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User's Guide for REFoffSpec Version 1.5.4

September 2011

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Computational Sciences and Engineering Division

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User's Guide for REFoffSpec Version 1.5.4
September 2011

ABSTRACT

This document is a user's guide for the IDL software **REFoffSpec version 1.5.4** whose purpose is to aggregate for analysis NeXus data files from the magnetism and liquids reflectometer experiments at the Oak Ridge National Laboratory Spallation Neutron Source. The software is used to scale and align multiple data files that constitute a continuous set for an experimental run. The User's Guide for REFoffSepc explains step by step the process using a specific example run. Output screens are provided to orient the user at each step. The guide documents in detail changes made to the original REFoffSpec code during the period November 2009 and January 2011. At the time of the completion of this version of the code it was accessible from the **sns_tools** interface as a beta version.

1. INTRODUCTION

REFoffSpec was designed for data reduction and aggregation of multiple data files for both the magnetism and liquids reflectometer experiments at the Spallation Neutron Source (SNS). The user specifies a set of run numbers comprising an experiment. These runs are analyzed using the parameters obtained from the Data Acquisition System (DAS) combined with a user selected region of a normalization beam(s) dataset which is sent to a remote processing code (refred_lp) which does the data reduction. The code then loads the reduced data files for further analysis. The code automatically aligns the datasets relative to their reflected beam pixel values (called RefPix values). The user then can select a spectral region to scale the datasets relative to a reference dataset (the longest wavelength dataset) and this scaling is applied to scale the two-dimensional data (intensity vs time-of-flight (TOF) and off-specular dimension). The code computes all shifting and scaling analysis for a chosen spin state (for example, Off_Off) and, in the last step, applies these uniformly to the other available spin states (On_Off, Off_On, and On_On). Finally, a plotting utility has been written and integrated into the code to plot reflectivity vs Q and scaled two-dimensional results for all spin states, as selected by the user.

Section 2 of the User's Guide for **REFoffSpec** provides information on how to access the software. The software is available through the **sns_tools** application. The operation of **REFoffSpec** is described in detail in Sect. 3. Each step in using the application is covered using a specific experimental run as example. Finally, details regarding the program, including the definition of parameters used to describe the datasets and the software configuration file, are described in Sect. 4.

2. ACCESS TO REFoffSpec

REFoffSpec is an IDL application that runs on servers or standalone machines with IDL installed. This description of the software will be based on using NX to connect from a desktop to PC to run REFoffSpec

on one of the SNS servers. Before starting launching REFoffSpec, the user should set up a directory structure for the results of the REFoffSpec data reduction. The user should create a directory **results** under the home directory. The data reductions, labeled by the reference run number, the run number for the longest wavelength or lowest Q data set, will appear in this directory.

The primary example used in this tutorial is the set of runs [5387, 5388, and 5389] for the magnetism reflectometer. The first run (5387) is the reference run. So the user should create the directory **5387** under the directory **results**. The structure would then look like (where ~ is user home directory):

>~/results/5387

2.1 LAUNCH sns_tools

To access the REFoffSpec code, go to the command prompt and type: **sns_tools**

The sns_tools application will launch (Fig. 1). Scroll to the bottom and click open **Beta Version** and select **REFoffSpec beta version**. Then click the bar that says: **LAUNCH APPLICATION**

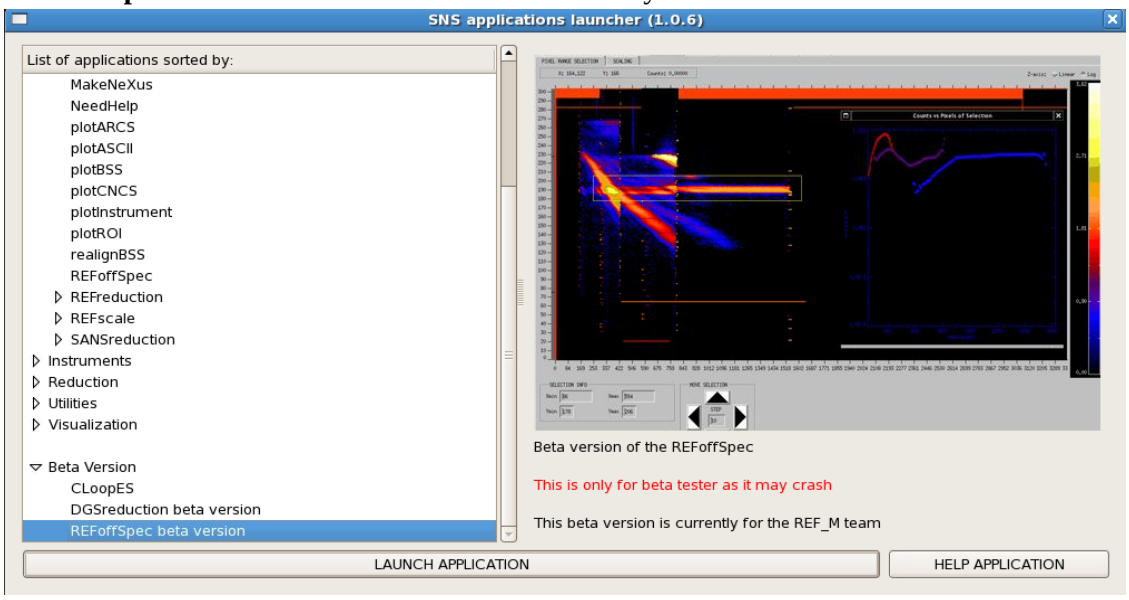


Fig. 1. Initial window of the sns_tools application.

This launches the IDL Virtual Machine. On the splash screen, click Click to Continue to launch REFoffSpec. This will launch the REFoffSpec first screen as shown in Fig. 2a.

2.2. INITIAL SCREEN

The initial screen of the application (see Fig. 2a) captures some important information from the user, including the type of data to be evaluated (REF_L or REF_M) and the screen resolution to choose (large for desktop, smaller for laptop). The laptop resolution is set for typical modern laptop and activates scroll bars for some windows.

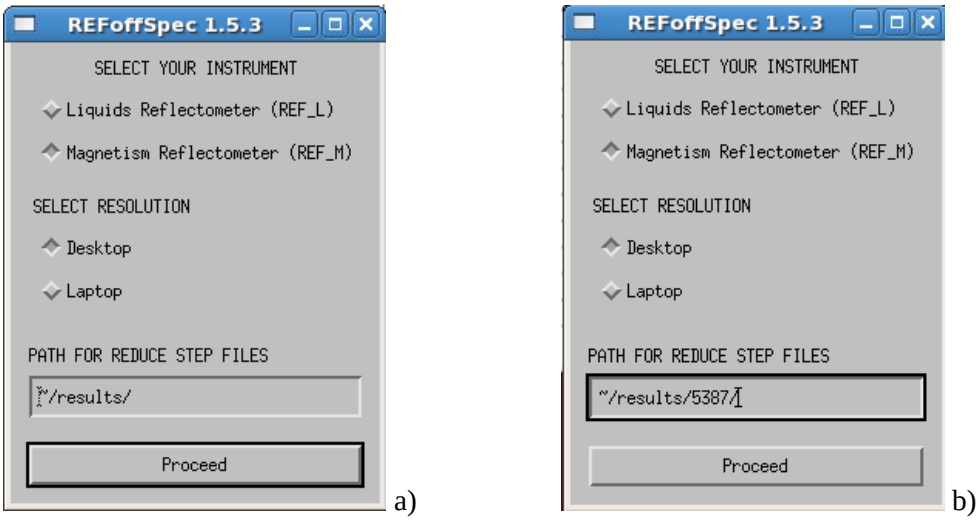


Fig. 2. a) Initial screen of the REFoffSpec application; b) The user enters reference run number 5387.

In addition, it is here that the user specifies the directory for data reduction files. The default value is ~/**results/**. If a subdirectory is desired, and we recommend that, specify it as shown in Fig. 2b. Note that the directory must already exist. All files associated with the data reduction process will go into this subdirectory (in this case **~/results/5387**/), including the ROI files. Note: While the user is presented with the ability to write the ROI files to other locations, we recommend not doing so. After specifying the directory for data reduction files click <Enter> or click Proceed to continue.

3. OPERATION OF REFoffSpec

Once REfoffSpec is launched, the user will see that there are 9 tabs across the top. These tabs, which should be selected in sequence, are: 1) Reduction, 2) Loading, 3) Shifting, 4) Scaling _1D, 5) Scaling_2D, 6) Output, 7) Options, 8) Log_Book and 9) Plot_Utility. The user is cautioned to proceed in numerical sequence of tabs 1-6. Tab 7 (Options) is used to set options prior to running the code. Tab 8 (Log_Book) is a log of the actions of the user while running the code. Tab 9 (Plot Utility) can be used at any time to plot results of the data reduction process. The operation of all of these tabs will be discussed in detail, starting with Tab 1, the Reduction step.

3.1 STEP 1: REDUCTION

The user will automatically enter the first of the three substep screens: REF_DATA. In this substep of **Reduction** for the specific set of runs of interest, the user will enter NeXus data files or browses for existing files with extension nsx on the computer. For magnetism reflectometer (REF_M) datasets, the user also will specify the RefPix values in the first substep. For both liquids and magnetism refelctometer dataset, the user enters normalization data files and selects the ROI of the direct beam for doing the normalization in the second **Reduction** step DIRECT. It is recommended that the user save the ROIs to

the **Reduction** step directory specified on launching the application (see Sect. 2). Finally, in the 3rd reduction step (NORMALIZATION) launches the remote job to execute the data reduction. Files from that process are written to the **Reduction** step directory. As the RefPix values for each Sangle are computed they are written to a file in the **Reduction** step directory. This file is later read during the **Shifting step.**

3.1.1 Step 1: Ref Data

Enter the run numbers (e.g., 5387—5389) in the textbox at the top of the REF_DATA screen (Fig 3) and hit the <Enter> key. These numbers can also be entered in sequence 5387, 5388, 5389. The archive is searched for these runs and the NeXus file names are written to a list. At the bottom of the REF-DATA screen (Fig. 3), select spin states to consider. In this case results will be computed for spin states "Off_Off" and "On_Off", using only the "Off_Off" direct beam data for normalization. The data files used for normalization are entered in the second reduction step. The screen will look as shown in Fig. 4, with the cursor bar highlighting the first data set (5387). User clicks VIEW/EDIT SANGLE to continue.

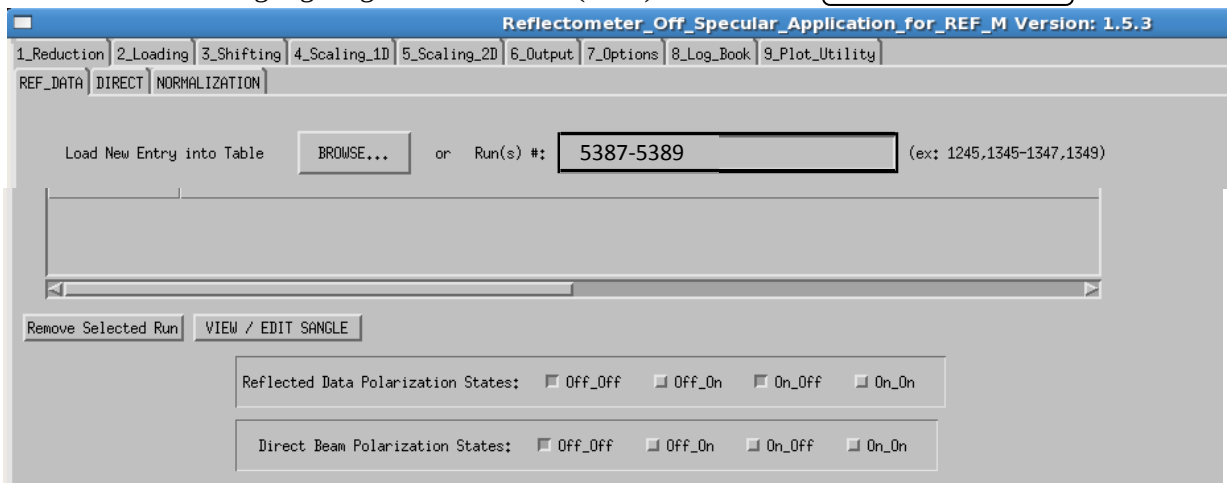


Fig. 3. Initial screen for reduction step with run numbers 5387 through 5389 entered and spin states "OFF_OFF" and "ON_OFF" selected.

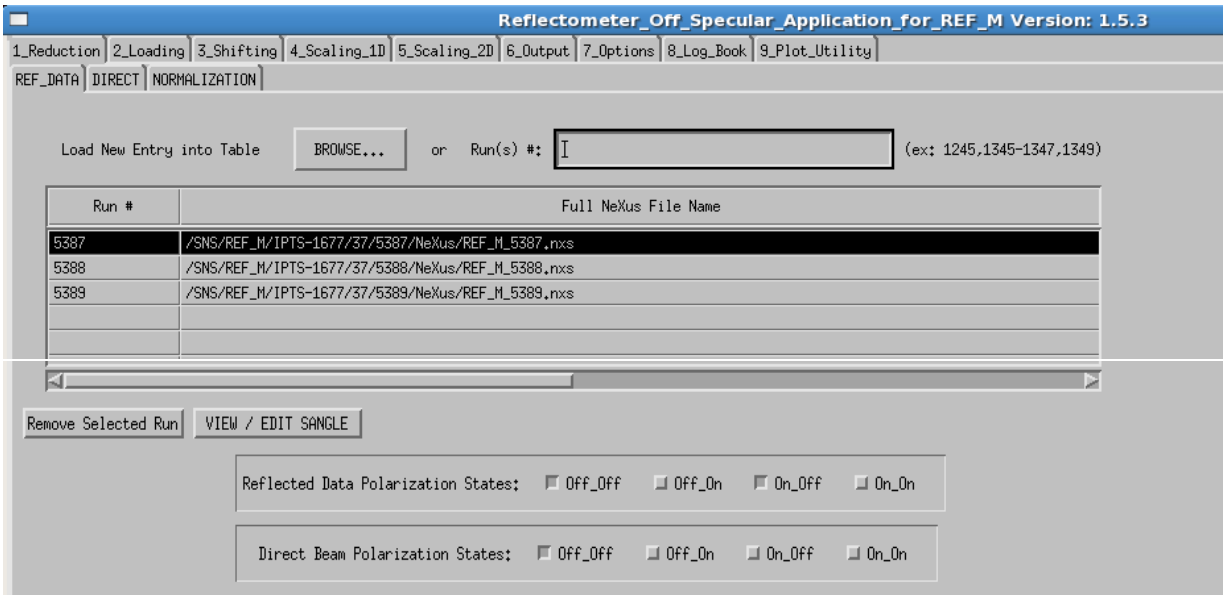


Fig. 4. Initial screen for reduction step with NeXus data files for runs 5387 through 5389 found.

3.1.2 Step 1: Ref Data — Sangle Calculation

In this screen the user can control all of the parameters associated with the experimental run. Most of these are populated from the Data Acquisition System (DAS). These include Dangle (radians), Dangle0 (radians), sample to detector distance, SDdist(m), and the sample angle, Sangle (radians). The direct beam pixel location (referred to as DirPix) also comes from the DAS. See Sect. 4.1 for detail on these parameters.

To perform the calculation of the scattering angle, the user will need to specify the reflected beam pixel location (referred to as RefPix) using the cursor. Place the cursor in the center of the reflected beam and click on the left mouse button (Fig.5). This establishes the RefPix value, drawing a *red* line through the center of the specular region of the reflected beam and simultaneously draws a red line through the correct RefPix pixel value in the "Counts vs pixel" plot in the lower left corner. The RefPix value can also be entered in the text box in the lower part of the right panel (blue arrow). The screen will then show an **asterisk** next to the selected run number in the upper left corner. To alter the RefPix value in the text box, the user must remove this **asterisk** by clicking Reset SANGLE flag of selected run number in the middle of the left-hand panel.

