

POWGEN User Manual for Data Reduction

This document contains a detailed description of how to reduce POWGEN data, including how to slice out data by time, temperature or other logged parameters. Instructions are also included for reducing POWGEN data into a format for pair distribution function (PDF) analysis. Data may be reduced using our analysis machines, either on-site via powgen (powgen.sns.gov) and powgen2 (powgen2.sns.gov), or outside ORNL via the analysis cluster (analysis.sns.gov).

Standard data reduction

Starting MantidPlot: All data is reduced using a program called MantidPlot. Type “mantidplot” in a terminal window on either the analysis cluster (<https://analysis.sns.gov>) or on the local analysis machines in the hutch (powgen and powgen2) to start the program. (See the side bar for instructions to make a shortcut to the terminal window.)

Reducing data with custom settings: Data are automatically reduced into gsas, fullprof and topas formats. If you want to rebins the data (different from what autoreduce creates) or do some special subtraction of background, you can re-reduce the data yourself using MantidPlot. In the main menu pick Interfaces→ Diffraction→ Powder Diffraction Reduction (Figure 1). This will launch the PG3 Reduction window (Figure 2). For a standard data reduction, enter the parameters on the Experiment Run Setup (Figure 2) and Advanced Setup (Figure 3) tabs, as indicated below.

Once all the parameters are entered correctly, simply press the Reduce button to start the reduction. The reduced data will appear as a workspace in the MantidPlot window, along with some additional workspaces, which may be deleted. You may view a plot of the data by right-clicking the workspace and selecting Plot Spectrum. Selecting multiple workspaces will overlay the plots.

Note that MantidPlot may begin to behave in unexpected ways when executing multiple operations in a row. In such cases, it may help to start fresh by selecting File -> Clear All Memory (Ctrl+Shift+L) or restarting MantidPlot. However, you will have to regenerate your workspaces.

Viewing metadata plots: You may view metadata associated with a run by right-clicking the workspace and selecting Sample Logs. Choose the desired variable and then press the Import Selected Logs button.

First Time?

If this is your first time using the analysis cluster, make a shortcut for a terminal on the desktop or launcher panel. To do this, click the start button , go to System Tools and right-click on MATE Terminal. Select either “Add this launcher to panel” or “Add this launcher to desktop”.

Once you start MantidPlot (by entering “mantidplot” in a terminal window), go to View on the toolbar and select Preferences. In the dialog box that pops up, select 2D Plots on the left, then the Options tab. Uncheck “Normalize histogram to bin width” and press the OK button. The program will automatically remember this setting the next time you open it.

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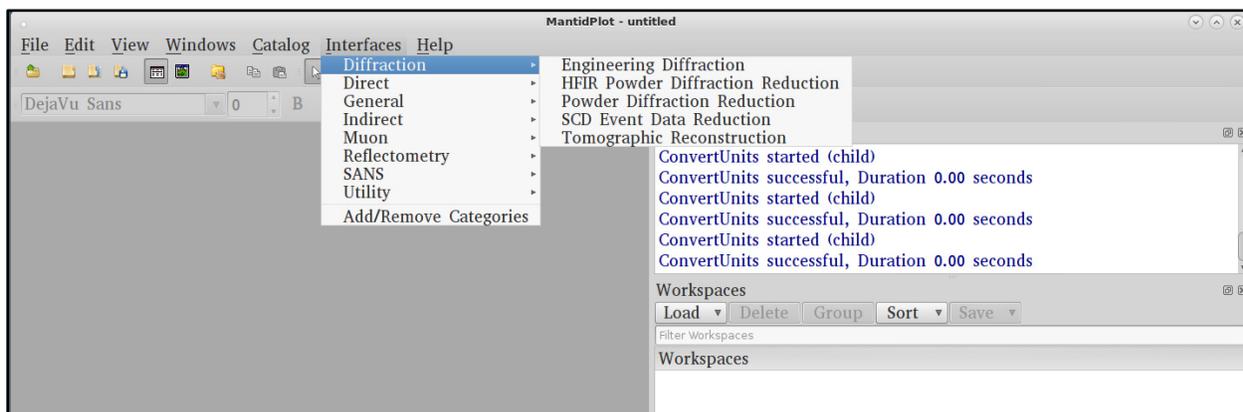


Figure 1. Opening the Powder Diffraction Reduction window.

