RZera 1.2 User Manual

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1. Main interface introduction

Figure 1. The main interface of RZera. (a) The “Diffraction” tab page. (b) The “PDF” tab page.

Fig. 1 is a screenshot of the main interface of RZera version 1.2. The main interface consists of two parts: on the left side, there is the software logo, the China Spallation Neutron Source logo, the English abbreviation of the multi-physics instrument (MPI), and a structural diagram. The right side features a Tab page which is the main part of the software. This Tab page has two tabs, "Diffraction" and "PDF", as shown in Fig. 1(a) and Fig. 1(b), respectively. These tabs are responsible for the reduction of experimental data in the diffraction mode and the total scattering mode of the MPI. Below, we will explain how to use these two tabs for data reduction.

2. Diffraction reduction mode

Data in diffraction mode is reduced on the "Diffraction" page. On this page, there are four sections: "Sample and Instrument Information", "Experimental Configure", "Vanadium and Hold Scale", and "Choose Bank and Set Rebin". Users need to import

or input the required files or parameters in these four sections. Below, each section will be explained in detail.

2.1 Sample and Instrument Information

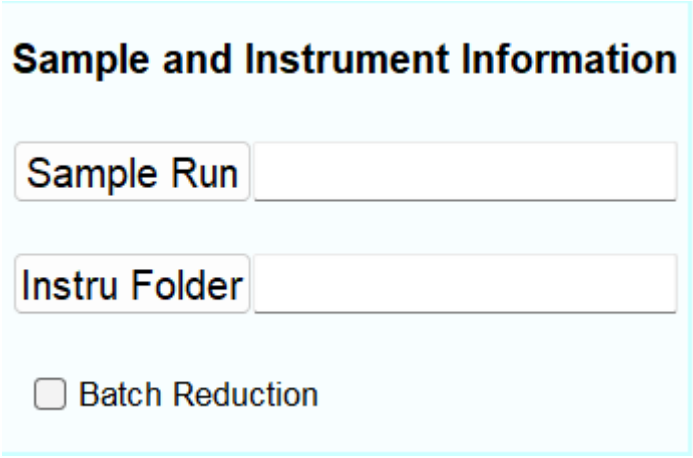

Figure 2. The section of “Sample and Instrument Information” in the diffraction tab.

In the "Sample and Instrument Information" section shown in Fig. 2, the "Sample Run" button is used to import the .nxs file (or files) of the sample. After clicking this button, a folder selection window will pop up, as shown in Fig. 3(a). By holding down the Shift key, users can select multiple folders and then click OK. The software will then search for files with the ".nxs" extension in the selected folders and present these files in a pop-up window for the user to choose from, as shown in Fig. 3(b). Users can select multiple .nxs files to import by left-clicking with the mouse, and then click OK to successfully import the files.

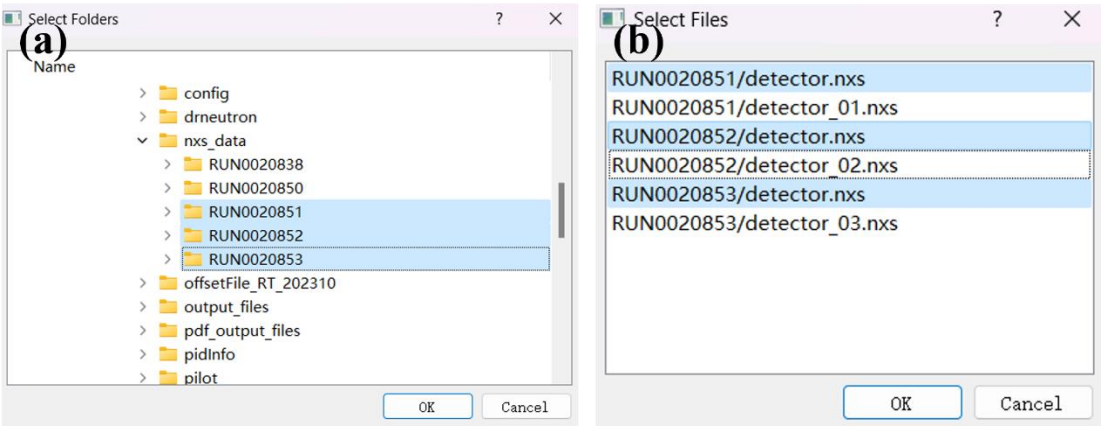

Figure 3. After clicking “Sample Run”, a folder selection window (a) will pop up. By holding down the Shift key, users can select multiple folders and then click OK. The software will then search for files with the ".nxs" extension in the selected folders and present these files in a pop-up window (b)

for the user to choose from.

