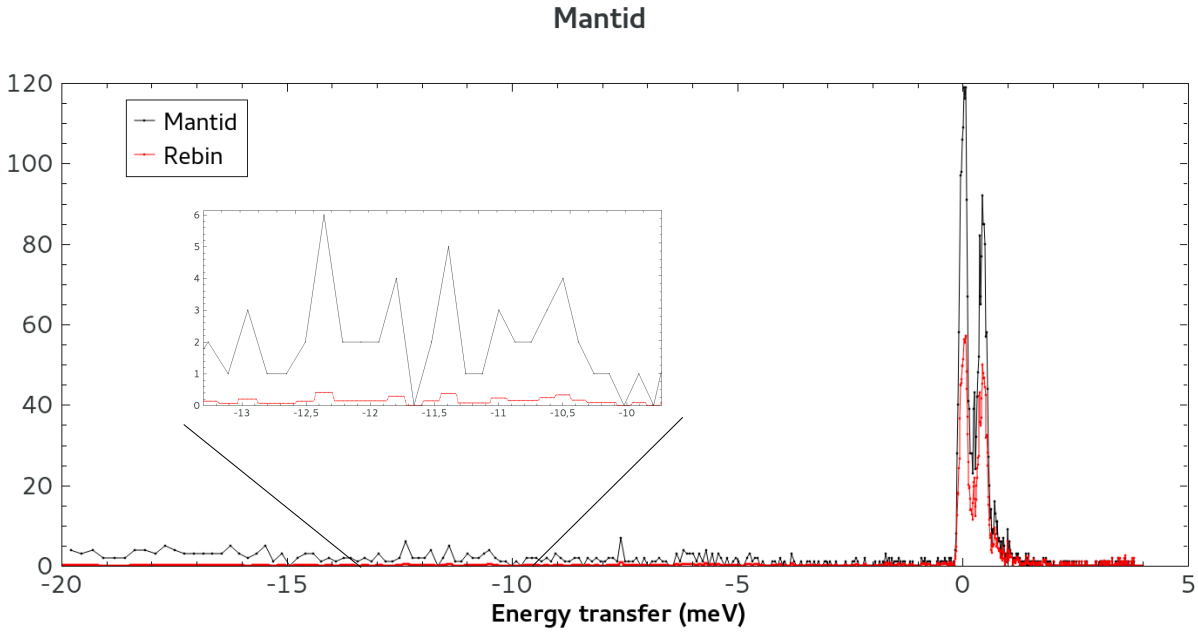


We can see that although the data-sets corrected in LAMP and MANTID are similar, there is still a small offset, whereas the two LAMP data-sets are strictly identical. To ensure that the correction was indeed taking place, we also added the standard t2e data.
We can conclude that while the t2e conversions are identical (as seen previously), the Detector Efficiency corrections are not. To ensure a relevant comparison, the Detector Efficiency correction was not included in later steps.

Rebin

When comparing the rebin of identical data in LAMP and MANTID, we get very different results.

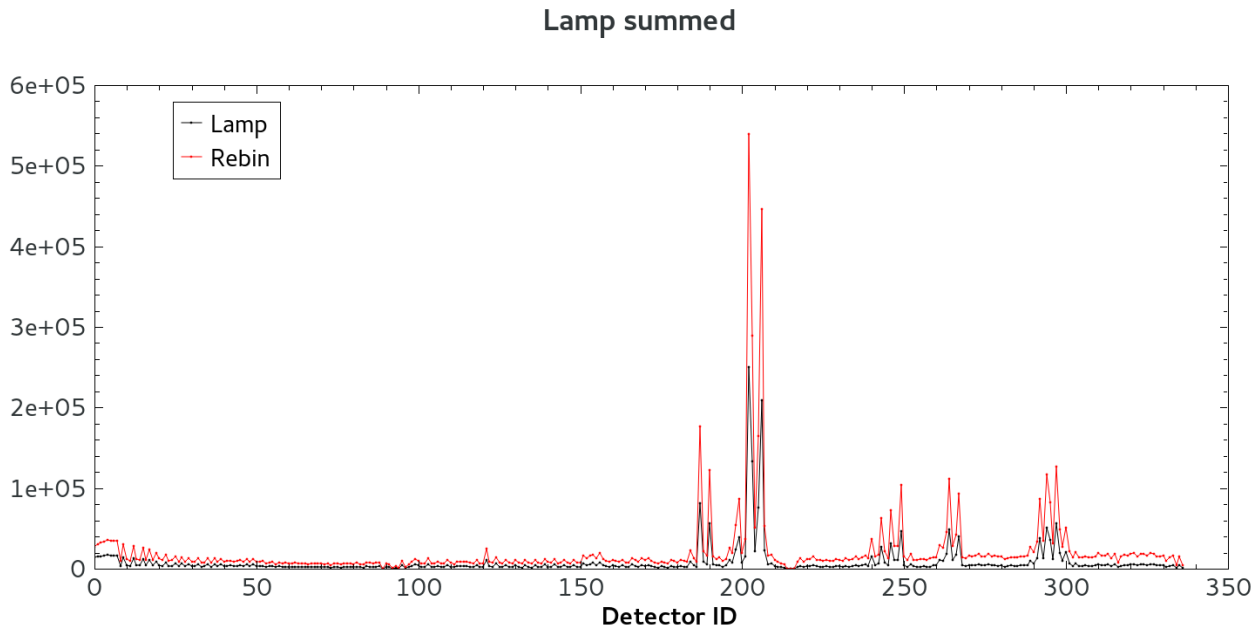


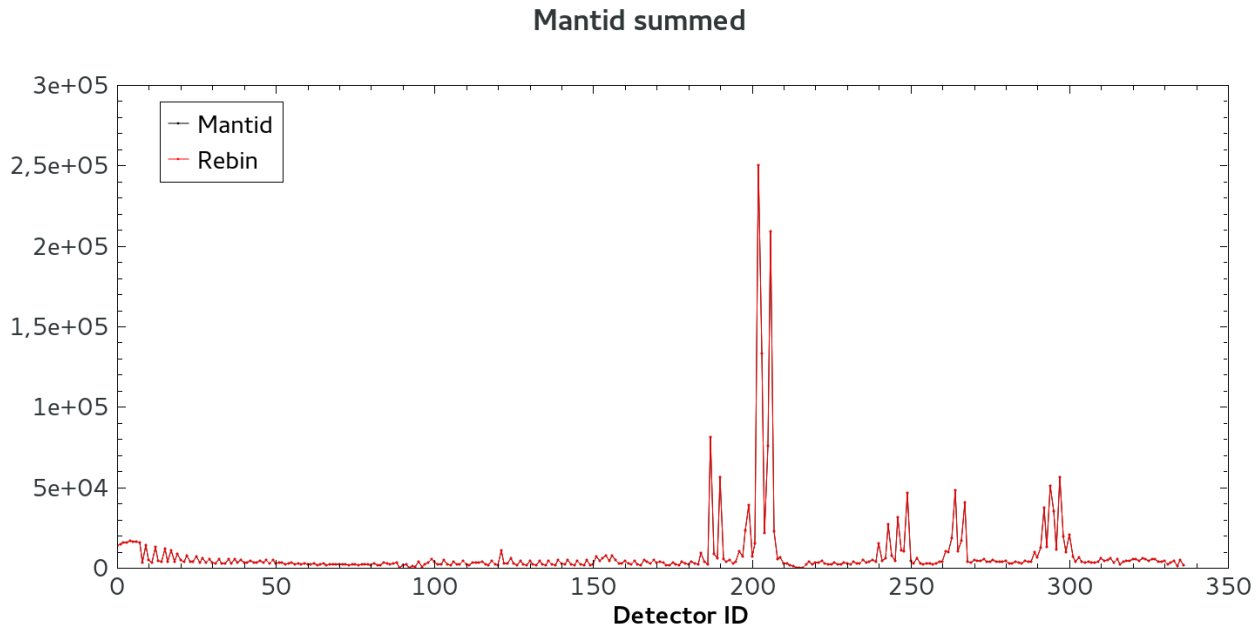


LAMP seems to extend the value of the nearest point to all the new points it has created to suit the new bin-width, whereas MANTID also rescales these data points as a function of the ratio between the number of points before and after the rebin. As the bin-width before the rebin is not constant in energy, the rescaling factor is not constant across the whole data-set.

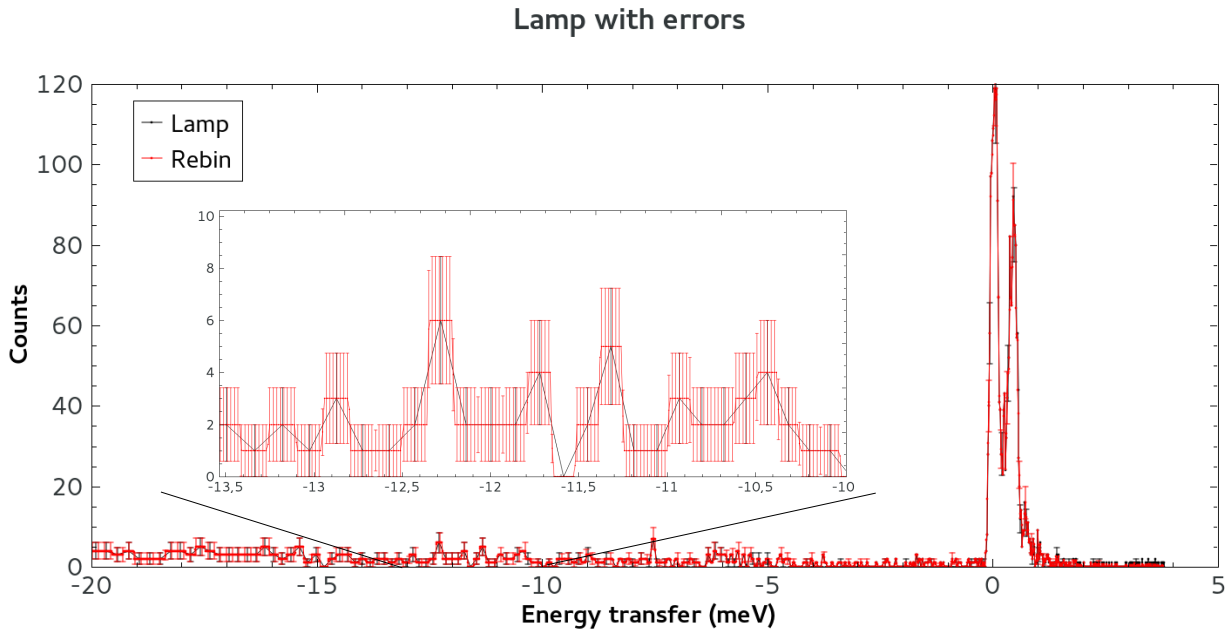
When looking at the sum over the detector ID, we can see that the MANTID rebinning algorithm conserves the total count (Σ Y(x)), whereas the LAMP rebin conserves the integral (Σ Y(x) dx).

