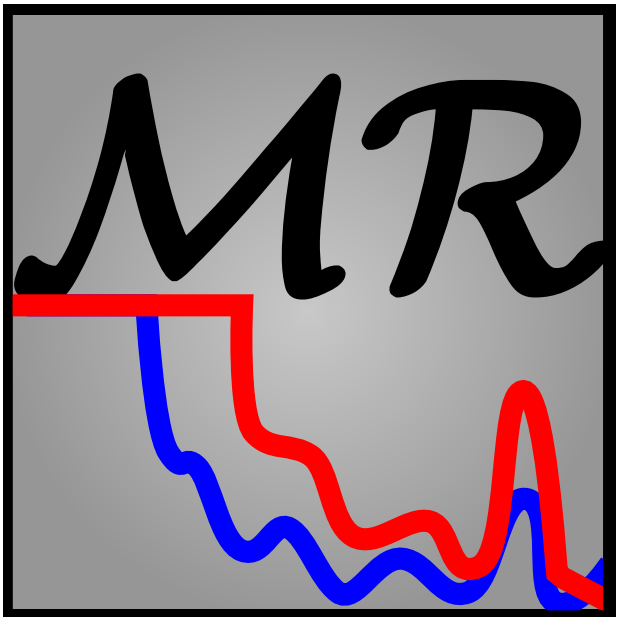
QuickNXS Users Manual

Version 0.5



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

Last updated February 5, 2013

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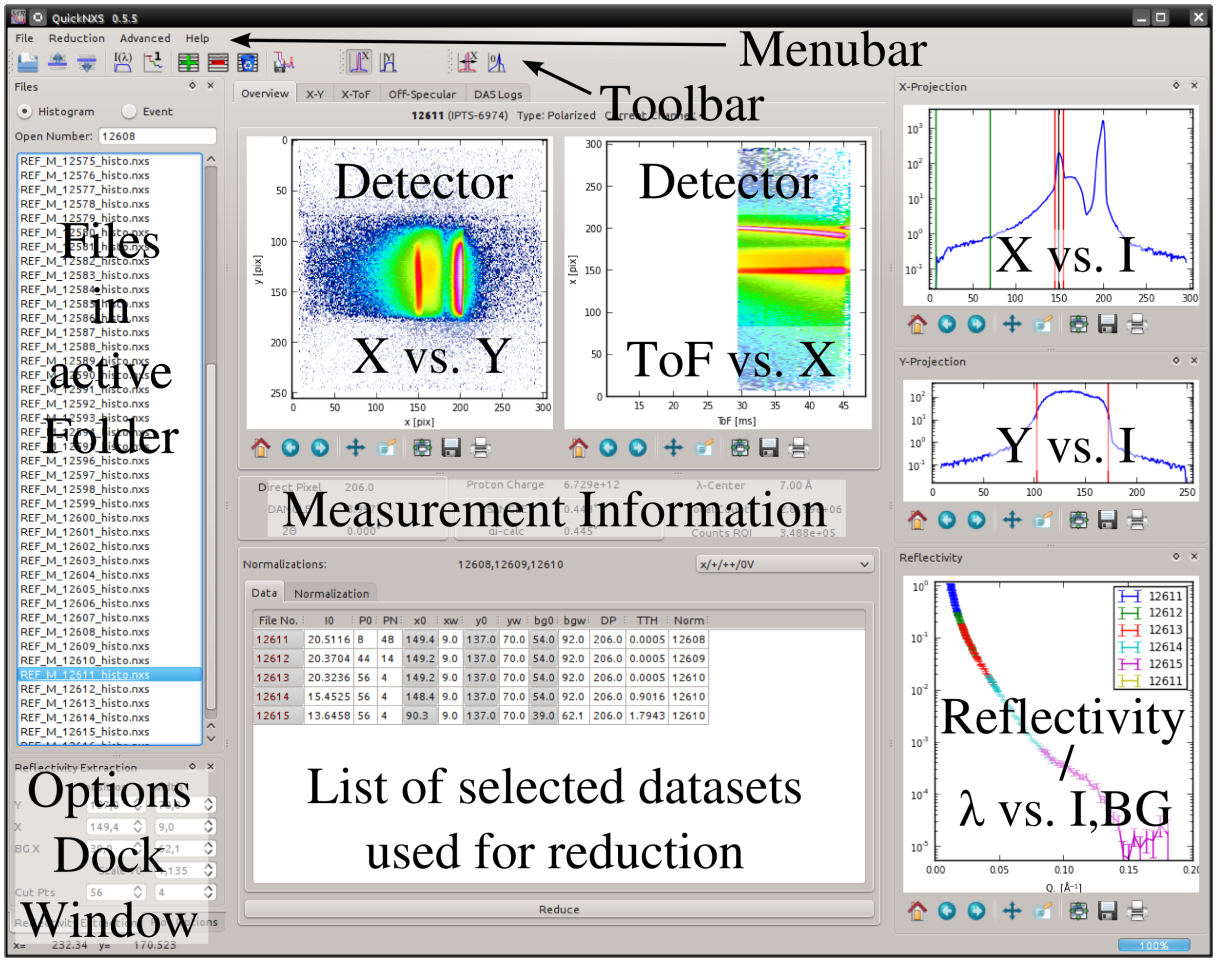
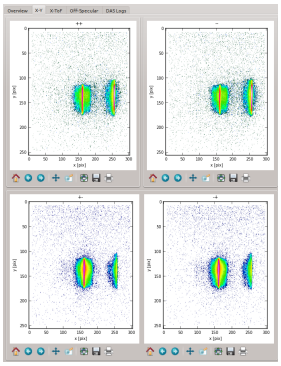
2.1 Overview