The "Instru Folder" button is used to import the folder path containing the pixel information files. These files include the spatial coordinate information of all the detector pixels in the MPI. After clicking this button, a folder selection interface will pop up. Once the target folder is selected, the import will be completed.

Checkbox "Batch Reduction": If this box is checked, each .nxs file will be reduced separately during the reduction process, and the output will consist of the same number of reduced results as the imported .nxs files. If the box is not checked, all .nxs files' data will be merged before reduction, and a single result will be output. Additionally, if this box is checked and all imported .nxs files have sequential numbers at the end of their filenames, the program will assume that the user intends to treat these data as experimental data collected at different times under the same experiment (time slicing). The program will mark the output result of each .nxs file with the same RUN number, which will be the same as the RUN number of the .nxs file with the lowest sequence number. However, they will be marked with different sequence numbers to distinguish that they were collected at different time periods.

2.2 Experimental Configure

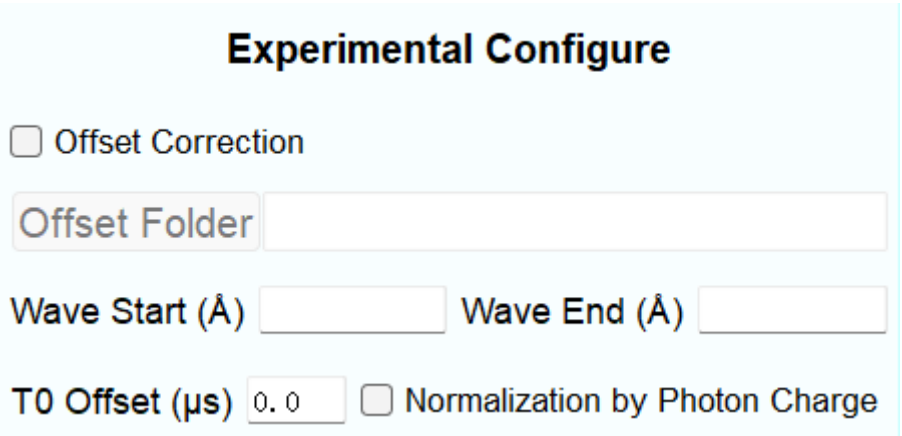

Figure 4. The section of "Experimental Configure" in the diffraction tab。

In the "Experimental Configure" section shown in Fig. 4, the function of the "Offset Folder" button is to import the offset files of the MPI, which contain the offset values for all pixels. If you do not wish to use these files, do not check "Offset Correction" (unchecked by default). If you wish to use these files, check the box.

Once checked, the "Offset Folder" button becomes available. Clicking this button will bring up a folder selection dialog, where you can select the folder containing the offset files.

"Wave Start" and "Wave End" limit the neutron wavelength range used during the reduction. These fields only allow the input of floating numbers, and the program will only use neutron data that satisfies this wavelength range during the reduction.

T0 Offset refers to the error between the recorded neutron flight time and the actual neutron flight time. This field only allows the input of floating numbers.

"Normalization by Photon Charge" indicates whether to normalize the data by proton charge. If checked, normalization will be performed; if unchecked, it will not be performed.

2.3 Vanadium and Hold Scale

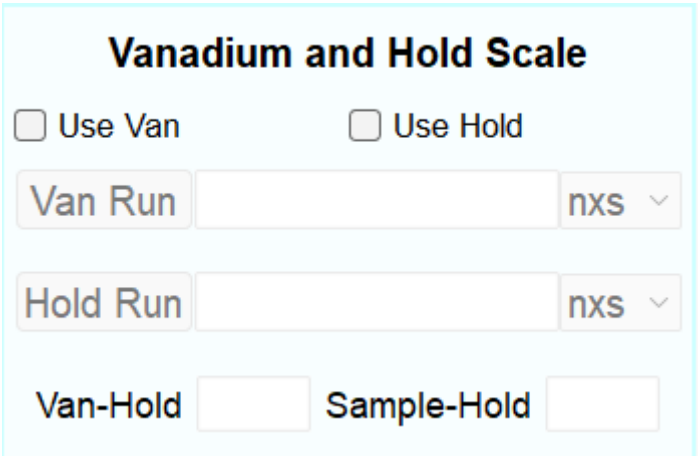

Figure 5. the section of “Vanadium and Hold Scale” in the diffraction tab.