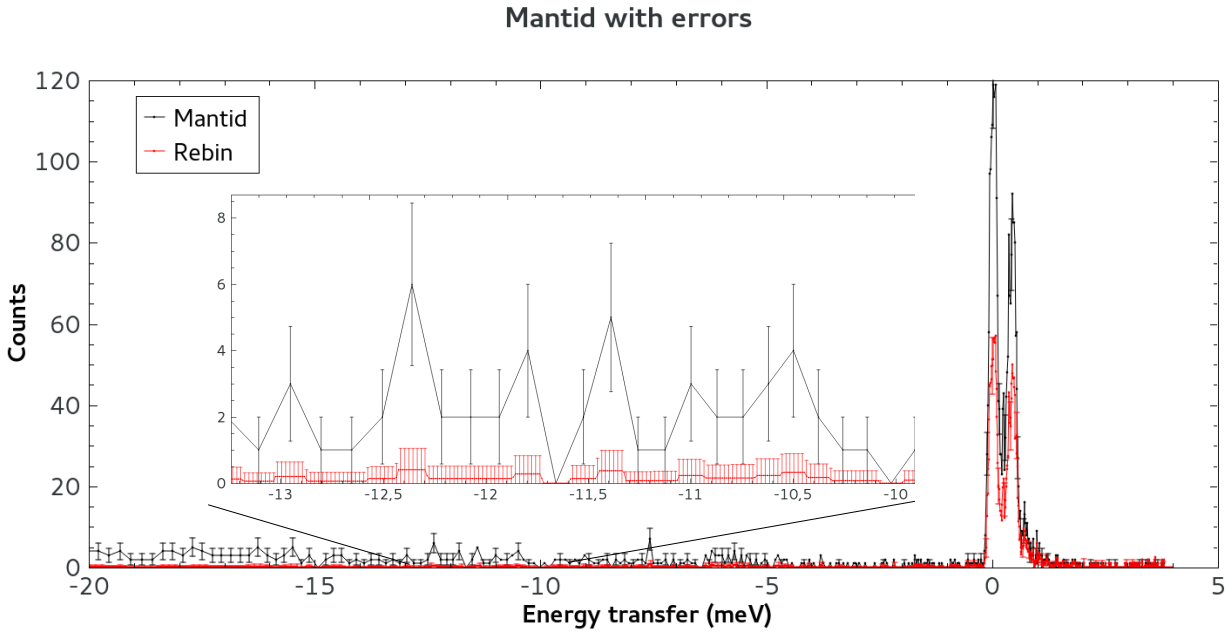
The result of summing over the energy channels in LAMP is an significant increase in the total count.





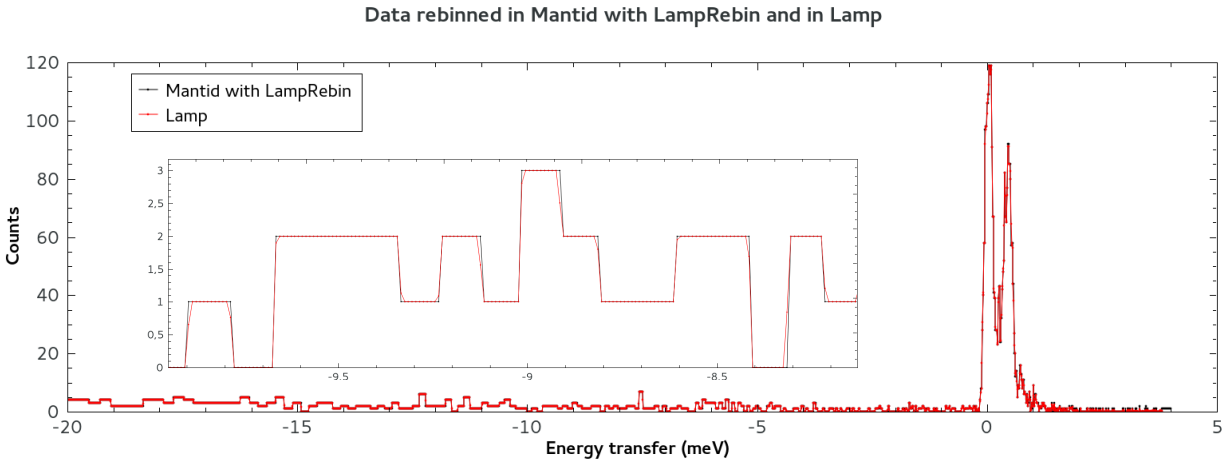
Concerning errors, the following figures show that the errors in LAMP are the same in all of the rebinned points as the point in the original data, however in MANTID the errors are scaled with the intensities.





We can see that the errors in lamp are the same in all of the rebinned points as the point in the original, which means that the total error is dramatically increased, however in Mantid everything is scaled so that the total error is the same, keeping the data in the same scope.

Using LampRebin, we are able to recreate the Lamp-style rebinning algorithm in Mantid for further comparing.

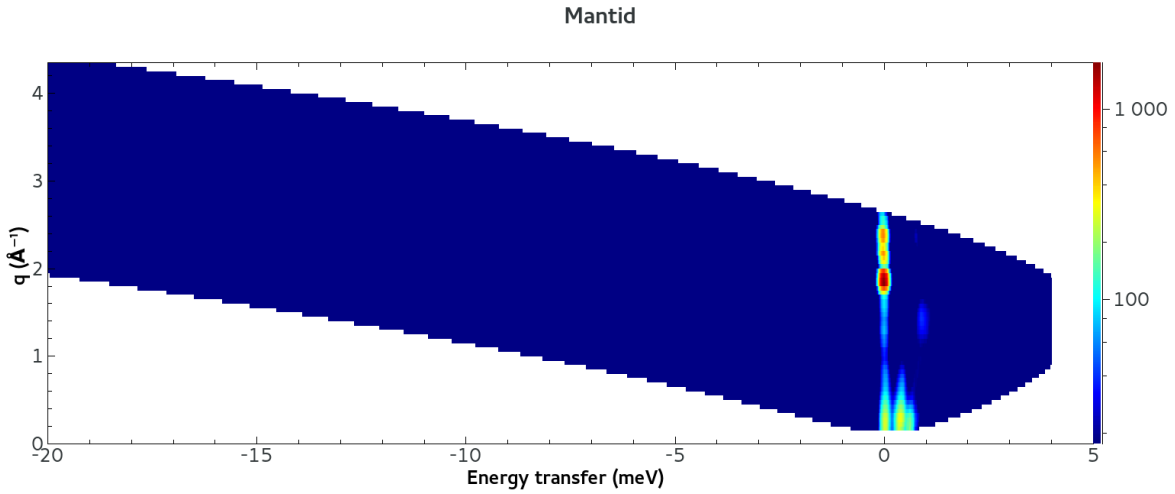


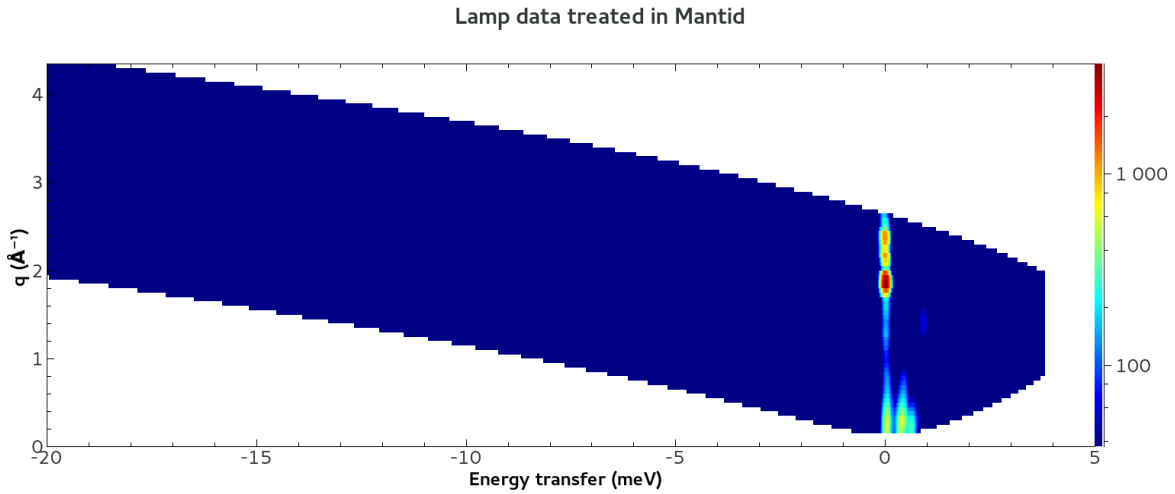
The data is thus almost the same, except for the data-points between two steps that are calculated and added by LAMP which are not implemented in LampRebin.

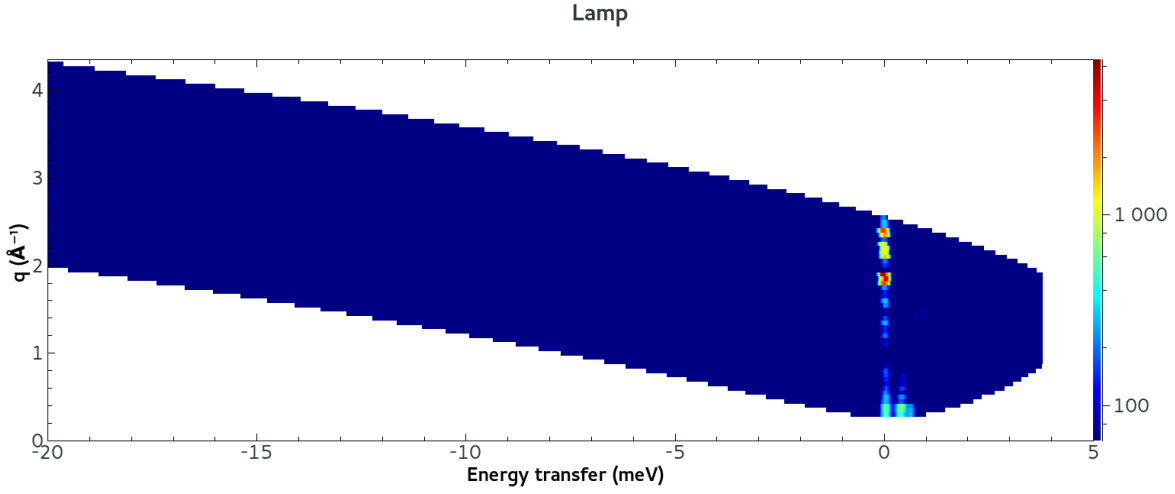
SofQW

For the best comparison possible, 3 data-sets were used :

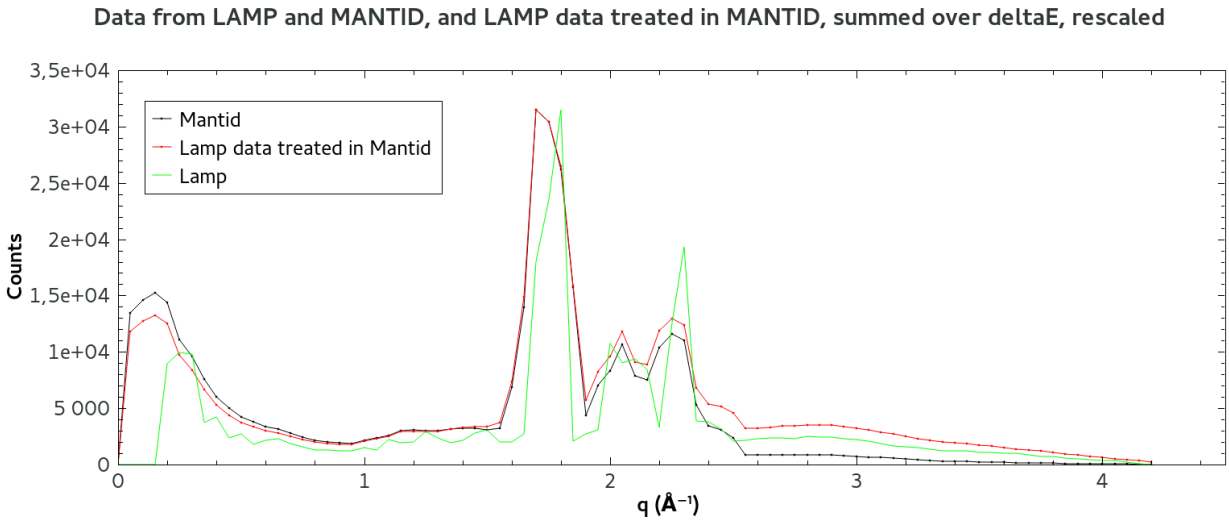
1. Data from LAMP, treated in LAMP
2. Data from LAMP treated in MANTID
3. Data from MANTID, treated in MANTID



