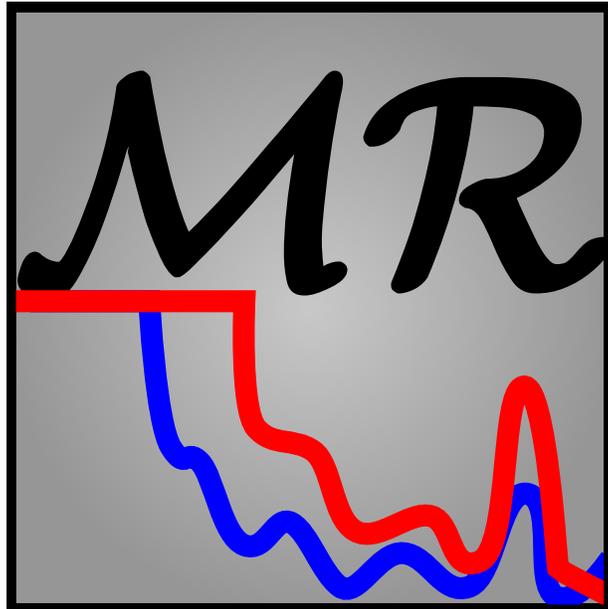


QuickNXS Users Manual

Version 1.0



Extraction software
of the
SNS Magnetism Reflectometer
Beamline - 4A.

Last updated October 29, 2014

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1 Introduction and Background

1.1 The data recorded at Beamline 4A

The raw data recorded at the magnetism reflectometer stores each detected neutron as one event, which includes information on the position on the detector, the relative time passed after the neutron pulse was created at the target, the absolute time of the according pulse and some instrument flags as the flipper ON/OFF state. After one run is finished this data is translated to the NeXus (.nxs) file format (which is based on the HDF5 standard) as two separate files, one with event information (flexible) and one with 3D histograms in X,Y and time of flight coordinates (fast).

While the X and Y position can be used in conjunction with the instrument motor positions to gain information about the scattering angle the time of flight (ToF) together with the moderator to detector distance allows to deduce the neutron wavelength. Combining these three degrees of freedom allows to transform the coordinates into reciprocal space coordinates (for reflectivity only the Q_z coordinate is relevant).

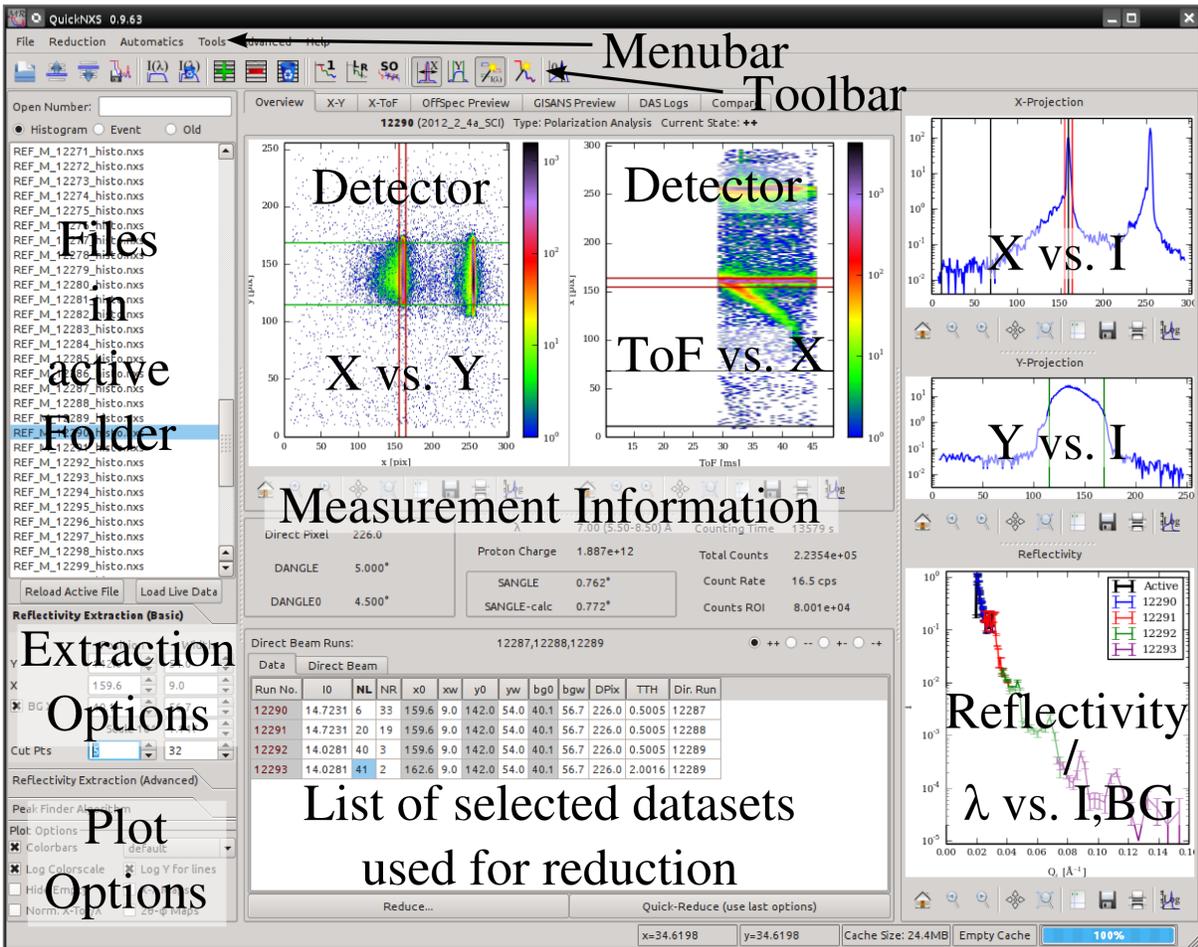
In order to derive the correct Q_z dependent intensities a normalization to the incident beam is necessary. For this the direct beam intensity of the same wavelength band and with the same instrumental setup is measured prior to the actual data. This measurement is later used as reference when calculating the reflectivity. When different incident angles are measured (as is most often the case), each incident angle takes a different part out of the direct beam and generally won't have the same overall scaling factor as the previous measurement. For the extracted reflectivity these different runs need to be combined.