In the "Vanadium and Hold Scale" section shown in Fig. 5, the function of the "Van Run" button is to import the scattering data files of the reference sample Vanadium, and the function of the "Hold Run" button is to import the scattering data files of the empty sample holder. On the right side of the row where these two buttons are located, there is a combobox for selecting the format of the imported files. This combobox has two modes available: "nxs" and "dat". In the "nxs" mode, the file import method is the same as shown in Fig. 3; in the "dat" mode, the file import method is the same as the "Instru Folder" in section 2.1 and the "Offset Folder" in section 2.2. Generally speaking, users should first import the Van Run and Hold Run data in the

"nxs" mode. During reduction, the program will reduce these two sets of data together. After saving the reduced data of these two sets as dat files, users can import the reduced Van Run and Hold Run data in the "dat" mode during the next reduction. This way, the program can directly read the reduced data without having to reduce them again, saving a significant amount of time. (Note: The name of the folder containing these dat files must be the RUN number, for example, "RUN0020850", and the filenames of the dat files should not be modified.)

"Van-Hold" is where you input the coefficient by which the scattering data of the empty holder is multiplied when subtracting it from the scattering data of V. This entry only allows the input of floating numbers. For example, if you input 0.5 here, the formula used for subtraction will be:

$$I_{Van} - 0.5 \times I_{Hold} \quad (1)$$

"Sample-Hold" works similarly, indicating the coefficient by which the scattering data of the empty holder is multiplied when subtracting it from the scattering data of the sample.

2.4 Choose Bank and Set Rebin

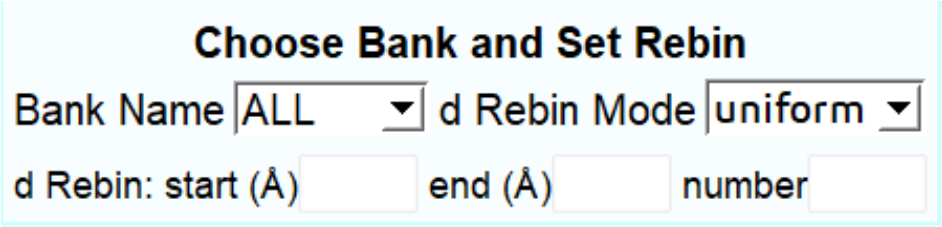

Figure 7. The section “Choose Bank and Set Rebin” in the diffraction tab.

The detector of the MPI is composed of 6 banks, from bank2 to bank7 (In the sample data folder, the nxs data only contains the data from bank 5 and bank3). In the "Choose Bank and Set Rebin" section shown in Fig. 6, the ComboBox "Bank Name" is used to select which bank's data to use for reduction. It offers 7 options: "ALL", "bank2", "bank3", "bank4", "bank5", "bank6", and "bank7". Selecting "ALL" will cause the program to reduce data from all banks; selecting any other option will cause the program to reduce data from the corresponding bank only (In the distribution version of RZera 1.2, only bank3 can be selected).

The three values for d Rebin—start, end, and number—define the number of data points from start to end when obtaining the I(d) curve through reduction. “start” and “end” only allow the input of floating numbers, while “number” only allows the input of positive integer. The ComboBox "d Rebin Mode" specifies the mode of data point division during d Rebin. There are three modes available: "uniform", "log_10", and "log_e". Selecting "uniform" will divide the data points evenly; selecting "log_10" will divide the data points according to a base-10 logarithm; selecting "log_e" will divide the data points according to the natural logarithm.

2.5 Save Configure and Load Configure

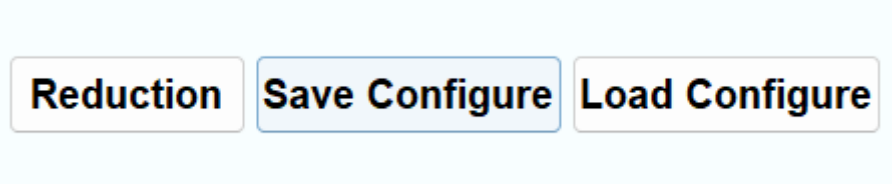

Figure 7. The “Reduction” “Save Configure” and “Load Configure” buttons in the diffraction tab.

On the right side of the "diffraction" tab, there are "Save Configure" and "Load Configure" buttons as shown in Fig. 7. The purpose of these two buttons is to help users quickly input configuration information. After the user has entered the reduction configuration information as previously described, they can click "Save Configure" to save this configuration information as a JSON file with a custom filename in the dialog that pops up. The next time the user uses RZera, they can click "Load Configure" and import the previously saved JSON file in the dialog that pops up. After importing, all the configuration information described in sections 2.1-2.4 that was saved in this JSON file will be reloaded onto the "diffraction" tab. This eliminates the need to re-enter the information, allowing the user to proceed directly with data reduction.