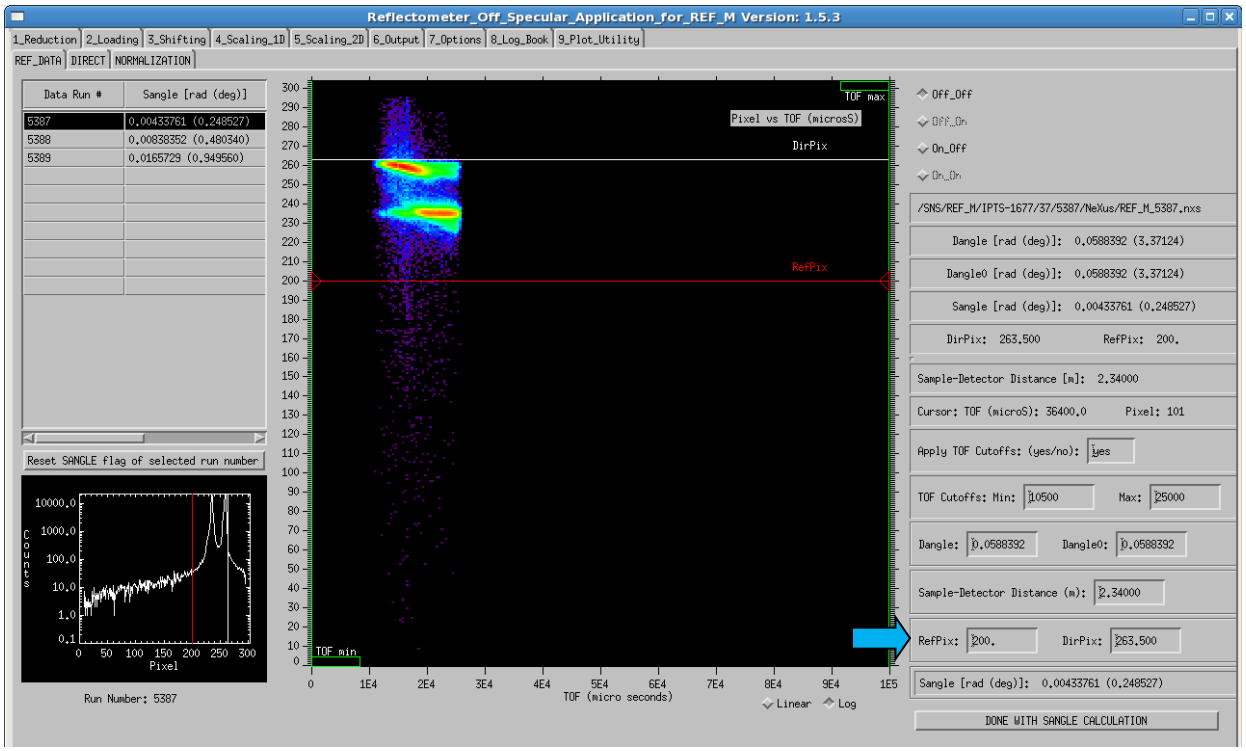


Fig. 5. The Sangle screen showing the first set of data, that for run 5387.

The user can also enter Time-of-Flight (TOF) min and max cutoff values which will strip spurious data points on either side of each dataset. To do so the value "yes" must appear in the field "Apply TOF Cuttoffs" and values must be entered for the min and max. Default values are specified in the configuration file (see Sect. 4) as shown in the screen above (Fig. 5). Before setting the RefPix value for the first (reference) dataset, the user can remove the TOF cutoffs by setting the "Apply TOF Cutoffs" entry to "no" or the user can change the value of the cutoff. These settings are retained for all other datasets.

Note that the value of Sangle in radians and degrees is shown for the first data set in the list provided at the upper left corner. An **asterisk** is placed next to this value after the user has completed this step. If the user is satisfied with the value of RefPix for the first dataset, they should click on the second entry in this list (run 5388 in this example) and the results of the second dataset will be displayed. To establish the RefPix value of the second dataset, click on the center of the spectral region of the reflected curve or type the value in the RefPix text box. Proceed likewise for the third data set (run 5389).

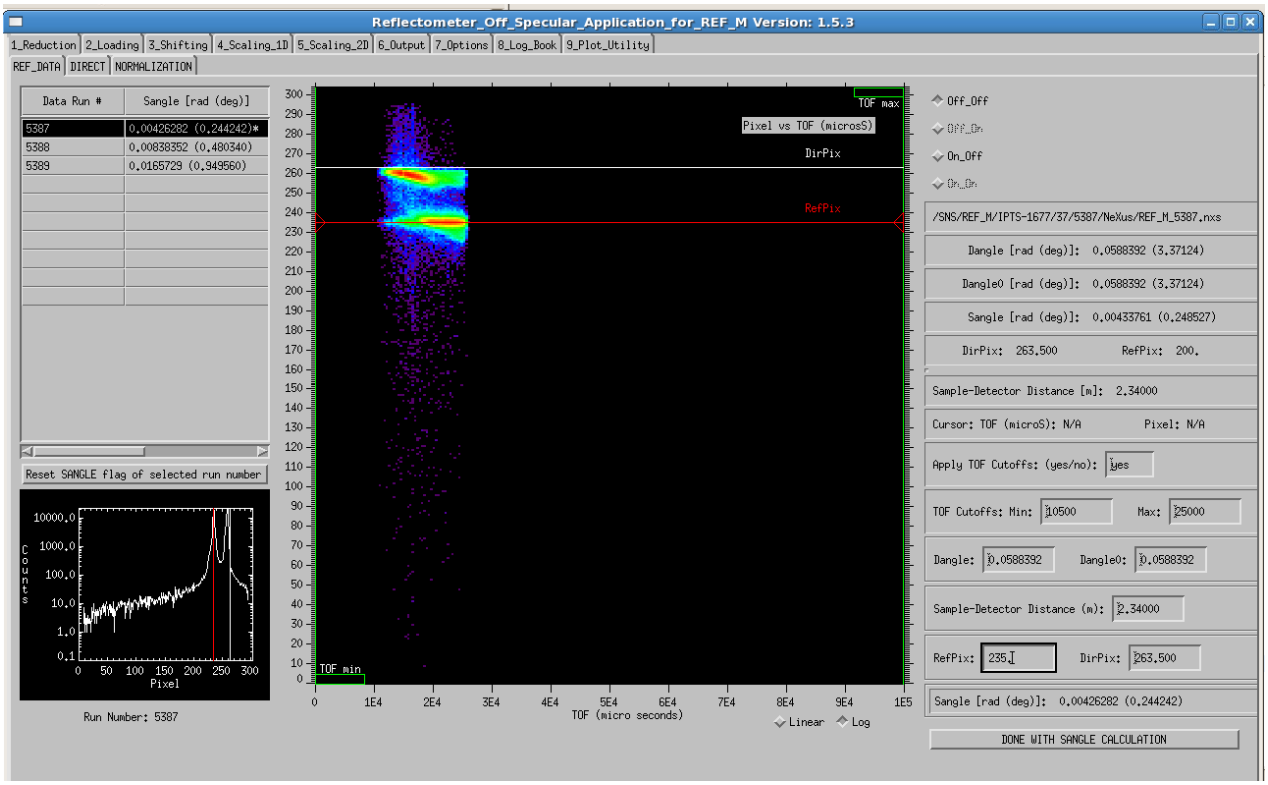


Fig. 6. Using the mouse, click on the screen to set the RefPix value (in pixels) for run 5387.

The screen will then show an **asterisk** next to each of the run numbers in the upper left corner, at which point the user is done with this step and clicks the button DONE WITH SANGLE CALCULATION in the lower right corner (Fig. 6).

3.1.3 Step 1: Direct

The user is then returned to the first screen (Fig. 4) and should select the "DIRECT" tab. In this step, the user selects the region of interest (ROI) of the direct beam (or beams) to use for normalization. In this case, a different direct normalization beam (5392—5394) is used for each reflected beam dataset (5392—5394). The user enters the run numbers in the screen (Fig. 7) followed by the <Enter> key. On the next screen (Fig. 8), when a separate normalization beam is used for each of the reflected data sets, the user should select these in the lower right corner. Then user should click Create/Modify? Visualize ROI File for each direct beam data. If the same direct beam is used to normalize all the datasets, the user only needs to do this once.

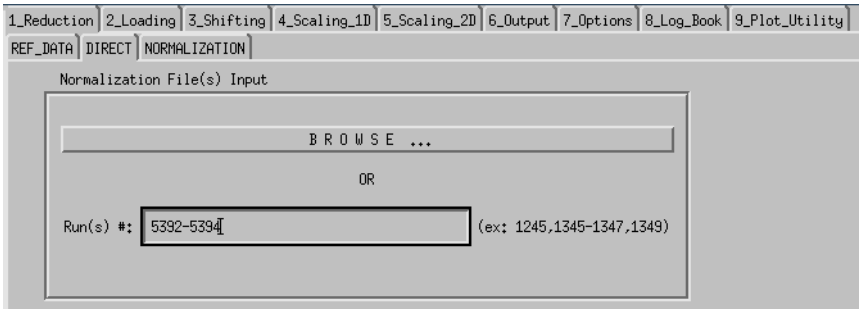


Fig. 7. Input screen for entering the direct beam run number(s).

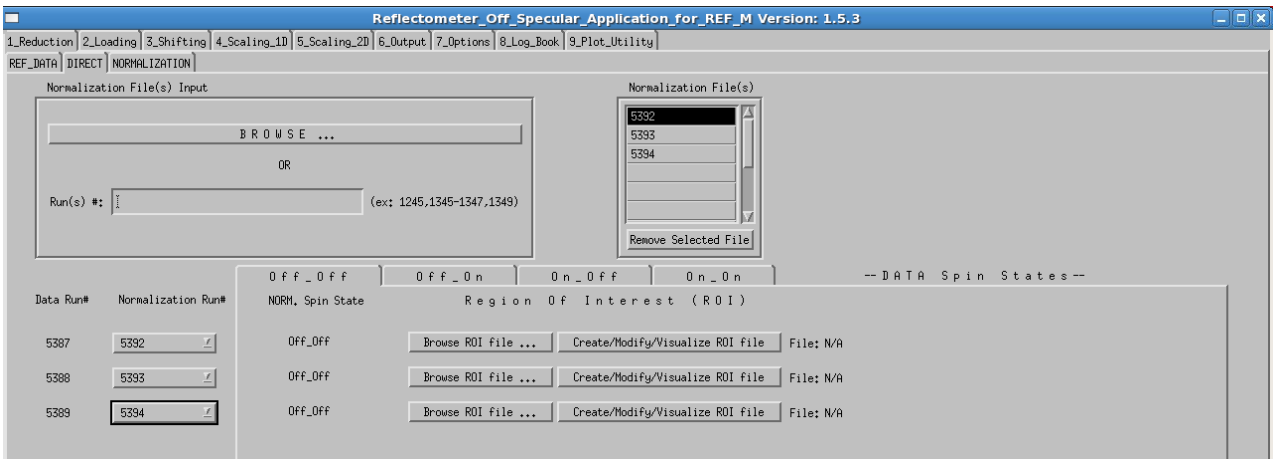


Fig. 8. Screen for entering the direct beam ROI associated with each of the reflected beams. A different normalization beam is used for each reflected beam. Select these using the pull downs (lower left).

After making this selection, the direct beam dataset (5392), which is used to normalize the 5387 dataset, is displayed. The user clicks on the upper pixel value for ROI with the left mouse. The user then clicks the right mouse button and selects the lower ROI value by clicking the left mouse button again. A screen will appear (see Fig. 9) showing the ROI selected. The user should then select SAVE ROI and RETURN TO TABLE is possible to change the location of the ROI file, it is NOT recommended. The user should click the button SAVE ROI as shown in Fig. 10.

The user should proceed as described for the two remaining direct beam data sets. The user does not need to select the ROI using the mouse if the same ROI is desired for each of the remaining datasets; simply click the button SAVE ROI and RETURN TO TABLE for each followed by clicking the SAVE ROI button. This creates ROI files in the REDUCE directory for each of the three direct beam data sets.

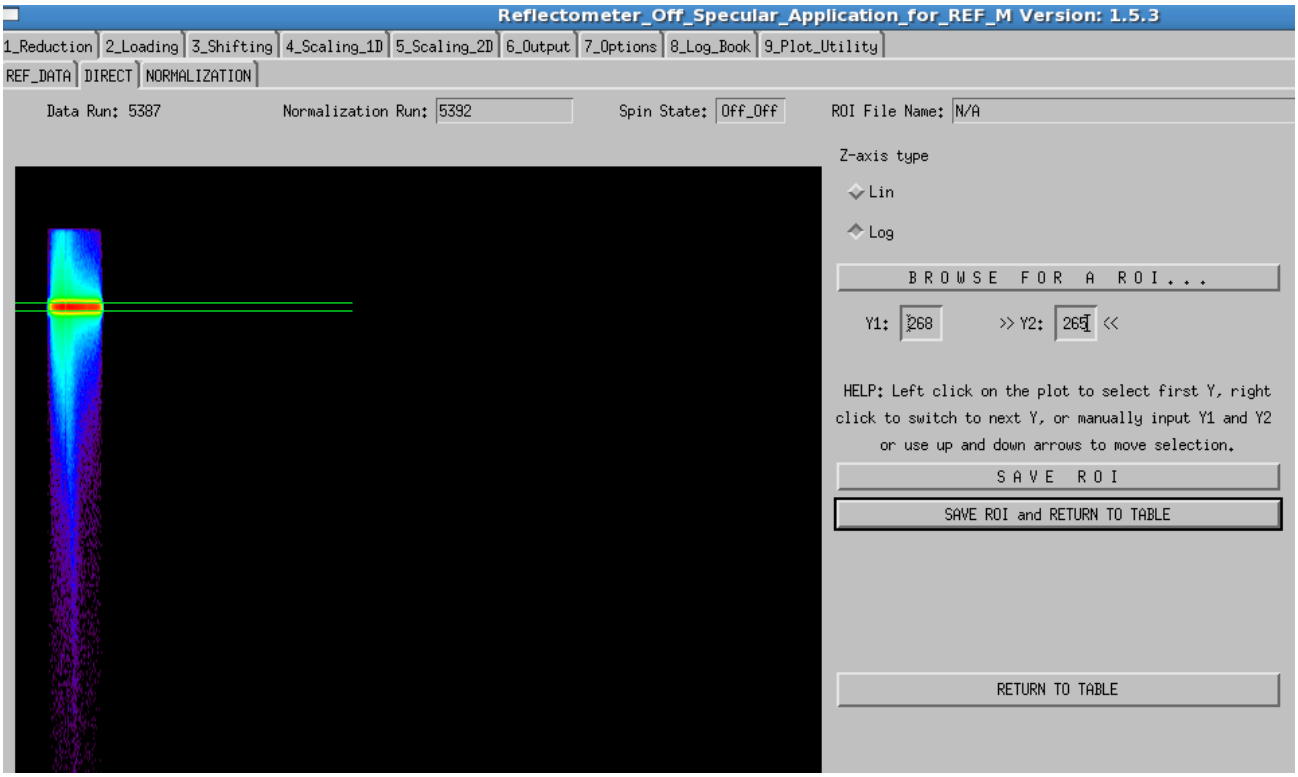


Fig. 9. Screen showing the selection of the ROI for the direct beam 5392 that determines the intensity used to normalize the reflected beam result for 5387.

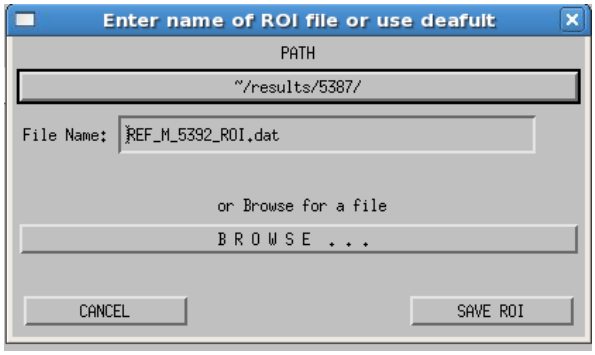


Fig. 10. Screen for saving the ROI for direct beam 5392.