1.2 What does QuickNXS data reduction do?

QuickNXS is a comprehensive tool to carry out the operations described above starting from the NeXus files and export the data in a form usable for plotting and fitting with reflectivity modeling software. The program includes real time plots of several projections of the raw file data and previews of the exported data. Several automated algorithms aid the process to improve the learning curve of non expert users and speed up the extraction process of normal datasets while keeping the flexibility to apply special treatments for more complicated cases. **For a quick start reflectivity extraction guide see section 3.3.**

2 User Interface

2.1 Overview



In addition to the default elements of a typical graphical user interface (GUI) like menu-, tool- and statusbar the QuickNKS program has a central area, which can be switch using the tab bar above, and several plot and option areas on the left and right side, always visible. Most users will work only with the "Overview" tab visible in the image above as it contains all valuable information about the current loaded dataset and the reduction parameters. The left and right

File -> Load Extraction... (CTRL+ALT+O) Reads the header of an exported dataset (.dat) to reconstruct the options and load the data files used for the reduction. This can be used to improve an already exported dataset.

 **Reduction -> Set Normalization (CTRL+W)** Use the data extracted from the current file as a direct beam dataset. You can add as many of these datasets as you like or remove them by activating this action again. The appropriate direct beam run is selected using the number of time of flight channels in the file and the central wavelength, if this is ambiguous a dialog is shown to select one dataset, unless the AutoNorm feature is active.

 **Reduction -> Clear Normalization (CTRL+SHIFT+W)** Empty the list of direct beam datasets.

 **Reduction -> Set Scaling (CTRL+S)** For the first dataset this tries to find the edge of total reflection and fits a constant to all points before it to normalize it to one. For subsequent datasets it fits a polynomial to the overlapping region of the active dataset and the closest one found in the reduction table to stitch them together. It is helpful to first define a suitable range of cut points to improve the results.

 **Reduction -> Cut Points (L/R) (CTRL+SHIFT+C)** Tries to select good cut points for the given wavelength band based on the corresponding direct beam measurement.

 **Reduction -> Keep Item in List (CTRL+Q)** Use the reflectivity from the current dataset and add it to the reduction list. Only works for dataset with direct beam run. The options in the reduction list can still be changed later.

 **Reduction -> Remove Line** Remove the selected line from the reduction list.

 **Reduction -> Clear List (CTRL+SHIFT+Q)** Clear the full reduction list to start a new reflectivity set.

 **Reduction -> Reduce...** Use the items and options in the reduction table to export a dataset. Shows a dialog to select how the export should be done.

Reduction -> Quick-Reduce... As Reduce but doesn't show the export dialog using the last set of options.

 **Automatics -> Automatic Peak Finder** If checked, the program runs a peak finder and peak fitting algorithm on the X-projection of the data each time a new dataset is loaded and sets the X-center parameter accordingly. This works very reliable in general and is activated by default.

 **Automatics -> Automatic Y Limits** If checked, the program detects the region, where the intensity in the Y-projection drops below a certain threshold and sets the Y-center and Y-width parameters accordingly. After adding the first dataset to the reduction table the option is switched off automatically to prevent issues at higher incident angle, where the

intensity is comparable with the background. Clearing the reduction list will reactivate the option.

 **Automatics -> AutoNorm** If more than one normalization datasets are defined that can be used for the current dataset the program will decide which to use based on slit settings.