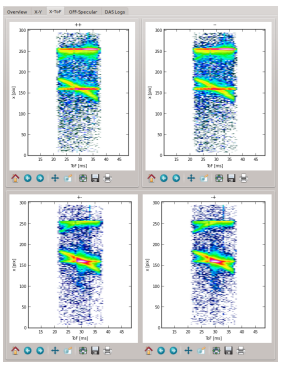


In addition to the default elements of a typical graphical user interface (GUI) like menu-, tool- and statusbar the QuickNXS program has a central area, which can be switch using the tab bar above, and several "Dock Windows" on the left and right side, always visible. Most users will work only with the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

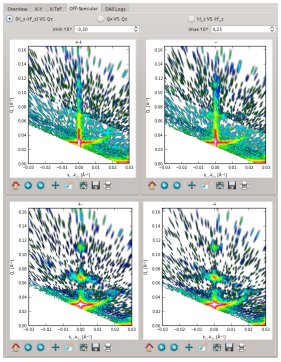
be customized as described in the according section and hold parameter entries for the reduction as well as the projection and reflectivity plot, most important for the extraction. The other tabs, shown below, allow a parallel view on the 2D maps of all channels in the active dataset as well as an preview of off-specular scattering and motor/controller logs from the current file.



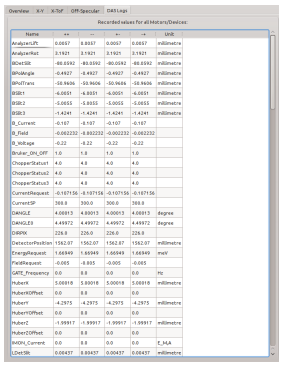
X-Y-Maps



X-ToF-Maps



Off-Specular



DAS Logs

Each of the plots has an own toolbar described in the plots section and show one specific aspect of your dataset. Often it is important to look not only on one of these plots to analyze the data, so it is good to familiarize with what you see there. All options available in the toolbar are duplicated somewhere in the menus, to make it easier to find, what you need. The most important actions have **keystrokes** assigned to them for convenience. The keys have been chosen to be accessible only with the right hand, so you can use them together with the mouse. **Most GUI elements have a tool tip** assigned, so you can always position the **mouse cursor** over **any element to get a more detailed description**, what it is used for.

2.2 Menu and toolbar actions

File -> Open... (CTRL+O) Shows a dialog to select a file to be loaded. The filename filter depends if "Histogram" or "Event" mode are selected in the Files Dock Window.

File -> Next File (CTRL+D) Opens the file below the active selection in the Files Dock Window.

File -> Previous File (CTRL+SHIFT+O) Opens the file above the active selection in the Files Dock Window.

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

Reduction -> Set Scaling (CTRL+S) For the first dataset it tries to find the edge of total reflection and fit a constant to all points before it to normalize it to one. For the second dataset 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 -> Keep Item in List (CTRL+Q) Use the reflectivity from the current dataset and add it the the reduction list. Only works for already normalized dataset. 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 Clear the full reduction list to start a new set of reflectivity.

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.

Advanced -> 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.

