Powgen User Manual for Mantid Workbench

This user manual covers how to use Mantid Workbench with Powgen data. Mantid Workbench may be used to view, slice and reduce Powgen data. (Autoreduced datafiles are automatically generated as data are collected at Powgen and are immediately ready for analysis. However, you may wish in certain instances to work with the raw data using the Mantid Workbench program.)

This manual starts with a basic introduction to Mantid Workbench, followed by instructions on how to proficiently use the program for expeditious plotting of Powgen data. Subsequently, it provides a detailed description of the standard data reduction process for generating autoreduced datafiles, accompanied by guidance for manual data reduction utilizing custom settings. This manual further encompasses detailed instructions on how to slice data based on parameters such as time, temperature, or other logged variables. Instructions are also included on how to reduce Powgen data into a format suitable for Pair Distribution Function (PDF) analysis and how to apply an absorption correction.

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1. Mantid Workbench Basics

Mantid Workbench may be accessed on our analysis machines, which are available on-site via dedicated machines (`bl11a-analysis1.sns.gov` and `bl11a-analysis2.sns.gov`) in the instrument hutch, or outside the ORNL network via the analysis cluster (`analysis.sns.gov`).

1.1. Starting Mantid Workbench

1.1.1. Log into the analysis cluster at https://analysis.sns.gov/, using your UCAMS username and password, the same as for the proposal system IPTS.

1.1.2. Right-click on the desktop and open the command line by selecting *Open Terminal*.

1.1.3. Type in `mantidworkbench`, then press enter.

1.1.4. Once the welcome window appears (Figure 1), select *SNS* as the Default Facility and *POWGEN* as the Default Instrument.

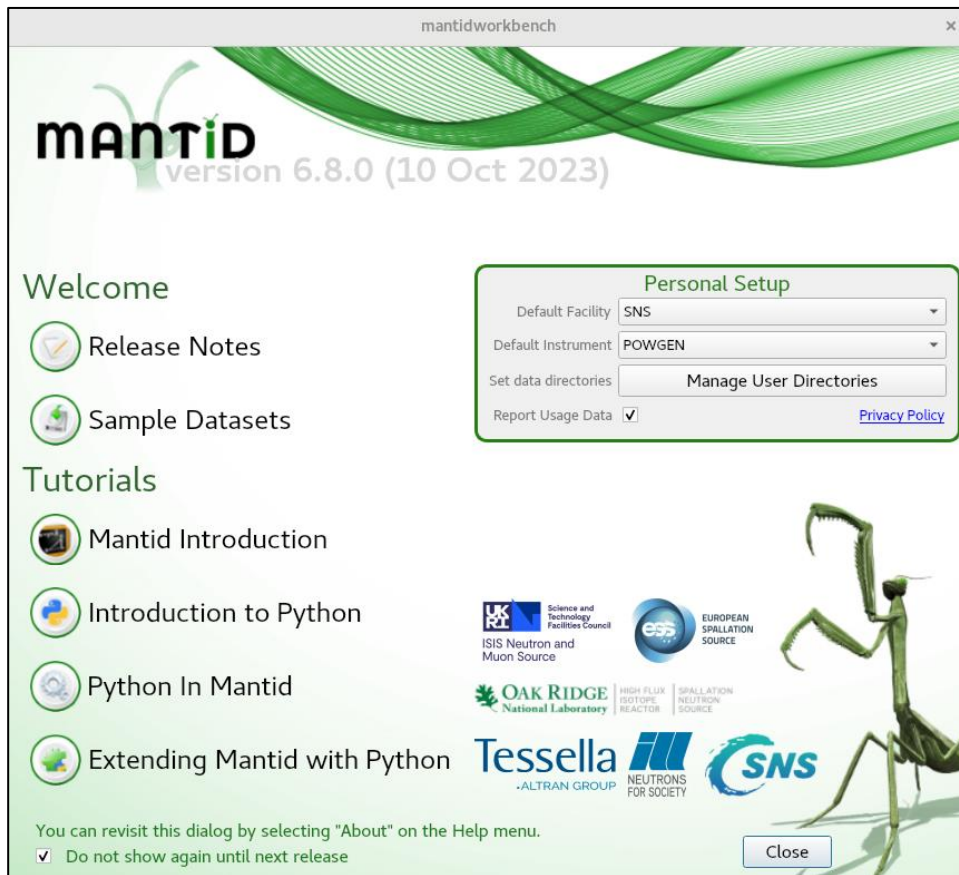1.1.5. Click the Close button in the welcome window to access the main interface of Mantid Workbench (Figure 2).

Figure 1. Mantid Workbench welcome screen. Select SNS as the default facility and POWGEN as the default instrument.

1.2. Main interface

1.2.1. The Workspaces pane is in the upper left. Once datasets are loaded, they will appear here.

1.2.2. The Algorithms pane is in the lower left. 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 pressing the Execute button.

1.2.3. The Plots pane is also in the lower left, accessible via the tab. As plots are generated, a list of them will appear here and you may show, hide or delete selected plots, as well as export image files.

1.2.4. The Editor/IPython pane is in the center. Most Mantid Workbench operations may be automated by writing Python-based scripts. Such scripts will not be covered in this document.

1.2.5. The Messages pane is on the right. As algorithms are run, any output or error messages will appear here.
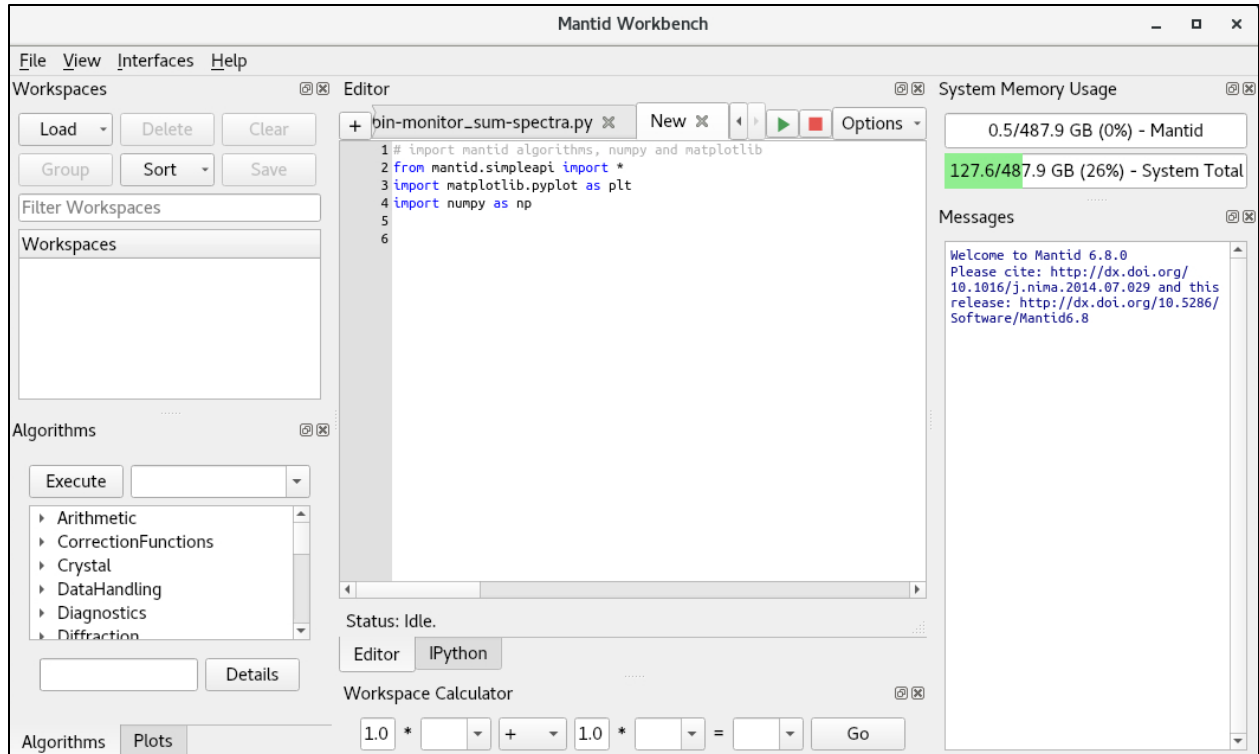
Figure 2. Mantid Workbench main interface, showing the Workspaces pane (upper left), Algorithms & Plots panes (lower left), Editor/IPython pane (center) and Messages pane (right).