 **Automatics -> Auto Reflectivity** When extracting several reflectivities with similar experimental setup the extraction parameters will likely be similar, as well. Activate this action at the total reflection run and it will use the current settings to subsequently scale and add all following datasets as long as the incident angle increases. Afterwards the **Strip Overlap** action is invoked. For good quality data this is a convenient way to reduce the full reflectivity very quickly.

 **Automatics -> Strip Overlap** This option can be invoked directly before reducing the data to remove overlapping points between subsequent runs. The points are removed from the lower Q_z run, as these normally will have much lower statistics.

Tools -> Open Compare Window... Open a dialog which allows the direct comparison of different reflectivity measurements, can be used several times and is equivalent to the Compare tab of the main window.

Tools -> Open Reduction Preview... Open a dialog which shows a preview of the extracted reflectivity with all spin states. Keeping this window open will slow down some actions.

Tools -> Filter Points... Allows you to post-process exported files by filtering specific data points.

Tools -> Search Database... This option is not always possible. It opens a dialog that allows the search for datasets based on specific parameters of the measurement.

Advanced -> Advanced Background ... (CTRL+B) Open a dialog with additional options for the background subtraction.

 **Advanced -> Adjust Direct Beam** For datasets where the direct pixel and or DANGLE0 values are not correctly defined, this action can take the current X-position of a direct beam measurement to set overwrite parameters accordingly.

Advanced -> Clear Overwrite This clears the overwrite parameters defined with "Adjust Direct Beam".

Advanced -> Polarization... Open a tool to plot polarization parameters of dedicated measurements. Not intended for users.

Advanced -> Raw Data Comparison... Show a dialog to compare the raw data of the current run (not divided by direct beam) with the direct beam measurement and background. Can be helpful to identify problems with the direct beam normalization or the extraction window.

Advanced -> Browse NXS file... (CTRL+N) Show a dialog that accesses the raw NXS file with it's folder structure. This is only intended for beamline staff.

Advanced -> IPython Console... Adds a new tab to the main window with an IPython interactive console, that can be used for advanced data treatment and scripting.

Advanced -> Debug Menu Useful things for program debugging.

Help Menu Online access to this manual and an about dialog.

2.3 The Overview Tab

This central tab shows information on the current dataset and the data reduction. A label at the top indicates the current file number, experiment ID, measurement type and the currently selected spin state. The two map plots below the label show the projected intensities on the horizontal and vertical detector axes (left) and on the time of flight and horizontal detector axes (right), in the same way as it is shown during data acquisition. In the center some important parameters, extracted from the datafile header, are displayed. The *SANGLE-calc* and *Counts ROI* parameters also depend on the selected X- and Y- region and are thus not directly read from the file. The mouse can be used to define the X- and Y-region in this plots similar as in the projection areas described below.

At the bottom you can find the reduction table and an additional tab with a list of defined direct beam datasets. These tables show the parameters used for the respective intensity extractions. The parameters in the Data tab can be edited afterwards and will be applied directly to the reflectivity curve shown in the Reflectivity area. Directly above the table is a label showing the numbers of all defined direct beam runs and radio buttons to select the current datasets spin state shown in the Overview, projections and reflectivity plots.

2.4 Plots and Options

The areas on the left and right of the window contain e.g. the projection plots and extraction parameters and are visible on any tab of the main interface. The left side contains option fields for the extraction parameters and file readout while the right side is dedicated for important plots. Here is a list of the available areas from top to bottom, first on the left and then on the right hand side.

Files A list of all datafiles in the current directory together with an entry to search for a file by number and select to extract either histogram or event mode data. In the event mode setting additional options will be displayed.

Reflectivity Extraction (Basic) The parameters used to extract the active reflectivity. When adding a dataset to the reduction list, these parameters are stored in the Data table.

Reflectivity Extraction (Advanced) Settings to change the extraction method or overwrite parameters otherwise read from the datafile. Options for the stitching algorithm can be found here as well.

Peak Finder Algorithm Settings for the peak finder algorithm not important for normal user operation.

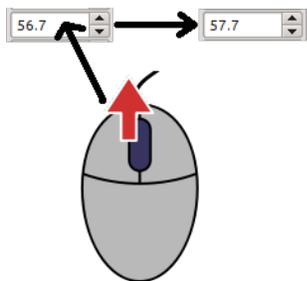
Plot Options Global settings for the shown plots, does not effect the data reduction in any way. Here you can also chose to show the 2D datasets in wavelength and angle coordinates instead of time of flight and pixel.

X-Projection A plot with the data of the loaded file projected on the detector X-axis. Black lines indicate the background region defined at the moment. The X-position is marked with a black line and the X-width with two red lines. The mouse can be used to change the background region and X-center using the left mouse button and set the X-width using the right mouse button.

Y-Projection An equivalent projection on the detector Y-axis, showing the selected Y-region with green lines. The mouse can be used to change the Y-region using left clicks.