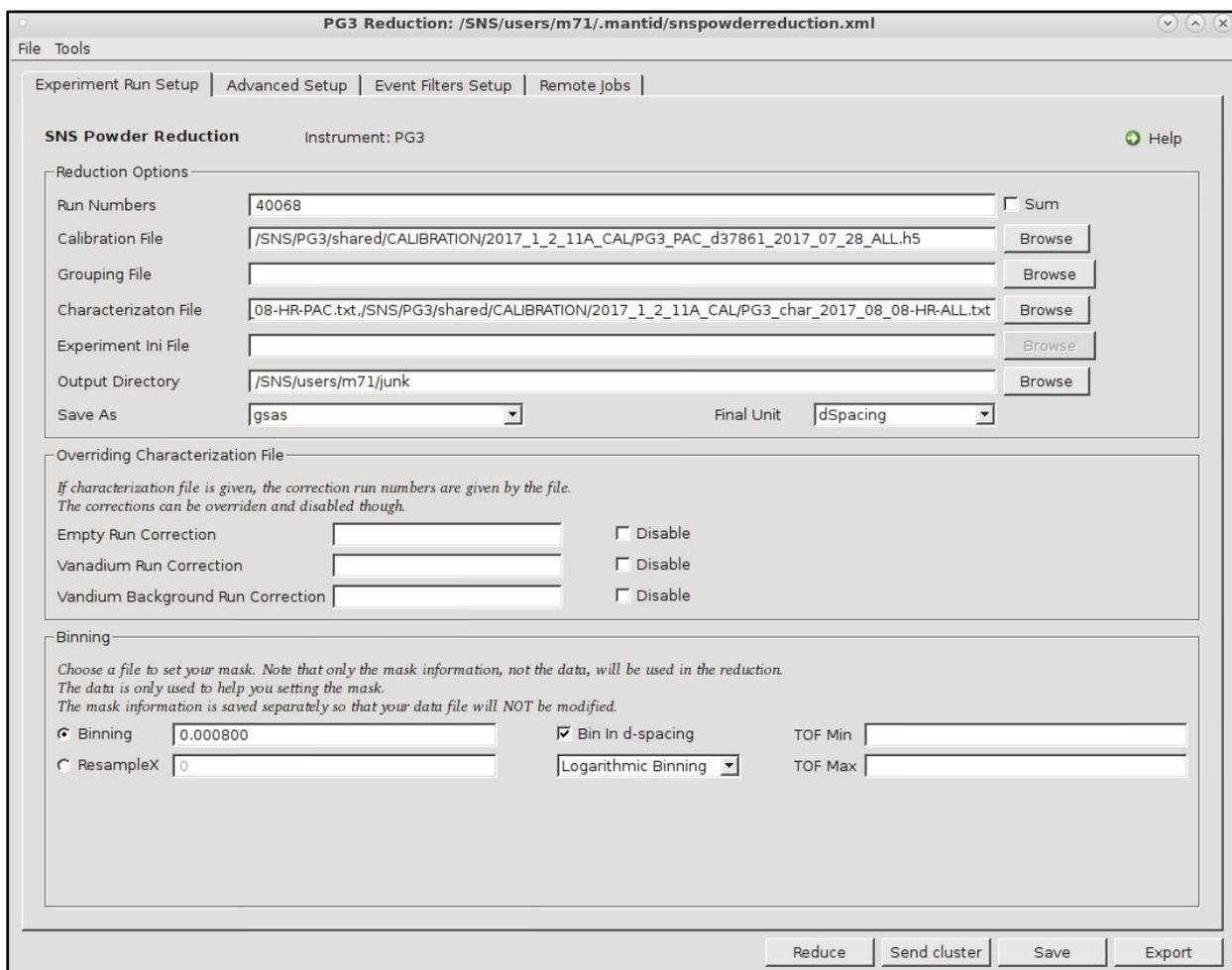


Figure 2. Main tab of the Powder Diffraction Reduction window.

SNS Powder Reduction → Experiment Run Setup tab (Figure 2):

- **Run Numbers:** This can be a single number or a range of numbers separated by a hyphen '-'. Multiple ranges separated by commas can also be entered. For example, "2346-2350, 2355, 2360-2365" is a valid entry. When the Sum box is checked, all the runs will be summed together into one file. When the Sum box is not checked, each run will be reduced separately.
- **Calibration File:** This file has an extension .h5 and is stored in the following folder: SNS/PG3/shared/CALIBRATION/cycle_1(2)_11A_CAL. The format of the filename is PG3_SE_dXXXXX_year_mo_day.h5, where SE represents the type of sample environment equipment used (e.g. PAC for the sample changer or OC for the cryostat) and XXXXX is the run number of the diamond run used for the calibration. Ask your local contact if you are not sure which calibration file to use.
- **Grouping File:** This should generally be left blank. Again, consult with your local contact if you want a special grouping of detectors.
- **Characterization File:** These are two simple text files, found in the same folder as the calibration file, that lists all the instrument standard Vanadium and Background data collected, as well as defining the time-of-flight ranges for each bank. You must select two characterization files, using the Shift or Ctrl key. The first is the file that ends in "-ALL.txt", and the second should be chosen to match the sample environment used (i.e. PAC, OC or JANIS). Ask your local contact if you are not sure which characterization files to use.
- **Experiment Ini File:** This should be left blank.
- **Output Directory:** Directory into which the reduced file will be saved. Use the Browse button to select the desired location.
- **Save As:** Use the dropdown menu to select the desired output file format(s): gsas, fullprof, topas, pdfgetn and/or processed nexus. The reduced files will be called PG3_run#.gsa for GSAS files, with the extension being *.dat for Fullprof and *.fxye for Topas files.
- **Final Unit:** Select dSpacing or MomentumTransfer (i.e. Q) as desired. The file will always be written in time-of-flight (TOF); the final unit is just for plotting the workspace.
- The fields in the "Overriding Characterization File" part should generally be left blank and unchecked. Empty Run Correction, Vanadium Run Correction and Vanadium Background Run Correction run numbers should be added only if you chose to not use the default run numbers set in the Characterization File. If you specify a run number in this box, that run number will override the run number specified in the characterization run. This is how you can do special background subtraction. If you check the Disable boxes, the algorithm will ignore the characterization file. This is a good way to generate a raw file without normalization and background subtraction.
- **Binning:** POWGEN uses logarithmic binning and the value here is $\Delta t/t$. A good starting point that works for most datasets is 0.0008. However, users can choose this value based on what is needed for their individual samples. To increase the number of points in a given peak use a smaller number and to decrease use a bigger number.