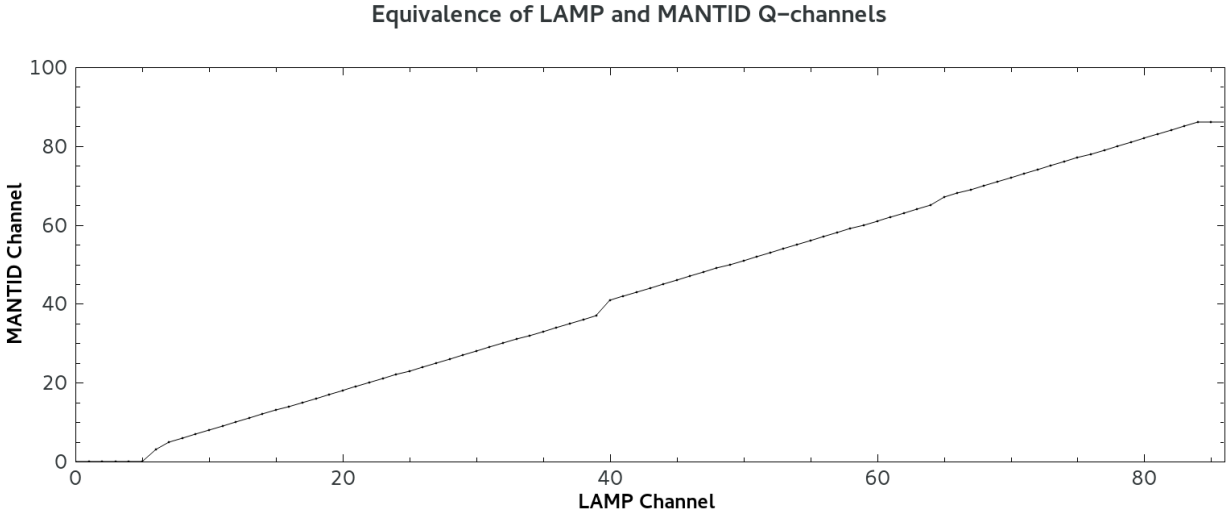




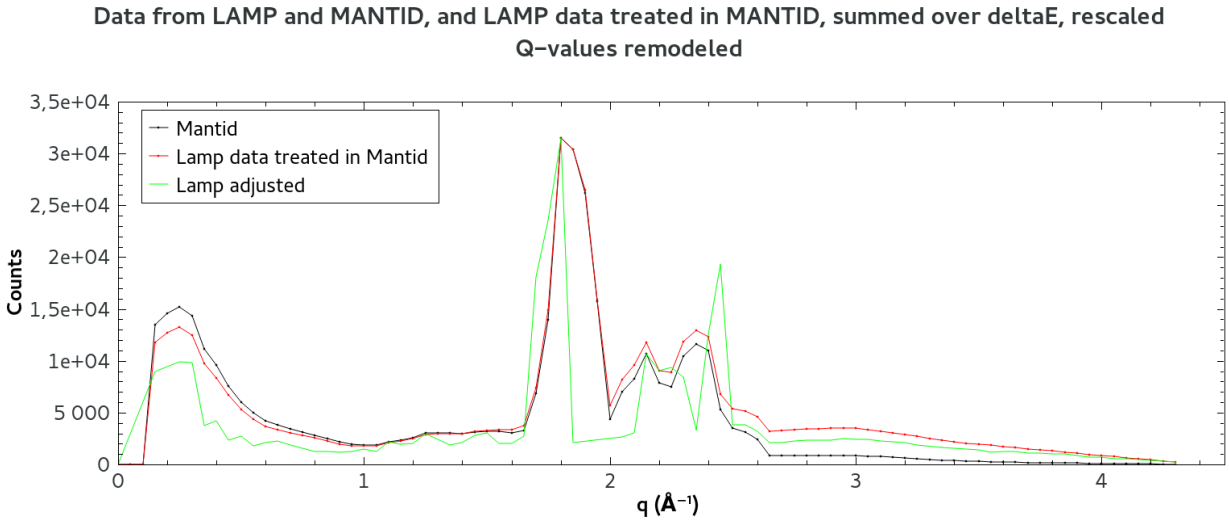
Comparison between 1 and 2 enabled us to compare the SofQW algorithms directly, on the exact same data, whereas comparison between 1 and 3 enabled us to compare total differences.



Looking at the 3 datasets summed over deltaE, we see that the peaks in MANTID and LAMP are not at the same Q-values. Comparing the start and end values of each Q-value in MANTID and LAMP, we were able to create a chart of which MANTID Q-channel was equivalent to which LAMP Q-channel.

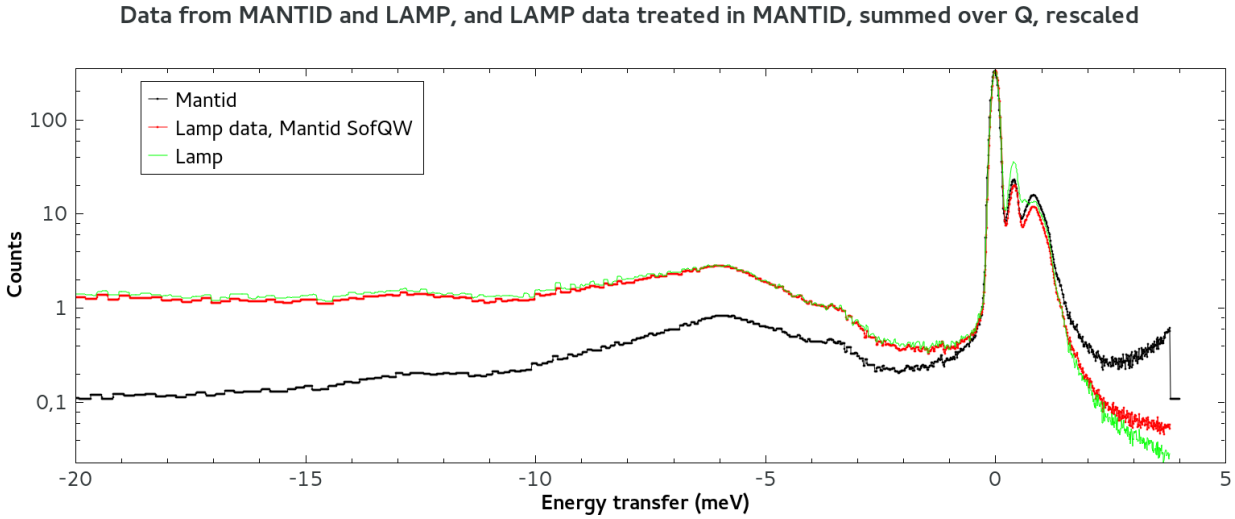


As we can see, the equivalence is not linear, or even 1-1. Using this equivalence chart, we were able to adjust the LAMP Q-values to be equivalent to the MANTID ones.



We see that both MANTID-treated data-sets have a similar shape, even though the input data has a different rebin (due to the differences between MANTID and LAMP), whereas the LAMP data treated in MANTID and LAMP have very different shapes, even though it is the exact same input data. This would indicate differences in the SofQW procedures.

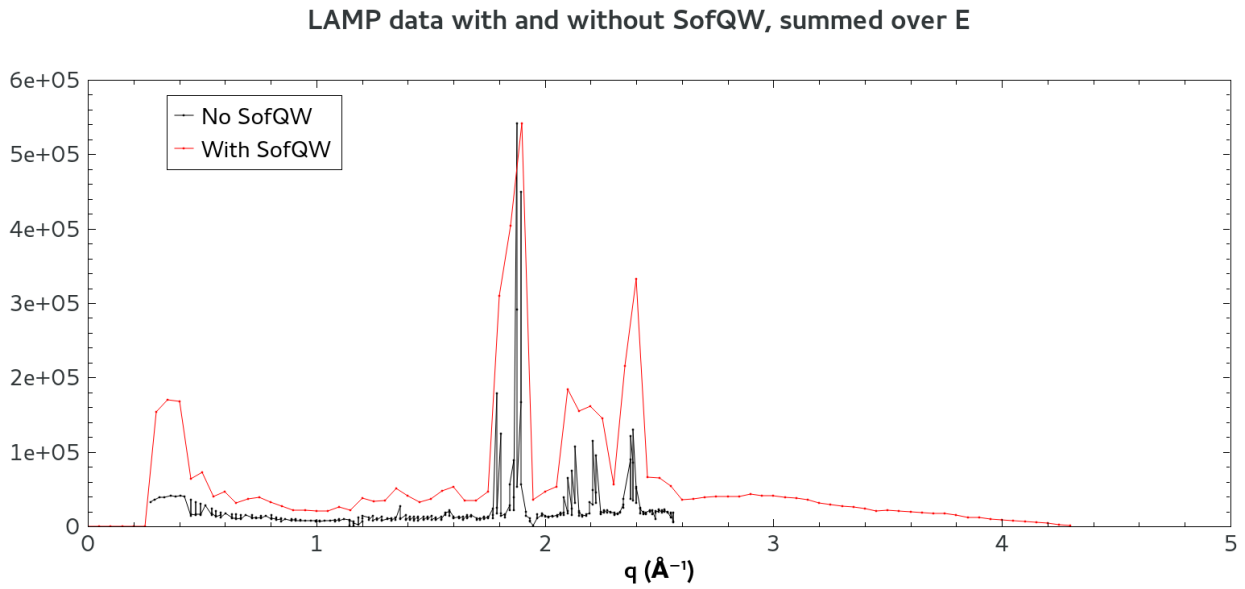
However, looking at the sum over Q, the results were different.