2.6 Reduction

After importing and inputting the necessary information for reduction as described in sections 2.1-2.4, pressing the "Reduction" button shown in Fig. 7 will initiate the data reduction process. If any required information is missing, a prompt window will appear, reminding the user to complete the information. As shown in Fig. 8(a), because the "Van Run" file was not imported, clicking "Reduction" will bring up a prompt

window saying "Please provide V run file". If all required information is complete, the software will display a progress bar window showing the current progress of the reduction. Meanwhile, the reduced sample data will be immediately displayed in the left column of the two list boxes at the bottom right as items. If the V and empty sample holder data are imported in "nxs" mode, their reduced data will be immediately displayed in the right column, as shown in Fig. 8(b). If they are imported in "dat" mode, their reduced results will not be displayed, because the data imported in "dat" mode are already reduced data.

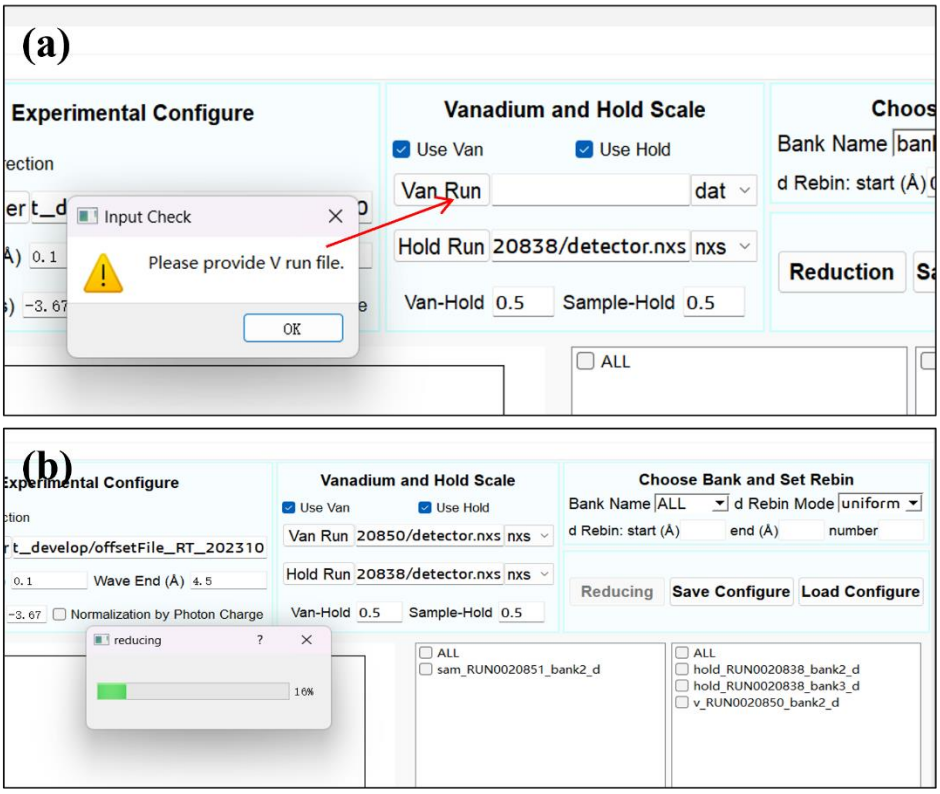

Figure 8. (a) because the "Van Run" file was not imported, clicking "Reduction" will bring up a prompt window saying "Please provide V run file". (b) After clicking "Reduction", a progress bar will appear, and the reduced data will be displayed as items in the two list boxes at the bottom right.

2.7 Plot、Save and Delete

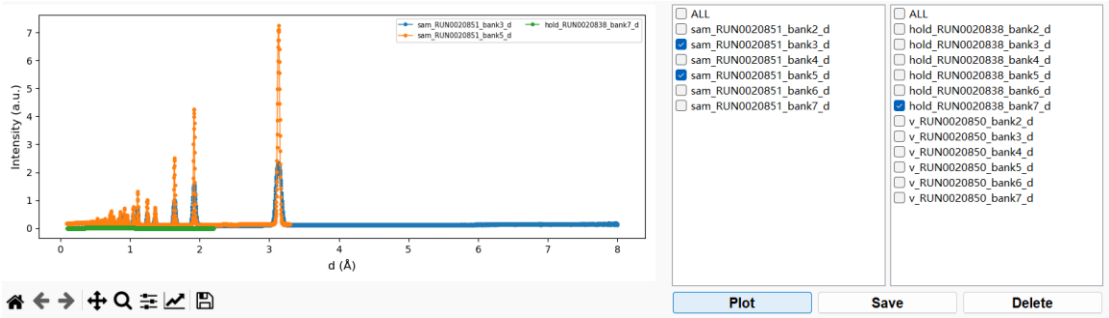

Figure 9.“Plot”, “Save” and “Delete” buttons operate the items in the two list boxes.