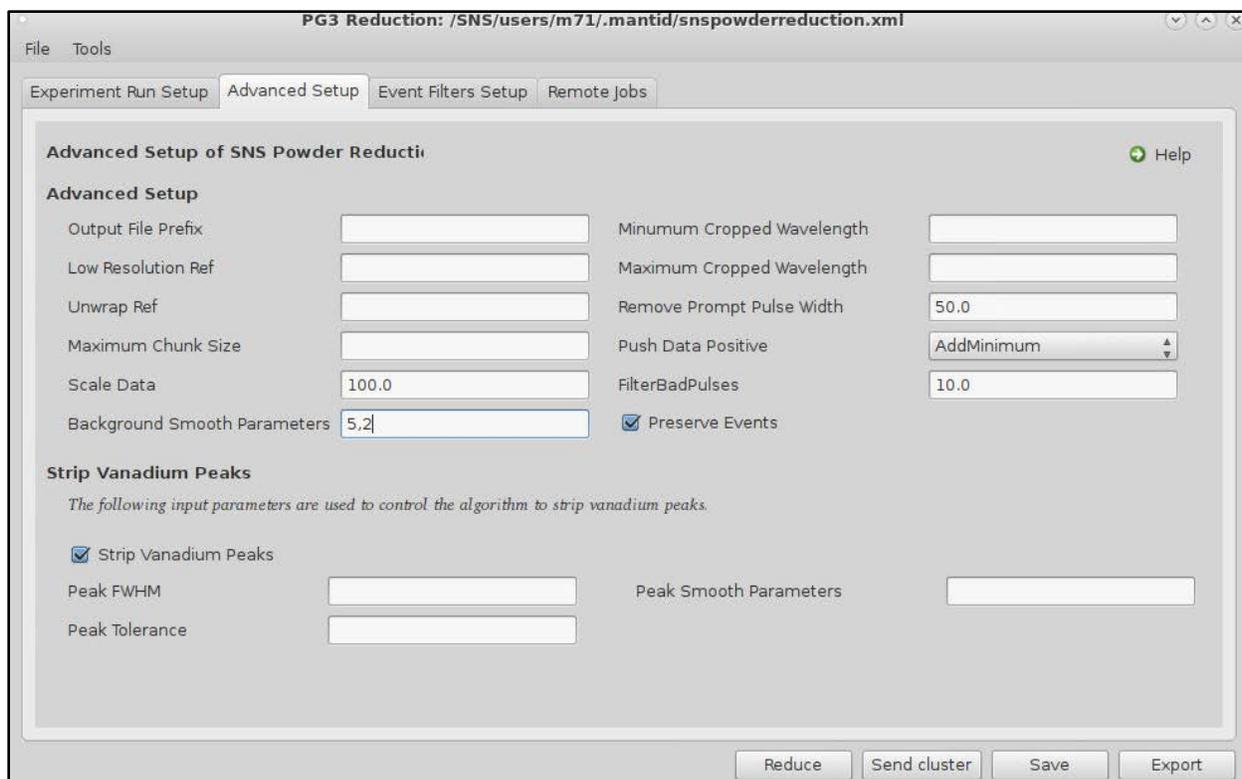


Figure 3. Advanced Setup tab of the Powder Diffraction Reduction window.

SNS Powder Reduction → Advanced Setup tab (Figure 3):

- Output File Prefix: If the Sum box on the first tab is checked to sum multiple datasets, this allows the user to specify the file name for the summed dataset.
- Scale Data: Some Rietveld programs have problems with plotting tick markers if the data is too close to the zero base line. By default (during autoreduction) we multiply by 100.
- Background Smooth Parameters: To apply smoothing to the background run. The parameter set of 5,2 works best for standard vanadium cans. For quartz tubes, we use 40,10.
- Remove Prompt Pulse Width should be 50.
- Push Data Positive: The intensities of individual data points can become negative due to background subtraction. In this case, we can either add a constant value to the spectrum so that all counts are positive (AddMinimum), reset those negative numbers to Zero (ResetToZero) or do nothing (None). Word of caution, there may be large negative spikes at the edges of data, in which case using AddMinimum can mess up goodness of fit parameters in Rietveld programs. In such cases, one should specify the spectrum range to exclude the spikes by setting the TOF Min and TOF Max values under Binning on the Experiment Run Setup tab.
- FilterBadPulses should be 10. This takes out any background collected during accelerator faults and down periods.
- Preserve Events should be checked.
- Strip Vanadium Peaks should be checked and the next several fields, which are associated with cutting out the vanadium peaks and a smoothing operation, should be left empty (default).

Slicing data by slow control log values or time:

You may also slice a single run into multiple datasets according to metadata, such as time, sample temperature or any other log value that is being recorded. You will need to use the tab titled Event Filters Setup (Figure 4) to setup the required slicing. You have various options to slice by time or by log value, e.g. temperature.

The General and Setup Assistant area offers options to help determine the slices needed. The Filter Start and Stop Times may be used to exclude data at the beginning and/or end of the run. For example, if you wanted to exclude data from the first five minutes of a run due to the sample temperature not being stable, you would enter a value of 300 (seconds) in the Filter Start Time box. If these boxes are left blank, no part of the dataset will be excluded.

The Filter Generator Assistant is useful for looking at metadata saved in the raw data file to decide where and when to slice the data. Type the run number in the Run Number box and then hit the Load button. After a moment, the dropdown box to the right will populate with all the metadata variable names. Most commonly, sample temperature is the variable of interest, for which the log name is SampleTemp. Select a variable, and then hit the Plot button. In the MantidPlot window, the value of that variable will be plotted as a function of time. The locations of the blue dotted lines will auto-populate the Filter Start and Stop Times; be sure to remove these values if they are not what you want.

The first slicing option is to divide the data into even slices by time. In the 'Filter By Time' area, check the box and enter the desired time interval in seconds. The algorithm will take the data and create a series of datasets with the time interval specified, which will appear in the Workspaces area of MantidPlot.