Advanced -> 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.

Advanced -> Refine X If checked, each time the user clicks on the X-projection plot to select another X-center position, a Gaussian fit is executed to refine the position.

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".

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 channel. 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 show during data acquisition. In the center some important parameters, extracted from the datafile header, are displayed. The αi, 2Θ and Counts ROI parameter also depends on the selected X- and Y- region and is 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 Dock Windows described below.

At the bottom you can find the reduction table and an additional tab with a list of defined normalization datasets. These tables show the parameters used for the respective intensity extractions. These parameters in the Data tab can be edited afterwards and will be applied directly to the reflectivity curve shown in the Reflectivity Dock Window. Directly above the table is a label showing the numbers of all defined normalization files and a drop-down selection for the current dataset channel shown in the Overview, projections and reflectivity plots. Selecting a channel not present in the current file will result in a fallback to the first channel.

2.4 Dock Windows

Dock windows are the the regions on the left and right of the window containing e.g. the projection plots and extraction parameters. They are visible on any tab of the main interface. These windows positions can be customized by the user anywhere around the center, on top of each other, detached from the main window or completely closed (will be saved on exit). Closed dock windows can be restored by right clicking any dock window title or the empty region next to the toolbar and menu. You can easily detach and reattach them by clicking the diamod button at the top right. Here is a list of available dock windows:

Files A list of all datafile 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.

X-Projection A plot with the data of the loaded file projected on the detector X-axis. Green 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 red lines. The mouse can be used to change the Y-region using left clicks.

Reflectivity Show all datasets already added to the reduction list and the currently selected one. For unnormalized datasets it show 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).

Reflectivity Extraction The parameters used to extract the active reflectivity. When adding a dataset to the reduction list, these parameters are stored.

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 instead of time of flight and pixel.

Advanced Background Additional parameters for the background subtraction, normally not in use.

Advanced Parameters Settings to change the extraction method or overwrite parameters otherwise read from the datafile.

Algorithm Parameters Settings for the peak finder and curve stitching algorithms.

Event Mode Readout Define the binning to be used when reading event mode data.

2.5 Convenient Parameter Alteration with the Mouse Wheel

You can use the mouse wheel when you 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 third icon from the left opens a dialog, which can be used to change the amount of freespace around the plot to fit the current window scaling. The last two icons can be used to save or print the plot. **Keep in mind that the X- and Y-projection 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

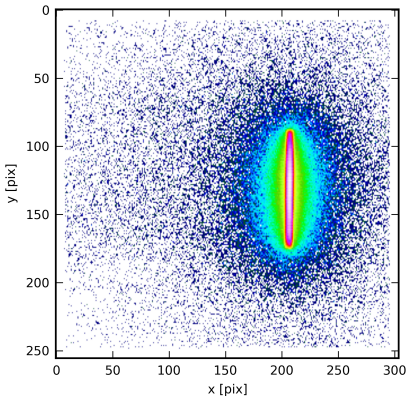
File No.	I0	P0	PN	x0	xw	y0	yw	bg0	bgw	DP	TTH	Norm
12611	20.5116	8	48	149.4	9.0	137.0	70.0	54.0	92.0	206.0	0.0005	12608
12612	20.3704	44	14	149.2	9.0	137.0	70.0	54.0	92.0	206.0	0.0005	12609
12613	20.3236	56	4	149.2	9.0	137.0	70.0	54.0	92.0	206.0	0.0005	12610
12614	15.4525	56	4	148.4	9.0	137.0	70.0	54.0	92.0	206.0	0.9016	12610
12615	13.6458	56	4	90.3	9.0	137.0	70.0	39.0	62.1	206.0	1.7943	12610

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 Dock Window there is a value for the direct pixel (DP) and detector arm position (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 Dock Window.