2. Data Plotting

2.1. To plot data vs d

2.1.1. In the Algorithm pane, type `LoadMultipleGSS` and click Execute.

2.1.2. In the LoadMultipleGSS input dialog box (Figure 3), use Browse to locate the folder with the autoreduced datafiles, typically `/SNS/PG3/IPTS-XXXXX/shared/autoreduce`, where XXXXX represents the proposal number.

2.1.3. In the FilePrefix field, enter PG3.

2.1.4. In the RunNumbers field, add one or more run numbers separated by commas, or use a dash to indicate a range of run numbers.

2.1.5. Click the Run button to load the datafiles, which will appear in the Workspaces pane.

2.1.6. Right-click a datafile and select *Plot*, then *Spectrum* to view the data as a function of d-spacing (Figure 4). Alternatively, you may select *Spectrum with errors* to plot the data with error bars.

2.1.7. To overplot multiple runs, use the Shift or Ctrl keys, as usual for multiple selections, to select all the desired datafiles, then right-click and select *Plot*, then *Spectrum*. You may also click and drag a workspace onto an existing plot.
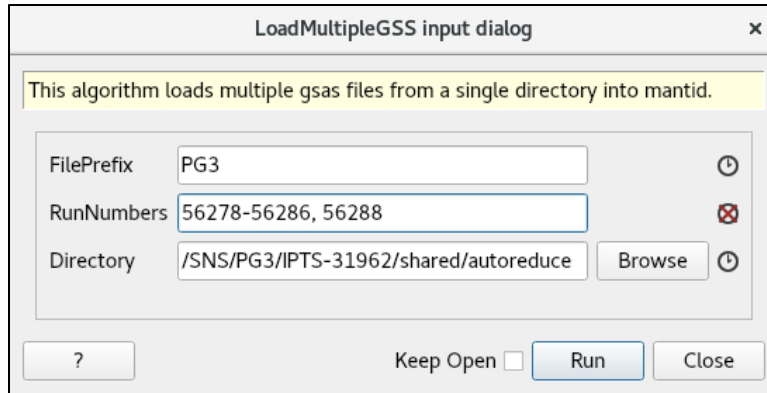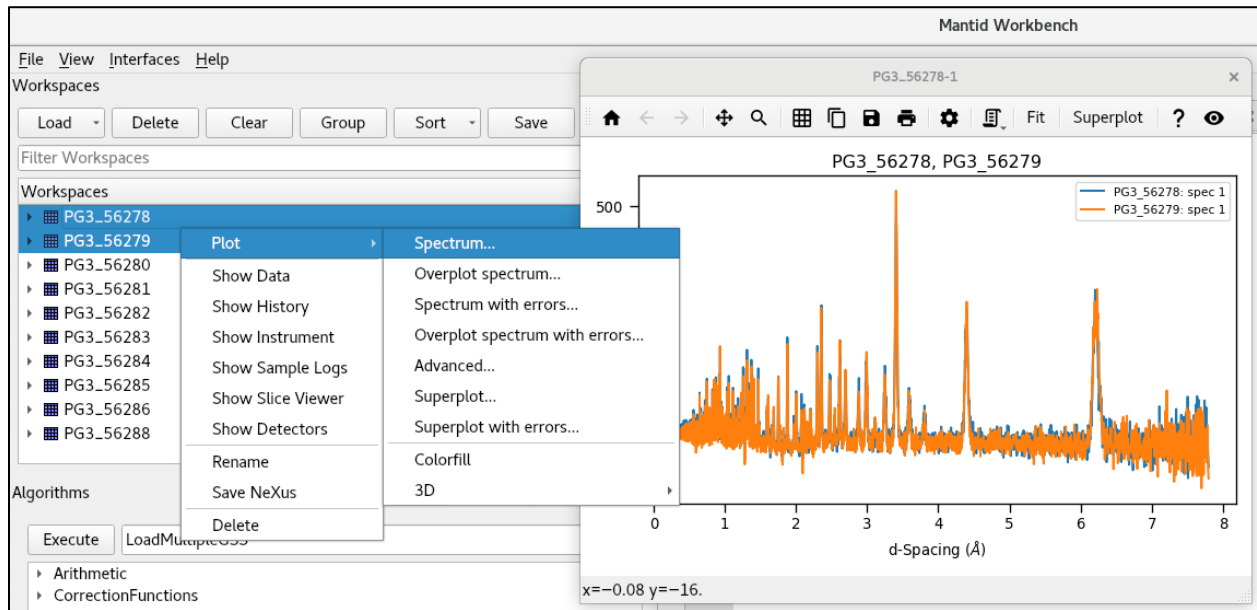
Figure 3. LoadMultipleGSS input dialog box.

Figure 4. Plot spectra by right-clicking selected workspaces and selecting *Plot* → *Spectrum*.

2.2. To plot data as a function of Q

2.2.1. In the Algorithms pane, type `ConvertUnits` and click Execute to open the ConvertUnits input dialog box (Figure 5).

2.2.2. Select the spectrum to be converted in the InputWorkspace field.

2.2.3. Give a name for the converted spectrum in the OutputWorkspace field. If this is the same as the InputWorkspace, the original spectrum will be overwritten.

2.2.4. Convert to Q by selecting *MomentumTransfer* in the Target field. Other parameters should be left at the default values.

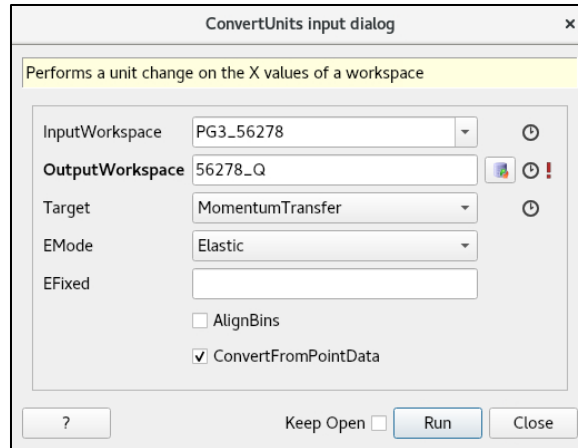2.2.5. Click Run to execute the algorithm.