Reflectivity Shows all datasets already added to the reduction list (colored lines) and the currently selected one (black line labeled 'Active'). For datasets without fitting direct beam runs it shows intensity and background vs. wavelength. Datasets in the reduction list can be scaled with the mouse wheel when at the right x-coordinates (faster scaling when CTRL is pressed while scrolling). Note that a dataset can be shown twice (as "Active" and with it's run number) when it is already in the reduction list and selected.

2.5 Convenient Parameter Alteration with the Mouse Wheel



You can use the mouse wheel when your cursor is on top of a value entry to increase or decrease the according parameter. This can be very convenient to see the result of e.g. changing the scaling factor for the current reflectivity. Holding down the CTRL key while scrolling increases the speed of the parameter changes. The same method can also be used to scale datasets in the reduction table, simply by moving the mouse at the curve in the reflectivity plot and scrolling with the mouse wheel.

2.6 Plots

Each of the plots described above are created with the same framework and have a toolbar below them:



The first 5 items allow the navigation on the plot, like zooming in and out or moving the current view position. The fourth icon from the left opens a dialog, which can be used to change the amount of free space around the plot to fit the current window scaling. The following two icons can be used to save or print the plot. The last button allows to toggle between logarithmic and linear plotting (this is not persistent after changing the dataset).

Keep in mind that the X- and Y-projections as well as the overview maps can be used to select the extraction parameters. This will only work when no scaling tool is selected from the plot toolbar.

2.7 Data reduction table

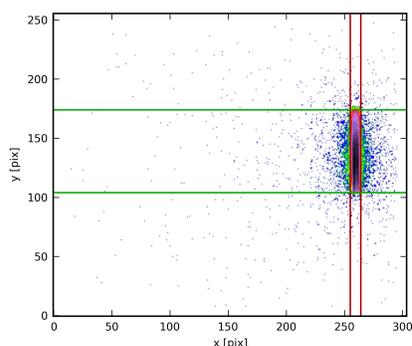
Run No.:	I0	NL	NR	x0	xw	y0	yw	bg0	bgw	DPix	TTH	Dir. Run
12290	14.7231	6	44	159.6	9.0	142.0	54.0	26	36	226.0	0.5005	12287
12291	14.7231	20	24	159.6	9.0	142.0	54.0	26	36	226.0	0.5005	12288
12292	14.7231	40	4	159.6	9.0	142.0	54.0	26	36	226.0	0.5005	12289
12293	16.6725	40	1	162.7	9.0	142.0	54.0	26	36	226.0	2.0016	12289

Each entry created in the reduction table shows all important parameters needed for reflectivity extraction. In addition to the parameters found in the Reflectivity Extraction area there is a value for the direct pixel (DPix) and relative detector arm position DANGLE-DANGLE0 (TTH) as well as the dataset and normalization file number. **Changing any of the reduction parameters** (except for the two file number columns) immediately recalculates the extracted reflectivity. All lines present in the reduction table are plotted together with the current dataset in the Reflectivity Extraction area.

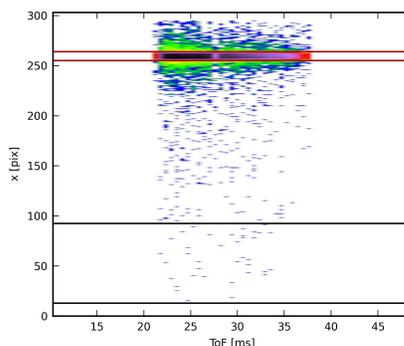
3 Data Reduction

3.1 Open and view a dataset

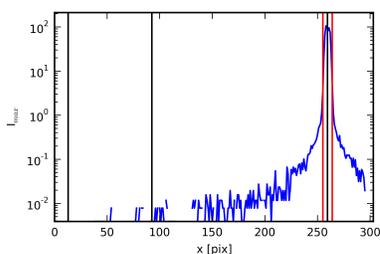
The first step to start with is to enter the number of a direct beam dataset in the "Open Number:" entry of the Files area and press enter. The program will now locate the file and open it. The Files area list will be populated with all files in your current proposal data folder and the plot windows should look similar to this:



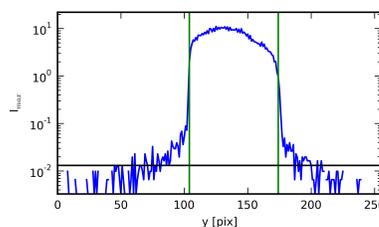
Overview X-Y



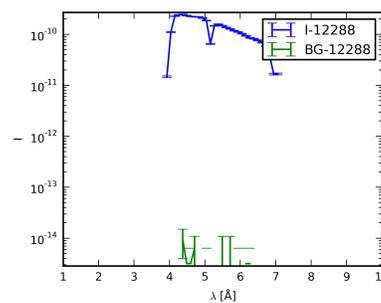
Overview ToF-X



X-Projection



Y-Projection



Reflectivity

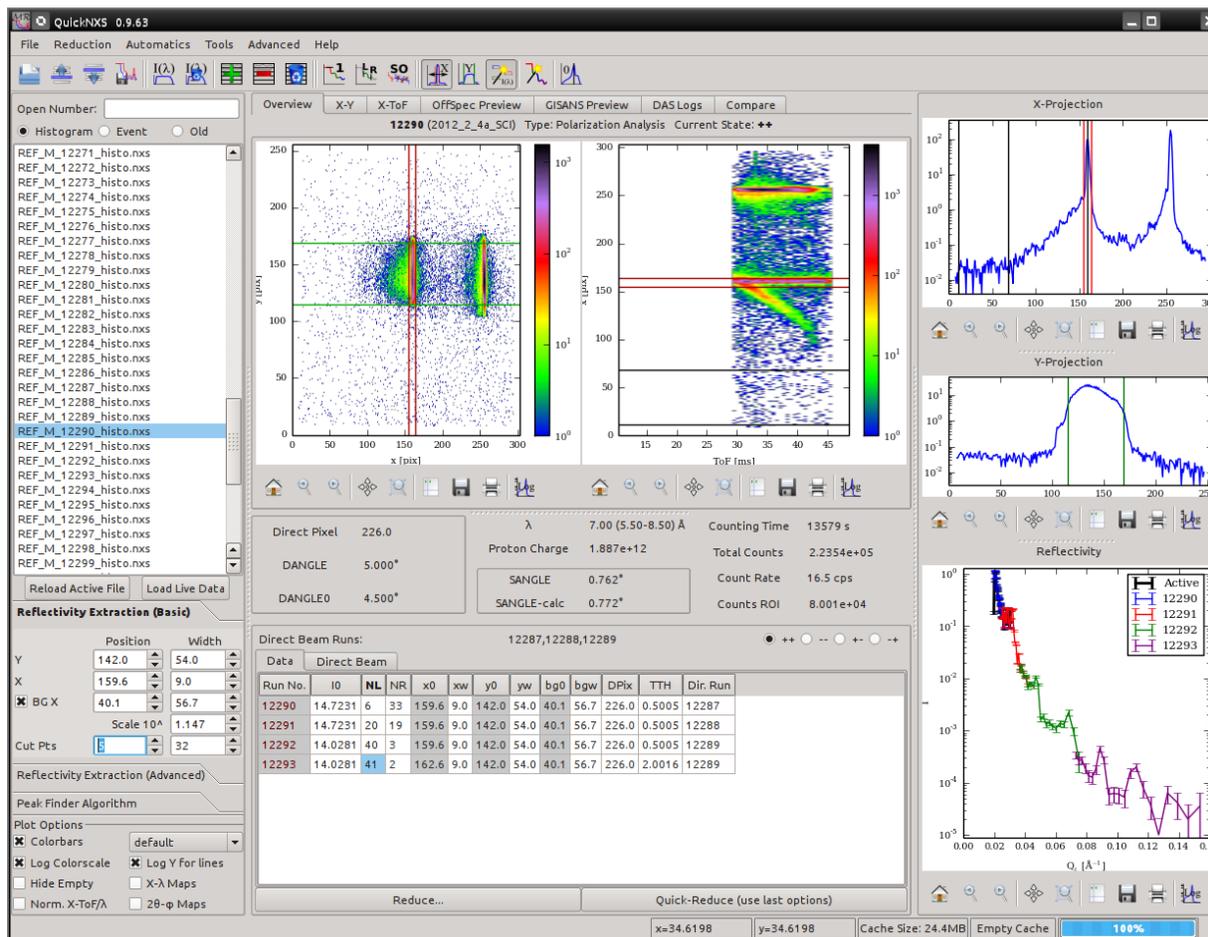
3.2 Go full-automatic: Reduction for dummies

For good quality data (enough intensity and narrow reflection) the program supports a fully automatized mode, where all reduction parameters are automatically calculated. This mode will be applied automatically when more than one dataset is selected at the File Open Dialog. The

3 Data Reduction

direct beam measurements have to have lower scan numbers than the actual measurements or need to be set in advance for this method to work.

The automatic algorithm performs the same steps as described in section 3.3, while trying to guess the best parameters. The datasets are read one-by-one and, depending on the reflection angle, they are either set as direct beam or reflectivity data in the reduction list. Here is an example how the interface might look after the algorithm has finished:



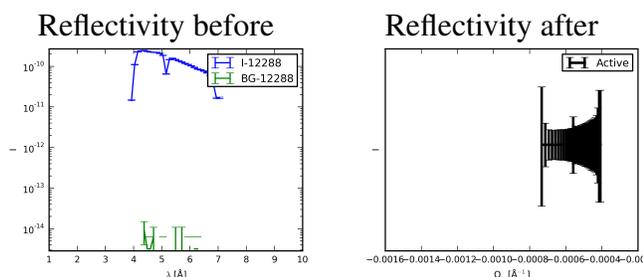
You can now scale individual datasets as described in 3.3.5, if the stitching was not performed optimally. When satisfied with the result, you can save the data as described in the export section 3.3.6.