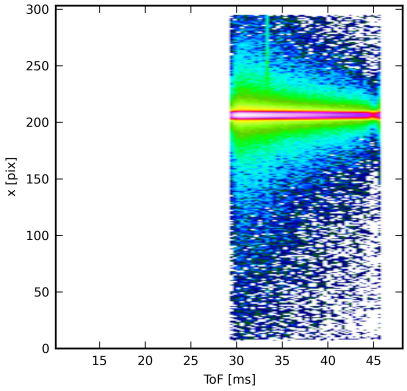
3 Data Reduction

3.1 Open and view a dataset

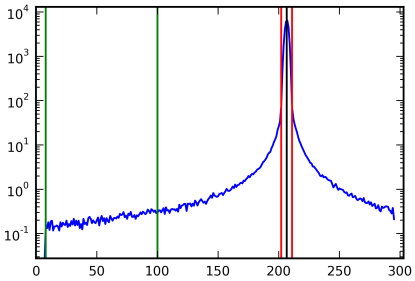
The easiest way to start with is to enter the number of a normalization dataset in the "Open Numbers:" entry of the Files Dock Window and press enter. The program will now locate the file and open it. The Files Dock Window list will be populated with all files in your current proposal data folder and the plot windows should look similar to this:



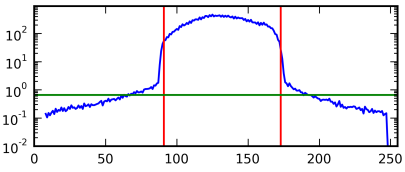
Overview X-Y



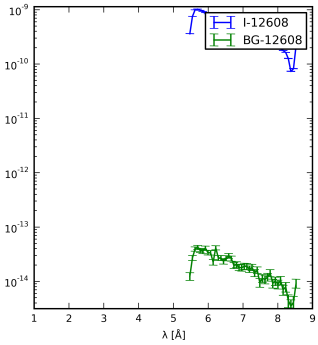
Overview ToF-X



X-Projection



Y-Projection

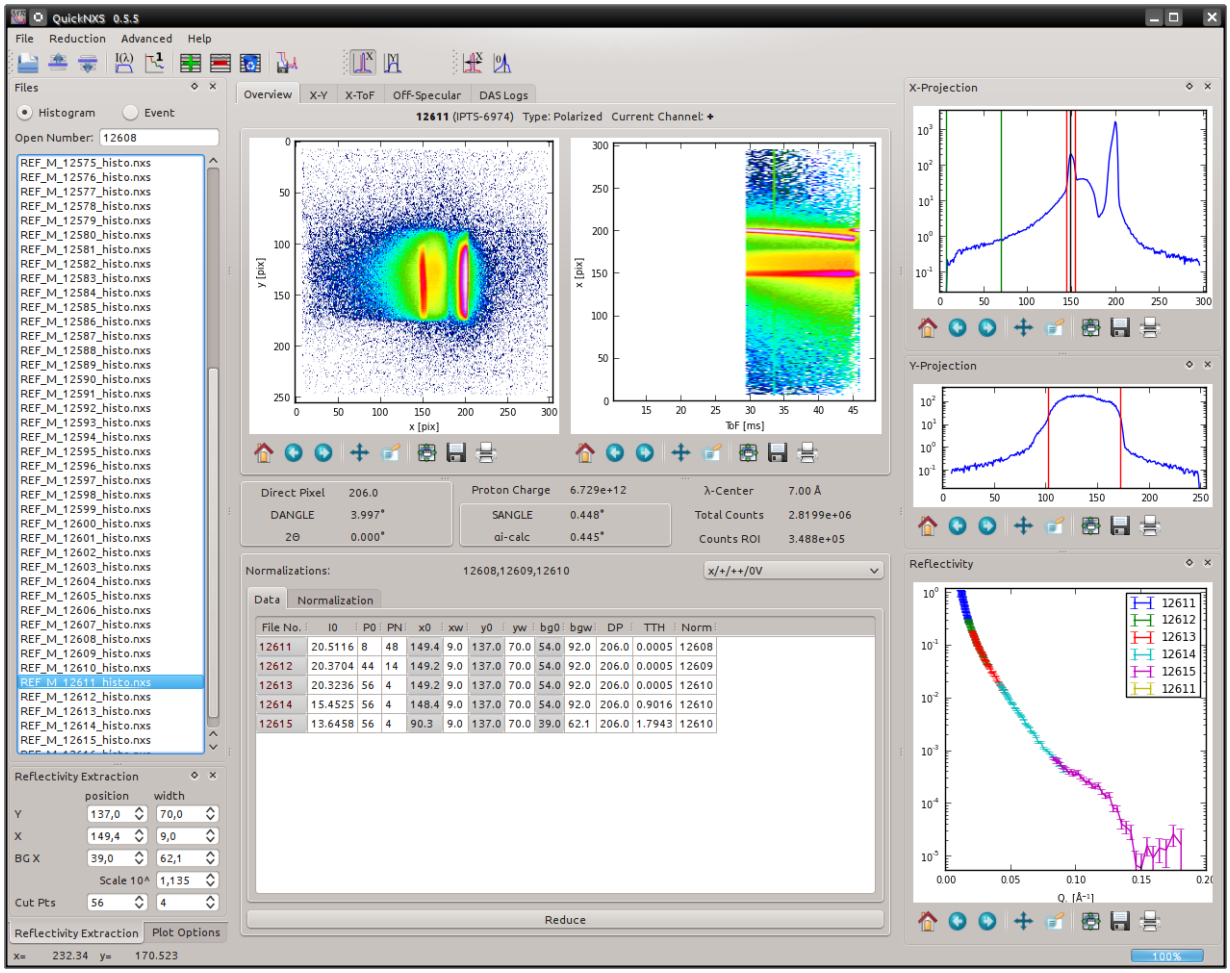


Reflectivity

3.2 Go full-automatic: Reduction for dummies

For good quality data 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 direct beam measurement 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 2θ-angle, they are either set as normalization 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.

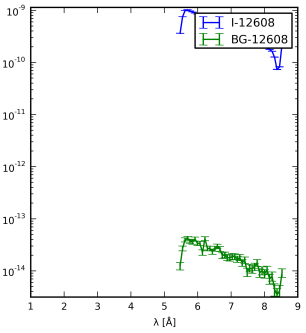
3.3 Quick start: Step-by-step standard reduction

For most datasets the reduction is done very similar to the fully automatized method but with more control of the user. Every dataset is examined by the operator to select the best extraction parameters.

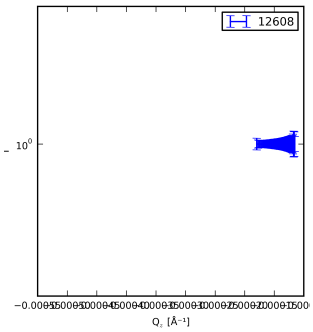
3.3.1 Step 1: Set wavelength normalization from direct beam