Figure 5. ConvertUnits input dialog box with options to convert to Q selected.

2.3. To make a waterfall plot

2.3.1. In the Workspaces pane, use the Shift or Ctrl keys to select the individual datasets you would like to plot together. Alternatively, if the datasets are already grouped, such as the output of data slicing as covered in section 4, just select the workspace group.

2.3.2. Right-click on a highlighted workspace and select *Plot → Advanced*.

2.3.3. In the Plot Advanced dialog box (Figure 6), next to Plot Type, select *Waterfall*.

2.3.4. Press the Plot All button, and a waterfall plot will be generated.

2.3.5. The x- and y-offset between curves may be changed with the *Adjust curve offset %* button |↔|, on the plot toolbar.
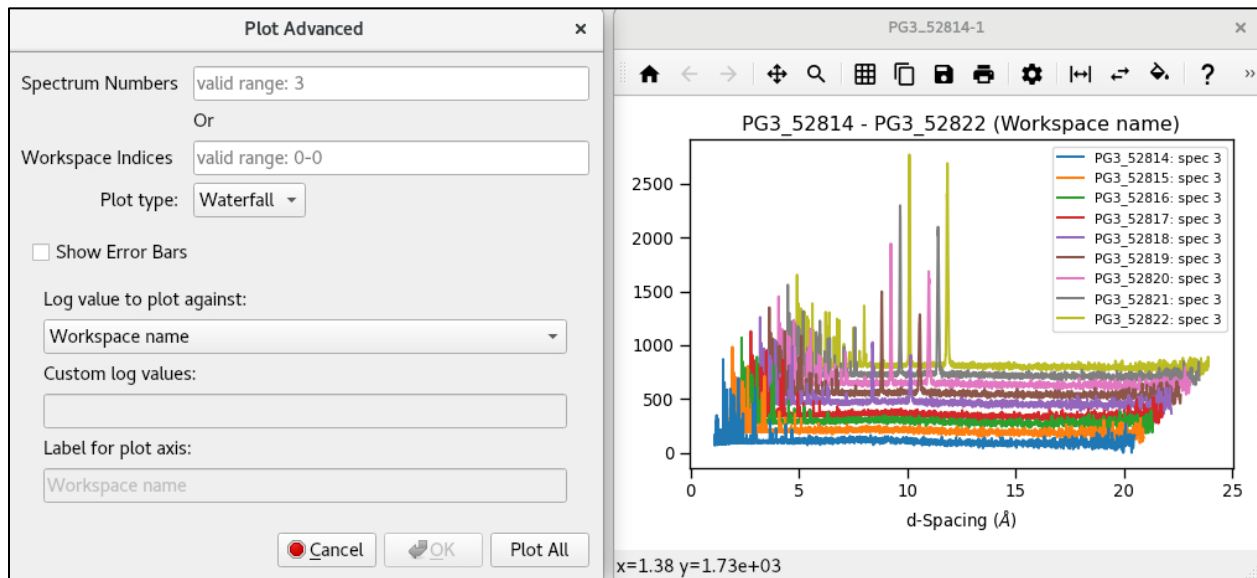

Figure 6. Plot Advanced dialog box (left) and example waterfall plot (right). Open the Plot Advanced dialog box by right-clicking the selected workspaces and selecting *Plot → Advanced*, then select *Waterfall* from the Plot type dropdown selector and press the *Plot All* button.

2.4. To make a colorfill plot

2.4.1. If the datasets you wish to plot are in individual workspaces, then in the Workspaces pane, use the Shift or Ctrl keys to select the individual datasets you would like to plot together.

NOTE: If the datasets you wish to plot are already grouped together, such as the output of data slicing as covered in section 4, you may skip to step 2.4.4.

2.4.2. In the Workspaces pane toolbar, press the *Group* button. The selected workspaces will be collected in a *NewGroup*.

2.4.3. Right-click on the *NewGroup* and select *Rename* to give it a meaningful name (Figure 7).

2.4.4. In the Algorithms pane, type `ConjoinSpectra` and click Execute to open the ConjoinSpectra input dialog box (Figure 8).

2.4.5. In the InputWorkspaces field, type the name of the workspace group containing the datasets to plot.

2.4.6. In the OutputWorkspaces field, give a name for the conjoined workspace.

2.4.7. Leave other fields at the default values. Press the Run button to run the algorithm. A new single workspace will be generated containing each dataset as a separate spectrum.

Figure 7. RenameWorkspace input dialog box.

Figure 8. ConjoinSpectra input dialog box.

2.4.8. Right-click on the new workspace and select *Plot* → *Colorfill* to generate a colorfill plot (Figure 9).

Figure 9. Colorfill plotting.

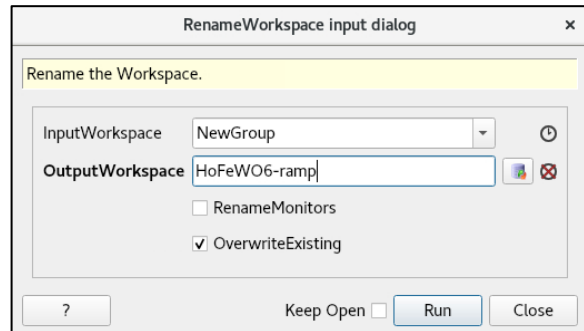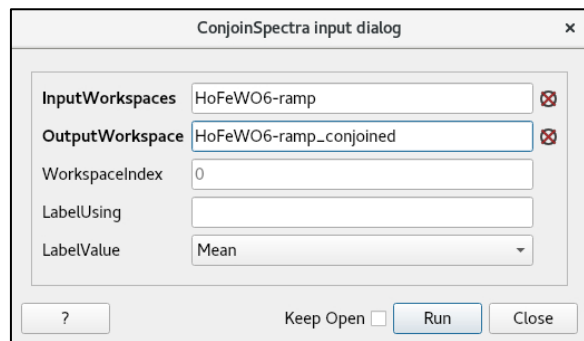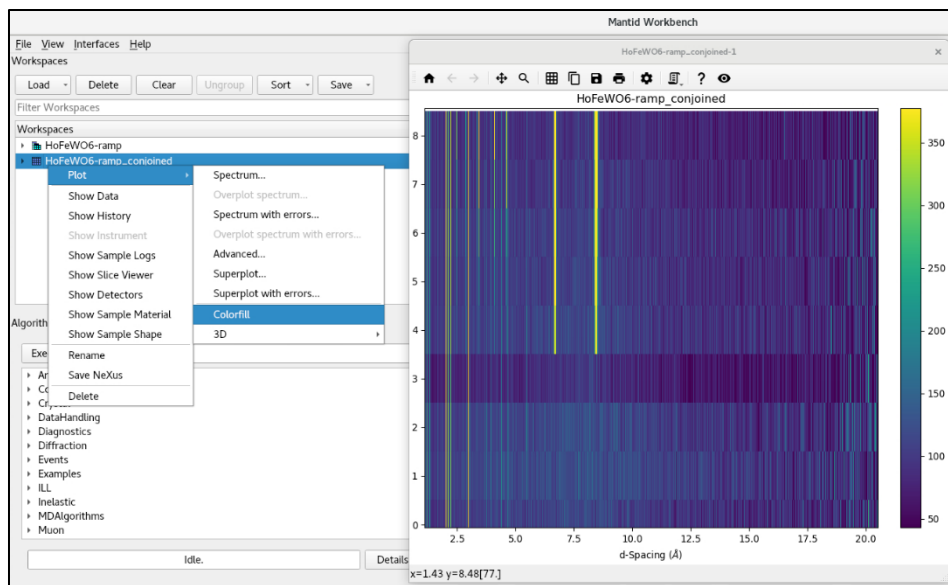## 2.5. To plot run metadata