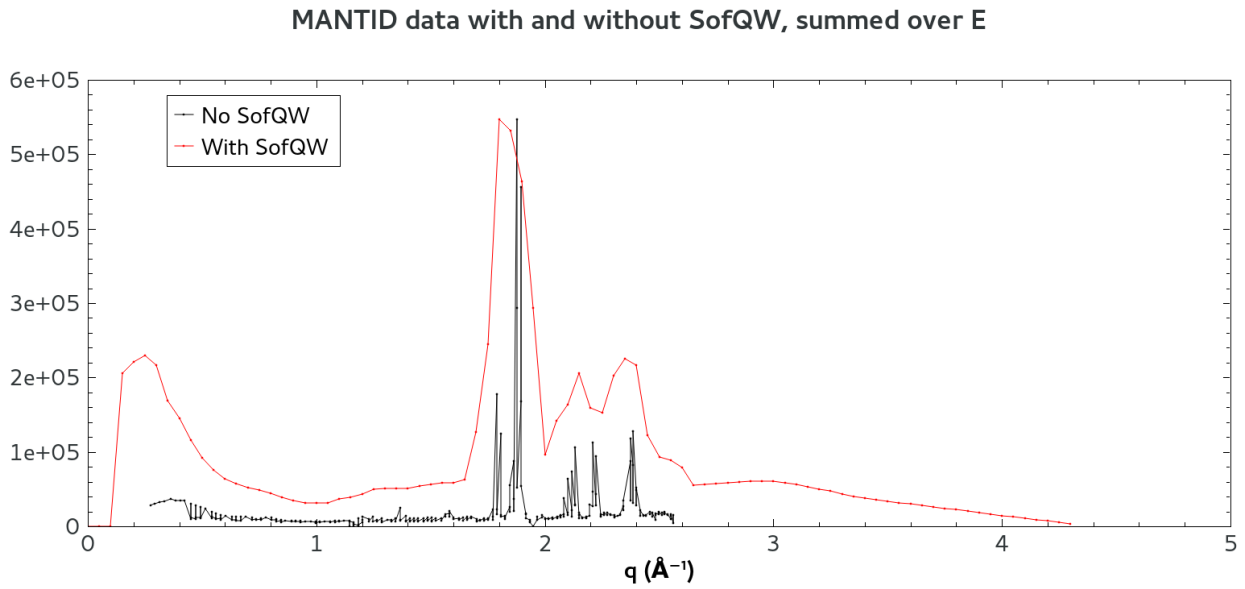


The results from the LAMP data treated in LAMP and MANTID (but with the same input data) were very similar, while the pure MANTID data was very different.

Thus it would appear that the SofQW procedures in LAMP and MANTID produce similar results when looking at the sum over Q, however they produce different results when summing over deltaE.

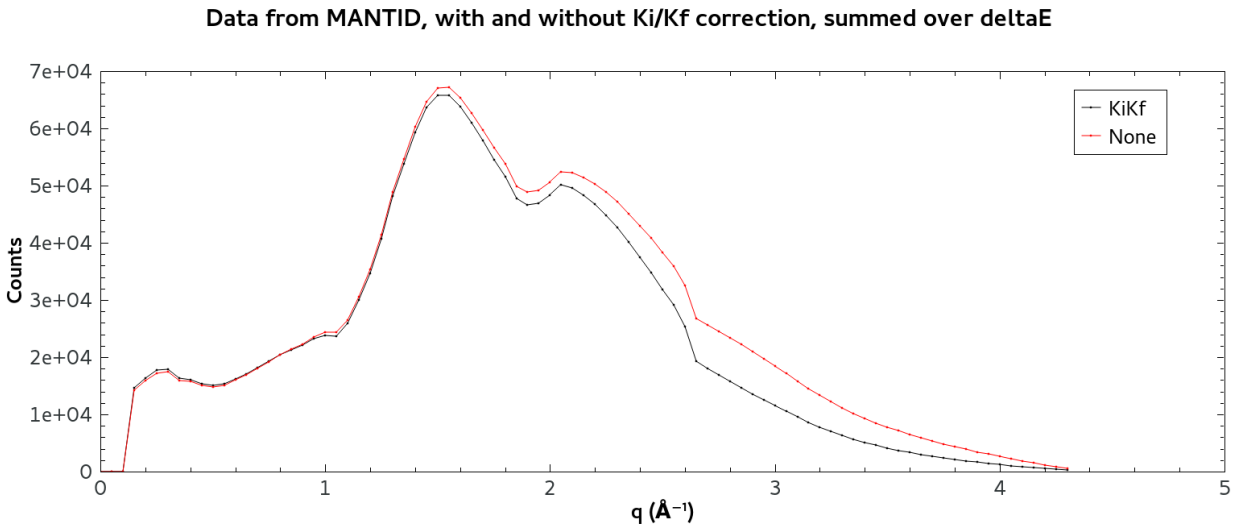
For further comparison, we looked at the data before SofQW, converted to Q using the detector angle, with the SofQW data in both LAMP and in MANTID with the LampRebin.

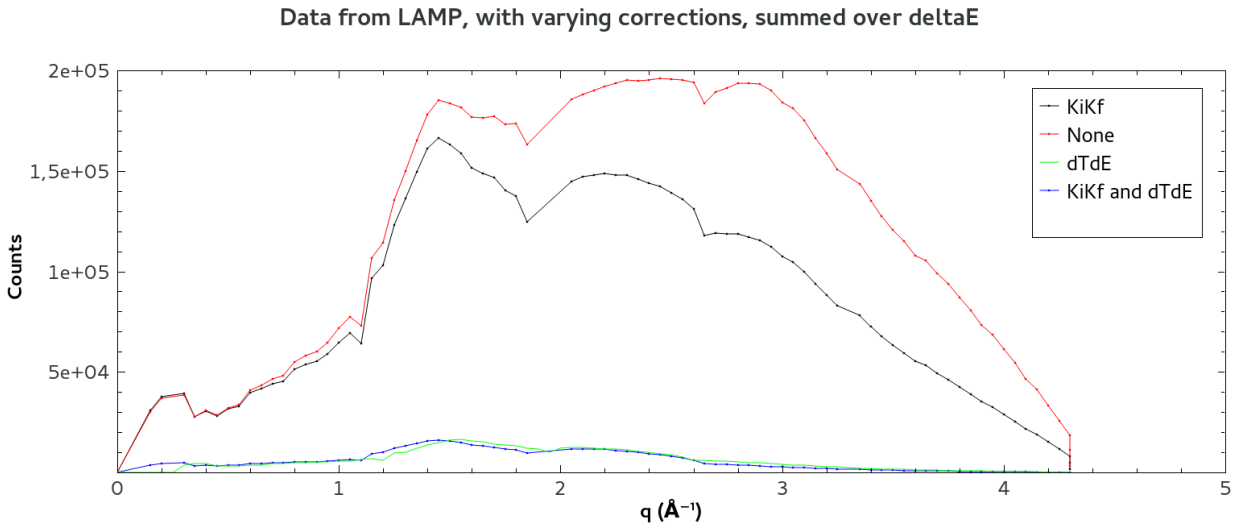


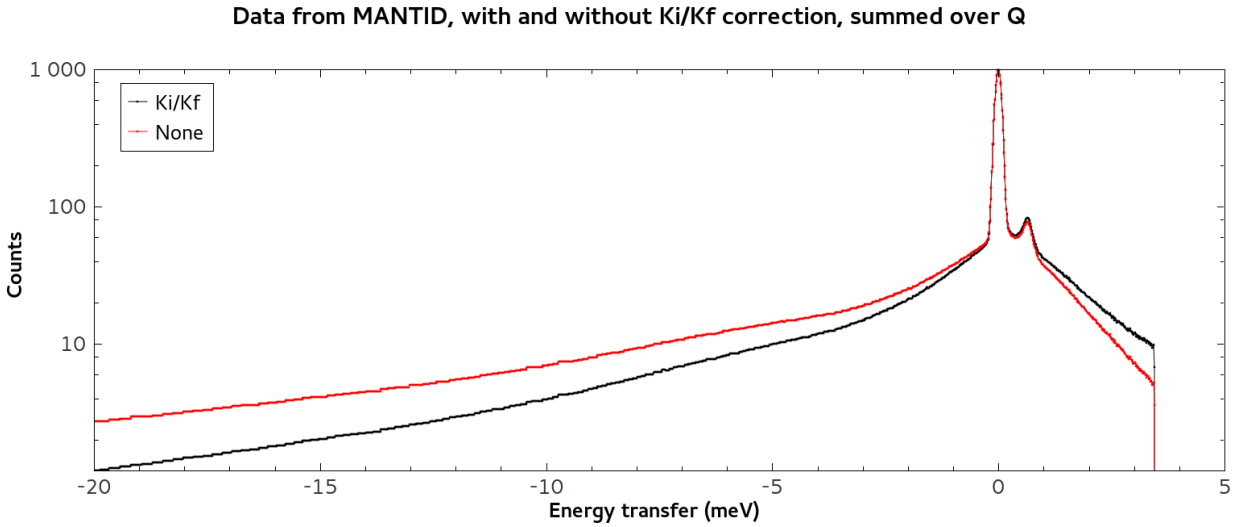


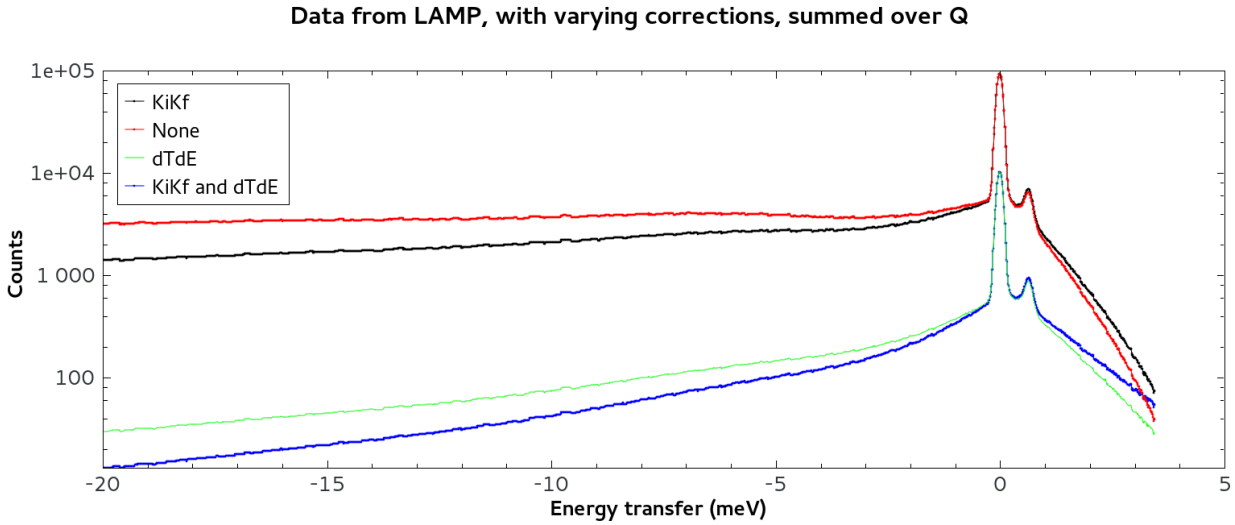
Comparing this pure formula conversion with the full SofQW, we see that LAMP seems to have a better fit.

To get a cleaner comparison, we looked at a data-set with cleaner data, namely 161389-161400. First, we looked at the data from LAMP and MANTID, with all possible combinations of corrections we could apply, and compared them.