Open your normalization file as described in section 3.1. Make sure the αi-calc value shown in the overview tab is close to zero the X- and Y-projections show the correct regions with the red indicators. Activate the **Set Normalization action** $I(\lambda)$ will add the current dataset to the "Normalization" list, the "Normalizations:" label will show the number of the dataset and the reflectivity will show the normalized intensities, which should all be one. Repeat this step for each normalization file needed for your dataset.

Reflectivity before



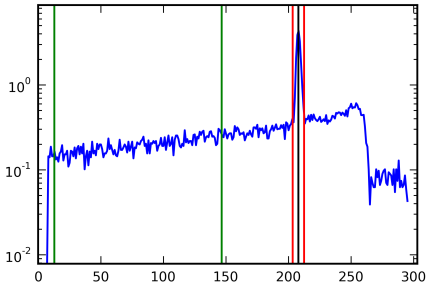
Reflectivity after



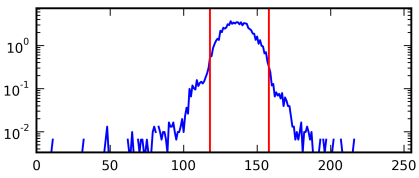
3.3.2 Step 2: Define a suitable background- and y-region

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, as there the signal to background ration is the lowest. 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 right detector slit for example). The Y-region, shown in the Y-projection of the first (low Q)

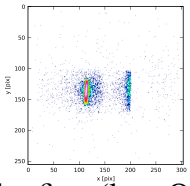
X-projection with background region (green)



Y-projection of small sample

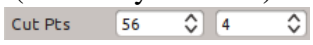


X-Y map

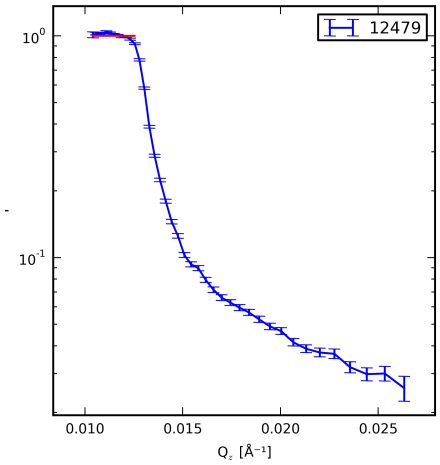


dataset, is often detected very well automatically. Just check that it fits to the reflected intensity area. For very small samples it can sometimes make sense to manually restrain the area to the sample reflection.