3.3 Quick start: Step-by-step standard reduction

For most datasets the reduction is done very similar to the fully automatized method but with more control by the user. Every dataset is examined by the operator to select the best extraction parameters. This description should work in almost all circumstances.

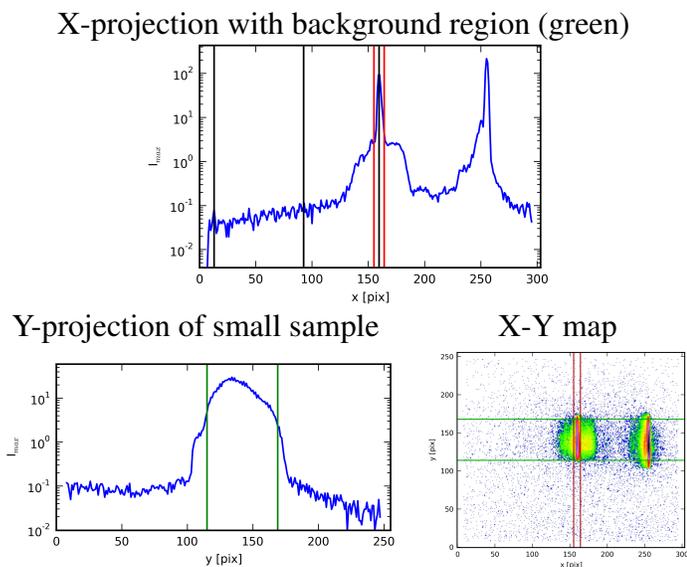
3.3.1 Step 1: Set direct beam runs

Open your direct beam file as described in section 3.1. Make sure the SANGLE-calc value shown in the overview tab is close to zero and that the X- and Y-projections show the correct regions indicated with vertical lines. Activate the **Set Normalization action** $I(\lambda)$. This will add the current dataset to the "Direct Beam" list and the "Direct Beam Runs:" label will show the number of the dataset and the reflectivity will show the normalized intensities, which should all be one. You can use the **Cut Points (L/R) action** $\left[\begin{array}{c} L \\ R \end{array} \right]$ here to already set reasonable parameters for the Cut Pts entries. Repeat this step for each direct beam measurement needed for your datasets.



3.3.2 Step 2: Define a suitable background- and y-region

Although it is in principle possible to define the extraction and background region for each dataset separately, it is recommended to use the same parameters for all files. From this perspective it is often a good idea to start with the dataset with the highest incident angle for the background, as the signal to background ration is the lowest there. To produce the best results you should select a large region (statistics), keeping enough distance from the reflected beam (especially when off-specular Bragg-sheets are present)



and to not include regions where the background drops (shadowed by the left detector slit for example). The Y-region, shown in the Y-projection of the first (low Q_z) dataset, is often detected very well automatically. Just check that it fits to the reflected intensity area. For very small samples it can sometimes make sense to manually restrain the area to the sample reflection using the right mouse button on the X-Y map.

3.3.3 Step 3: Normalize to total reflection and add the first dataset

Go to your dataset starting at the lowest Q_z value and remove points which are not reasonable from the low Q_z region with the **Cut Pts parameters**:

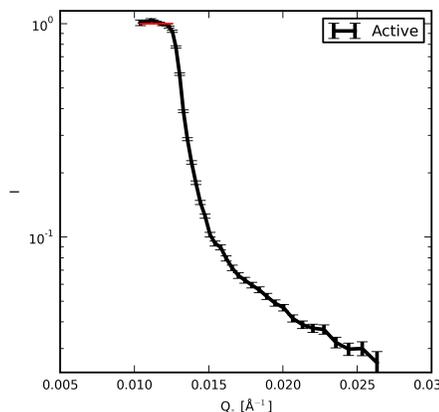
Cut Pts 56 4

(can be done automatically with the **Cut Points (L/R)**  action if not already performed after direct beam selection).

Then activate the **Set Scaling action**  to normalize the total reflection to one.

This should now look like the image on the right. Next add the dataset to the refinement list using the **Keep Item in List action** , copying the current parameters to the list. This will automatically switch off the **Automatic Y Limits** , so all datasets will be reduced with the same Y-range.

This is important for the high Q_z region as the background often inhibits a good automatic detection of the Y-region.