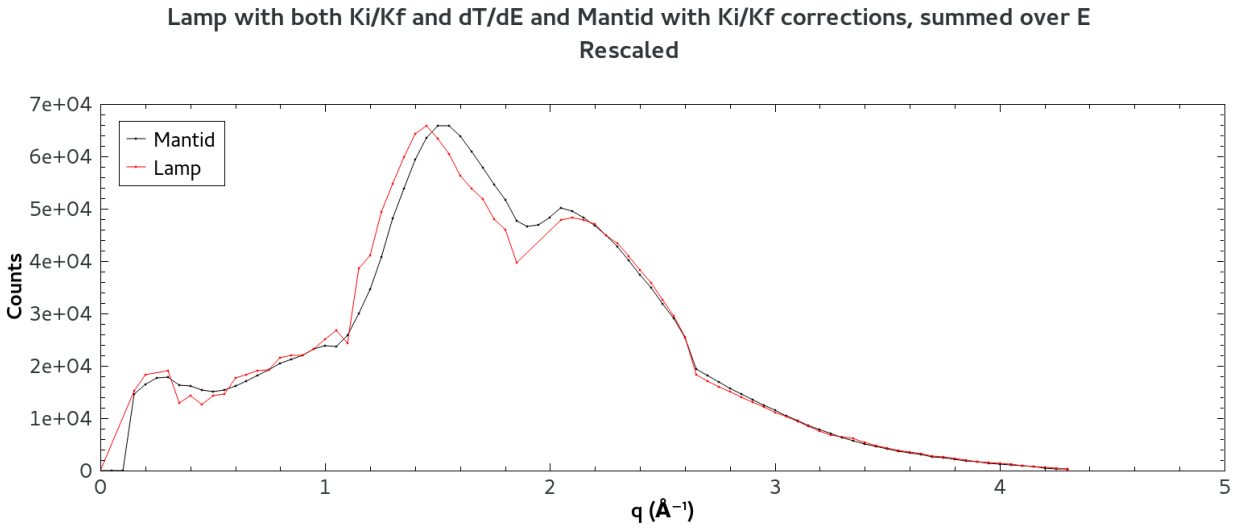


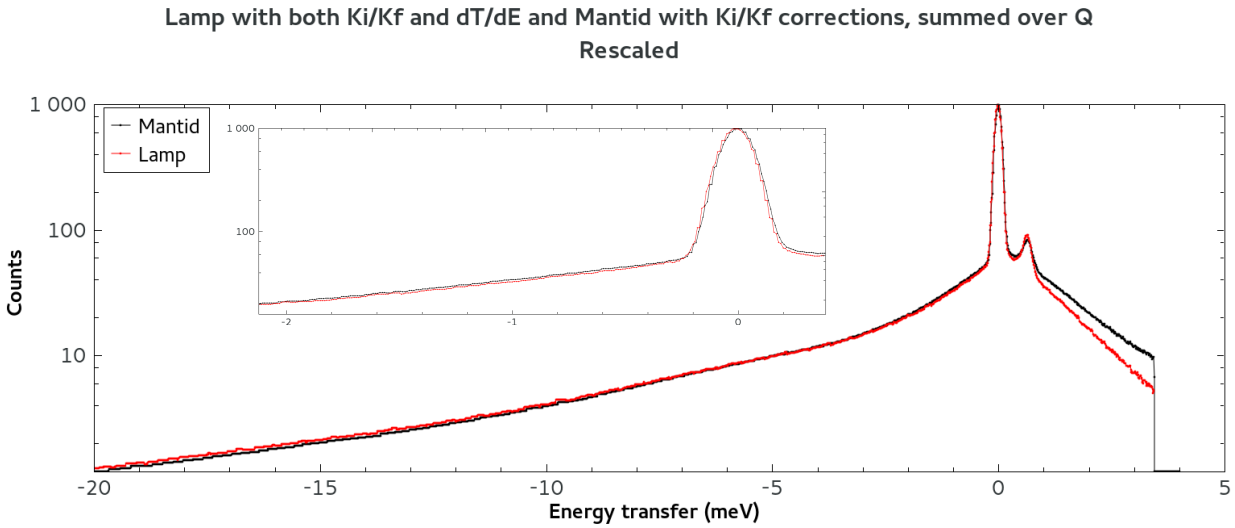




It is obvious that the corrections in LAMP are a lot more significant than in MANTID. When we look at the sum over Q in LAMP, we see that the symmetry of the elastic peak is lost when the dTdE correction is not applied to the data, however both MANTID curves have the symmetry, which would indicate that the dTdE correction present in LAMPs t2e routine is present in MANTIDs SofQW routine.

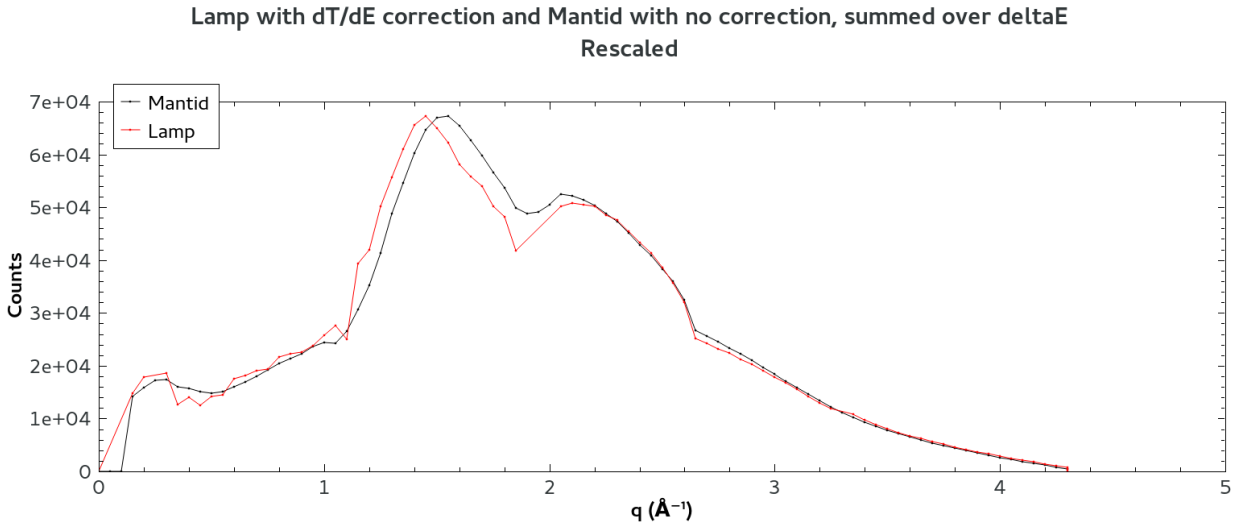
After looking through all the data-sets carefully, we saw that the LAMP data with both corrections was closest to the MANTID data with Ki/Kf correction.

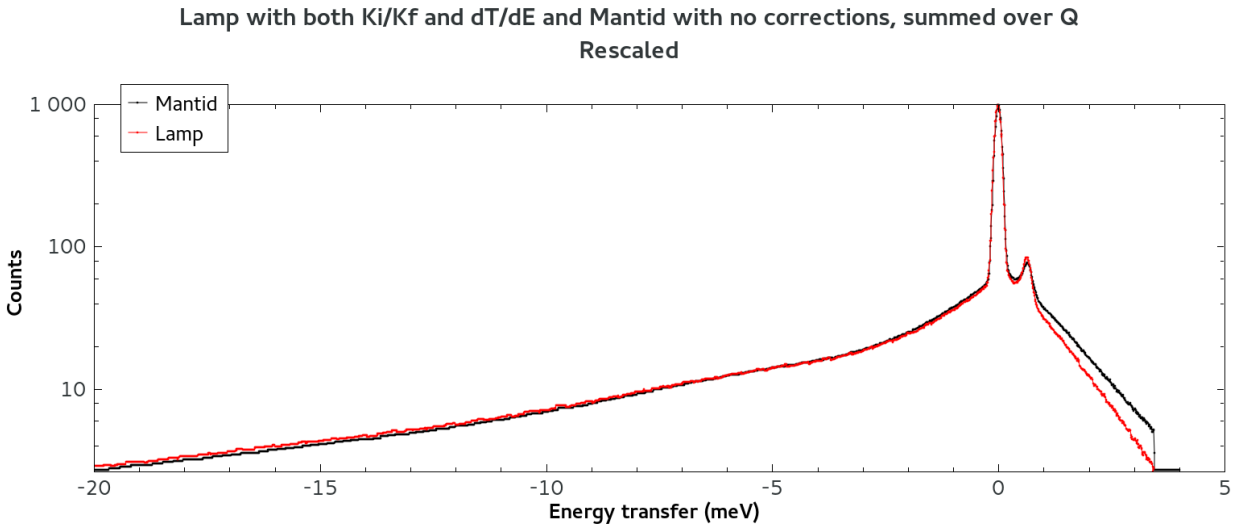




Thus, we believe that the main differences between the SofQW in MANTID and LAMP come from MANTID correcting for the differences in the previous steps, namely that the SofQW in MANTID has the dT/dE correction which is in the t2e command in LAMP.

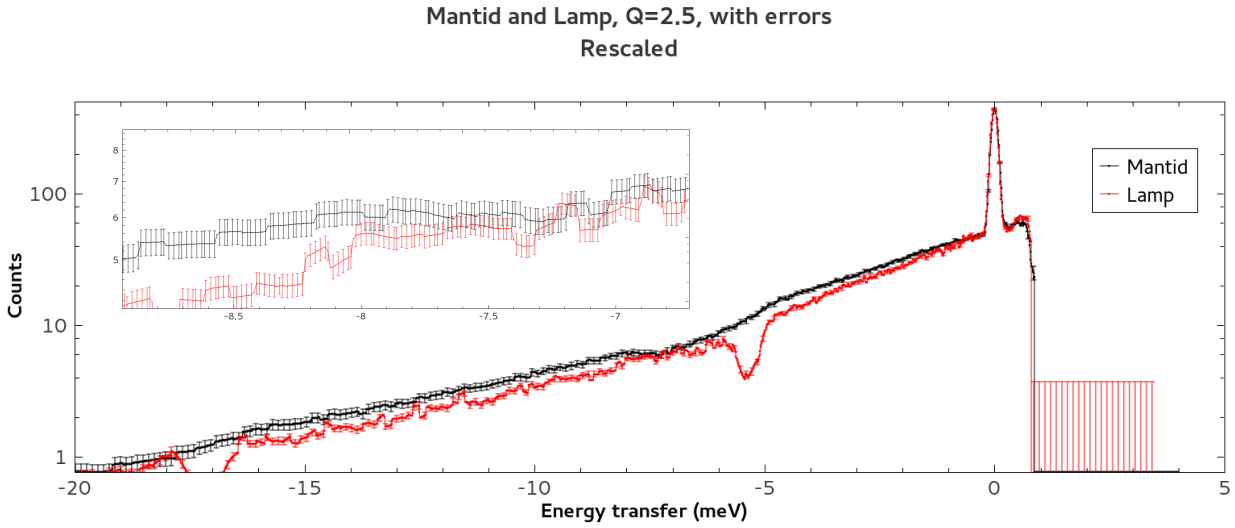
If we look at the data-sets with no Ki/Kf correction, but leaving the dT/dE correction in LAMP, we see similar results as well.





This would tend to confirm our theory that MANTID includes a dT/dE correction in SofQW.

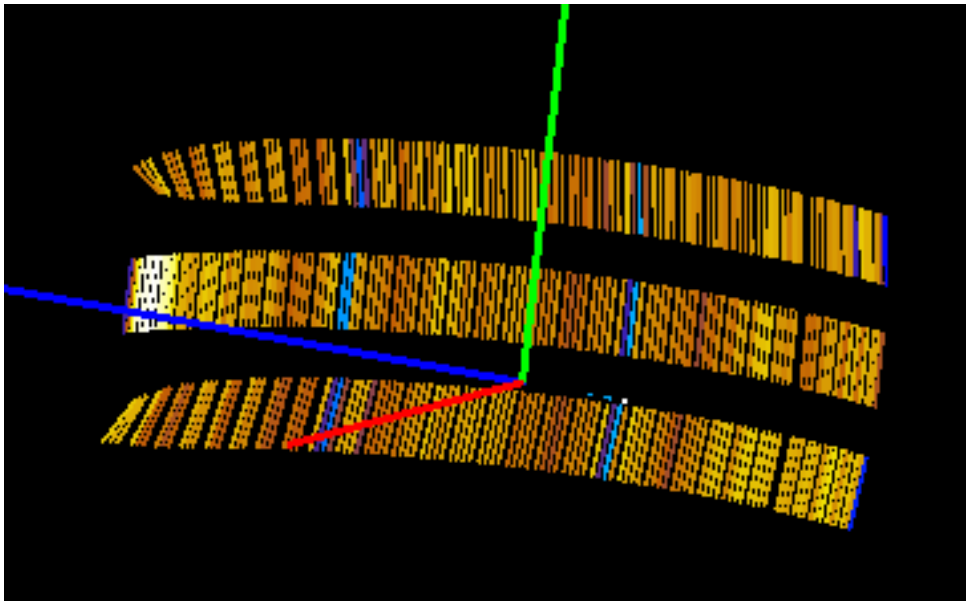
However, when looking at a single Q-value, we see slight differences.