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

Go to your datasets starting at the lowest Q_z value, remove points from the low Q_z region, which are not reasonable (not always needed) with the **Cut Pts parameters**: 

Than 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**  to add the dataset with the current parameters in 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.

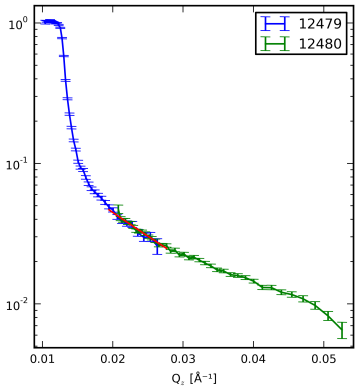


3.3.4 Step 4: Add additional datasets and stitch them together

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 are the **Cut Pts** and **Scaling** values. If the scaling of subsequent datasets does not fit, activate the **Set Scaling action**  again. This fits a parabola to the logarithmic data of both adjacent datasets including a scaling factor for the second, which is than used for the scaling after the fit. The error weighted χ^2 used for this refinement is:

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

$$\text{with } p(Q) = a \cdot Q^2 + b \cdot Q + c$$



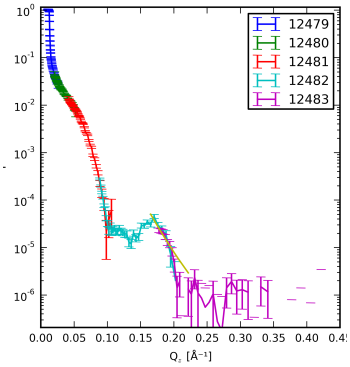
The resulting fit function is shown in the reflectivity plot together with the scaled data as can be seen in the two figures on the right.. For some datasets with very sharp features like multilayer Bragg-peaks this method will not work, in those cases you need to change the **Scale 10^** parameter manually until the datasets fit together nicely. For polarized measurements it can sometimes be helpful to switch back and forth between different polarization channels as the variation in

contrast can lead to smooth transitions, where the other channel 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 of belonging to this measurement.

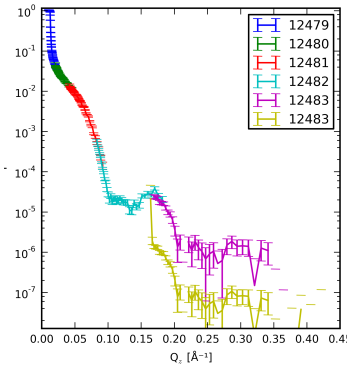
3.3.5 Step 5: Refine the dataset scaling and cutting

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 move the mouse **cursor on top of the curve** you want to scale and **move the mouse wheel**. To remove unwanted point you need to change the values of the **P0** and **PN column** entries as they define the number of points cut from the low- and hight-Q side respectively. If the number of time of flight channels in the histogram dataset is larger than the wavelength window used for the measurement it is possible that large values are needed (<=60) to see changes in the dataset.

As added to reduction list

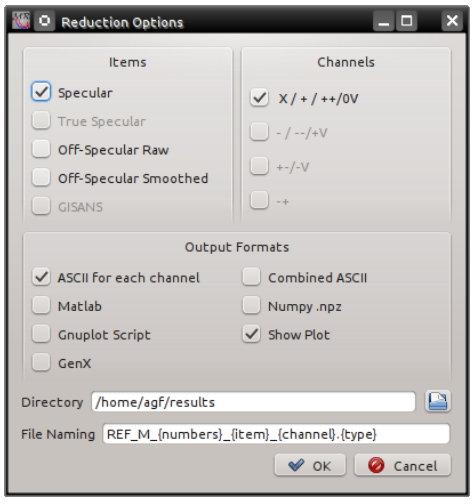


With changed cut points



3.3.6 Step 6: Export your data

Now you are ready to export you reflectivity! Activate the **Reduce... action** from the menu, toolbar or the button below the reduction list. The reduce dialog as several options for the export of the dataset. You can select which reductions should be stored, choose the channels 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 channels, 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.



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 problems to be aware of

4 Advanced Usage

4.1 GUI Customization

4.2 Event mode data

4.3 Re-reduction of already exported data

4.4 Overwrite direct beam parameters

4.5 Advanced background subtraction

4.6 "Fan"-Reflectivity

4.7 Off-specular scattering