Another option is to divide the data according to another variable, in the 'Filter By Log Value' box, which allows data to be sliced by any logged value embedded in the raw data. To use this mode, the box in this area must be checked. Log Name is the name of the variable by which to slice the data, e.g. SampleTemp for the sample temperature. Value Change Direction may be used to only consider changes where the log variable is increasing or decreasing. Log Step Size determines the coarseness of the slicing. For example, when slicing by sample temperature, entering a value of 5 will divide the data into individual datasets each covering 5 degrees of temperature range. The Log Boundary may be either Centre or Left. The other fields may be left blank to use the default values.

Take Note

Be aware of the interaction between the Log Boundary and the Minimum and Maximum Log Values and check the sample logs of the generated workspaces to ensure that the log value ranges covered are as desired. For example, using a step of 5K with a centre log boundary and a minimum log value of 10K will produce a first slice with T_{\min} of 7.5 and T_{\max} of 12.5, even if no data exists below 10K.

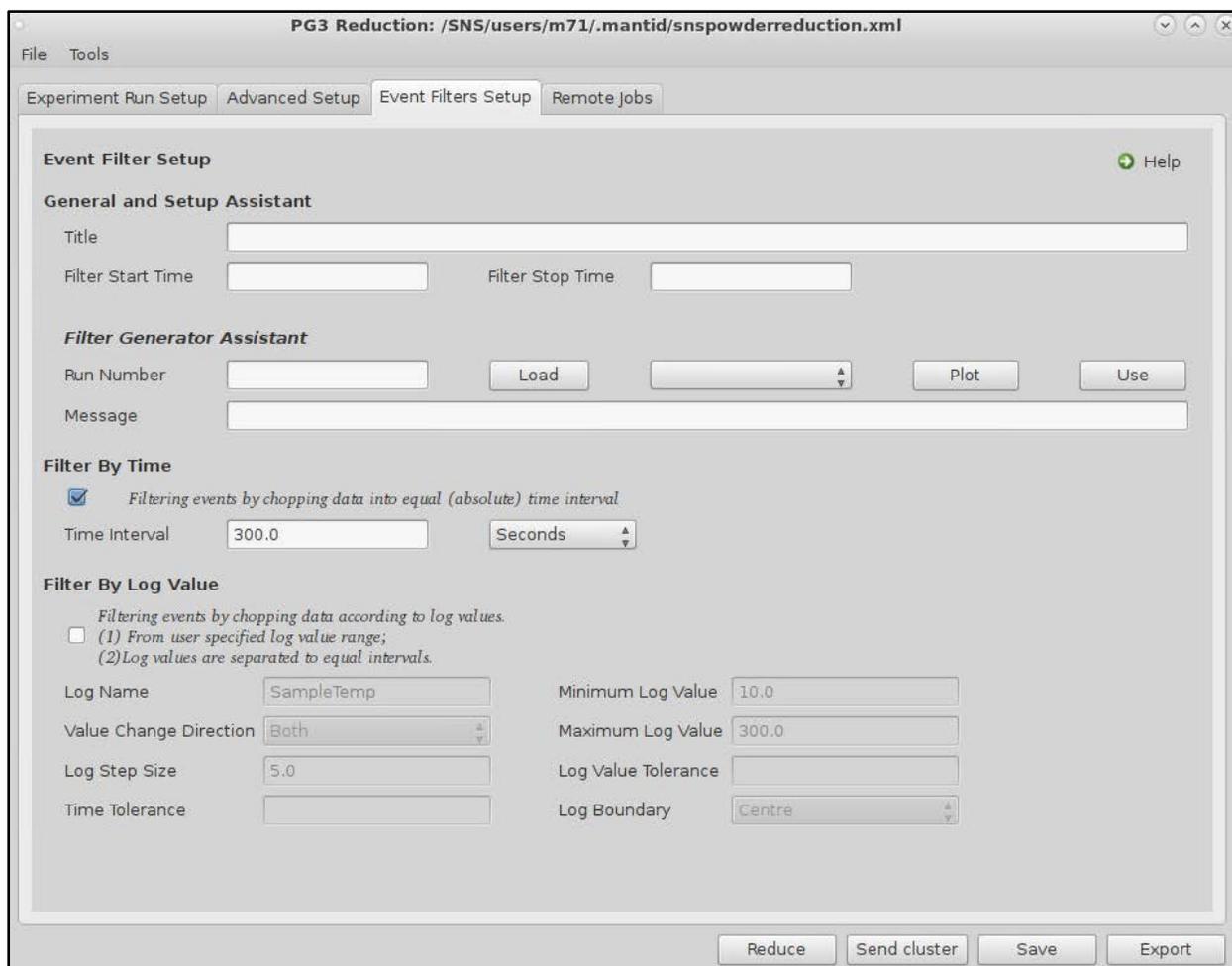


Figure 4. Event Filters Setup tab of the Powder Diffraction Reduction window.

No matter which slicing technique is used, the datafiles produced will appear as a split workspace in MantidPlot, under PG3_run-number_0_split (Figure 5). The individual slices will have _1, etc. appended to the run-number in order of increasing log value (not time) and may be viewed by expanding the split workspace with the + button. To plot an individual slice, right click on the desired slice and select Plot Spectrum. Currently, the intensities in the datafiles produced by slicing are not renormalized by proton charge correctly, so they may need to be rescaled (using the Mantid algorithm Scale) for comparison or an appropriate value for scaling used in the Advanced Setup pane. Multiple slices may be viewed in the same plot by right-clicking the split workspace and selecting Plot Spectrum for a simple overlay plot or Plot Advanced for more complex options, including waterfall, tiled, surface and contour plots, as discussed below.