2.5.1. Sometimes you may want to look at the sample logs during the run, for example the sample temperature. To view metadata associated with a run, first load the raw data (not autoreduced data) by typing `LoadEventNexus` in the Algorithms pane. (Note that workspaces generated by manual reduction, as in section 3, will also contain metadata. In this case, you may skip to step 2.5.5.)

2.5.2. In the LoadEventNexus input dialog box (Figure 10), select the appropriate *.nxs.h5 file with the Browse button, typically in the folder `/SNS/PG3/IPTS-XXXXX/nexus/`.

2.5.3. Make sure that the LoadLogs option is checked. Other options can be left at the default values.

2.5.4. Click the Run button to load the data.

2.5.5. Right-click the run in the Workspaces pane and select Show Sample Logs.

2.5.6. Select the desired metadata from the list on the left in the sample log window that pops up (Figure 11). For sample temperature, this is *SampleTemp*. A plot of the metadata vs time will appear on the right side of the window, along with some statistical data.

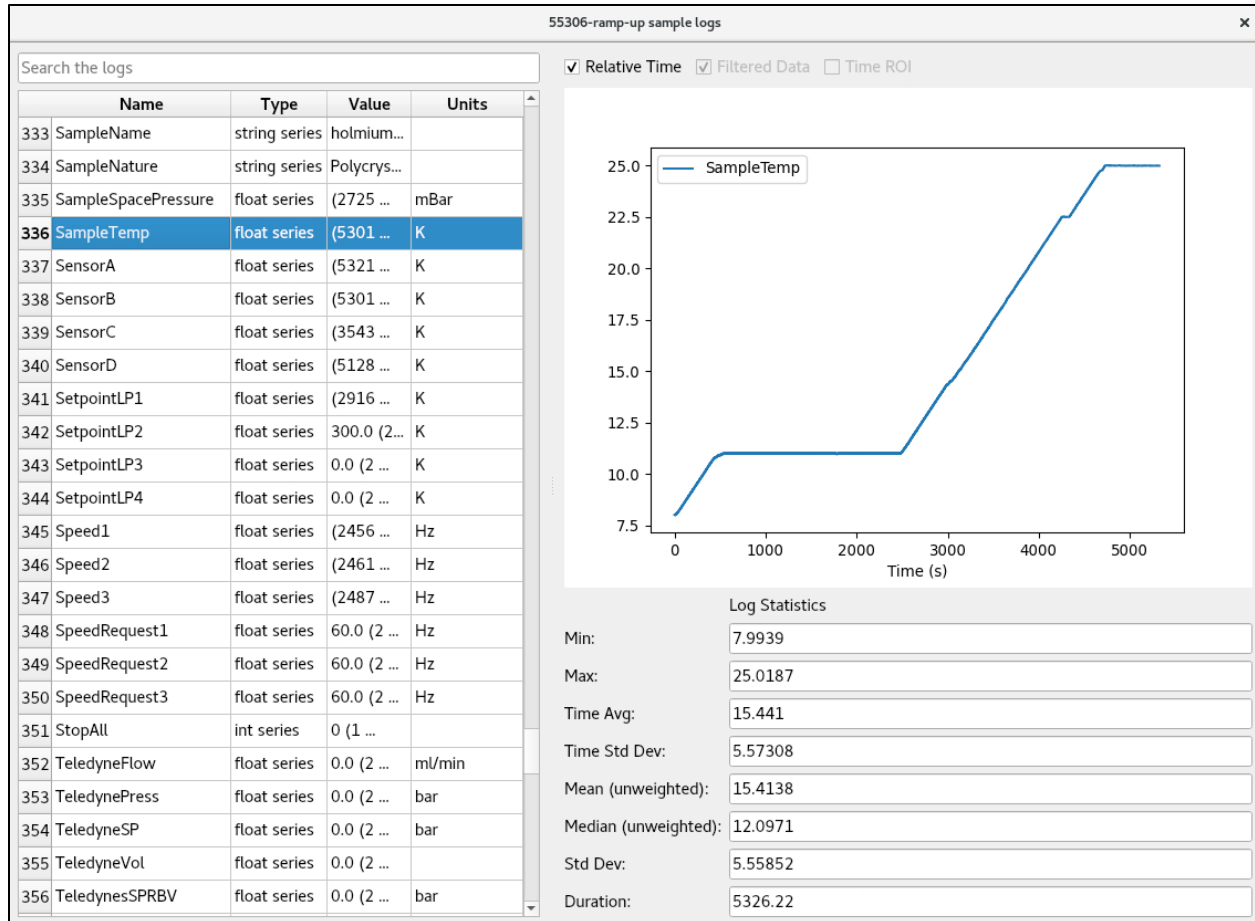Figure 10. LoadEventNexus input dialog box.

Figure 11. Sample logs dialog box, showing the list of metadata on the left side and a plot of the selected parameter on the right with some statistical data.

3. Manual Data Reduction

3.1. Power Diffraction Reduction interface

3.1.1. On the top menu bar in Mantid Workbench, select *Interfaces*, then *Diffraction*, then *Powder Diffraction Reduction* (Figure 12). This will launch the PG3 Reduction window.

3.1.2. Enter the appropriate parameters in the Experiment Run Setup tab (Figure 13), as outlined in section 3.2 below.

3.1.3. If desired, enter parameters in the Advanced Setup tab (Figure 14), as outlined in section 3.3 below.

3.1.4. Press the Reduce button. The reduced data will appear as a workspace in the Mantid Workbench window, along with some additional workspaces generated by the normalization procedure. You may plot the data or view metadata as explained in section 2.5 above.