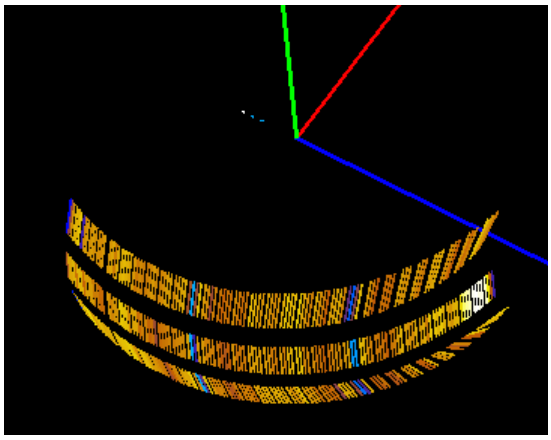


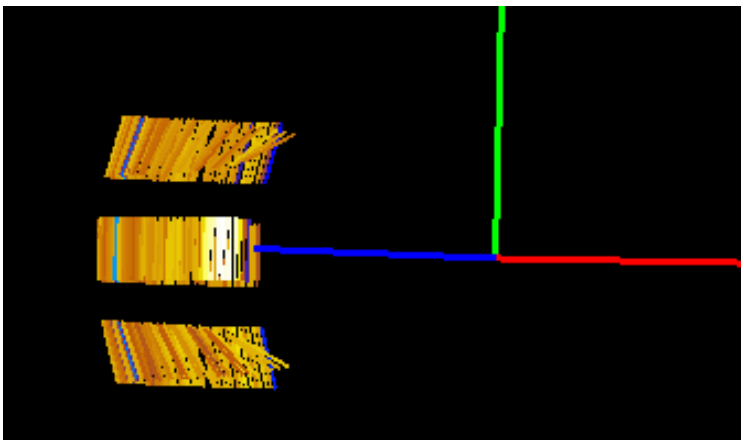
There seems to be slightly more fluctuation in the LAMP data, however the general shape is conserved. Concerning errors, we can see that they are similar.

Instrument View

Concerning the instrument view, the one in version 3.2.1 seems to have issues regarding resizing and moving the window, but they have been fixed in the latest version (3.4).

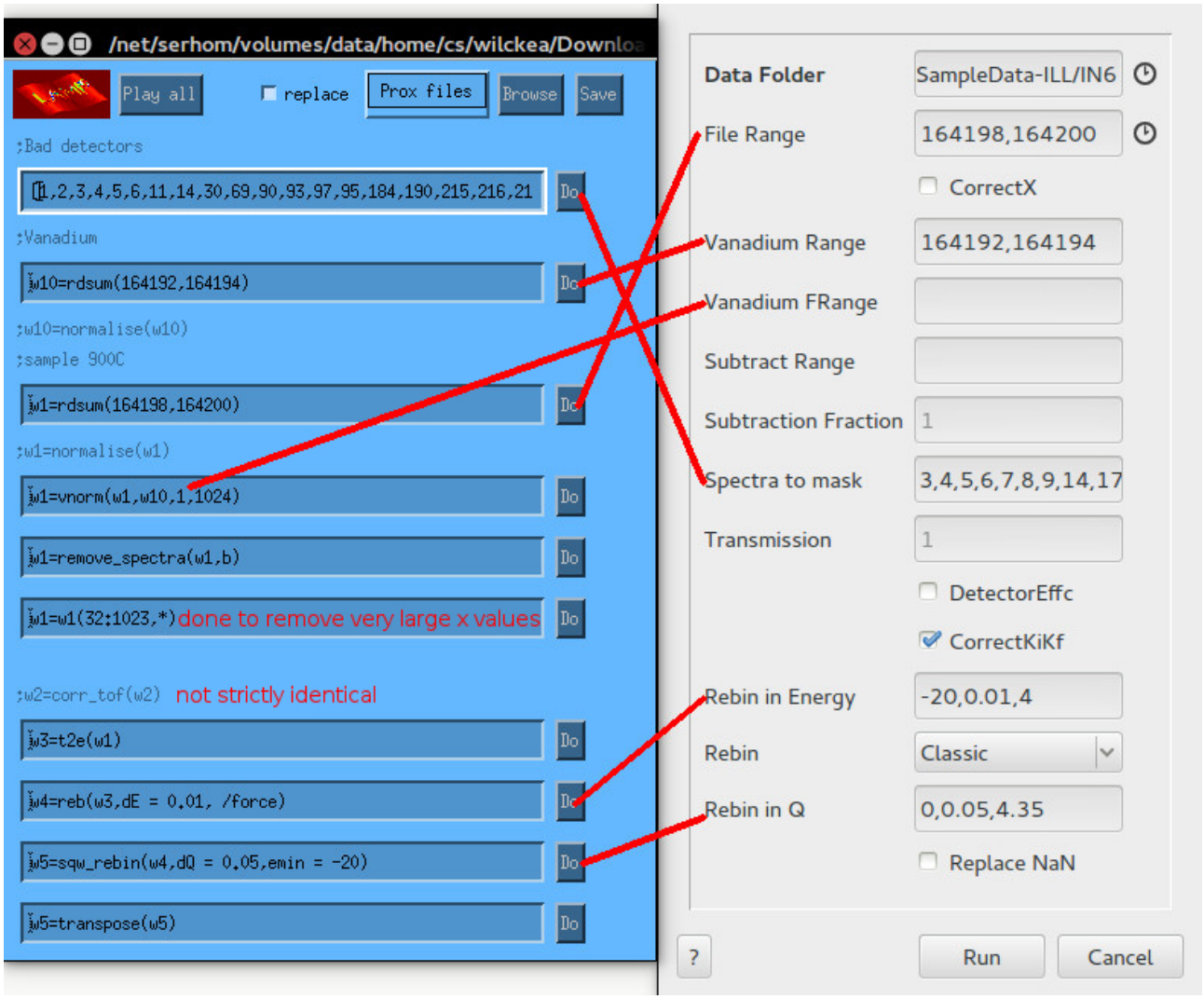




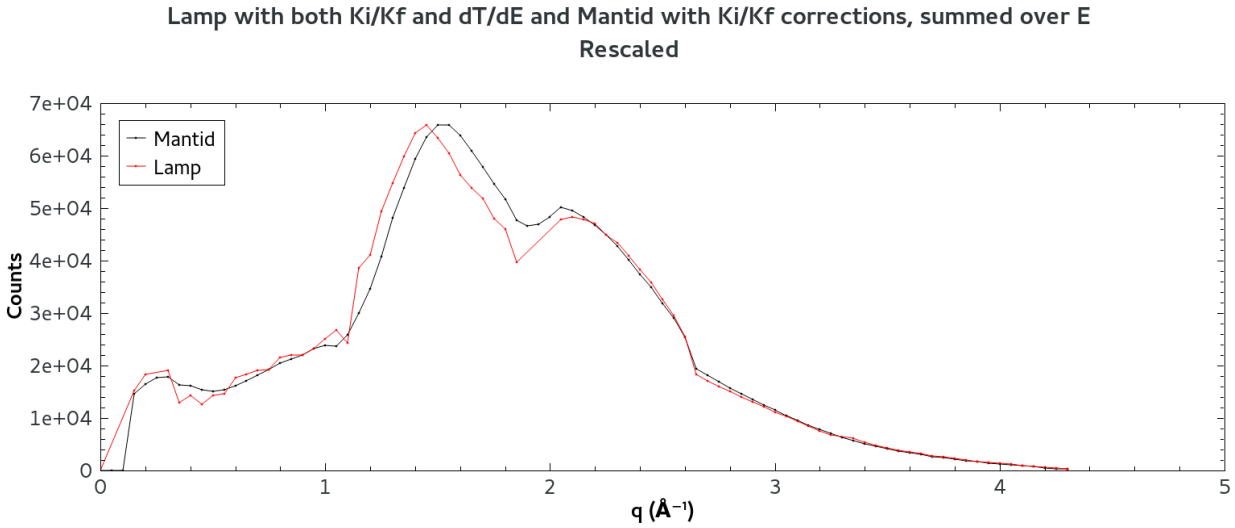


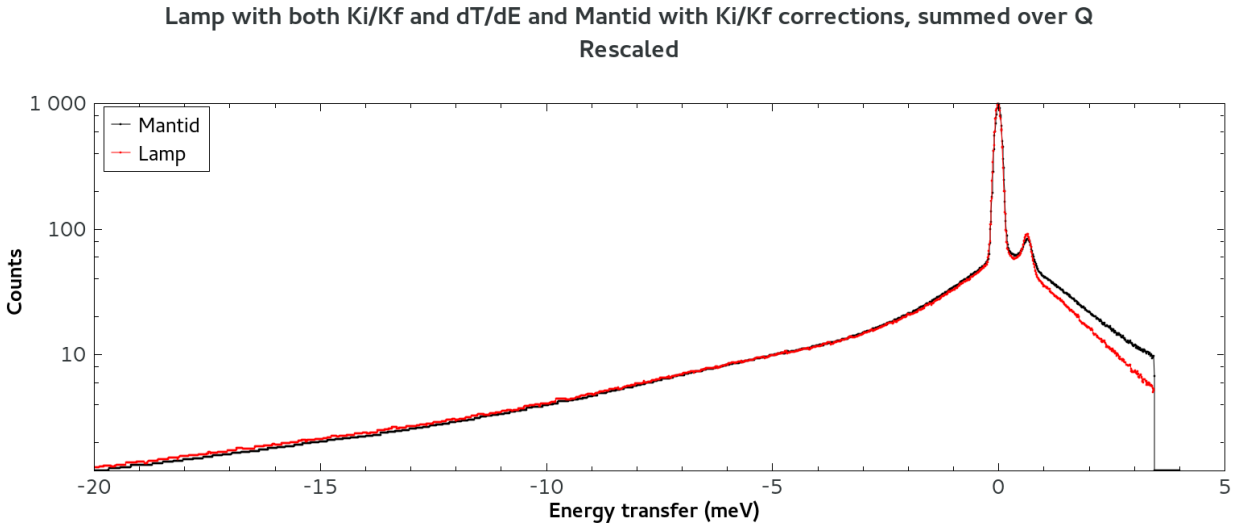
Operation	Comparison
Read	MANTID keeps the 3 monitor detectors in the data whereas LAMP deletes them, which created a 3-spectra offset between the data. As MANTID plots data using end-points and LAMP using midpoints, there is a channel difference between the data as well.
Vanadium normalisation	There is a scaling factor difference. In the default script, LAMP normalised both data-sets to Scattering Angle, which is not done in MANTID.
Masking	LAMP removes spectra completely whereas MANTID sets all the data of the selected spectra to 0. The list of spectra to mask in MANTID should be increased by 3 for each spectrum, because of the 3 monitor workspaces at the beginning. In the default MANTID script, making occurs directly after the data has been read, whereas in LAMP it occurs after the normalisation.
Tof to Energy conversion	The default LAMP t2e operation has a Ki/Kf correction built-in whereas MANTID does not. The separate Ki/Kf correction in MANTID is also different from the one in LAMP, as LAMP includes a dT/dE correction.
Detector Efficiency	The detector efficiency correction is not done at the same point in the script in MANTID and LAMP. LAMP does it before the t2e, whereas MANTID does it after. It also appears that the correction is not strictly identical.
Rebin	MANTID rescales each point as a factor of how many points were created from a single original point, whereas LAMP keeps the original magnitude of all points.
SofQW	Procedures are different, it seems that the Mantid SofQW includes the dT/dE correction, making the final result similar. There is also a non-linear equivalence between spectra in LAMP and MANTID data.