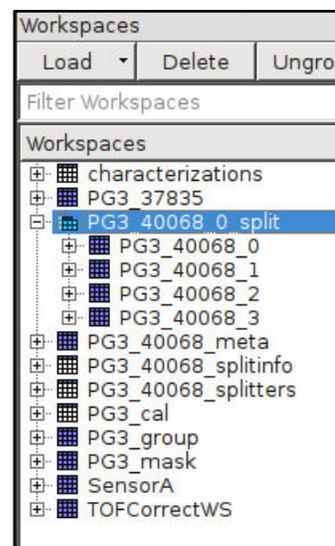


Figure 5. Workspaces list.

Data reduction for Pair Distribution Function (PDF) analysis:

You may also use MantidPlot to reduce data from Powgen into a format appropriate for pair distribution function (PDF) analysis. This procedure will use the Algorithms box in MantidPlot (Figure 6). Algorithms are small bits of code that typically take a few inputs and execute a single step. They are run by typing the algorithm name in the box and hitting the Execute button.

1. Execute the “LoadGSS” algorithm (Figure 6) in MantidPlot by typing the name in the algorithm box and hitting the Execute button. In the pop-up box, use the Browse button to navigate to the autoreduce folder for your proposal and select the desired autoreduced *.gsa data set. Give the dataset an appropriate name in the OutputWorkspace box and hit the Run button.
2. Execute the “ConvertUnits” algorithm (Figure 7). The InputWorkspace will be what you just loaded in step 1 above. If the OutputWorkspace is set to the same as the InputWorkspace, that workspace will be overwritten. If that is not desired, change the OutputWorkspace to something different. The Target should be **MomentumTransfer** and the EMode should be **Elastic**.
3. Plot the converted data by right-clicking on the workspace and selecting Plot Spectrum.
4. Press the Select Multiple Peaks toolbar icon , on top of the panel. The Fit Function sidebar will open, as in Figure 8.
5. Right-click on the plot and select Add background using a FlatBackground type (Figure 8). Drag the vertical blue dotted lines to set the fitting range to 30 to 50 Å⁻¹. Press the Fit button and select Fit to fit the background.
6. On the Fit Function sidebar, under f0-FlatBackground, record the fitted value A0 (Figure 9).
7. Execute the “Scale” algorithm (Figure 9) to divide the data by A0 (by multiplying by the inverse). The InputWorkspace should be the converted workspace from step 2 above. Give the OutputWorkspace a different name if you do not wish to overwrite. The Factor should be a value equal to 1/A0 and the Operation should be **Multiply**. This should result in a spectrum that goes to a value of 1 in the range of 30-50 Å⁻¹.
8. Execute the “PDFFourierTransform” algorithm (Figure 10). InputSofQType should be **S(Q)** and PDFType should be **G(r)**. Select appropriate values of Qmin and Qmax. Using the Keep Open checkbox will allow you to easily test different values of Qmin and Qmax.
9. Execute the “SavePDFGui” algorithm (Figure 11), which will generate a *.gr file formatted for the PDFGui program with the relevant header for neutron data.

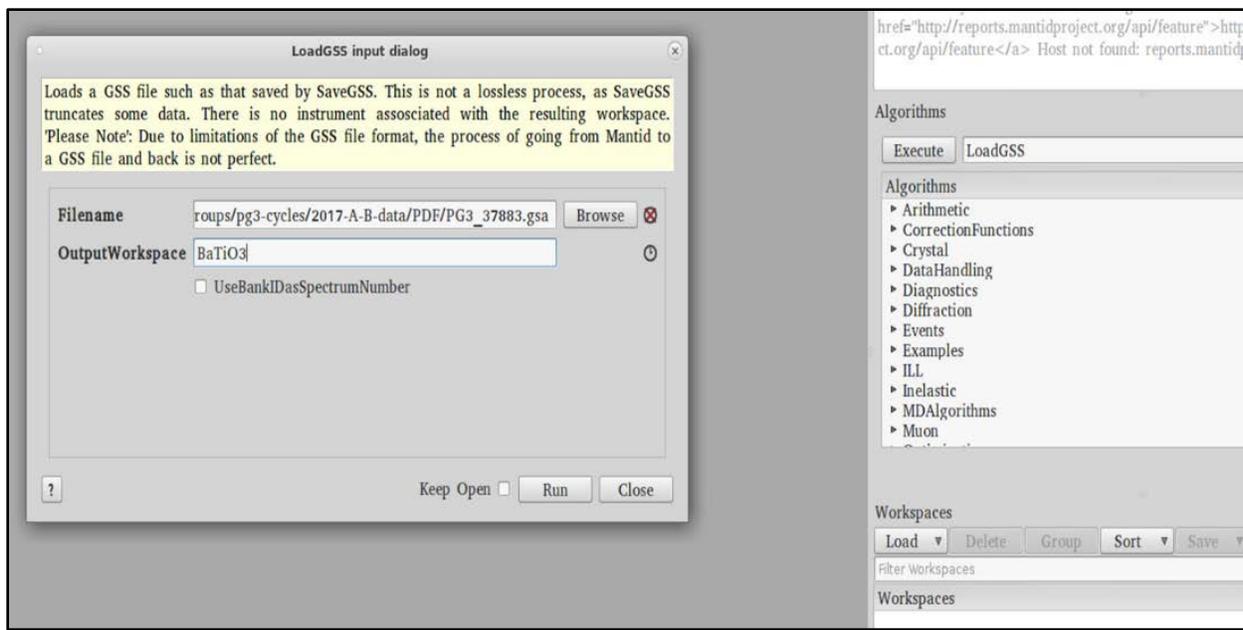


Figure 6. Main MantidPlot window, showing the Algorithms box on the right and the LoadGSS dialog box.