Note:
Mantid Workbench 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 by restarting Mantid Workbench. However, you will have to regenerate your workspaces.
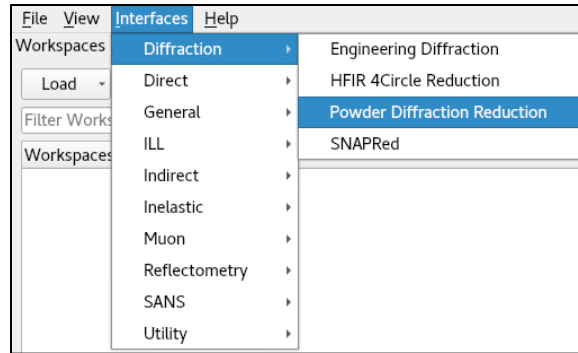
Figure 12. Select Interfaces --> Diffraction --> Powder Diffraction Reduction.
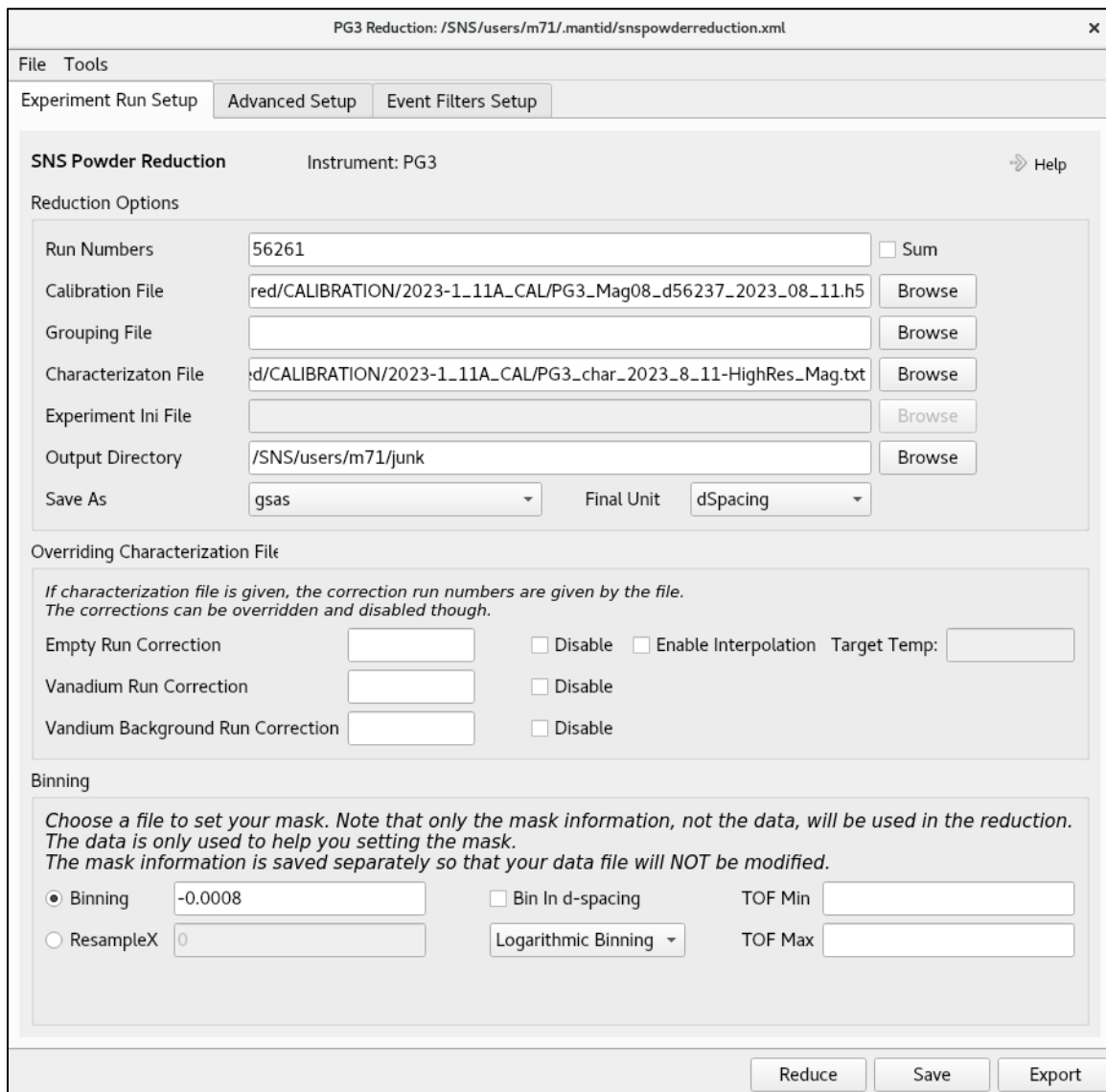

Figure 13. Powder Diffraction Reduction input dialog box, Experiment Run Setup tab.

3.2. Experiment Run Setup tab

3.2.1. *Run numbers*: This can be a single number, multiple numbers separated by commas and/or a range of numbers separated by a hyphen. For example, "`2346-2350, 2355`" is a valid entry. The Sum box should be unchecked to reduce each run separately. To sum multiple runs together, refer to section 3.4 below.

3.2.2. *Calibration File*: This file has an extension .h5 and is stored in the following folder: `/SNS/PG3/shared/CALIBRATION/ 20XX_[Cycle]_11A_CAL/PG3_[SE]dXXXX_date.h5`, where `20XX_[Cycle]` links to the time of the experiment with `[Cycle]` taking a value of 1 (A cycle) or 2 (B cycle), `[SE]` represents the sample environment equipment used (e.g. PAC for the sample changer or OC for the cryostat) and XXXX is the diamond calibration run number. Ask your local contact if you are not sure which calibration file to use.

> **Note:**
> Run numbers may be found from ONCat (https://oncat.ornl.gov, select *SNS*, then *PG3*, then search for your IPTS number) or from the runsummary files on the analysis cluster (`/SNS/PG3/IPTS-XXXXX/shared/ autoreduce/ runsummary.csv`).

3.2.3. *Characterization File*: There are two simple text files, in the same folder as the calibration file, that list all the instrument standard vanadium and background information, as well as defining the time-of-flight ranges for each bank. The first file should be chosen to match the sample environment used (e.g. PAC or OC) and the second one has a filename that ends in `_[SE]_limit.txt`. You must select both characterization files, using the Shift or Ctrl key, and click Open. Both filenames will be loaded into the Characterization File field. Ask your local contact if you are not sure which characterization files to use.

3.2.4. *Output Directory*: The directory into which the reduced file will be saved.

3.2.5. *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#]`, with extensions according to Table 1.

Table 1. Options for saving reduced data.

Save As	Analysis Program	Filename
fullprof	FullProf, JANA	`PG3_[run#].dat`
gsas	GSAS-II	`PG3_[run#].gsa`
nexus	-	`PG3_[run#].nxs`
pdfgetn	PDFgetN	`PG3_[run#].getn`
topas	TOPAS	`PG3_[run#].xye`

3.2.6. *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 specified here is only for plotting the data within Mantid Workbench.

3.2.7. *Binning*: Powgen uses logarithmic binning and the value here is log ($\Delta t/t$).

- *Binning*: A good starting point that works for most datasets is -0.0008. (In the Mantid framework, a negative bin size indicates logarithmic binning.) You can choose the value based on what is needed for your individual samples. To increase the number of points in each peak (finer bin, at the cost of statistics), use a smaller number (e.g. -0.0004) and vice versa for a coarser bin.
- *Bin In d-spacing*: This should be unchecked.

- *Linear/Logarithmic Binning* dropdown: *Logarithmic Binning* should be selected.
- *ResampleX*, *TOF Min* and *TOF Max*: These should be left blank.