3.1.4 Step 1: Normalization

The user should then click on the "NORMALIZATION" tab on the main screen (Fig. 4). The user will then see a screen (Fig. 11) that lists the reflected beam datasets, the direct beam (NORM) data sets, and the ROI files (with extension dat). In this third step of the data reduction process, the files are passed via a script to the program **refred_lp**, which does the data reduction. Each set of data is run as a separate process on remote machine specified in the configuration file. To launch these remote jobs, the user should click **RUN JOBS and PLOT** at the bottom of the screen (Fig. 11).

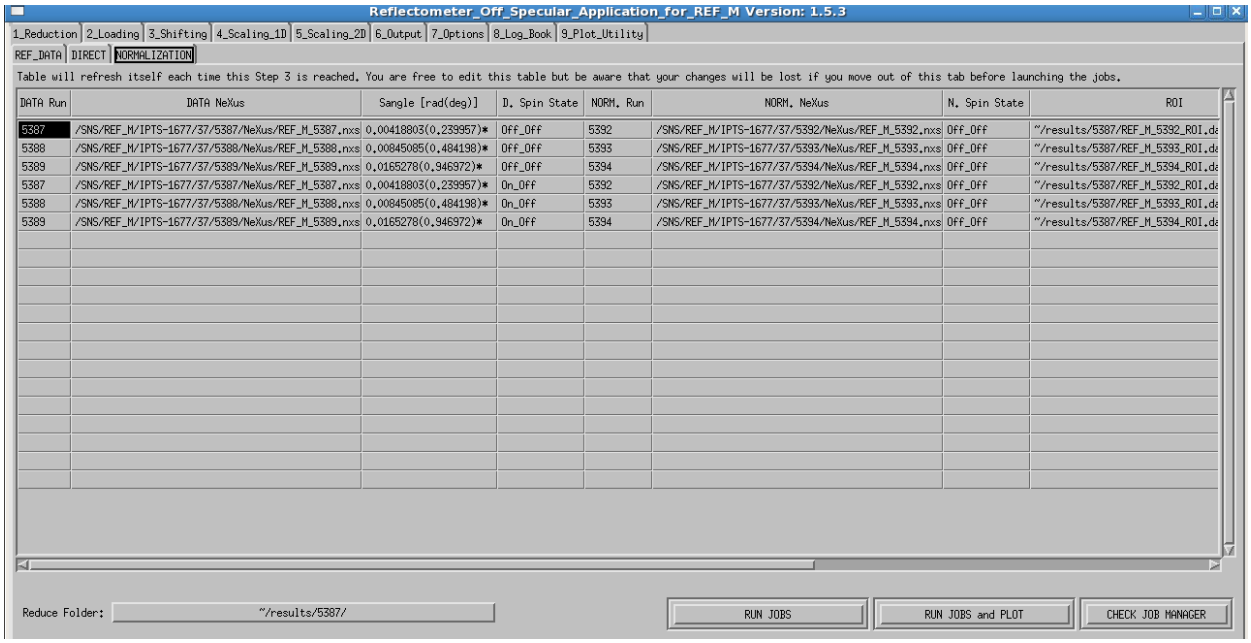


Fig. 11. Screen shows a table of the reflected data to be reduced, the normalization data, and the ROI files for each data set to be processed.

In the terminal window where **sns_tools** was launched, the user will see the command strings for each of the remote jobs. For example, for run 5387 and normalization run 5392 the command string is:

```
================================================================================
cmd:
sbatch -p heater refred_lp --inst=REF_M  /SNS/REF_M/IPTS-
1677/37/5387/NeXus/REF_M_5387.nxs --data-path=/entry-Off_Off/bank1,1 --
omega=0.00418803,0.0,units=radians --norm=/SNS/REF_M/IPTS-
1677/37/5392/NeXus/REF_M_5392.nxs --norm-data-paths=/entry-Off_Off/bank1,1 --
norm-roi-file=~/results/5387/REF_M_5392_ROI.dat --tof-cut-min=10500 --tof-
cut-max=25000

remove old output file rm ~/results/5387/REF_M_5387_Off_Off.txt
remove old rmd file rm ~/results/5387/REF_M_5387_Off_Off.rmd
================================================================================
```

Note also that the program tells the user if old versions of the output files and rmd files are deleted to make way for new files. These files are deleted so that REFoffSpec program will wait not just for completion of the remote jobs but also for writing of these output files before proceeding.

The user can continue to analyze the results for either the reduced Off_Off spins data (selected as shown above) or the reduced On_Off spin data (not selected), as specified in the succeeding window (Fig. 12a). On selecting the default of "Off_Off", the user sees the next window (Fig. 12b).

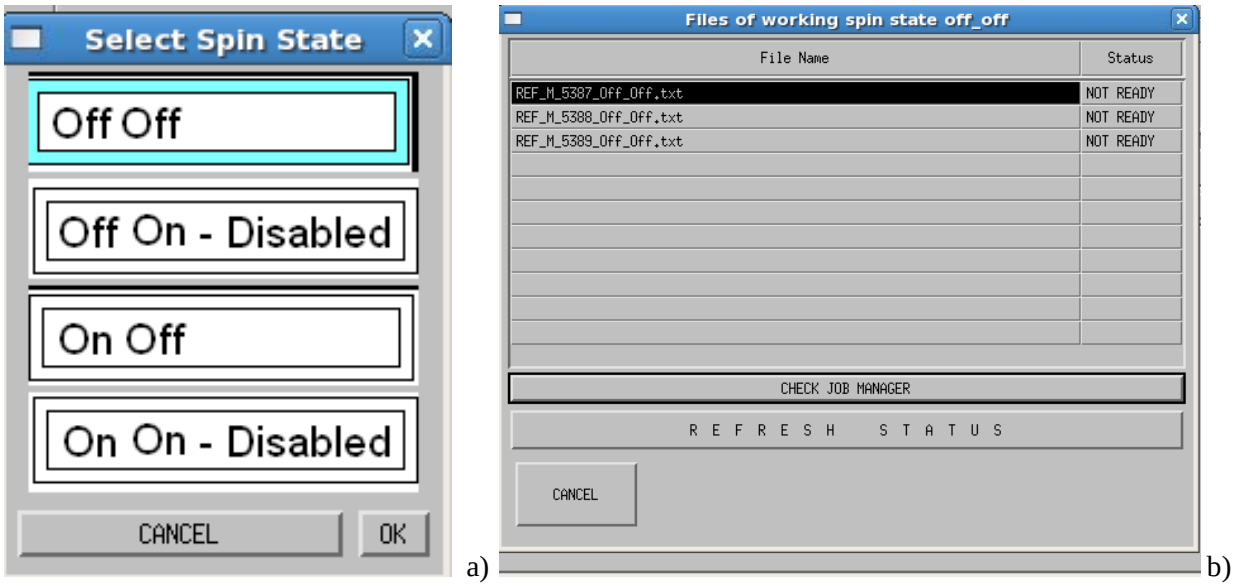


Fig. 12. a) Screen for selecting the spin state to be processed (in this case "Off_Off"); b) Screen showing the reduced data sets to be created by the remote data reduction step.

The user can check the status of the remote calculations two ways. The status can be checked by continually clicking the REFRESH STATUS button. The user can also launch the Job Manager, which launches the "Job Status Page" from the nuetronsr.us web page. The URL for this web page is: https://neutronsr.us/applications/jobmonitor/squeue.php?view=all.

When the remote program has completed AND the reduced files have been written to the users select area (in this case **~/results/5378/),** then the user will see the button as shown in the next figure. Upon clicking the REFRESH STATUS , the user will see the MOVE ON TO THE NEXT STEP button if the remote reduction step is complete. On clicking this button , the user is led to the second step of the application, the **LOADING step**, in which all reduced datasets are displayed on the same plot.

3.2. STEP 2: LOADING

This step displays all the reduced data files on the same screen. If the user has started at the Reduction step (Step 1), then one is automatically led to this step. If the reduce files are already created and stored in the **Reduction** step directory, one can start at this step. In that case, click the BROWSE ASCII button and select the reduced data files (those with extension **txt**) to analyze. For example, in this case the user might select the Off_Off spins state results as shown in Fig. 13., resulting in display shown in Fig. 14.

There is no action required by the user on the **Loading** step. The user should simply proceed on to the next step by clicking the **Shifting** tab on the top bar of the screen**.**

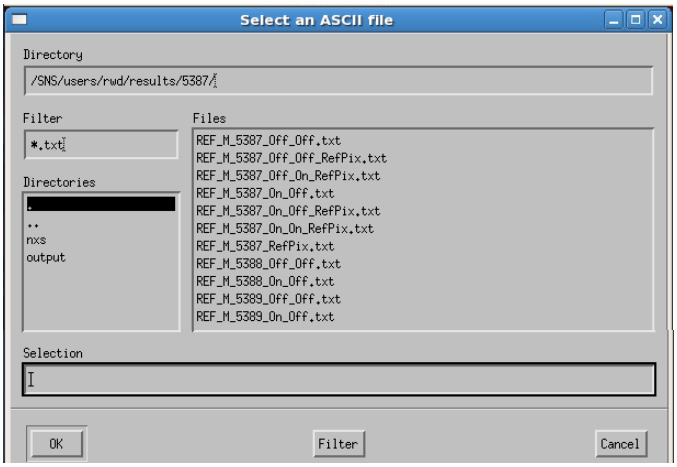


Fig. 13. Screen for selecting a set of reduced (ASCII) data files for processing. This screen appears when the user enters REFoffSpec at the Loading step.

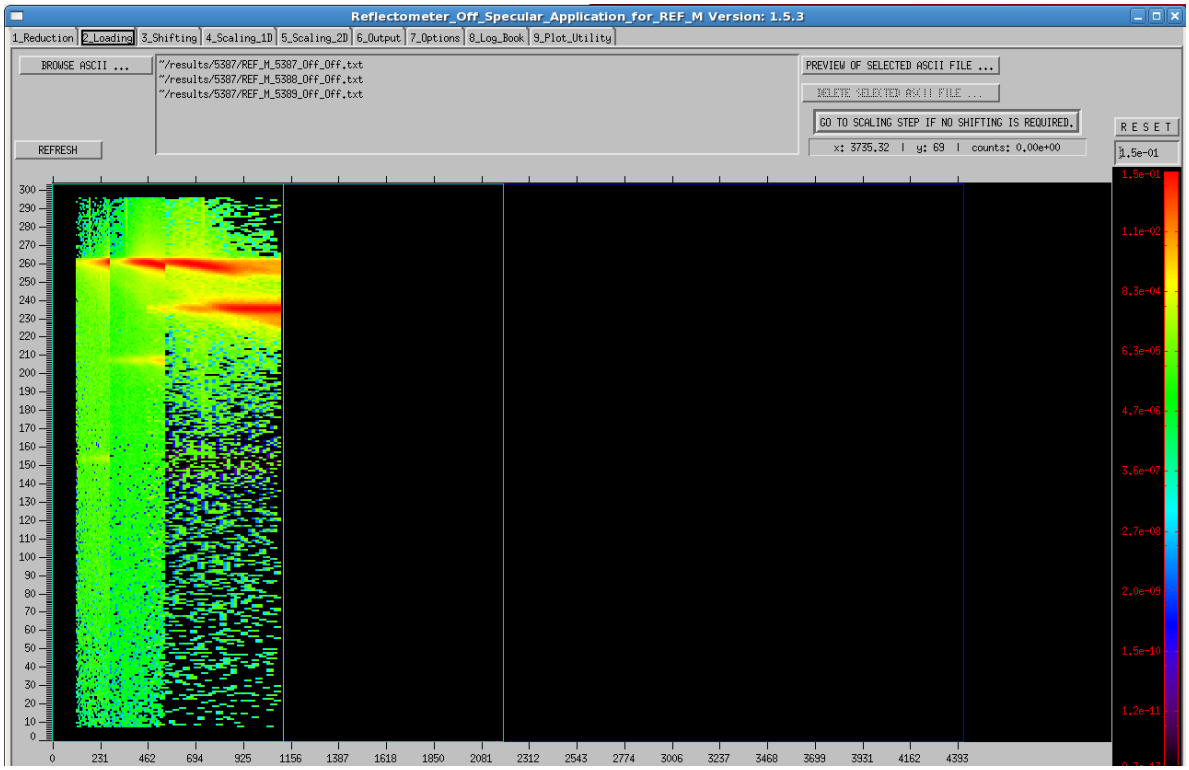


Fig. 14. The reduced datasets 5387—5389 are loaded during the Loading step. This screen automatically appears if the user arrives here from the Reduction step.

3.3 STEP 3: SHIFTING (Magnetism Reflectometer Only)

In the **Shifting** step, the RefPix values for each dataset will be used to shift the data so that the spectral line of the reflected is aligned. This step is needed only for datasets obtained from the magnetism reflectometer instrument. If the user is evaluating datasets from the liquids reflectometer instrument, this step can be skipped. In that case, the user can go directly to step 4: **Scaling_1D**. Since we are evaluating magnetism reflectometer data (runs 5387—5389), we continue on with the **Shifting** step. Since the

RefPix values are saved in a file, they will automatically be displayed here for the data considered as shown in Fig. 15 below.

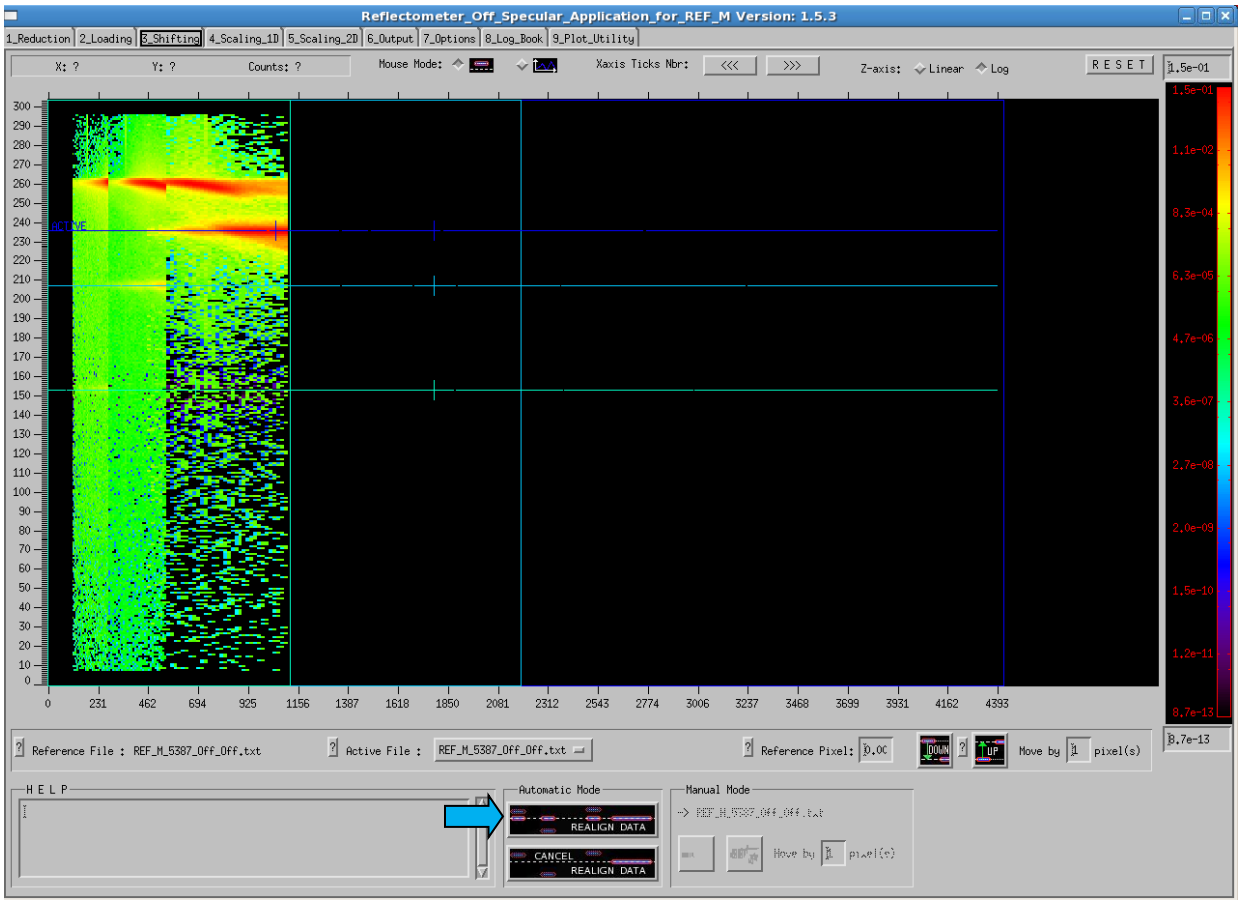


Fig. 15. Screen for Shifting step displays the datasets with the RefPix values indicated by horizontal colored lines through the spectral peaks.