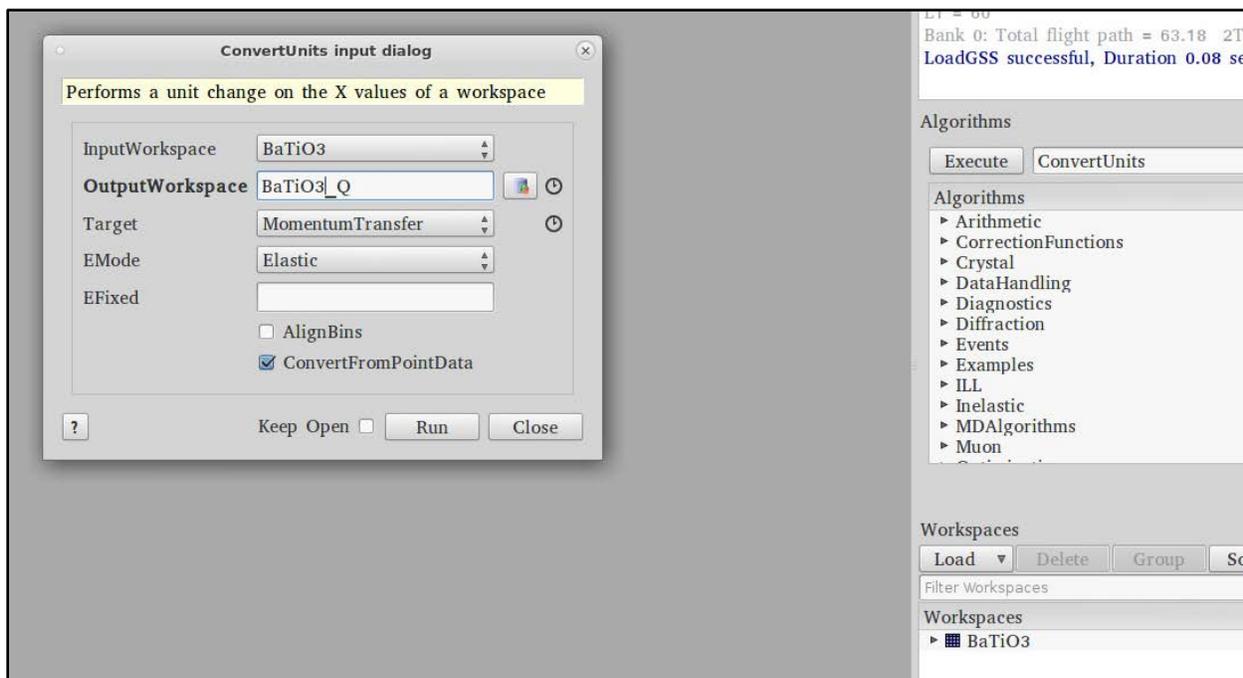


Figure 7. ConvertUnits dialog box.

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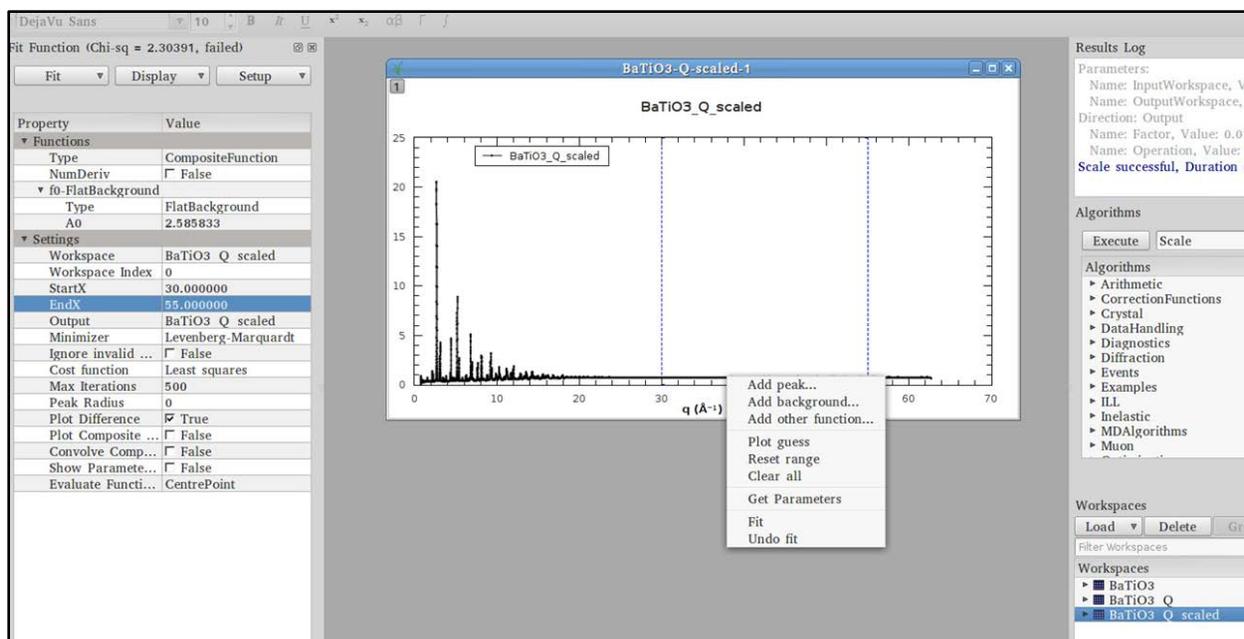


Figure 8. Fit function sidebar and plotted data.