The MANTID parameters that were found to create the closest results were the following:



With these parameters, we were able to get results that were similar, in both Q and deltaE.



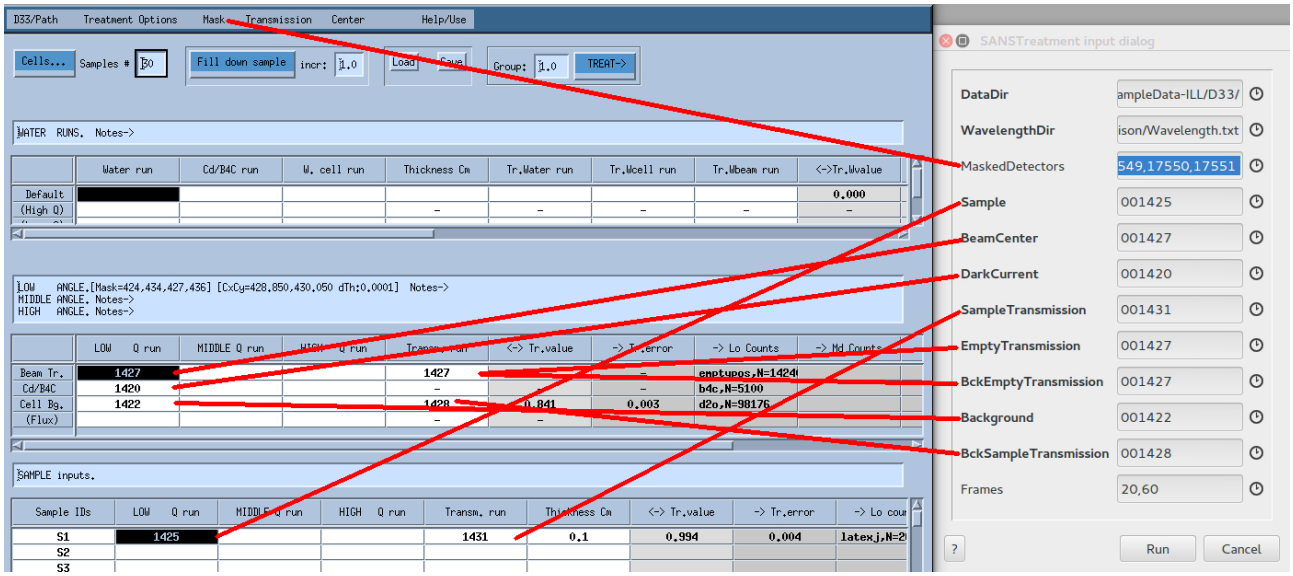


SANS

Introduction

Contrary to the TOF data, the SANS treatment procedure is not done in identifiable steps, but one single one, where all the data is plugged in at the beginning and the software handles everything. This made comparison slightly more difficult, as we could only vary the parameters and not look inside to see when the differences occurred. To make a more thorough comparison, we also used a third program, GRASP.

The equivalence between LAMP and MANTID parameters is presented below.



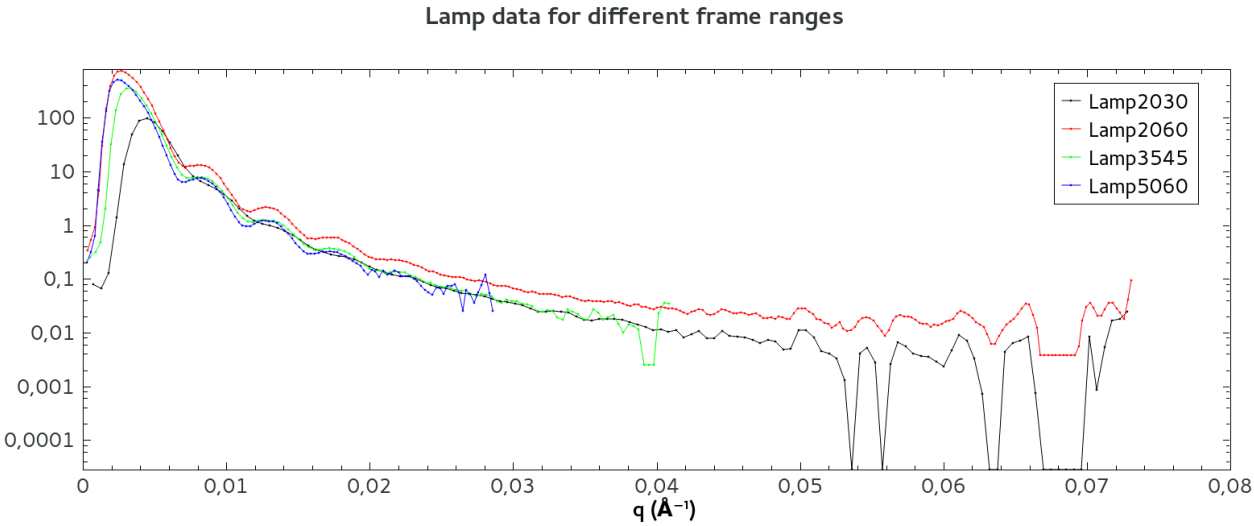
As MANTID selects data based on wavelength, and LAMP and GRASP select it based on frames, a file with the frames and their equivalent wavelengths must be given to MANTID (WavelengthDir).

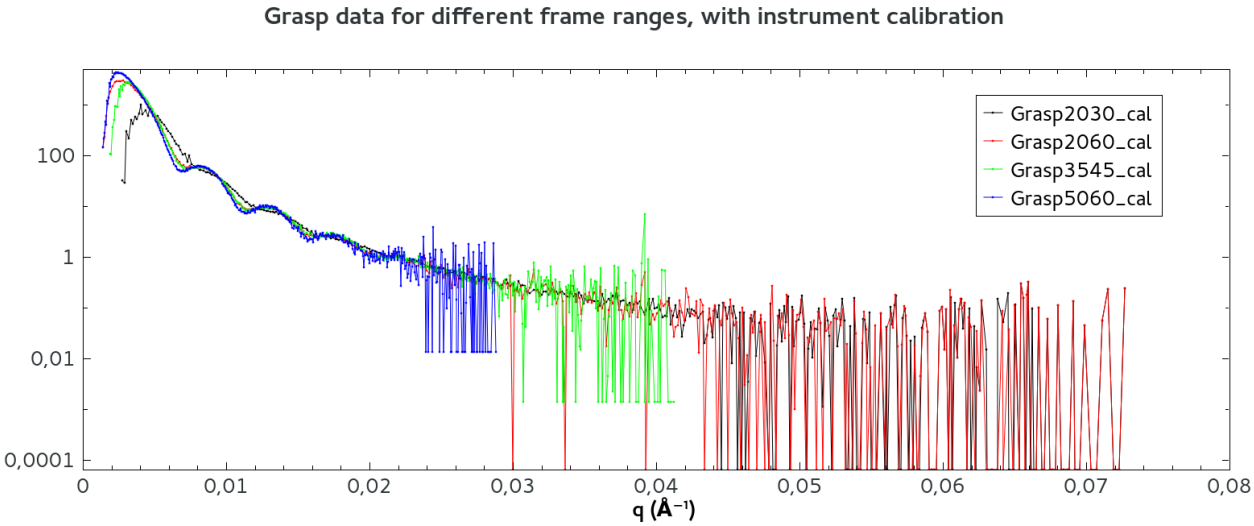
The comparison was done using 4 frame-ranges:

1. 20-30
2. 35-45
3. 50-60
4. 20-60

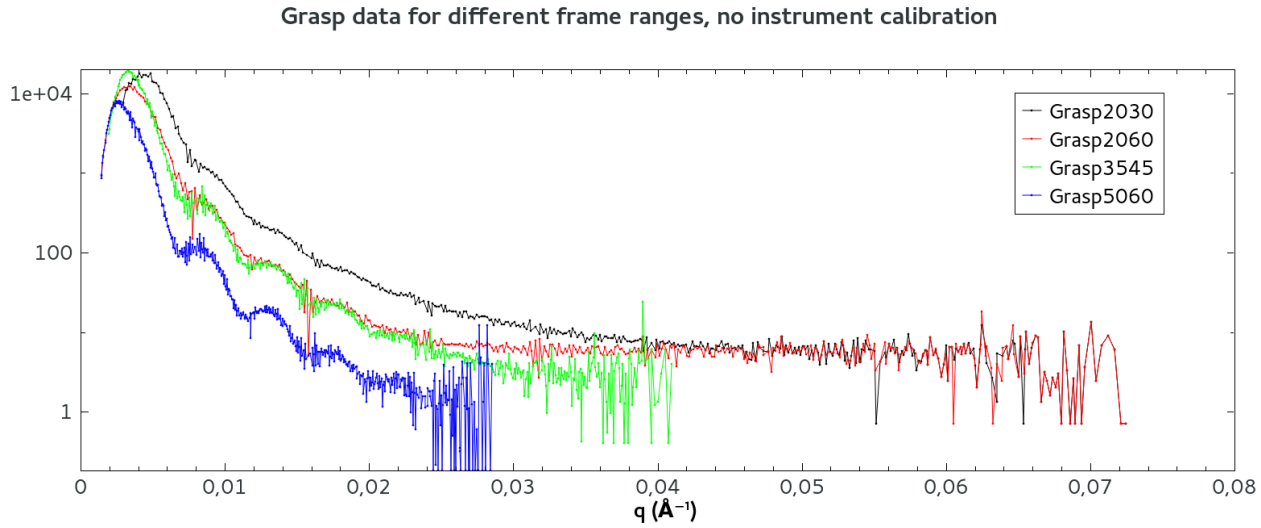
Comparison

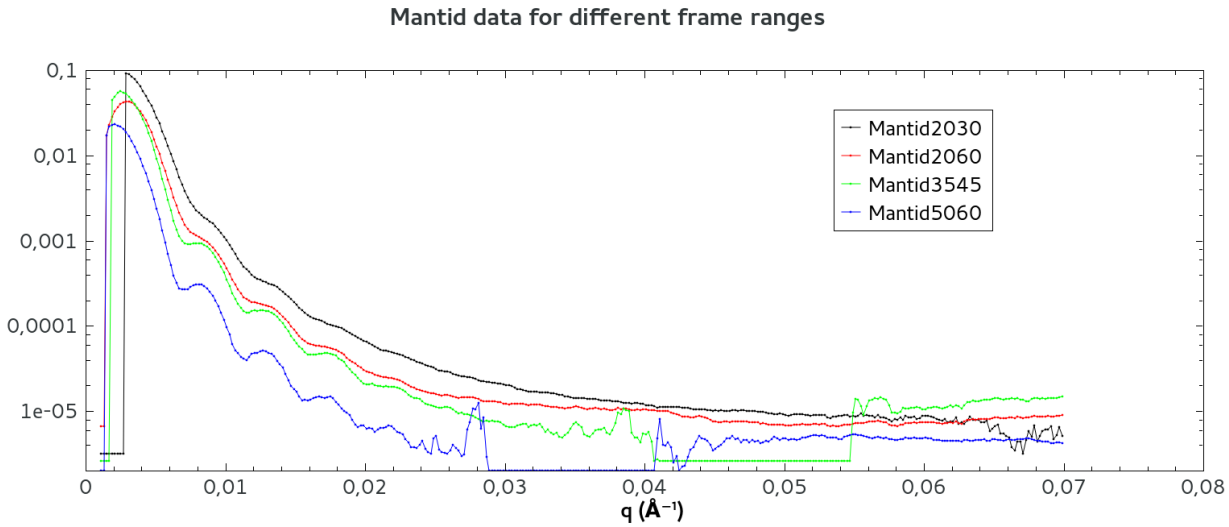
First we compared the different frame ranges in the 3 programs, to see how each program treated variable frame ranges.