The user clicks the Realign Data button (blue arrow) at the bottom of the screen. This aligns all the RefPix values together, aligning the specular peaks for each of the dataset (see Fig. 16.)

The user can manually alter the RefPix values for each dataset by the following procedure. First select the dataset by selecting the "Active File." The RefPix value is specified by either 1) using the mouse and clicking on the location on the screen, 2) entering the value in the text box adjacent to the label "Reference pixel," or 3) using the Move Up or Move Down buttons by the specified number of pixels. If the 3rd approach us used, the user MUST click in the text box displaying the RefPix value for that to properly register and be saved in the RefPix output file. After setting all the values manually the user must click the Realign Data button to complete the alignment. The adjustments in the RefPix values will be stored in the RefPix.txt file so that they can be properly recalled at the Loading step.

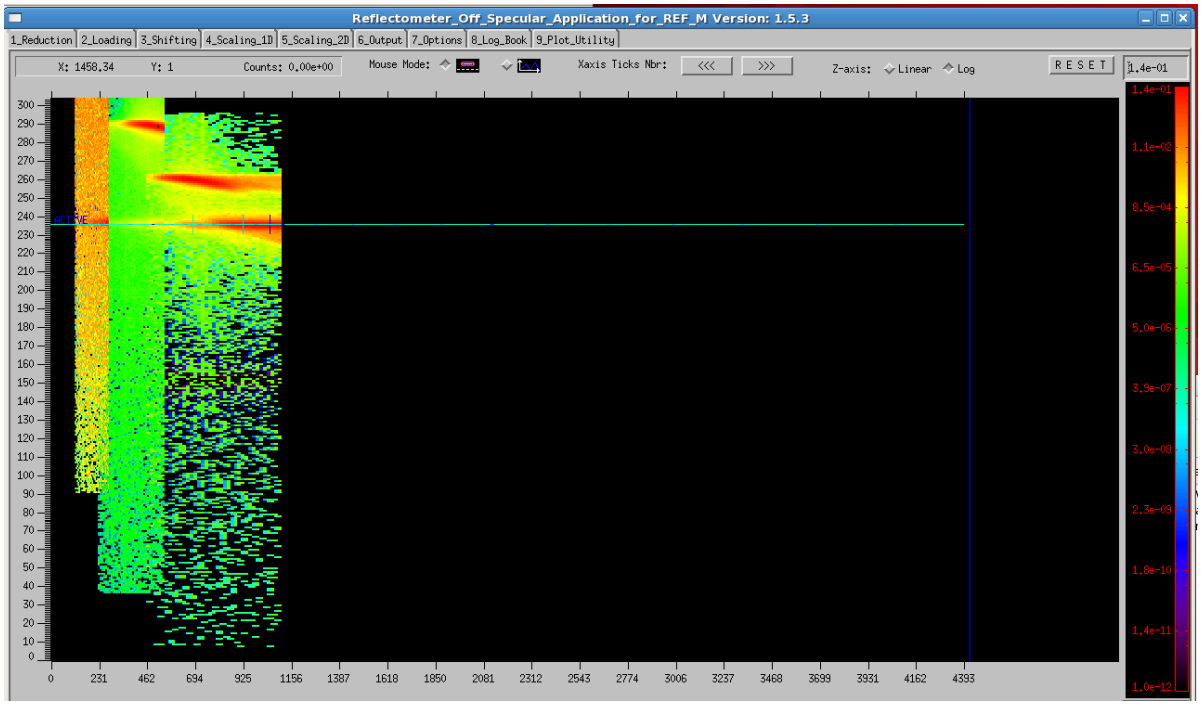


Fig. 16. The 5387—5389 datasets are aligned using RefPix values saved from the Reduction step.

3.4 STEP 4: SCALING 1D

In this step the results are scaled across all datasets using a selection of pixels about the RefPix value. This step consists of two steps: 1) selection of the pixel range and 2) scaling the dataset.

3.4.1 Step 4: Pixel Range Selection

After aligning the datasets, the user selects the **Scaling_1D** tab at the top of the screen. On the screen, the mouse is used to draw a horizontal window across the spectral potion of the data (Fig. 17). After the window is drawn, the user should refine the ymin and ymax (see bottom right corner of the screen) so that difference is 3 – 4 pixels centered on the spectral peak by entering values into the text boxes. For the example datasets (5387—5389), the optimum vertical window size is [234:236]. Enter these values in the text boxes and, while still in one of the text boxes, press the enter button. The application will then redraw the selection window as show in Fig. 17. In the process of drawing the window selection, a plot of the unscaled datasets is made in a separate window (Fig. 18). Each set of data is drawn with a different color symbol. The user proceeds to the second step in the **Scaling_1D** step, **SCALING**, where the reduced data is scaled using the values of the data in the pixel range selected in this first step.

3.4.2 Step 4: Scaling

The **SCALING** step of Step 4 consists of three steps: a) **ALL FILES**, b) **CRITICAL EDGE** and c) **SCALING OTHER FILES**. Selecting **ALL FILES** shows all the datasets prior to scaling. In the **CRITICAL EDGE (CE)** step, the user selects the range of the data at the critical edge of the reference dataset and scales that to 1. In the **SCALING OTHER FILES** step, the user scales the remaining files to the reference dataset.

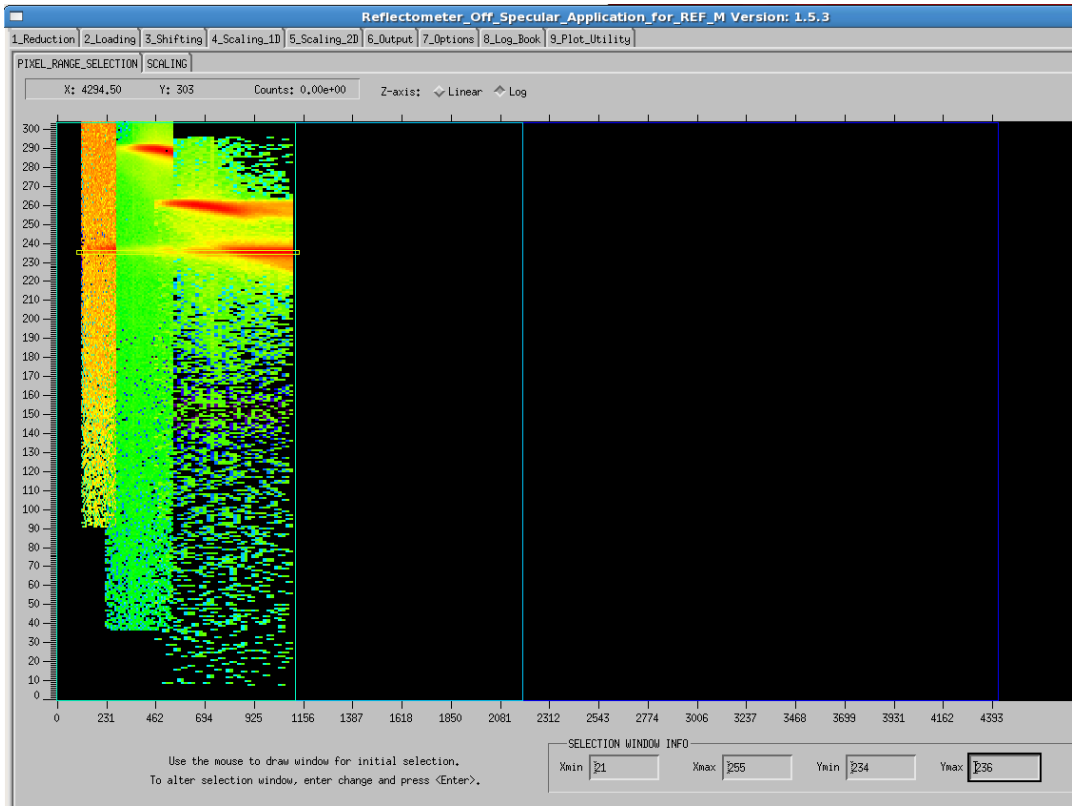


Fig. 17. Selection window is drawn across the specular peak, completely encompassing that region in the wavelength range. The text boxes at the bottom of the screen are used to refine ymin/ymax values for this example to [234:236].

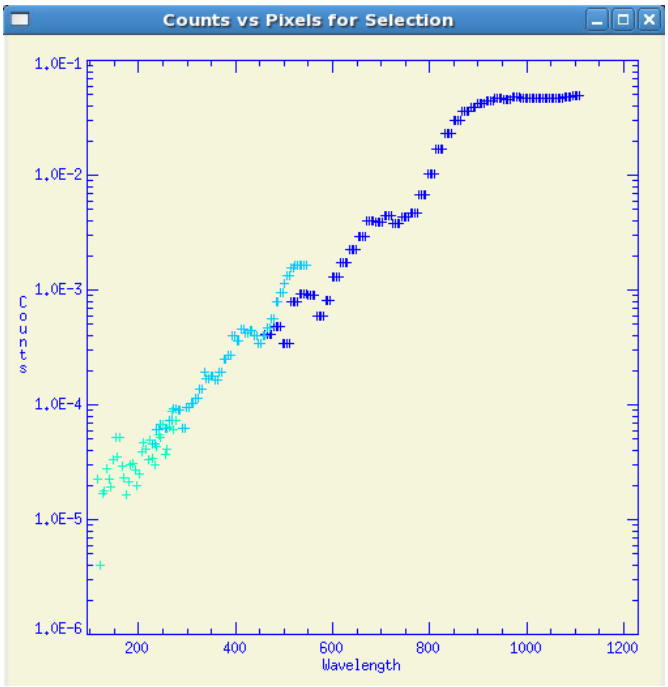


Fig. 18. Plot of the unscaled data for each of the datasets (runs 5387—5389) displayed as counts vs λ perpendicular (Å).

Figure 19 is a screen shot of the **ALL FILES** step showing all the datasets prior to scaling. The user should proceed to clicking the tab **CRITICAL EDGE**, which will show just the reference of lowest Q data set (Fig. 20**). The user the selects the region for scaling the CE, this region will be scaled to** unity (Fig. 21). The selection region is chosen by first placing the cursor on one edge of the region and clicking on the LEFT mouse button, then clicking the RIGHT mouse button to reset, and then placing the cursor on the other edge of the region and clicking the LEFT mouse button. The dataset is scaled to unity by clicking AUTOMATIC FITTING and RESCALING. Alternatively, the user can manually scale the dataset by entering a scaling factor in the text box and clicking the button Manual Scaling of CE.

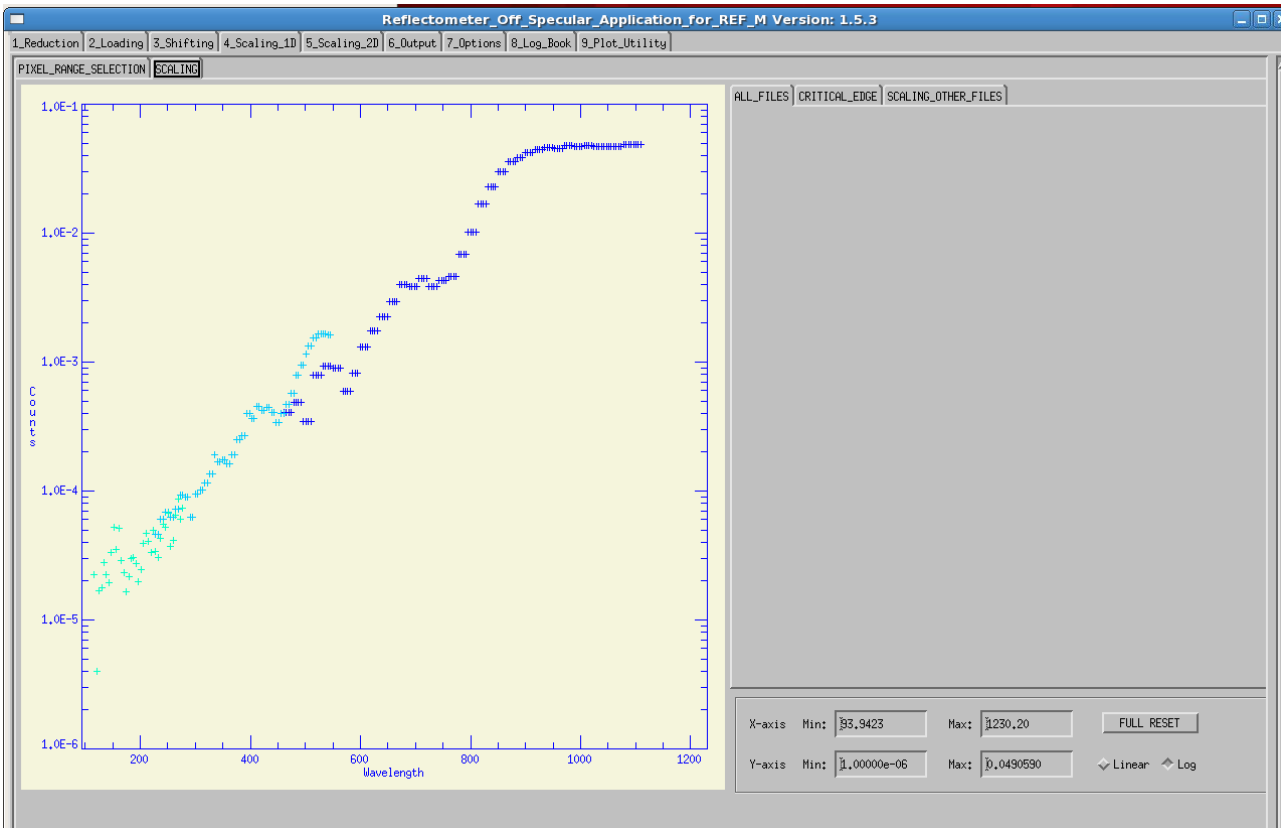


Fig. 19. The ALL FILES tab of the Scaling_1D step shows all datasets prior to scaling.

The user then selects the tab **SCALING OTHER FILES** and the screen shows the remaining datasets as well as the scaled reference dataset (Fig. 22). By clicking AUTOMATIC RESCALING the user can automatically scale these datasets to the reference dataset (Fig. 23).