3.2.8. Other fields: Other fields should generally be left blank to use the default values.

3.2.8.1. *Grouping File*: By default, all detectors are included. But a grouping file may be specified to include only a sub-set of detectors. For example, for the very highest resolution (at the expense of intensity), one can include only the in-plane detectors. Consult with your local contact if you want a special grouping of detectors.

3.2.8.2. *Experiment INI File*: This should be left blank.

3.2.8.3. *Overriding Characterization File*: These should generally be left blank and unchecked in order to use the values specified in the characterization files. If you specify a run number in the Empty Run Correction, Vanadium Run Correction and Vanadium Background Run Correction boxes, that run number will override the value given in the characterization file. Situations in which this is necessary include when the background runs are non-standard, e.g. quartz tubes in a vanadium can, or for temperature dependent runs in AGES. If you check the Disable boxes, the reduction algorithm will skip those steps entirely, generating a file without normalization and/or background subtraction.

3.3. Advanced Setup tab

3.3.1. *Output File Prefix*: You may specify a prefix to be added to the reduced data filename. This can be useful for differentiating datasets reduced with different settings.

3.3.2. *Scale Data*: Some Rietveld programs have issues with plotting tick marks if the data are too close to the zero baseline. Therefore, during autoreduction, the output intensity is multiplied by 100. You may specify a different multiplier value here.

3.3.3. *Background Smooth Parameters*: These parameters apply smoothing to the background run (i.e. the empty vanadium measurement, not the sample data). The parameter set of "5, 2" works best for standard vanadium cans. For AGES with quartz tubes, a parameter set of "40, 10" typically works best.

3.3.4. *Remove Prompt Pulse Width*: This should be 50, to eliminate the effect of very high energy epithermal neutrons on the data.

3.3.5. *Push Data Positive*: The default setting is *None*. Due to background subtraction, the intensities of individual data points can become negative, especially with highly absorbing samples or poor statistics. To counter this, you can either add a constant value to the spectrum so that all counts are positive (*AddMinimum*) or reset those negative numbers to Zero (*ResetToZero*).

3.3.6. *Offset Data*: This will add a constant value to the data and should generally be left at 0.

3.3.7. *FilterBadPulses*: The standard value is 95. This will filter out events measured while the proton charge is less than 95% of the average proton charge. You may use a lower value to filter out fewer events if the neutron beam power was not stable during the data collection.

> **Caution:**
> Using AddMinimum or Offset Data can alter the Rietveld goodness-of-fit parameters by effectively raising the background level for the whole pattern. In cases where there are large negative spikes at the edges of the data due to poor statistics, you should instead adjust the spectrum range to exclude the spikes by setting the TOF Min and TOF Max values, under Binning on the Experiment Run Setup tab.

3.3.8. *Preserve Events*: This should be checked.

3.3.9. *Strip Vanadium Peaks*: This should be checked. The next several fields, which are associated with cutting out the vanadium peaks and a smoothing operation, should be left empty (default).

3.3.10. *Absorption Correction*: This will apply an absorption correction to the data, particularly useful if your sample has moderately- to highly-absorbing elements. For more details, see section 6.

3.3.11. Other fields: Other fields should generally be left blank to use the default values.

- *Low Resolution Ref* & *Unwrap Ref*: These relate to time-focusing.
- *Maximum Chunk Size*: This sets the max chunk size during processing.
- *Mimumum* & *Maximum Cropped Wavelength*: These parameters change the neutron wavelengths to be included in the reduction. This is useful, for instance, when the resonance of elements (e.g. In, Ir or Er) in the sample is close to the incident spectrum.
- *Caching Options*: These relate to the calculations for the absorption correction.

Figure 14. PG3 Reduction input dialog box, Advanced Setup tab.

3.4. To sum scans together

With the Powder Diffraction interface, you may easily sum together multiple runs collected at the same conditions to improve the statistics. Follow the procedure in section 3.1.1 above, with the following changes.

3.4.1. In the Experiment Run Setup tab, in the Run Number field, input the run numbers you wish to sum together and check the box labeled Sum. As before, use commas and/or dashes to indicate ranges of run numbers.

3.4.2. In the Advanced Setup tab, in the Output File Prefix field, it is particularly important to input a filename prefix when summing runs to avoid overwriting other datafiles and causing confusion. If no prefix is specified, it will use the default filename of PG3_[run], where [run] is the <u>first</u> run listed in the Run Number field.

3.4.3. Also in the Advanced Setup tab, in the Push Data Positive field, it is important to select *None* when summing datafiles to keep the background consistent.

4. Slicing the Data by Time or Log Value

You may also slice a single run into multiple datasets according to metadata, such as time, sample temperature or any other log value that has been recorded.

4.1. Event Filters Setup tab

4.1.1. Open the Powder Diffraction Reduction interface (section 3.1) and complete the Experiment Run Setup (section 3.2) and Advanced Setup (section 3.3) tabs, as for standard data reduction.

4.1.2. Switch to the Event Filters Setup tab (Figure 15) to input parameters for data-slicing.

4.1.3. The Title field should be left blank.

4.1.4. 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 (units are seconds) in the Filter Start Time box.

> **Caution:**
> The values in the Filter Start and Stop Time boxes will be applied when filtering by time or by log value, or when doing a standard data reduction without slicing. If you do not want to exclude any data, please be sure to leave these two boxes blank.

4.1.5. The Filter Generator Assistant area is a useful tool for looking at metadata to decide where and when to slice the data.

4.1.5.1. Type the run number in the Run Number box. Note that this run is only used for the Filter Generator Assistant. The run listed on the Experiment Run Setup tab is what will be reduced and/or sliced.

4.1.5.2. Press the Load button. After a minute, the dropdown box to the right will populate with all the tracked variable names. The log name for sample temperature, the most common variable of interest, is *SampleTemp*.

4.1.5.3. Select a variable, and then press the Plot button. In the Mantid Workbench window, the value of that variable will be plotted as a function of time. The blue and green dotted lines are set by Filter Start Time and Filter Stop Time, respectively; only data between the dotted lines region will be processed.

4.1.5.4. To use the selected variable for data slicing by log value (as covered in section 4.3), press the Use button. The variable name will be copied to the Log Name field.
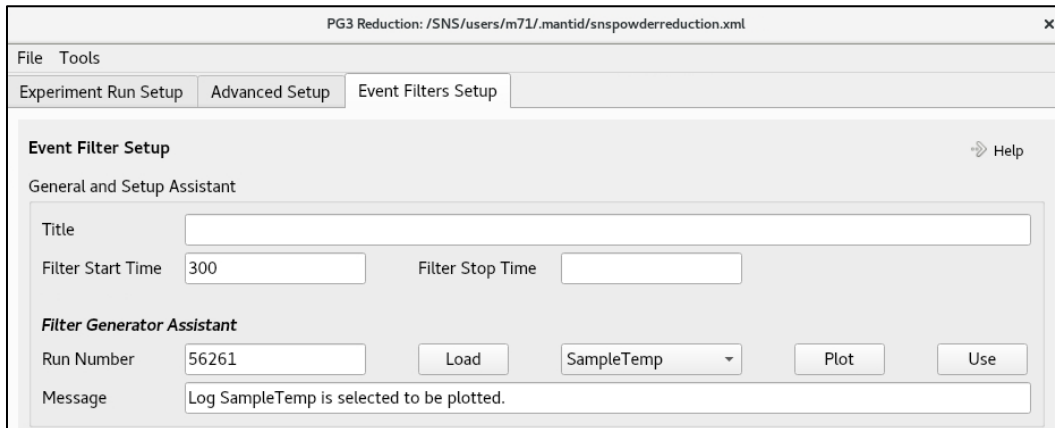

Figure 15. Top section of the Event Filters Setup tab of the PG3 Reduction input dialog box.