We see that both LAMP and GRASP treat different frame ranges in the same way, with all ranges being roughly superimposed.



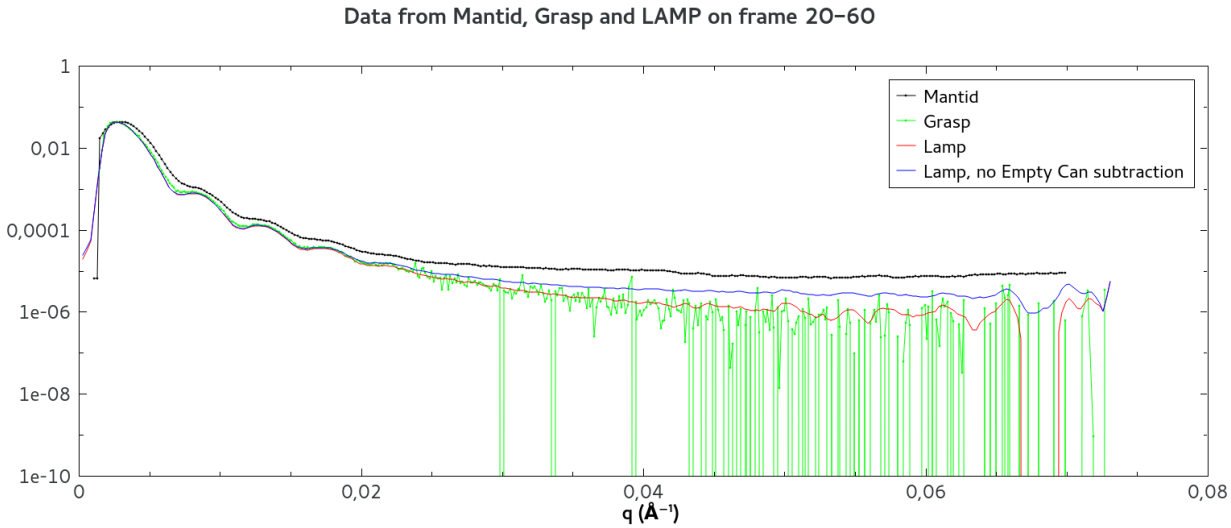


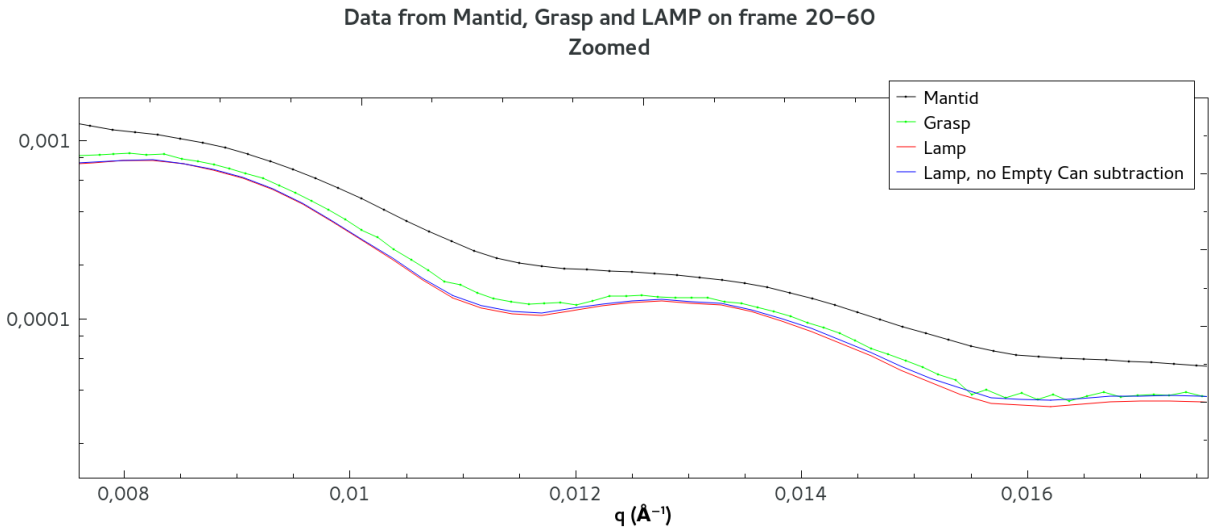
For the higher frame-ranges in MANTID, the data does not end like in GRASP and LAMP because the side-panels of the detector were not ignored.

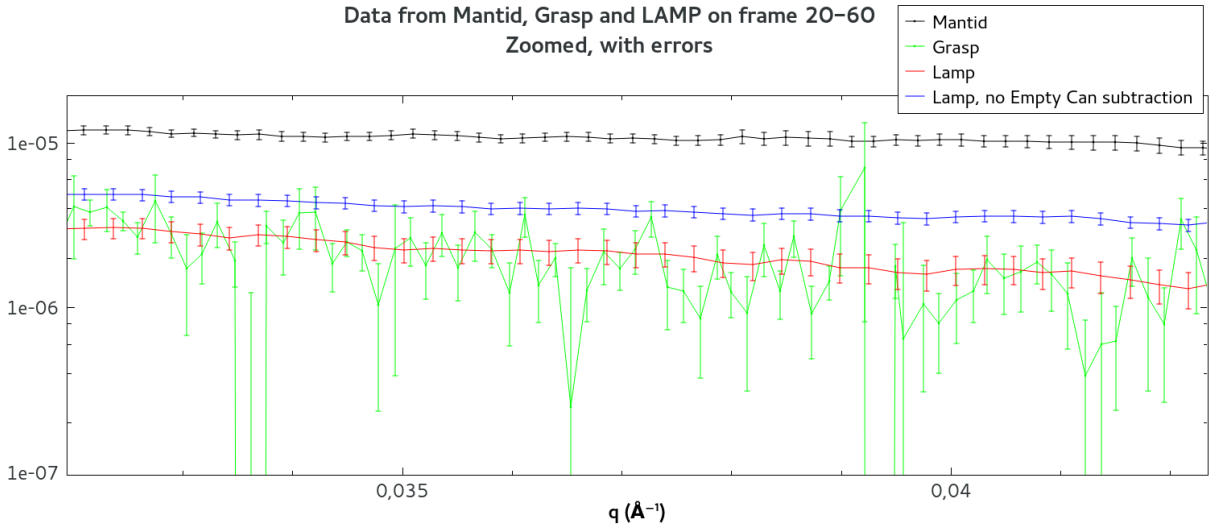
We can see that MANTID and GRASP treat different frame ranges in roughly the same way when GRASP does not account for instrument calibration. Indeed the different ranges have the same arrangement in both MANTID and GRASP without calibration, with the 2030 being above the others, the 3545 and 2060 in the middle, with the 2060 slightly higher, and the 5060 frame range below the others.

This lead us to believe that MANTID might not have an instrument calibration in its SANS routine.

In order to get a better idea of the comparison, we cropped the first peak, to look at the remaining data. We compared the data on frames 20-60 for all programs together.



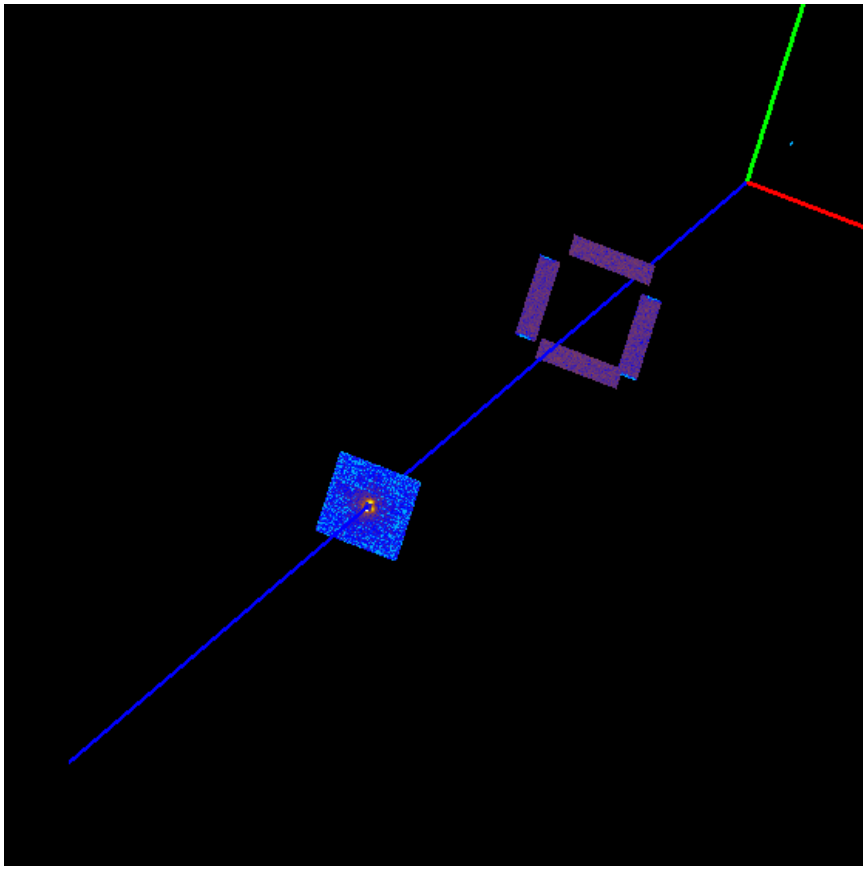




We can see that the closest match to MANTID is the LAMP data with no empty can subtraction, be it from the general shape or the size of the errors.

Instrument View

The instrument view for D33 has the same issues in Mantid 3.2.1 as that of IN6, which indicates that the issue is with Mantid/Paraview and not with the actual Intrument Definition File. In Mantid 3.4 everything works perfectly.



Conclusion

It would appear that the SANS treatment in MANTID produces significantly different results than the one in LAMP and GRASP. Whether this is due to the wrong parameters being given in MANTID or whether it is a difference in the treatment algorithm itself is unclear, and looking over the results and methods with a SANS specialist could help in finding the source of the differences. As it stands, it looks like MANTID does not have the instrument calibration that is applied in LAMP and can be applied in GRASP, which would explain the differences in general shape of the I(Q) curve.

The errors in the MANTID data are also similar to those in LAMP when no Empty Can subtraction is done, which should not be the case as the Empty Can data is passed to MANTID, so the errors should be slightly higher as a result of this subtraction.