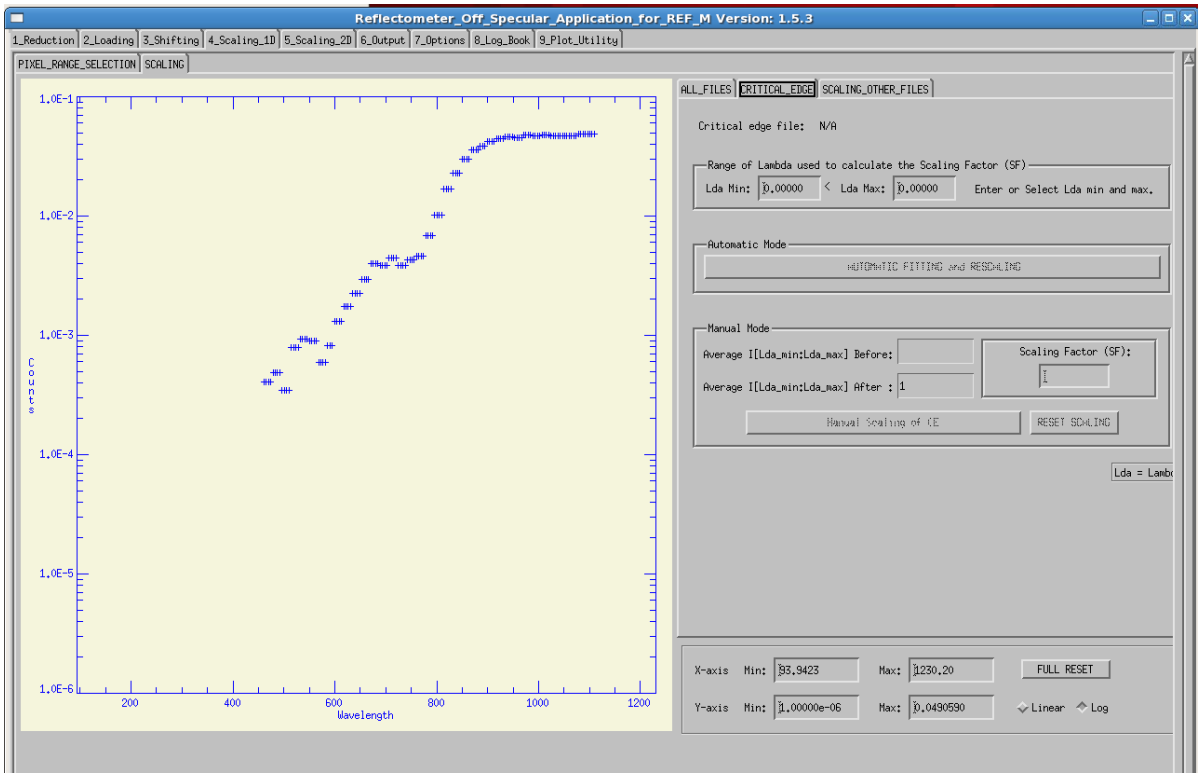


Fig. 20. The CRITICAL EDGE tab of the Scaling_1D step shows the longest wavelength dataset (lowest Q) prior to scaling.

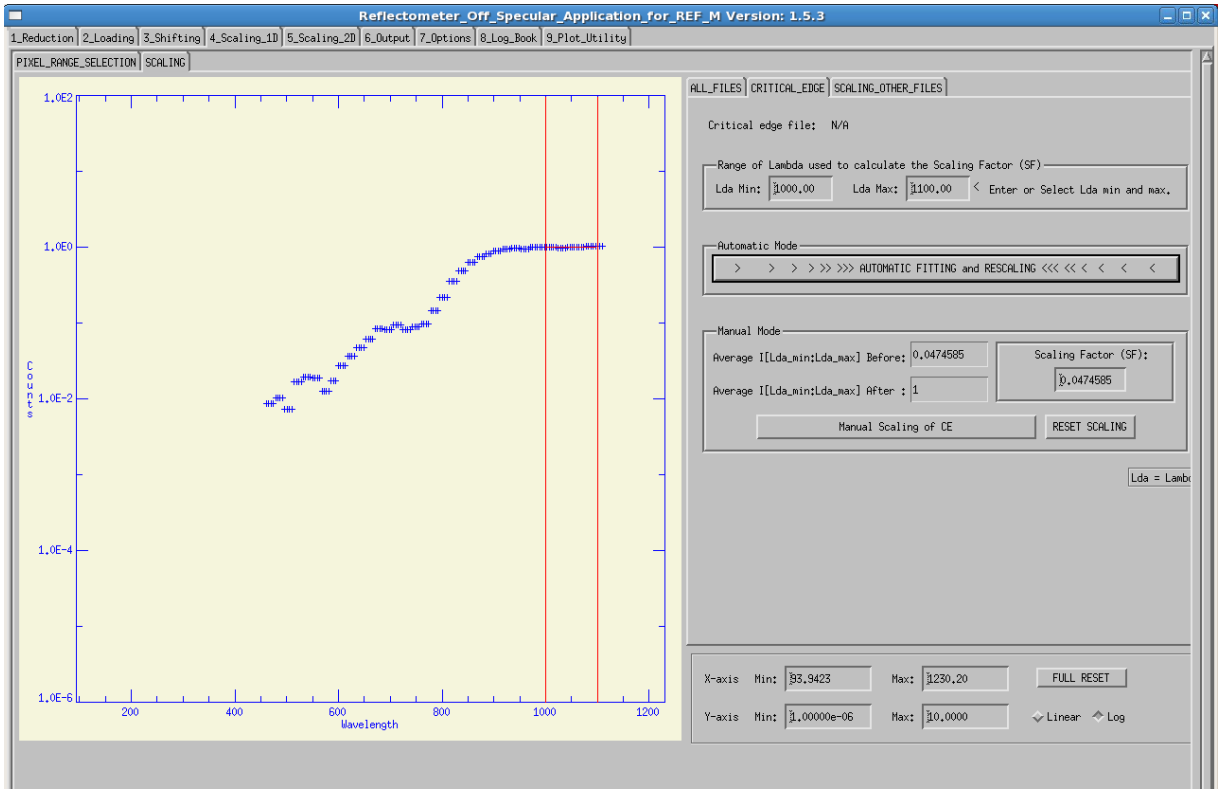


Fig. 21. The CRITICAL EDGE (CE) tab of the Scaling_1D step shows the region of the CE selected to be scaled to unity.

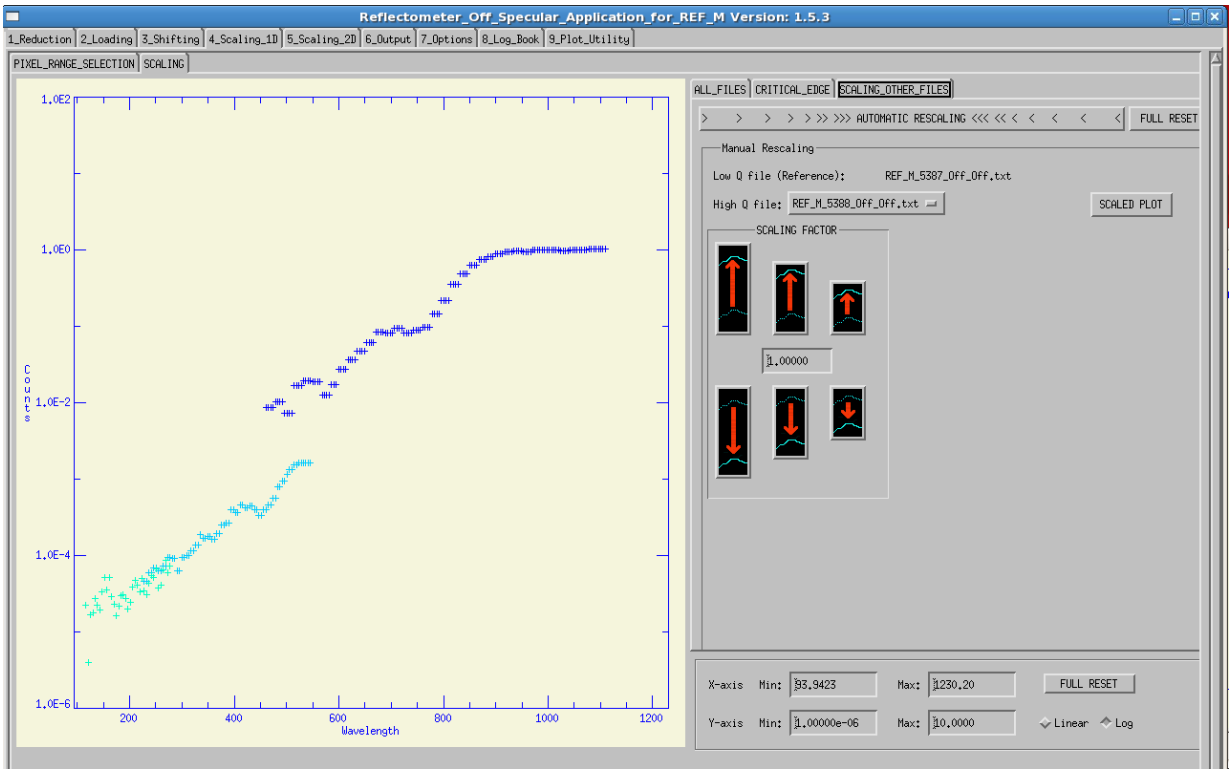


Fig. 22. The SCALING OTHER FILES of Scaling_1D step shows all datasets prior to scaling.

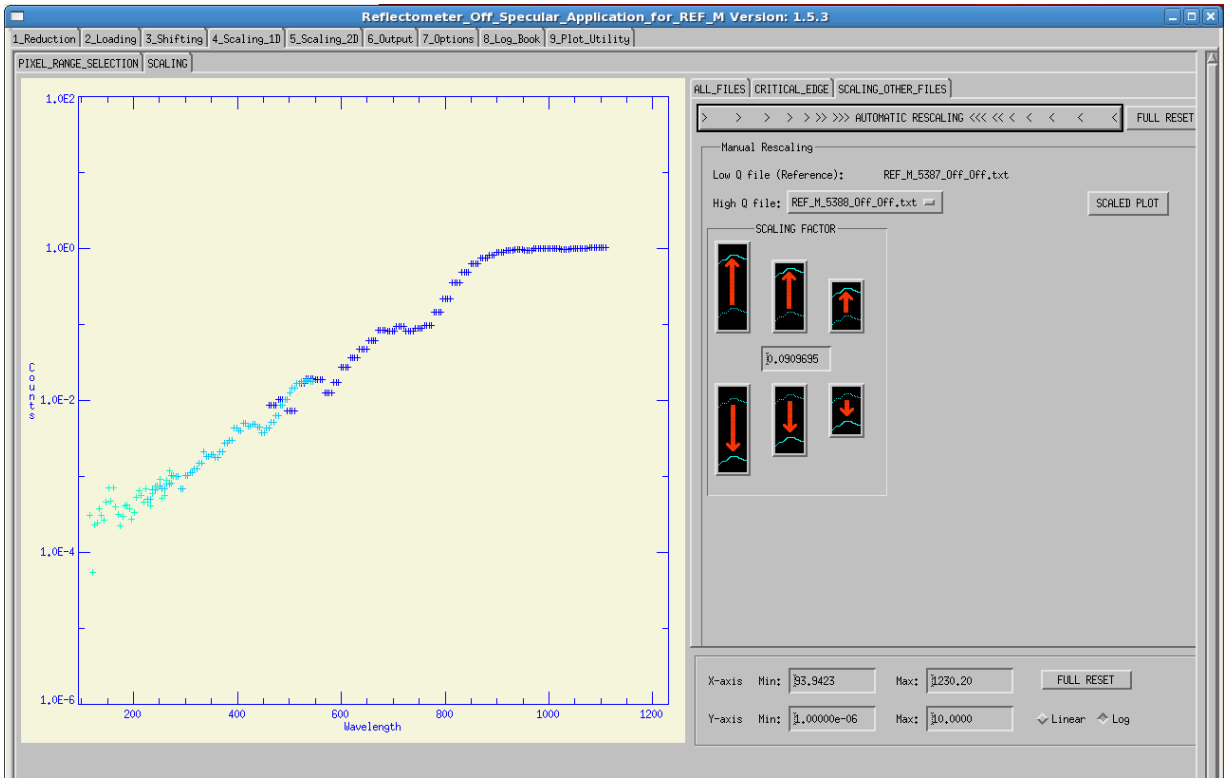
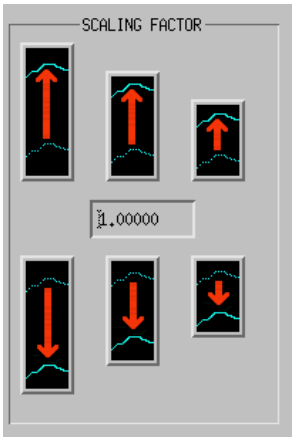


Fig. 23. Screen showing datasets after choosing automatic scaling.

The other datasets can be **manually** scaled to the reference data set by selecting the data set (High Q file) and the using the arrows in the middle of the panel to adjust the curve up or down as described in Fig. 24.



Large arrow: Scale (divide) curve by factor of 0.2

Medium arrow: Scale (divide) curve by factor of 0.5

Small arrow: Scale (divide) curve by factor of 0.6667

Large arrow: Scale (divide) curve by factor of 5

Medium arrow: Scale (divide) curve by factor of 2

Small arrow: Scale (divide) curve by factor of 1.5

Fig. 24. Buttons used to control manual scaling of datasets.

After scaling the other files to the reference data set, the user can click the button labeled Scaled Plot to produce a plot of the scaled datasets in a separate window for comparison later to the reflectivity plots created later in the next step (Step 5).

3.5 STEP 5: SCALING 2D

On proceeding to this step, the user will see the scaled 2D data (Fig. 25). The selection window chosen in the previous step is redisplayed on the plot. It is highly recommend that one NOT alter this selection window. Altering this window will affect the scaling of the results.

The user selects either to plot the Reflectivity (intensity) versus Q($Å^{-1}$) or λ perpendicular(Å). When one of those options is selected, a button appears at the bottom which allows the user to select an output (working) directory. It is recommended that the user do so. This directory MUST also already exist. So prior to the launching REFoffSpec or before reaching Step 5, the user should create this subdirectory. For example, in the case of the dataset: [5387, 5388, 5389], an example working directory would be **~/results/5387/output**.

Prior to generating the plots the user should select the manner in which the data will be spliced. There are two choices: higher Q datasets override lower Q datasets (default) or maximum value in the two datasets is taken. This option is selected in the upper right corner of the screen (outlined in this image by a red box) near the RESET button (see Fig. 25). In this example, the default is taken, as this tends to produce better results, since higher Q data tends to have better resolution.

The scaled 2D data is plotted in counts versus λ perpendicular. The box that was used in Step 4 (Scaling_1D) appears automatically. The user is advised to use this box, but the height and width of the box can be changed by entering values into the text boxes below the plot. Results will be most consistent if this selection window is not altered.