4.1.6. There are two options for slicing data, by time (covered in section 4.2) or by metadata (covered in section 4.3). Fields in one of these two areas must be completed to slice the data.

4.1.7. After pressing the Reduce button, the algorithm will execute, and several new entries will appear in the Workspaces pane. The datafiles will appear as a grouped workspace with the name PG3_[run#]_0_split. The workspace *_splitinfo records the correlation between index in the *_0_split workspace and the filtered values. The workspace *_splitters records the correlation between index in the *_0_split workspace and the log time, with nanoseconds as the unit.

4.2. Filtering by time

The first slicing option is to divide the data into even slices by time. In the *Filter By Time* area (Figure 16), check the box and enter the desired time interval. Make sure the appropriate unit is selected in the adjacent dropdown field. The algorithm will divide the run into a series of datasets with the time interval specified.
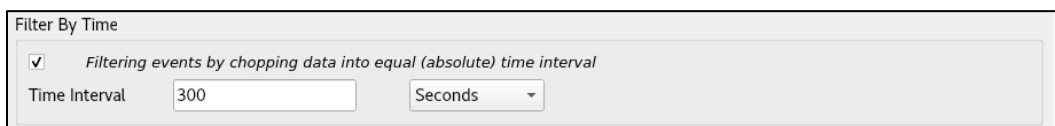
Figure 16. Filter By Time section of the Event Filters Setup tab of the PG3 Reduction input dialog box.

4.3. Filtering by log value

The second slicing option is to divide the data according to metadata, such as sample temperature. The slicing parameters are set in the Filter By Log Value area (Figure 17).

4.3.1. The box in this area must be checked to slice by metadata.

4.3.2. *Log Name*: This is the name of the logged variable to be filtered. The full list of names can be found using the Filter Generator Assistant as described in section 4.1.5 above.

4.3.3. *Value Change Direction*: There are three options: *Both*, *Increase* and *Decrease*. *Increase* will only slice the data when the log value increases, i.e. d(log value)/dTime is positive. *Decrease* will only slice the data when the log value decreases, i.e. d(log value)/dTime is negative. *Both*, which is the default value, will slice the data when the log value changes in either direction.

4.3.4. *Log Step Size*, *Minimum* & *Maximum Log Value*, *Log Value Tolerance*: These parameters combined control the log binning, i.e. how many and with what size the data slices are constructed. The Log Value Tolerance (default setting is blank) shifts the bin boundary further to the left. If no Tolerance is inputted, it defaults to half of the Log Step Size. Table 2 below provides a few examples. Please refer to this documentation on the Mantid algorithm [GenerateEventsFilter v1](#) for more detailed information.

Table 2. Examples of parameters for Filtering by log value.

Step Size	Min	Max	Log Value Tolerance	Log Bins
5	10	15	0	[10,15)
5	10	15	2.5	[7.5,12.5) [12.5,17.5)
5	10	15	blank (default to half step size, 2.5)	[7.5,12.5) [12.5,17.5)

4.3.5. Log Boundary: This should be set to *Left*.

4.3.6. Time Tolerance: This should be left as default, i.e. blank.

Figure 17. Filter By Log Value section of the Event Filters Setup tab of the PG3 Reduction input dialog box.

5. Manual Data Reduction for Pair Distribution Function (PDF) Analysis

Typically for unit-cell based analysis of PDF data, the autoreduced PDF data (*.getn) are ready for use. If you would like to re-reduce your data with different parameters, such as Qmin and Qmax, than the default values, you can follow the below procedure.

> **Caution**: A supercell-based approach following the reverse Monte Carlo routine usually requires an absolute scale, requiring further post-processing of the data that will not be covered in this manual. Users are strongly encouraged to read the following post to learn more about such post-processing. https://rmcprofile.ornl.gov/data-pre-processing-for-rmcprofile/

5.1. Execute the `LoadGSS` algorithm in Mantidworkbench by typing the algorithm name in the algorithm box and hitting the Execute button. In the LoadGSS input dialog box (Figure 18), use the Browse button to navigate to the autoreduce folder for your proposal and select the desired `*.gsa` file. The checkbox should be left unchecked. Give the dataset an appropriate name in the OutputWorkspace box and hit the Run button.
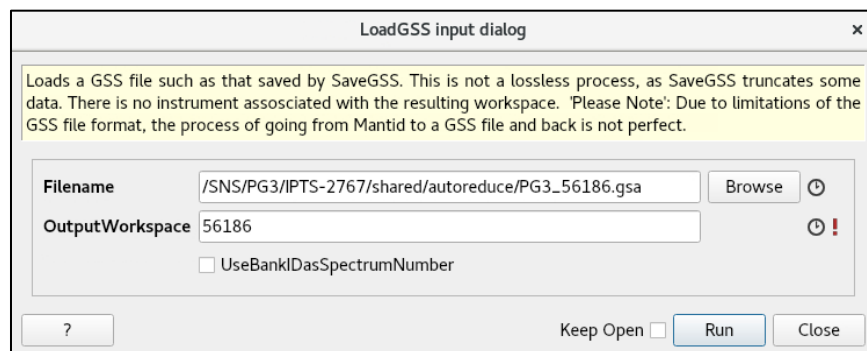

Figure 18. LoadGSS input dialog box.

5.2. Execute the `ConvertUnits` algorithm (Figure 5). The InputWorkspace will be what you just loaded in the step above. If the OutputWorkspace is set to the same as the InputWorkspace, it 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*. Other parameters should be left at the default values.

5.3. Execute the `Scale` algorithm (Figure 19). The InputWorkspace should be the converted workspace from the step above. Again, give the OutputWorkspace a different name if you do not wish to overwrite. The Factor should be `0.01` and the Operation should be *Multiply*. The purpose of this step is to reverse the scaling automatically applied during autoreduction as discussed in section 3 above.
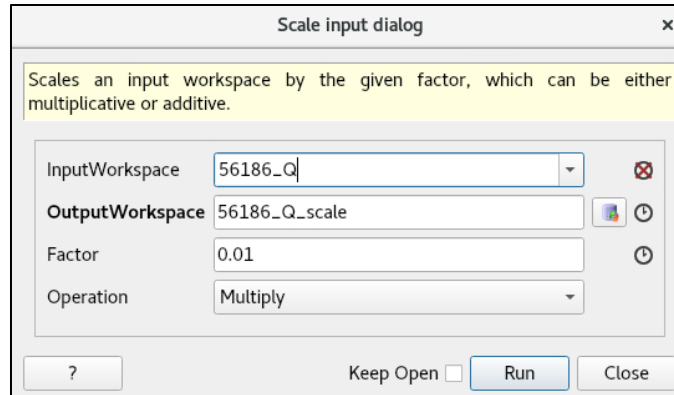
Figure 19. Scale input dialog box.