Below the list boxes, there are three buttons: "Plot", "Save", and "Delete". By selecting the reduced data items in the list boxes and clicking "Plot", the software will plot the I(d) curves of the selected items on the canvas on the left side, as shown in Fig. 9. Users can use the toolbar at the bottom left to operate the curves on the canvas.

Clicking the "Save" button will bring up a save dialog. After the user selects a folder, the software will create subfolders in this folder using the RUN numbers of the selected data and save the selected data in these subfolders according to their respective RUN numbers. For sample data in the left list box, the software will save each data item in three formats: ".dat", ".gsa", and ".histogramlgor", and the saved data will be I(tof) curves, not I(d) curves. For sample data in the right list box, the software will only save them in the ".dat" format as I(d) data. These data can be used as "Van Run" and "Hold Run" files imported in "dat" mode in subsequent reductions.

Clicking the "Delete" button will delete the selected items from the list boxes (Can’t recover!).

Each list box has an "ALL" item, which is designed to facilitate batch selection. Selecting the "ALL" entry will select all entries in that box, and deselecting it will simultaneously deselect all items in that box.

3. PDF reduction mode

The data of the total scattering mode is reduced on the "PDF" tab. On this tab, before obtaining the sample's S(Q) data through reduction, you need to complete the information in "Sample Information" and "Experimental Information". After obtaining the S(Q) data through reduction, these data can be stitched together to obtain a single S(Q) dataset with the highest possible resolution and the widest possible coverage. Then, a Fourier transform can be performed on this dataset to obtain the final Pair Distribution Function (PDF). The reduction process will be explained step by step below.

3.1 Sample Information

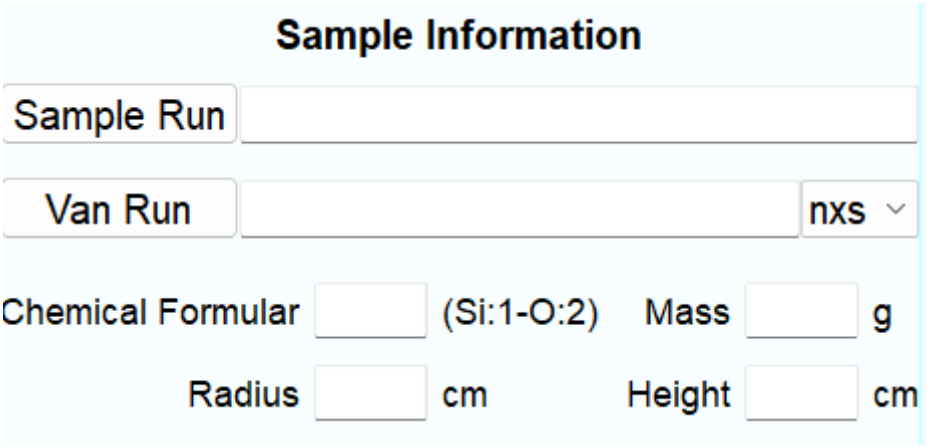

Figure 10.The section “Sample Information” in the PDF tab.

Under the "Sample Information" section, there are two buttons: "Sample Run" and "Van Run", as shown in Fig. 10. Their usage is exactly the same as the "Sample Run" and "Van Run" in the diffraction mode described in Section 2. The "Chemical Formula" in this section requires the input of the sample's elemental composition ratio in the specified format. For example, Fe2O3 should be entered as "Fe:2-O:3", and pure silicon should be entered as "Si:1". The "Mass" requires the input of the sample's mass. The "Radius" requires the input of the sample's radius, which is generally the inner diameter of the cylindrical sample holder. The "Height" field requires the input of the sample's vertical size.