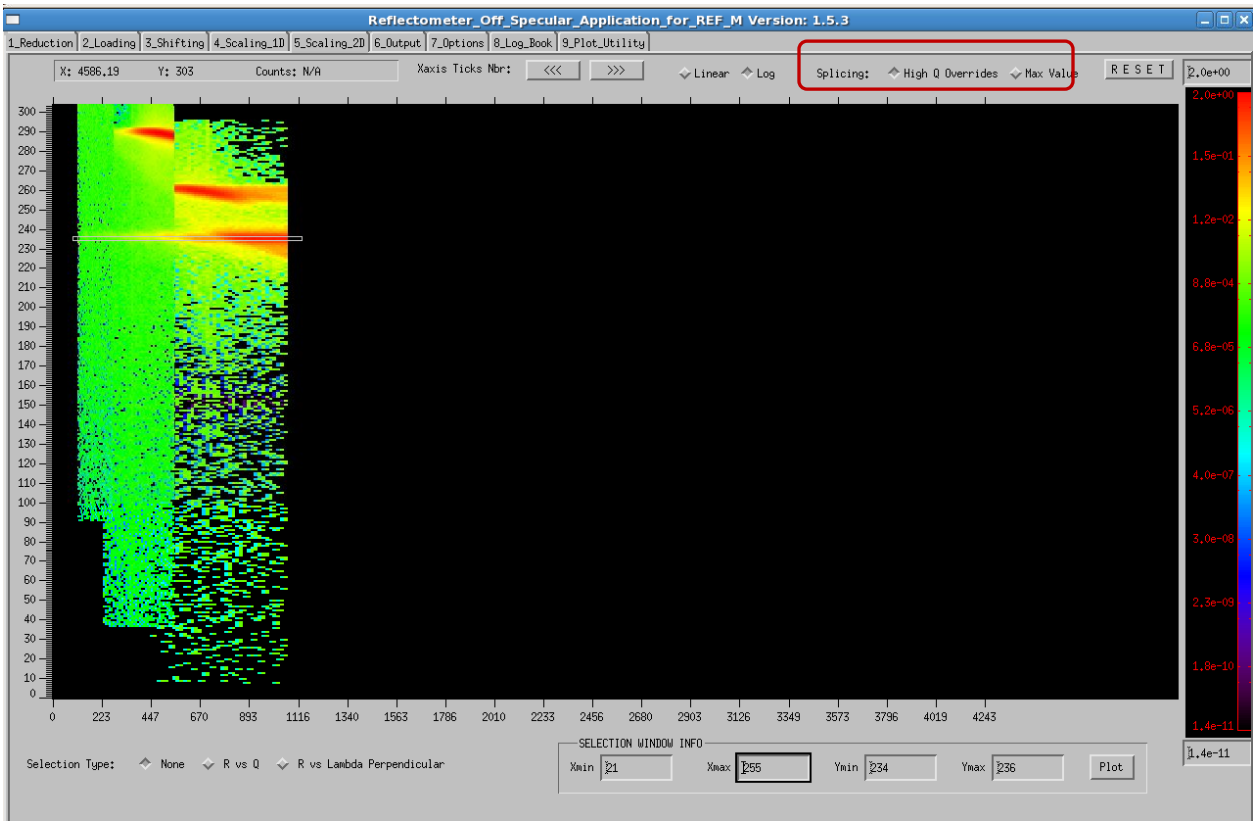


Fig. 25. Scaled 2D results for the three datasets 5387—5389. The selection window chosen in the Scaling_1D step (Step 4) is automatically displayed on entering this step.

Now the user can plot and save the reflectivity data to the chosen output directory. The user can plot either Reflectivity(R) vs either λ perpendicular or Q($Å^{-1}$). Figure 26 shows the results for R vs λ perpendicular. This plot can be compared to the "SCALED PLOT" produced in Step 4. The user should return to the previous screen by clicking the button Select New Data Range the upper left corner.

On the screen shown in Fig. 25 the user should then select the radio button "R vs Q" in the lower left corner and click Plot. The user will then see the plot of reflectivity vs Q as shown in Fig. 27.

After selecting to plot R vs Q, the user should now select a working directory for saving the results. Click on the path bar (which shows **~/results/5387/** in Fig. 26), and select a working directory, e.g**. output**. This directory must be created before running REFoffSpec or, at least, before reaching this point in the program. It is recommended that this directory be different than the one used for the Reduce directory (where RefPix, ROI, and ASCII data files are saved). In addition to a directory in the user's area, a SHARE directory could be used. The resulting output directory (**~/results/5387/output**) appears in the path bar (see Fig. 27 and details in Fig. 28). The user should then click the button Save R vs Q to save the results to the output directory. Note that if reflectivity data are to be saved for the other spin states (e.g., On_Off, etc.) in the Output Step (i.e., Step 6), then data must be saved for the working spin state (e.g., Off_Off) in this step.

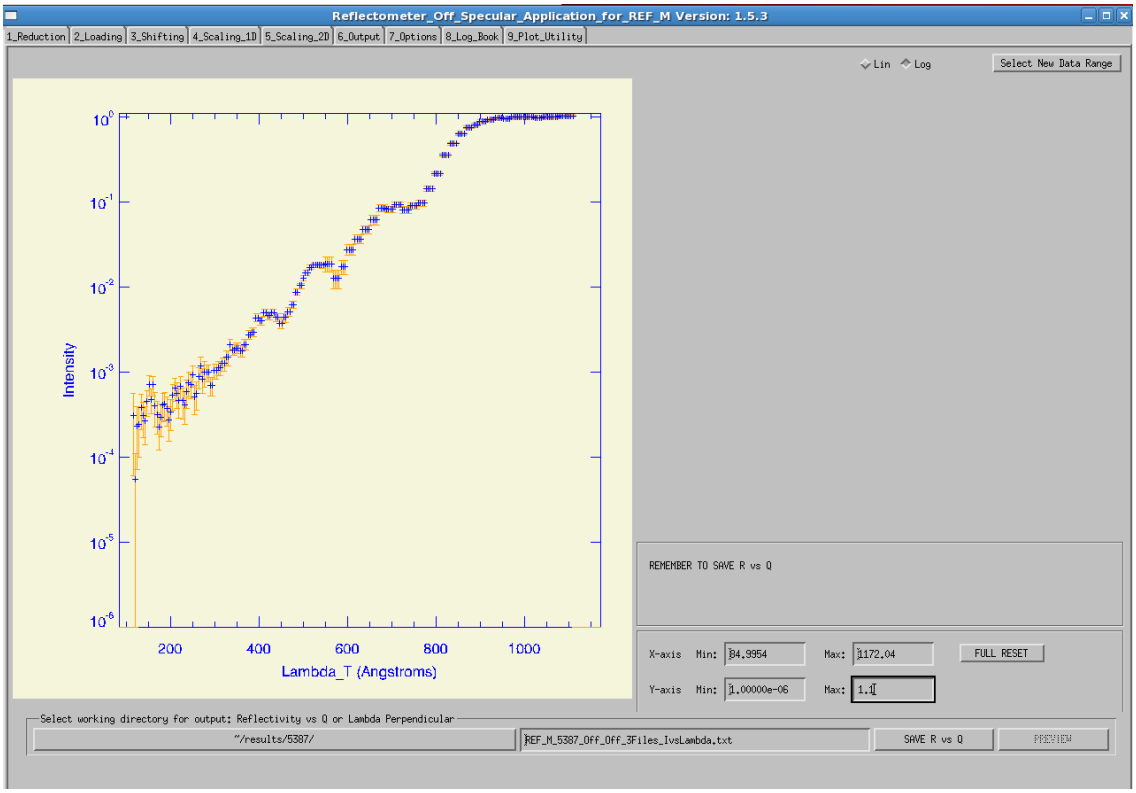


Fig. 26. Reflectivity vs λ perpendicular as plotted in the Scaling_2D step.

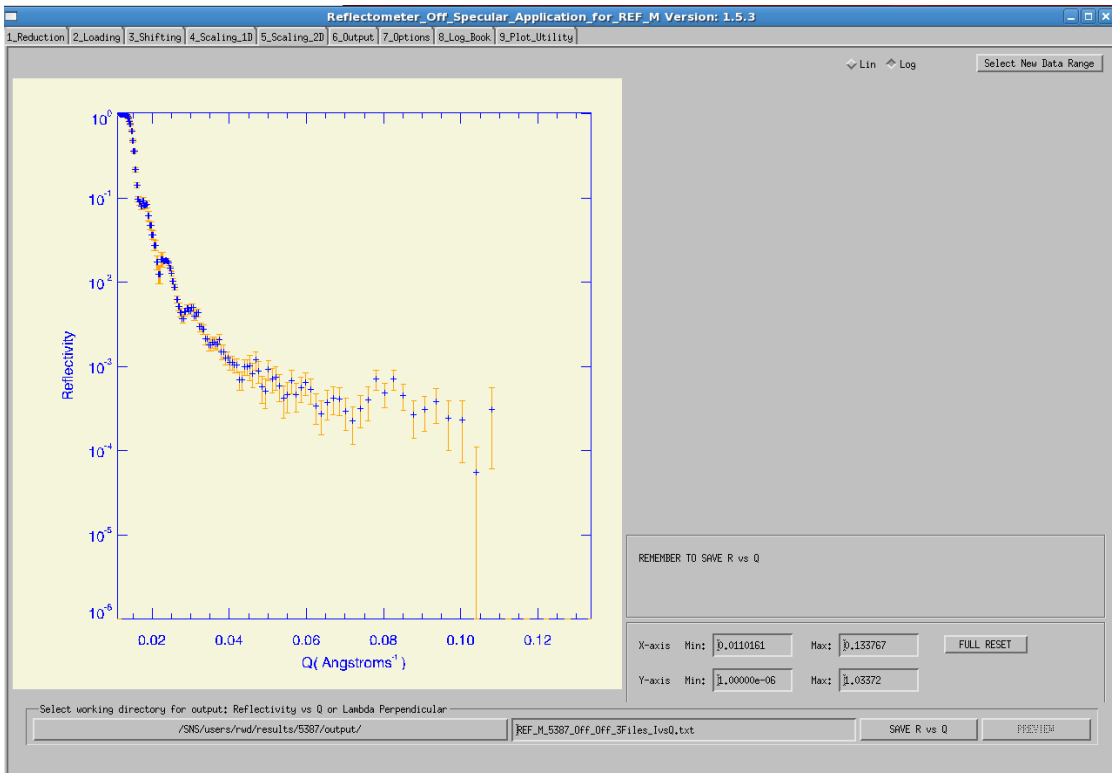


Fig. 27. Reflectivity vs Q (Å $^{-1}$) as plotted in the Scaling_2D step.

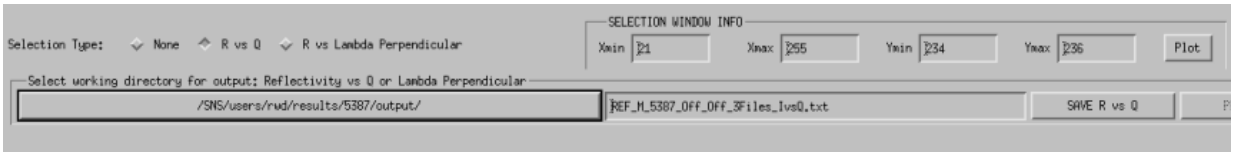


Fig. 28. Detail of selecting output directory for Reflectivity vs Q and Scaled 2D results.

3.6 STEP 6: OUTPUT

In Step 6, the application automatically computes the shifting, scaling and stitching of the specular data for the other spin states and applies that to scaling the 2D data. This step (see Fig. 29) uses the same output directory for writing the scaled 2D data for all spin states including that computed in Step 5. The user can change the directory, if desired, but we do not recommend this. The user should exclude spin states for which there is no input data, by clicking the **Exclude** check box at the top left corner of each data set listed.

The user then proceeds to click the button CREATE OUTPUT FILE in the middle of the left side panel (see blue arrow). This step will analyze results for each of the remaining spin states, writing all the files to the same directory chosen on Step 5 (Scaling_2D) for writing the reflectivity data (i.e., the working directory). The steps processed are shown in the Status box below that button (see enlarged view of that in Figure 30). If processing is OK that is indicated; if not the user will see "FAILED" and the reason will have to be discerned. One reason might be that the **Exclude** checkbox was not checked when there was no data to be processed for that spin configuration (e.g., Off_On in the case shown). This is not an error however, just a warning to the user that there was no data for this spin case.

3.7 STEP 7: OPTIONS

By selecting this tab the user can set various options prior to running the program. Those options and the default settings are shown in Sect. 4.3 below.

3.8 STEP 8: LOG BOOK

The Log Book keeps a record of the user's selections and code responses during execution. This log can be copied into a file and saved in the directory for the run along with the reduction step files. A future version will automatically write this log as a file in that directory. The Log Book for the example (runs 5387—5389) is shown in Fig. 31.

It is recommended that the user cut and paste the output of the Log Book into a file in the output (working) directory. A future version should provide an option to write the contents of the Log Book to a file in the output directory.

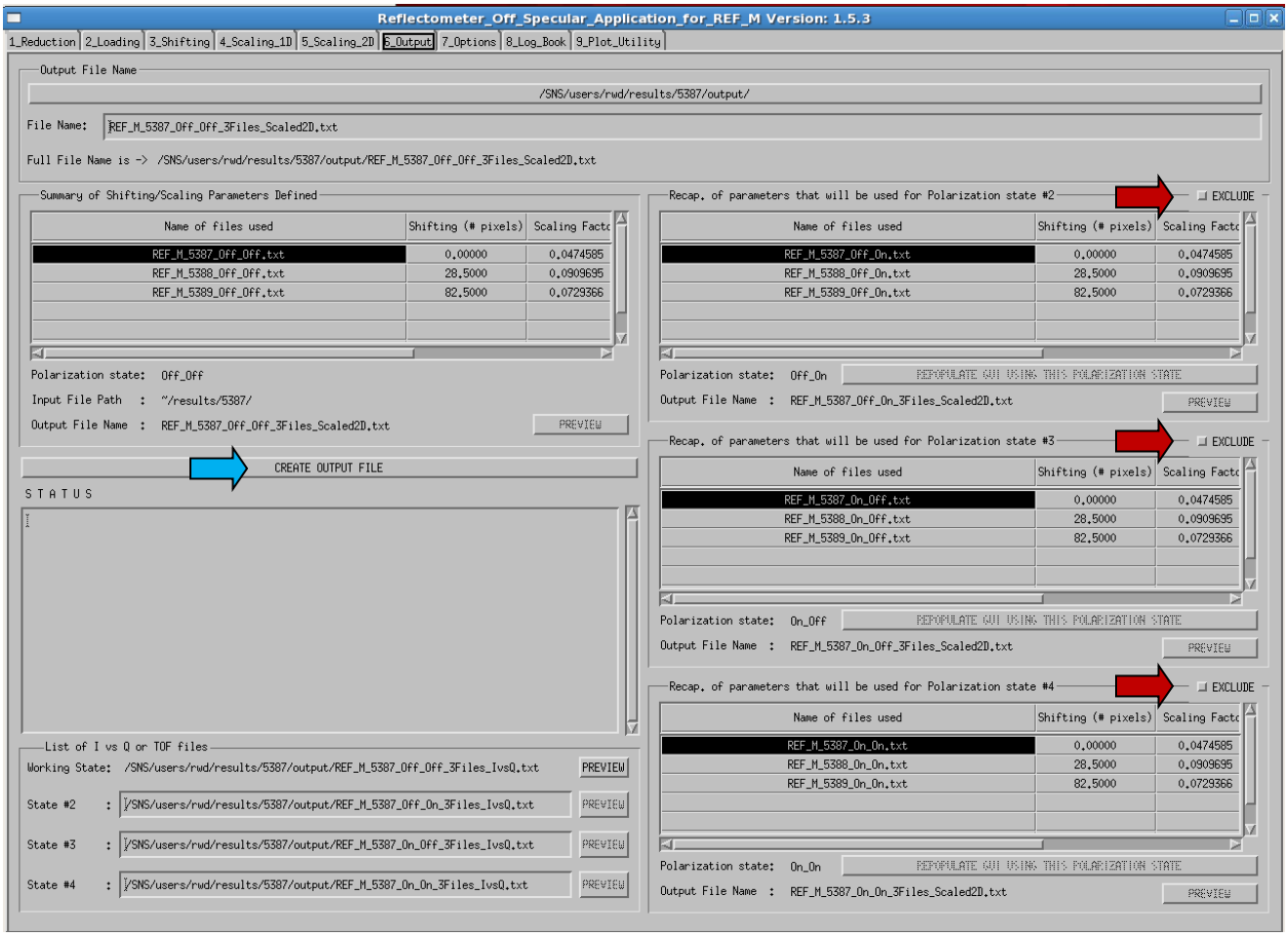


Fig. 29. Output step screen for the 5387—5389 example. Exclude buttons are noted on right using red arrows and the "Create Ouput File" button is noted with a blue arrow.