5.4. Plot the converted, re-scaled data by right-clicking on the workspace and selecting *Plot →
Spectrum*.

5.5. On the top of the plot panel, press the Fit button. The Fit Function sidebar will open (Figure
20). Right-click on the plot and select *Add background*, selecting a *FlatBackground* function
from the resulting dialog box. Drag the vertical green dotted lines to set the fitting range to 30
to 50 Å^{-1}. Press the Fit button and select *Fit* to fit the background.

5.6. On the Fit Function sidebar, under f0-FlatBackground, record the fitted value A0. Execute the
`Scale` algorithm again, this time to multiply the data by `1/A0`. This should result in the data
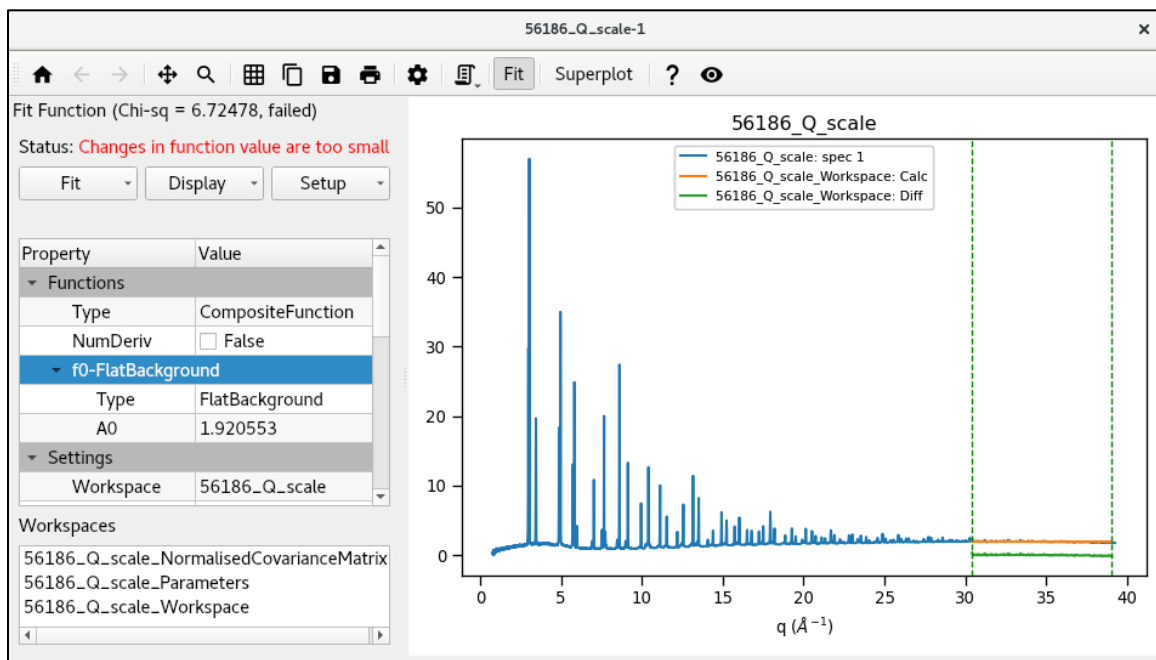going to a value of 1 in the range of 30-50 Å^{-1}.

Figure 20. Fit Function sidebar on spectrum plot, showing the FlatBackground fit.

5.7. Execute the `PDFFourierTransform` algorithm (Figure 21). InputWorkspace should be that
generated in the previous step. Give a name in the OutputWorkspace box. The field called
SofQType should be *S(Q)* and PDFType should be *G(r)*. Select appropriate values of Qmin and

Qmax. The other parameters should be left blank to use the default. Using the Keep Open checkbox will allow you to easily test different values of Qmin and Qmax.

Figure 21. PDFFourierTransform input dialog box.

5.8. Execute the SavePDFGui algorithm (Figure 22), which will generate a *.gr file formatted for the PDFGui program with the relevant header for neutron data.

Figure 22. SavePDFGui input dialog box.

6. Absorption Correction

Applying an absorption correction to your data is especially important for samples with elements that have significant absorption. The absorption correction can be applied during manual data reduction, on the Advanced Setup tab, in the Absorption Correction box (Figure 23). For more details, see https://powder.ornl.gov/bragg_diffraction/data_reduction/powgen.html#absorption-correction.

> **How absorbing is my sample?**
> Some common elements with moderate-to-high absorption include Li, In, Ag, Au, B and most of the lanthanides. Neutron absorption strengths for different elements may be found on the Addie website https://addie.ornl.gov/scatteringinspector.

6.1.1. *Sample Formula*: The elemental composition of your sample, with the elements separated by dashes. Isotopes are indicated by parentheses; otherwise, natural abundance will be assumed. For example, `La-(B11)6` indicates lanthanum hexaboride made with the ^{11}B isotope. Other examples of valid entries would include `C-H3-O-H` and `Ti-Al5.5-V4.5`.

6.1.2. *Measured Mass Density*: In units of g/cm^3.

6.1.3. *Number Density*: Theoretical number density, in units of Å^{-3}, which you may calculate from crystallographic information, e.g. from a CIF.

6.1.4. *Packing Fraction*: This is not an editable field. When both the measured mass density and the number density are given, the packing fraction field will be automatically calculated.

6.1.5. *Container Type*: Dropdown selection of the standard sample containers, which will read in the geometry information required for the absorption correction. *PAC06* is the standard 6mm diameter vanadium PAC cans, for example.

6.1.6. *Type of Correction*: Dropdown selection of alternate methods to calculate the absorption correction. The option *SampleOnly* is recommended for general use.

6.1.7. *Sample Height*: In units of cm. If no value is given, the program will attempt to read the value from the sample log metadata.

6.1.8. *Vanadium Rod Radius*: Radius in cm of the vanadium rod used for data normalization. The standard value at Powgen is `0.3175` cm.

Absorption Correction				
Sample Formula	Ba-Ti-O3	Measured Mass Density (g/cc)	3.23	Help
Number Density	0.0775	Packing Fraction	0.53816	
Container Type	PAC06	Sample Height		
Type of Correction	SampleOnly Help	Vanadium Rod Radius	0.3175	

Figure 23. Absorption Correction box on the Advanced tab of the PG3 Reduction interface.

7. Appendix

7.1. Frequently used algorithms

- `LoadGSS`: This will load an autoreduced GSAS file, plotted as a function of TOF.
- `LoadMultipleGSS`: This will load one or more autoreduced GSAS files, plotted as a function of d-spacing.
- `LoadEventNexus`: This will load the raw data, including metadata, and allows one to look at any recorded log value (e.g. sample temperature) as long as Load Logs is checked.
- `Rename`: This will change the name of a workspace.
- `ConvertUnits`: This will change the x-axis of a loaded run, between TOF, d or Q.
- `Scale`: This will either multiply all data points in a run by a constant value or add a constant value to all data points.

Many other algorithms are available. To learn more, go to the Mantid website.
https://www.mantidproject.org