3.2 Experimental Information

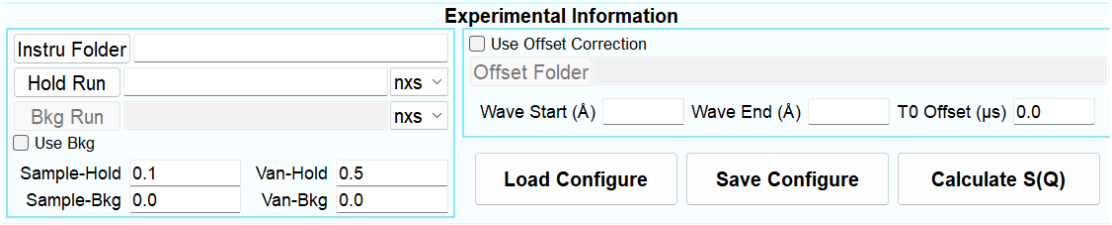

Figure 10. The section “Experimental Information” in the PDF tab.

The "Experimental Information" section requires a lot of information to be input and is divided into left and right parts by two boxes.

In the left part, you first need to import the "Instru Folder" and "Hold Run". Their import methods are exactly the same as the "Instru Folder" and "Hold Run" in the diffraction mode described in Section 2. This part has an optional import item "Bkg

Run". If you check "Use Bkg", you can import this item, and the import method is the same as "Hold Run". However, the current RZera 1.2 version does not support the "Bkg Run" processing function, so it is not necessary to import this item at the moment. The last part includes "Sample-Hold", "Van-Hold", "Sample-Bkg", and "Van-Bkg". Their functions and usage are the same as the "Sample-Hold" and "Van-Hold" described in Section 2.3.

The right part has an optional "Offset Folder" import item. Its function and usage are the same as the "Offset Folder" described in Section 2.2. "Wave start", "Wave end", and "T0 Offset" are also exactly the same as described in Section 2.2.

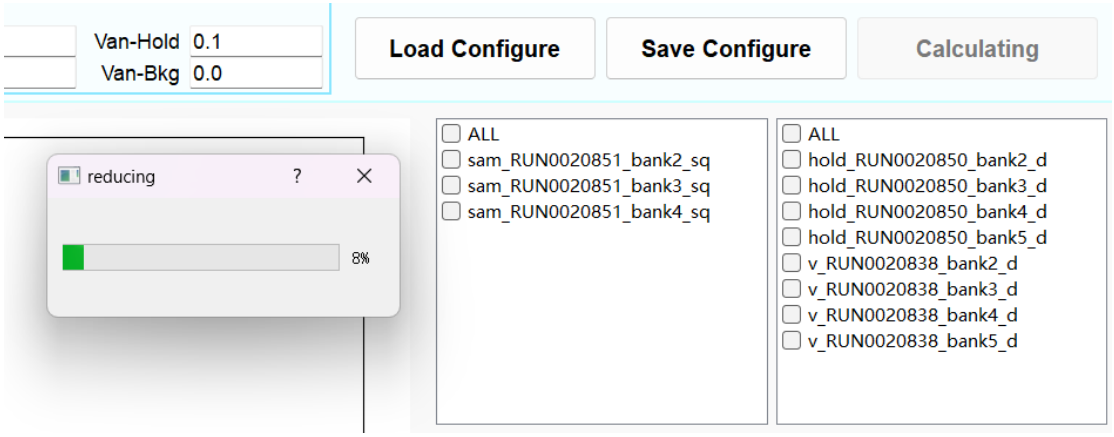

Figure 11. After clicking "Calculate S(Q)", a progress bar will appear, and the reduced data will be displayed as items in the two list boxes below.

At the end of the "Experimental Information" section, there are two buttons: "Load Configure" and "Save Configure". Their functions are the same as those described in Section 2.5 and are used to load and save the configuration information of the "PDF" page. In addition to these two buttons, there is also a "Calculate S(Q)" button. Its function is similar to the "Reduction" button in Section 2.6, but it calculates the S(Q) data obtained from the reduction of all banks and all modules (components of the banks) of the MPI (left list box). Additionally, if the Van Run and Hold Run are imported in "nxs" mode, it will calculate the I(d) data obtained from the reduction of the Van Run and Hold Run (right list box), as shown in Figure 11.

3.3 Processing S(Q) data （Plot S(Q), Merge S(Q), Save, Delete）

Below the list boxes that display the reduced data, there are four buttons, as shown

in Figure 12. These buttons are used for further processing of the S(Q) data. The "Plot S(Q)" button is used to plot the selected items on the canvas on the left side. Note that if there are selected items in the left list box, the "Plot S(Q)" button will not plot the selected items in the right list box. This is because the horizontal axis coordinates of the data in the two list boxes are not consistent, and therefore, they are not suitable to be plotted together.