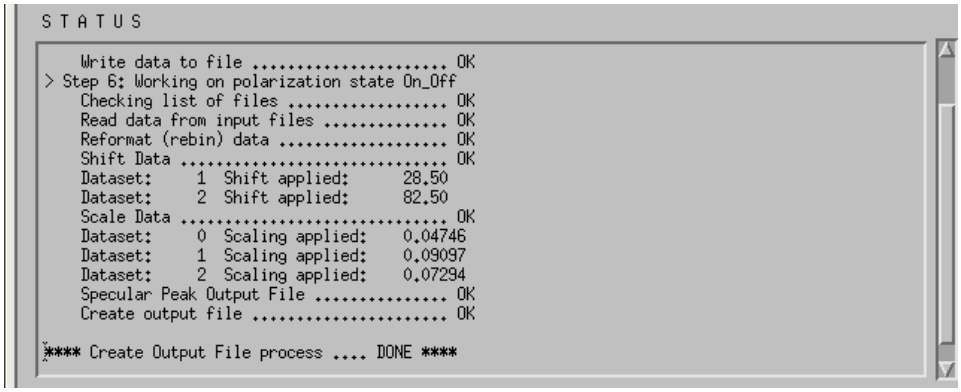


Fig. 30. Portion of the output status box for the 5387—5389 example. The run is complete.

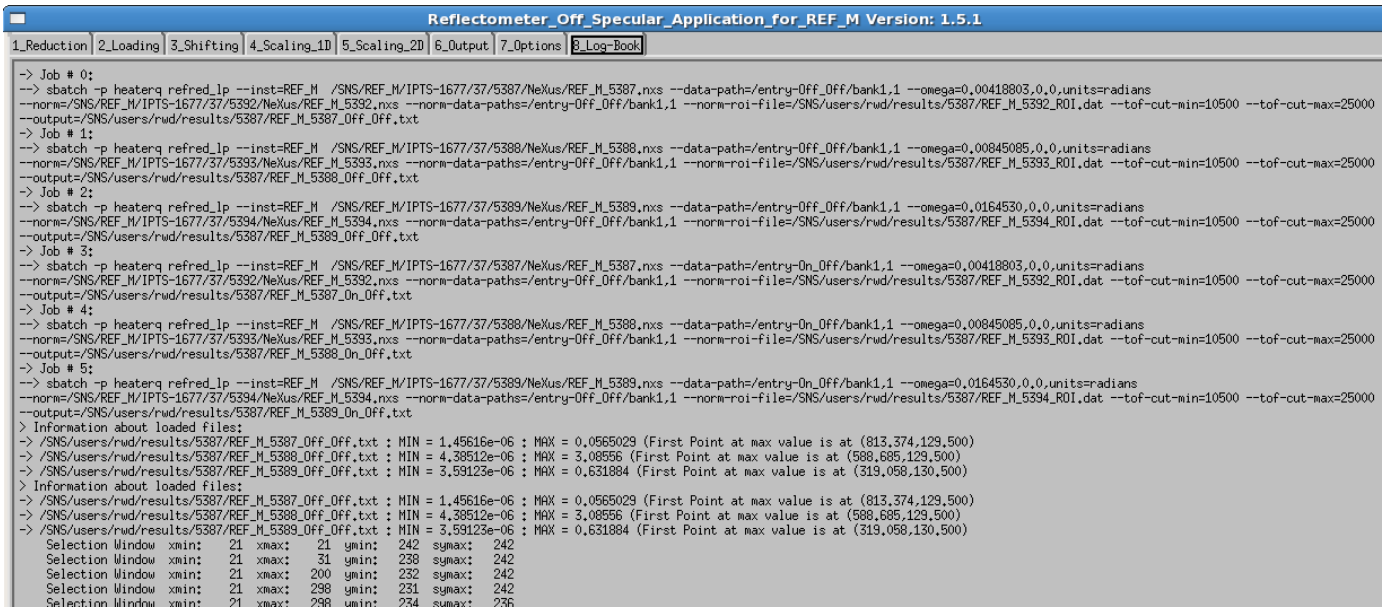


Fig. 31. Portion of the Log Book for the 5387—5389 example.

3.9 STEP 9: PLOT_UTILITY

The last tab, the **Plot_Utility** tab, provides the user the opportunity to plot all the results generated (see Fig. 32). Two types of plots are available: 1) Reflectivity plotted vs Q (Å -1) and 2) the scaled 2D results. The user clicks the button selects the files from a picklist (Fig. 33).

After selecting the desired output directory, the user selects the Plot Reflectivity vs Q button or the Plot Scaled 2D Results to create plots the desired spin state (Off_Off or On_Off). Clicking the button activates a picklist for the user to the specific files to plot. An example of the picklist for Reflectivity vs Q is shown in Fig. 34 and the plot of the selected results (Off_Off) is shown in Fig. 35.

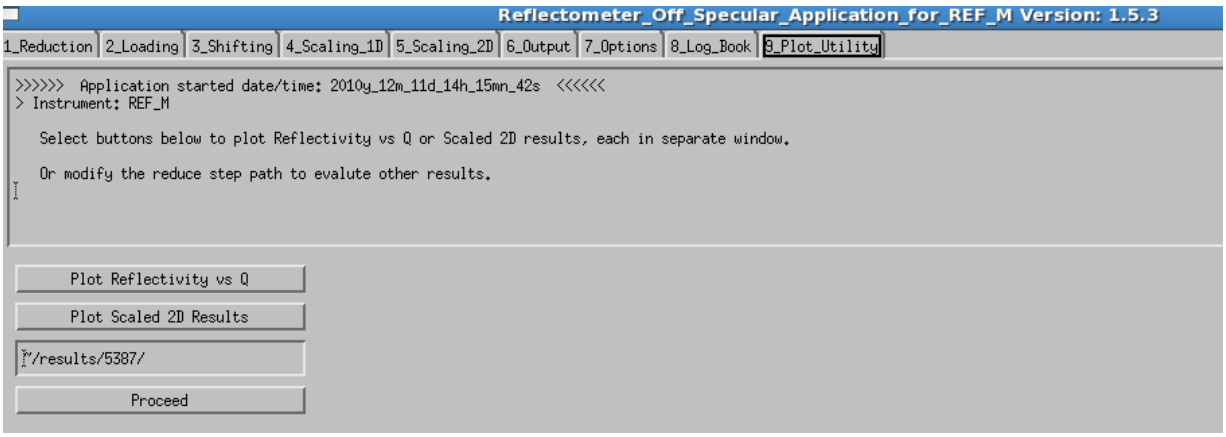


Fig. 32. The Plot_Utility screen.

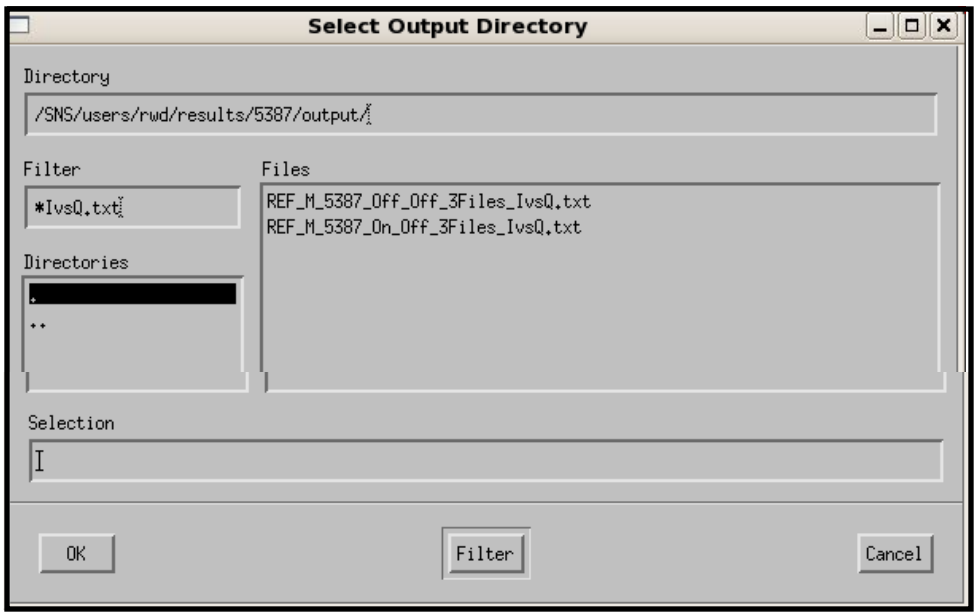


Fig. 33. Picklist to select results for plotting Reflectivity vs Q. There are two choices, one for Off_Off and one for On_Off, for the experimental runs we are evaluating.

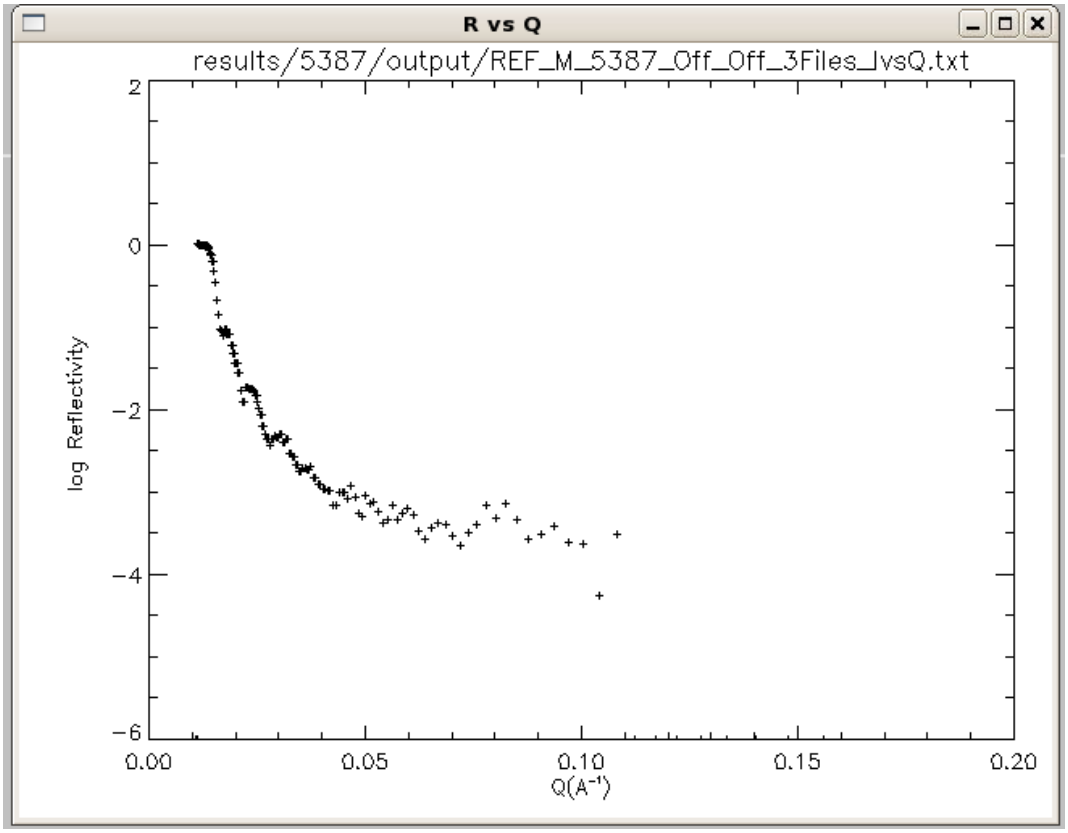


Fig. 34. Reflectivity vs Q for REF_M_5387_Off_Off datasets.

To compare results, you can place plots for the Scaled 2D results side by side with plots for Reflectivity vs Q (Off_Off on the top and On_Off on the bottom) as shown in Fig. 35.

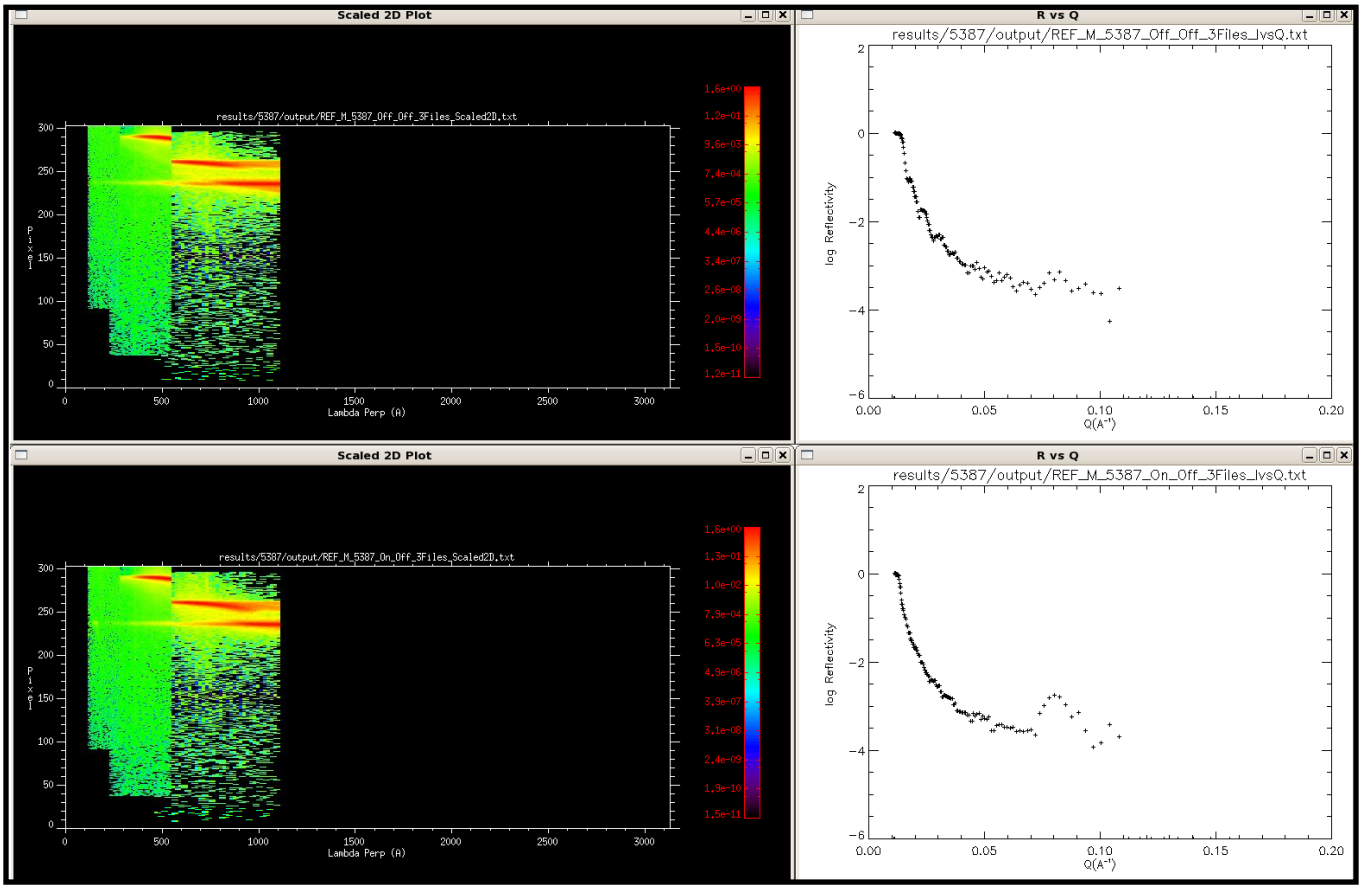


Fig. 35. Scaled 2D plots (left) and Reflectivity vs Q (right) for Off_Off (top) and On_Off (bottom) spin states for runs 5387—5389.

3.10 CHANGING THE RESULTS DIRECTORY

The user can examine other results that have already been processed by simply entering the results directory in the entry box on the Plot Utility screen. The user enters reference run number (e.g., **~/results/6183/** as shown below in Fig. 36) for the already processed data. In this case the program does not know the particular output directory to use, so the user is presented with a picklist of output directories for the run 6183, as shown in Fig. 37. On selecting the output directory (in this case "output"), the user then proceeds as described above to select and plot Reflectivity vs Q or Scaled 2D results for this case.