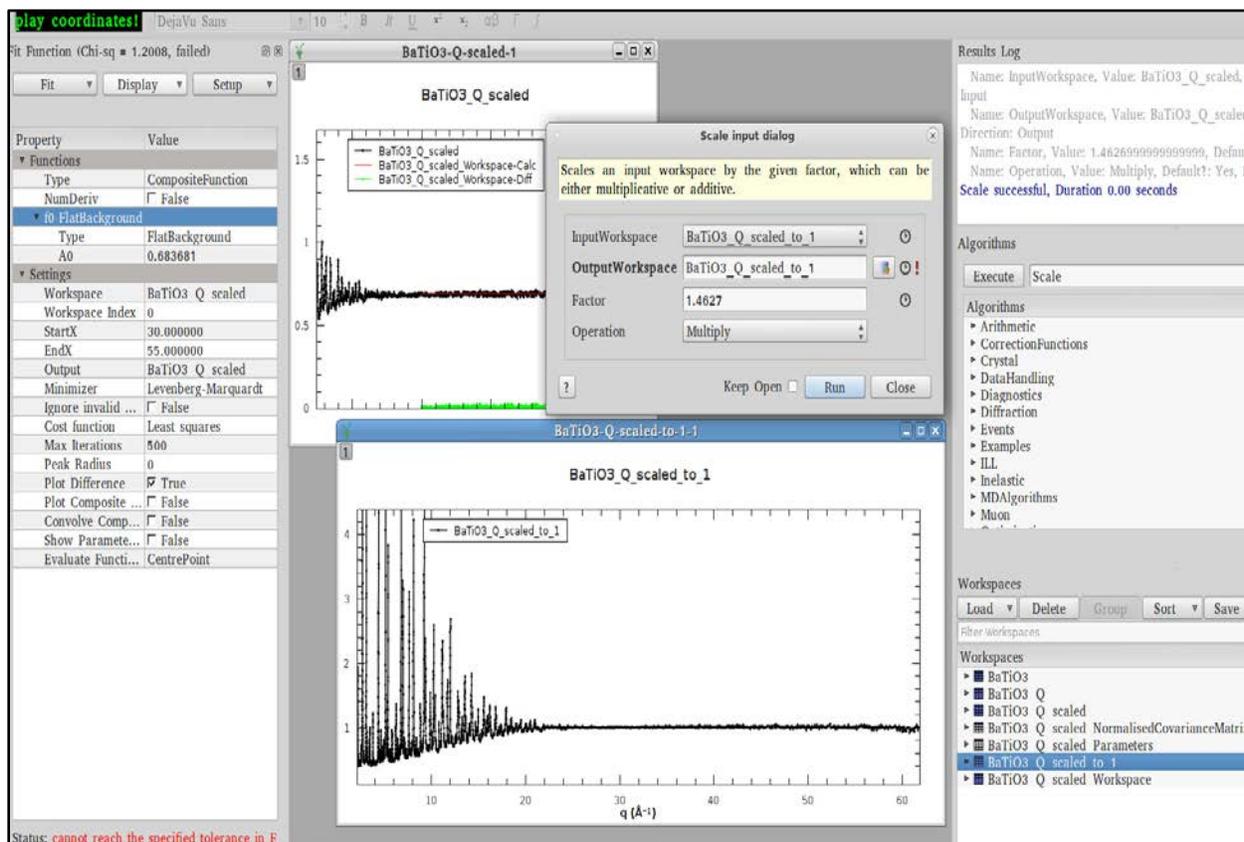


Figure 9. Scaling the data according to the background fit.

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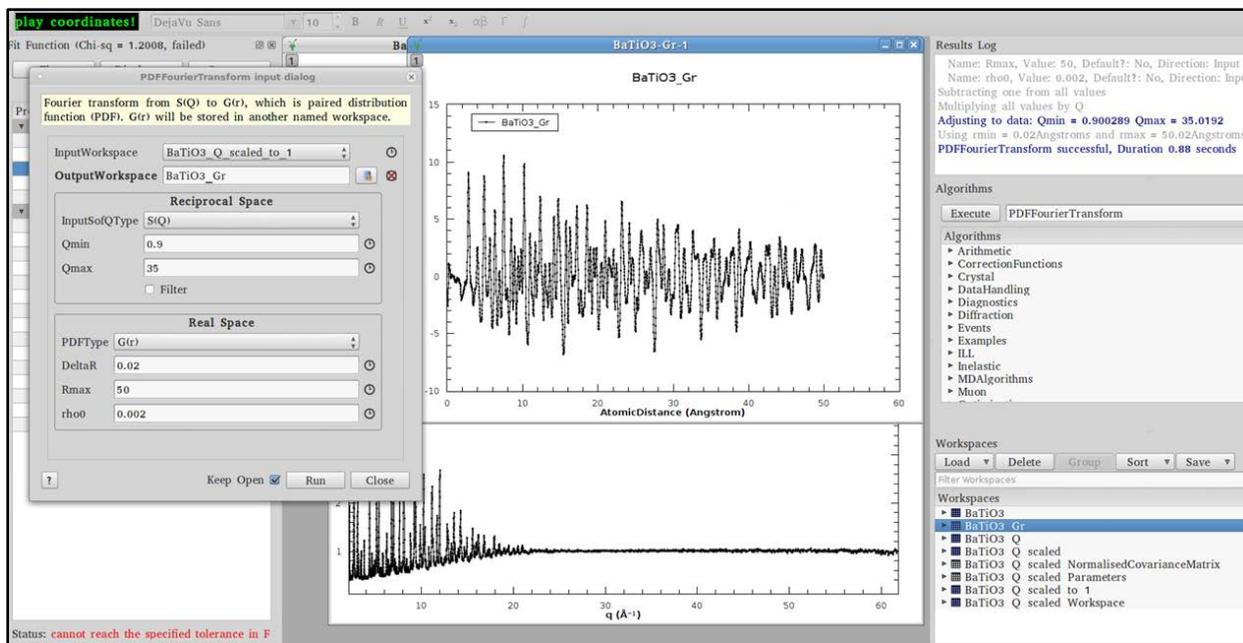


Figure 10. PDFFourierTransform dialog box.