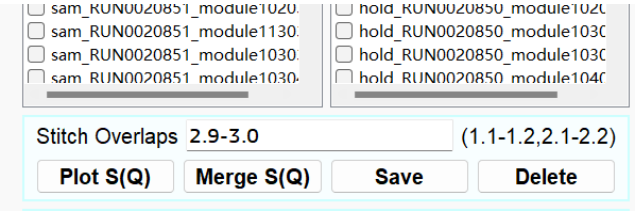

Figure 12. The four buttons Plot S(Q), Merge S(Q), Save, and Delete below the list boxes.

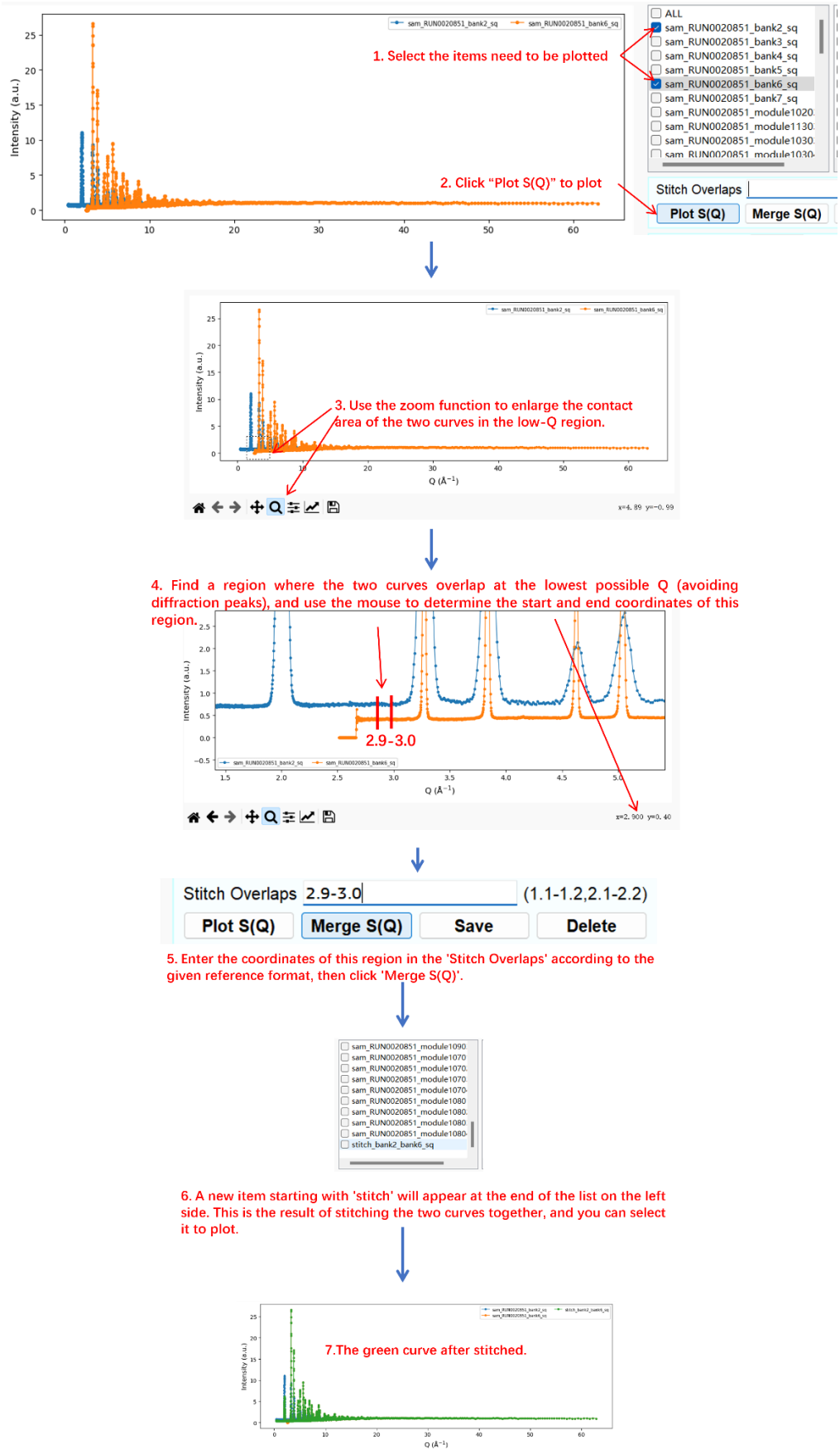

Figure 13. Detailed flowchart for stitching two S(Q) curves.