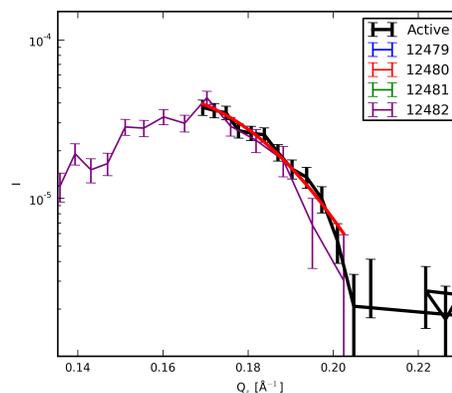


3.3.4 Step 4: Add additional datasets and stitch them together

Now you can continue adding each subsequent dataset one after another. If nothing goes wrong, the only thing that needs to be changed from dataset to dataset is the **Scaling** parameter. If the scaling of subsequent datasets does not fit, activate the **Set Scaling action**  again. This fits a polynomial to the logarithmic data of both adjacent datasets including a scaling factor for the second, which is then used for the scaling after the fit. The error weighted χ^2 used for this refinement is:

$$\chi_{stitch}^2 = \sum_{DS1} \frac{(\log(I_i) - p(Q_i))^2}{(\delta I_i / I_i)^2} + \sum_{DS2} \frac{(\log(I_j \cdot scale) - p(Q_j))^2}{(\delta I_j / I_j)^2}$$

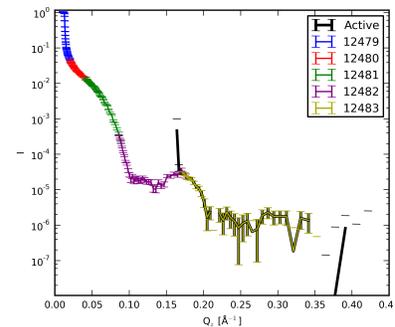
with $p(Q) = a \cdot Q^2 + b \cdot Q + c$ for polynomial order 3



The resulting fit function is shown in the reflectivity plot together with the scaled data as can be seen in the figure on the right. For some datasets with very sharp features like multilayer Bragg-peaks this method will probably not work, in those cases you need to change the **Scale** 10^x parameter manually until the datasets fit together nicely. For polarized measurements it can sometimes be helpful to switch back and forth between different polarization states as the variation in contrast can lead to smooth transitions, where the other state has a sharp feature. Now add the dataset to the reduction list with **Keep Item in List** action  again and repeat the procedure for all datasets belonging to this measurement.

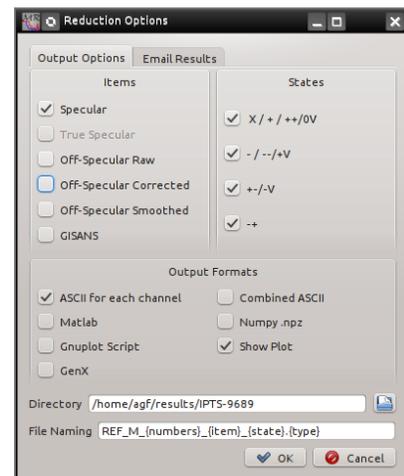
3.3.5 Step 5: Refine the reflectivity scaling and cutting

When all datasets of one measurement have been added, as can be seen in the image on the right, you can try to improve the scaling of the different parts, if needed, and change the cutting parameters. To change the scaling of one dataset you can either change the value of the **I0** column entry in the reduction list or put the mouse cursor on top of the curve you want to scale and **move the mouse wheel**. To remove unwanted points you need to change the values of the **NL** and **NR** column entries as they define the number of points cut from the low- and high-Q side respectively. If the number of time of flight channels in the dataset is larger than the wavelength window it is possible that large values are needed (≤ 60) to see changes in the dataset. (Removing of overlapping points with low statistics can be done with **Strip Overlap** )



3.3.6 Step 6: Export your data

Now you are ready to export your reflectivity! Activate the **Reduce...** action  from the menu, toolbar or the button below the reduction list. The reduce dialog has several options for the export of the dataset. You can select which reductions should be stored, choose the spin states to export and define which data formats should be created. As a default, the specular reflectivity of all available channels will be exported to separate ASCII files and a dialog with a plot of the resulting data will be shown afterwards. Additional output options are a combined ASCII file containing all states, a matlab or numpy datafile for later processing, a Gnuplot script and image file to plot the ASCII data and a GenX reflectivity modeling template already containing the measured data. If you



want to send the resulting data to your email address you can use the **Email Results** tab to enter your address and select which and if the data should be send after the export.

3.4 Examples

This section will give three example datasets, which you can use to try the reduction yourself and compare the result with the images in this manual.

3.5 Common complications to be aware of

Bend/Twisted samples Samples which do not have a flat surface can produce "fan"-like or split reflections. In these cases the peak fitting can result in different extraction areas for different incident angles. Use a small X window and/or the "**Fan**" **Reflection** option (see section 4.5) from the **Reflectivity Extraction (Advanced)** tab and define the reflection position manually.