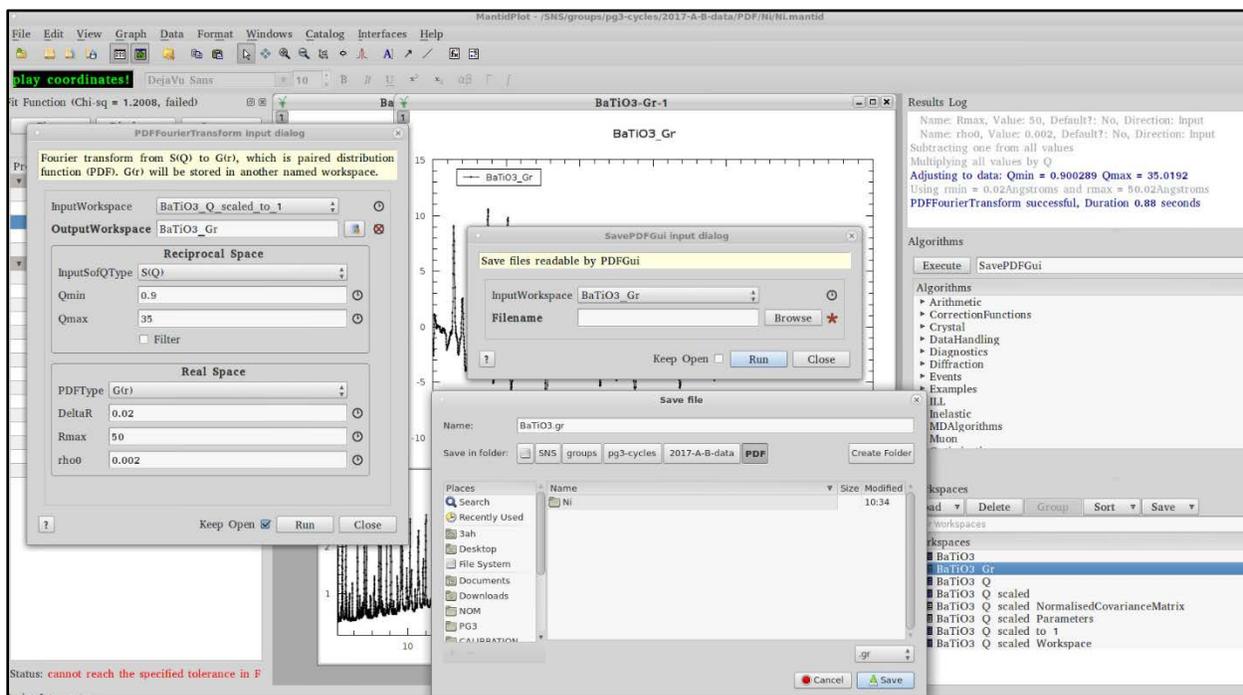


Figure 11. SavePDFGui dialog box.

Plotting in MantidPlot:

Once runs have been reduced in MantidPlot, they will appear as workspaces in the Workspace list on the right side of the MantidPlot window. From here they may be easily plotted to look at the data. Right-click on the workspace and select Plot Spectrum (Figure 13). To overlay multiple plots, use the Shift or Ctrl keys to select multiple workspaces. Or you may simply drag and drop onto an existing plot. For navigating the plot, the plotting toolbar (shown below) contains the following options (left to right): select, pan, zoom in, zoom out, full zoom out, crosshairs, peak fit, add label, add arrow, add line, add function and add legend.



More advanced options are available for displaying multiple runs in the same plot. In order to simplify analysis, you may group the runs together. Select all the runs and press the Group button. For sliced data, the runs will already be grouped. Select either the group or all the individual workspaces, then right-click and select Plot Advanced. Under Plot Type, select one of the available options. The first option, 1D Plot, is a standard overlay plot. Waterfall Plot displays the plots with adjustable offsets in the X- and Y-axes. Tiled Plot will generate separate subplots for each run. Surface Plot generates a 3D plot. Contour Plot generates a 2D color fill plot.

Other useful commands:

Other useful commands are below. In the Algorithms panel type in the following commands and hit return or click Execute.

- LoadGSS: This will load a GSAS file, plotted as a function of tof.
- ConvertUnits: To change the x-axis, e.g. to d-spacing.
- LoadMultipleGSS: Here a series of runs can be specified and plotted as a function of d spacing.
- LoadEventNexus: To look at any recorded log value (e.g. sample temperature), load the Nexus raw data file. Make sure to check Load Logs.
- Scale: To multiply all data points in a run by a constant value, or to add a constant value.

Many other algorithms are available. To learn more, go to the Mantid website.

http://www.mantidproject.org/Main_Page

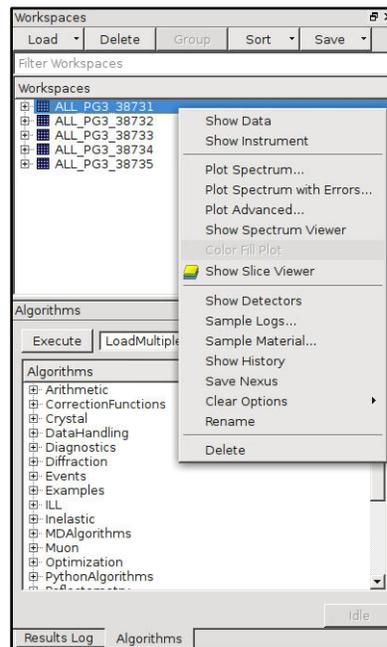


Figure 12. Plotting from the Workspaces list.