After obtaining the S(Q) data, in order to get a dataset with the widest possible coverage while ensuring the resolution, it is generally necessary to perform a “merge” operation on two or more datasets (i.e., stitching them together). This function is implemented by the "Merge S(Q)" button. Fig. 13 shows the detailed process of stitching two S(Q) curves together. Following this procedure, users can also stitch multiple curves. If stitching N curves, you need to find N-1 overlapping regions and enter them into "Stitch Overlaps" according to the reference format.

The "Save" and "Delete" functions are basically the same as those described in section 2.7. It should be noted that the data in the left sidebar is saved in a different format here compared to section 2.7; it is saved as ".txt" file format S(Q) data.

3.4 Calculating the pair distribution functions

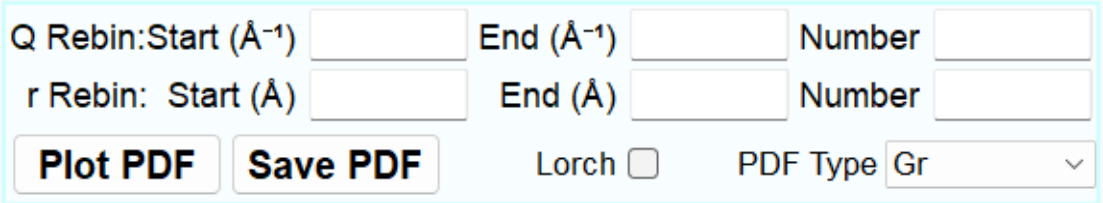

Figure 14. The plotting and saving PDF function section at the bottom right corner of the 'PDF' tab, used to obtain the PDFs from the S(Q) curve.

The section shown in Fig. 14 is used to plot and save the PDFs from the S(Q) curve. By clicking the "Plot PDF" button, the software will rebin the selected S(Q) data using the "Start," "End," and "Number" values in the Q rebin of this section. The rebin mode is "uniform," and unlike in section 2.4, other modes cannot be selected. Note that the start and end values for Q Rebin must fall within the Q value range of all the selected S(Q) curves. If even one curve does not meet this requirement, "Plot PDF" will not be successful. This section provides the "Lorch" function, and if the user selects Lorch, the software will add the Lorch filter function when calculating the PDF curve. Additionally, this section offers the "PDF Type" option, allowing users to choose to calculate G(r), gr, or RDF curves according to their needs. After rebinning the S(Q) data, the software will plot the user-specified type of PDF curve on the left canvas based on the "Start," "End," and "Number" values in the r Rebin section, and whether Lorch is selected, as shown in Fig. 15.

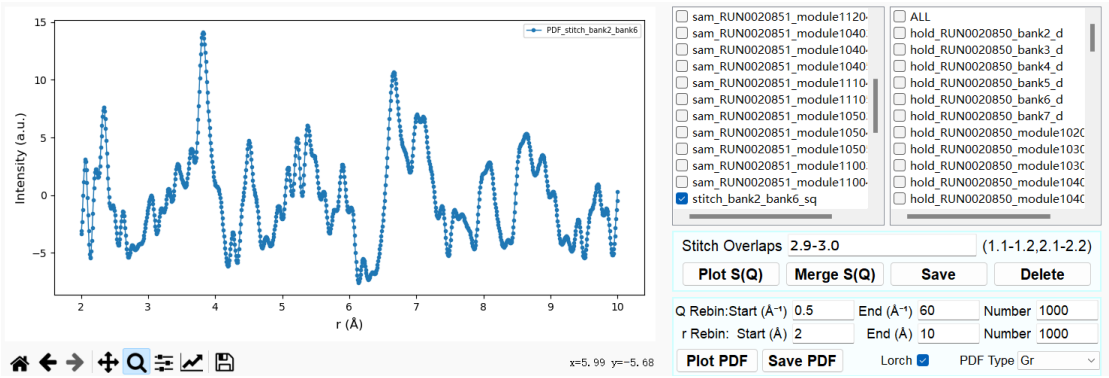

Figure 15. Click 'Plot PDF' to plot the PDF curve G(r) for the selected S(Q) curves.

By clicking the "Save PDF" button, the software will, just like when clicking "Plot PDF," rebin the selected S(Q) data using the "Start," "End," and "Number" values in the Q rebin function of this section. It will then bring up a dialog box to save the file. The PDF curve will be saved as a .dat file in the specified path based on the "Start," "End," and "Number" values in the r Rebin section. Similarly, the start and end values for Q Rebin must fall within the Q value range of all the selected S(Q) curves. If even one curve does not meet this requirement, "Save PDF" will not be successful.