Runs don't fit together This often is caused by one of two reasons: One possibility is that there are very sharp features in the reflectivity which are measured differently for the different angles, as the resolution changes with the angle. In this case the only possibility is to try to merge the datasets manually as good as possible. If the measurement is polarized, take a look at the other spin state, sometimes the feature won't be as pronounced and make it easier to find the scaling factor. The other possibility is that the direct beam position, which should be measured before the experiment and written to the datafile, is not correct. This can be checked with the according direct beam run. If the **SANGLE-calc** value for the direct beam run is not close to zero you can use the **Adjust Direct Beam action**  to overwrite the values read from the datafile. Afterwards it should be possible to extract the reflectivity normally. Don't forget to reset this overwrite afterwards using **Clear Overwrite** (see section 4.3).

4 Advanced Usage

4.1 Event mode data

When the event mode is selected for file import, additional options for the desired binning are shown. You can define the number of **Bins**, the bin steps (constant ΔToF , ΔQ or $\Delta\lambda/\lambda$ steps) and split datasets in time. In all other aspects event mode data is not treated differently from histogram data. To be able to use a direct beam measurement, it needs to be extracted with the same binning as the actual measurement.

4.2 Re-reduction of already exported data

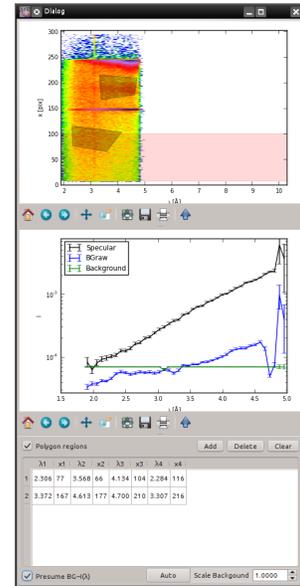
You can read all datasets and options from an already exported reflectivity using the **File->Load Extraction...** menu and select an ASCII file. Afterwards the options in the reduction table can be changed as desired.

4.3 Overwrite direct beam parameters

If the the direct beam position was not saved correctly during instrument alignment all calculated Q_z -values for the reflectivity will be wrong. To correct this there are two parameters to overwrite it in the **Reflectivity Extraction (Advanced)** area, **Direct Pixel** and **Dangle0**. These parameters are ignored if they have the values -1 and None. To overwrite the correct values you can open a direct beam dataset and activate the **Adjust Direct Beam action**  to save the current DANGLE as **Dangle0** and the fitted X-position as **Direct Pixel**.

4.4 Advanced background subtraction

There are a few cases where you could need additional control over the subtracted background, for this case you can use the **Advance Background...** action to open a dialog with more options. An example is shown on the right. The upper plot shows the X vs. λ plot of the current dataset, indicating the areas taken to calculate the background data. The lower plot shows the extracted data and background as wavelength vs. intensity plot. You can use Polygons to define the extraction area for the background precisely, these polygons are than shown in the X vs. λ plot as gray areas. The normal extraction region defined by the main window parameters is shown in red. For each λ channel the average value of all pixels in the gray areas is taken as background. If, for a given value of λ , no points are defined with a polygon the red area is taken. As an additional option it is possible to presume a background that is directly dependent on the incident intensity to reduce the error bars.



4.5 "Fan"-Reflectivity

Some samples have a wavy or bent surface and reflect the neutron beam into different angles. Treating these as one reflection will destroy the Q_z resolution of you measurement or needs to be restricted to a small X-region, which reduces the statistics. For these cases the **Reflectivity Extraction (Advanced)** area has a **"Fan"-Reflectivity** option, which treats each pixel on the detector separately to calculate $I(Q_z)$ and combines these reflectivities afterwards to get better statistics. In this case you can widen the red area on the X-projection plot to take your full reflectivity into account. The underlying algorithm reduces the total width of a selected dataset in Q_z so it can be possible that for lower angles you do not get overlapping areas to stitch the data together. In this case you should select a smaller area for the lower angle measurements and/or extract two regions in X for one dataset.

4.6 Off-specular and GISANS scattering

Off-specular scattering can easily be extracted when the specular reflectivity is already defined in the reduction table. You can take a look at the **OffSpec Preview** tab to preview it in advance (does not show the active dataset, only the reduction table entries). The reduction dialog has a

4 Advanced Usage

separate option to export the off-specular data, where *Raw* refers to the data as extracted, *Corrected* applies an algorithm to reduce detector artifacts from high intensity areas and *Smoothed* will interpolate the data to a regular grid with Q_z -dependent Gaussian smoothing (parameters are defined in a separate dialog when exporting).

*The scaling factors to combine datasets for off-specular extraction will only be correct if the **full reflectivity** is within the X-width and if you **keep the X-width constant!** These conditions need not to be fulfilled when only specular data is extracted.*

For GISANS measurements another dialog appears when exporting, where you can define the wavelength bands, which will be combined in one image.