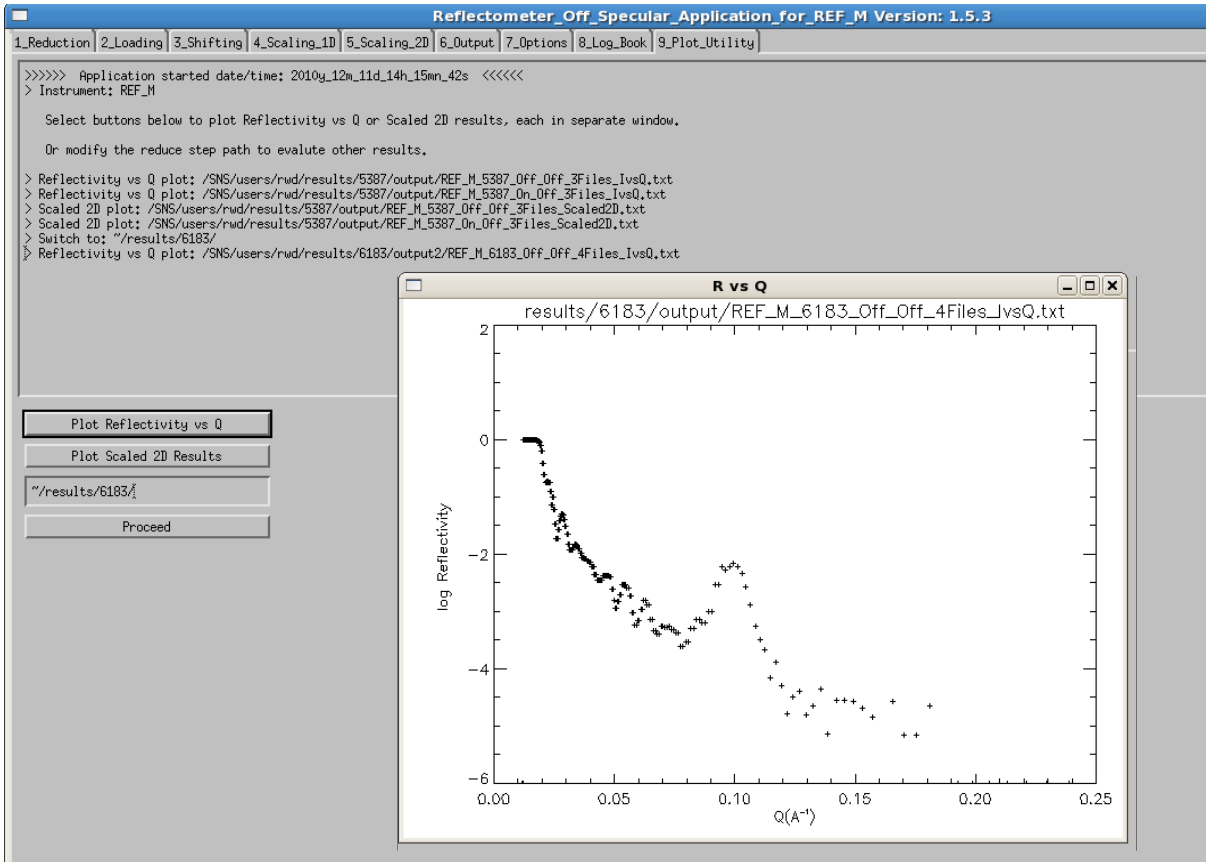


Fig. 36. The user has changed the directory from 5387 to 6183. Clicking the Plot_Utility tab results in a picklist associated with this new reference dataset directory.

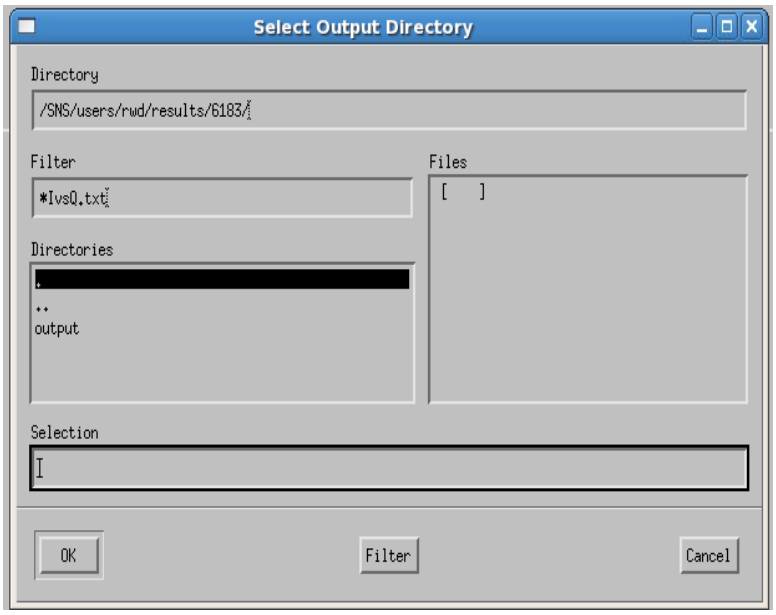


Fig. 37. Picklist for output directory when switching to new reference run number.

3.11 RETURNING TO START OF APPLICATION

The user can start the application over from the **Loading step** by entering a new reference run number (directory must already exist) into this text entry box on the Plot_Utility screen. However, when going back to the start of the code, the user must exercise the following precautions.

1. On returning to the **Loading step (see Sect. 3.2)**, the user **must delete the files** showing in the reduction step screen by selecting all the files and then clicking the button DELETE SELECTED ASCII FILE.
2. Then load the files of interest for the set of runs by clicking the BROWSE ASCII button and selecting files.
3. Proceed then to the **Shifting step** as describe previously and select Realign Data to realign the data.
4. The user should continue by clicking the **Scaling_1D** tab. The old pixel selection range box will show. Simply ignore that and draw the new selection box as desired. Again adjust the ymin/ymax to the desired values and continue to scale the CE and scale the other datasets to the reference dataset. When completed, continue on to **Scaling_2D** tab.
5. At this point, user **must** click the RESET button in the upper right corner to repaint the screen. The selection box will show as set in the Scaling_1D step. Continue on to selecting the type of plot and click the working directory button to select the output directory. Note that the button will show the old working directory of the previous example. **This must be altered or the output files will go into the wrong directory!** Proceed to plot the Reflectivity vs Q and save the plot to the output directory.
6. Continue on to the **Output** step and proceed as usual to process the other spin states and save the data. Lastly, select the **Plot_Utility** tab and plot desired results.

Note that you CANNOT return to the Reduce Step and process a new set of runs! The application must be stopped and started over to process a new data reduction.

3.12 USE FOR LIQUIDS REFLECTOMETER RESULTS

REFoffSpec was designed to reduce and analyze datasets for both the liquids and magnetism reflectometer experiments. To process REF_L data, login to LRAC and launch the application using sns_tools. On the front screen select the **Liquids Reflectometer (REF_L)** check box. Then proceed as described for REF_M datasets. The difference is that the user will not need to set RefPix values and can skip from the **Reduce Step** direct to the **Scaling_1D** step. In addition, since the magnetic spin of the neutrons is not involved, there will be a single result.

4. DETAILS OF REFoffSpec

4.1 Experimental Parameters

Sample to Detector Distance (SDdist): Distance between the sample and the detector (m)

Detector Angle (Dangle): The angle determined by the relative position of the detector as it travels on the arc during the measurement. (See Fig. 38).

Initial Detector Angle (Dangle0): The angled determined from the relative position of the detector when the direct beam position (DirPix) is determined. (See Fig. 38).

Directed Pixel value (DirPix): Direct beam pixel values

Reflected Pixel value (RefPix): Reflected beam pixel values

Sample Angle (Sangle): Sample angle (radians) is computed from:

A = (Dangle – Dangle0)/2.0
B = (DirPix – RefPix) *7.0E-4
C = 2. SDdist
Sangle = A + B/C (rad)

Time of Flight (TOF) cutoffs: Minimum and maximum time of flight cutoffs (μsec).

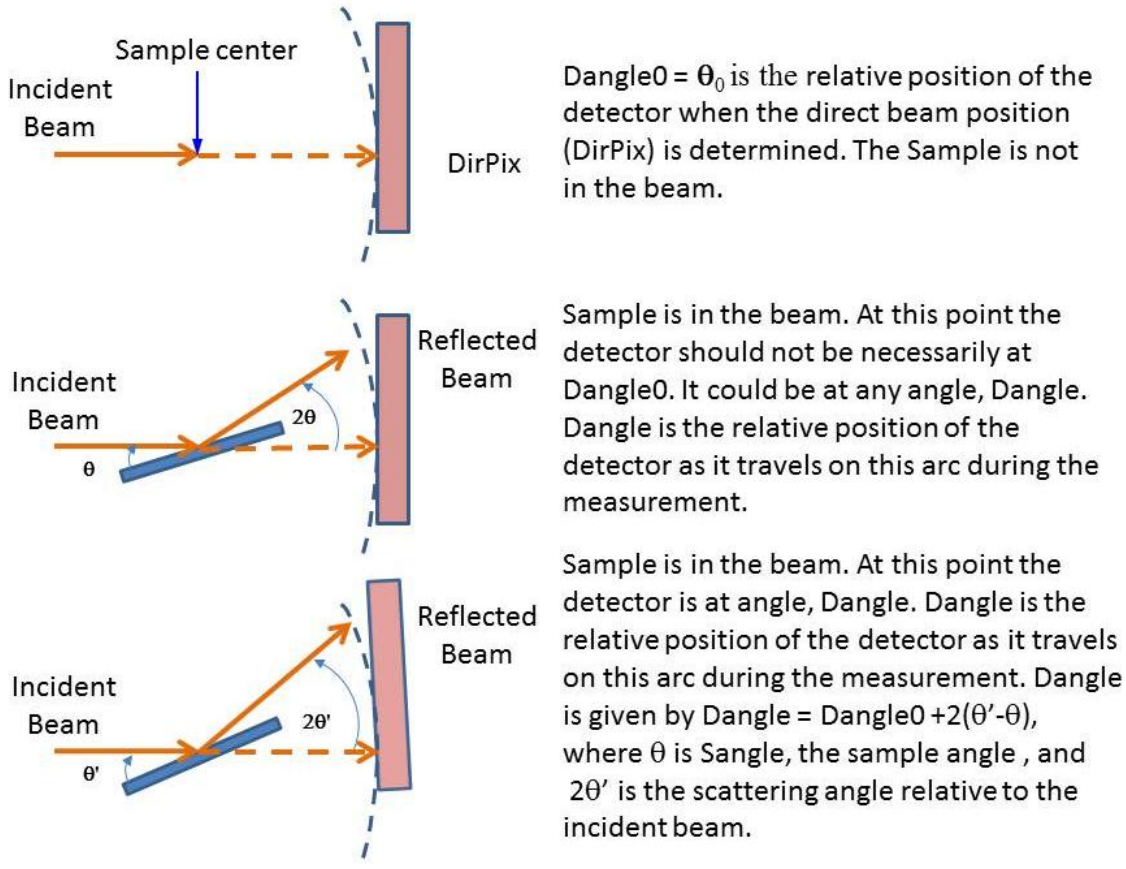


Fig. 38 Definitions of Dangle and Dangle0.

4.2 REFoffSpec Configuration File

The REFoffSpec configuration file (ref_off_spec.cfg), an XML file that contains parameters for configuring the code, is as follows.

```
<configuration>
      <application>REFoffSpec</application>
      <version>1.5.4</version>
      <debugging default='no'>no</debugging>
      <faking>
         <data default='no'>no</data>
      </faking>
      <testing default='no'>no</testing>
      <scrolling default='no'>no</scrolling>
      <checking_packages default='yes'>yes</checking_packages>
      <am values='[slurm,oic]'>slurm</am>
      <browser>/usr/bin/firefox</browser>
   <MainBaseTitle>Reflectometer_Off_Specular_Application</MainBaseTitle>
   <MainTabTitles>
      <step1>1_Reduction</step1>
      <step2>2_Loading</step2>
      <step3>3_Shifting</step3>
      <step4>4_Scaling_1D</step4>
      <step5>5_Scaling_2D</step5>
      <step6>6_Output</step6>
      <step7>7_Options</step7>
      <step8>8_Log_Book</step8>
        <step9>9_Plot_Utility</step9>
    </MainTabTitles>
    <ReduceTabNames>
      <name1>REF_DATA</name1>
      <name2>DIRECT</name2>
      <name3>NORMALIZATION</name3>
    </ReduceTabNames>
    <ScalingTabNames>
        <sname1>PIXEL_RANGE_SELECTION</sname1>
      <sname2>SCALING</sname2>
    </ScalingTabNames>
    <ScalingLevel3TabNames>
        <sl3name1>ALL_FILES</sl3name1>
      <sl3name2>CRITICAL_EDGE</sl3name2>
      <sl3name3>SCALING_OTHER_FILES</sl3name3>
    </ScalingLevel3TabNames>
    <RefPix>
      <InitialValue>200.</InitialValue>
      </RefPix>
      <DataPlot>
      <ColorTable>13</ColorTable>
      <YSizeDraw>608.</YSizeDraw>
      <XSizeDraw>600.</XSizeDraw>
        <BoxColors>
          <BoxColor0>60</BoxColor0>
            <BoxColor1>100</BoxColor1>
            <BoxColor2>120</BoxColor2>
            <BoxColor3>135</BoxColor3>
            <BoxColor4>150</BoxColor4>
```

```
            <BoxColor5>175</BoxColor5>
            <BoxColor6>200</BoxColor6>
            <BoxColor7>225</BoxColor7>
            <BoxColor8>250</BoxColor8>
        </BoxColors>
      </DataPlot>
      <CurvePlot>
          <BackgroundColor>Beige</BackgroundColor>
      <CESelect>
            <VerticalLineColor>Red</VerticalLineColor>
            <SelectColor>Yellow</SelectColor>
      </CESelect>
      </CurvePlot>
      <Detector>
            <Pixels_YNumber>304</Pixels_YNumber>
            <Pixels_XNumber>256</Pixels_XNumber>
            <Pixels_YSize units='m'>7.E-4</Pixels_YSize>
            <Number_of_Sangle>10</Number_of_Sangle>
      </Detector>
    <TOFCutoffs>
        <ApplyTOFCutoffs>yes</ApplyTOFCutoffs>
      <TOFCutoffMin units='microsec'>10500</TOFCutoffMin>
      <TOFCutoffMax units='microsec'>25000</TOFCutoffMax>
    </TOFCutoffs>
    <Reduction>
      <Queue>heaterq</Queue>
    </Reduction>
    <ReflectivityPlot>
         <DataColor>Blue</DataColor>
         <ErrorColor>Orange</ErrorColor>
         <ZoomBoxColor>Yellow</ZoomBoxColor>
         <VerticalColor>Red</VerticalColor>
         <HorizontalColor>Red</HorizontalColor>
         <AverageColor>Yellow</AverageColor>
    </ReflectivityPlot>
    <Shifting>
      <RefPixLoad>yes</RefPixLoad>
    </Shifting>
    <Recap>
        <SplicingAlternative>0</SplicingAlternative>
    </Recap>
</configuration>
```

4.3 REFoffSpec Options

The REFoffSPec options tab allows the following items to be set up prior to or during code operation.

4.3.1 Step 3: Shifting

Use non-active file attenuator. Options: **Yes, No** Default: **No**

If yes then, entry for transparency coefficient (numerical value)

Reference Pixel Selection Options: **Y, X and Y** Default: **X and Y**

Fast Pixel Selection Mode. Options: **Yes, No** Default: **No** (User must select active file)

Plot 2D Selection Style. **Options: _ _ _ _ _ . . . . . .–.–.– – – – . .** **. – – – – – – – –** Default: **_ _ _ _ _**

4.3.2 Step 4: Scaling

Plot data with error bars. Options**: Yes, No** Default**: No**

Precision in pixel of mouse click selection (move resize). Default value: **5**

Plot2D Symbols**.** Options: **Plus sign, Asterisk, Period, Diamond, Triangle, Sphere, X**
Default**: Plus sign**