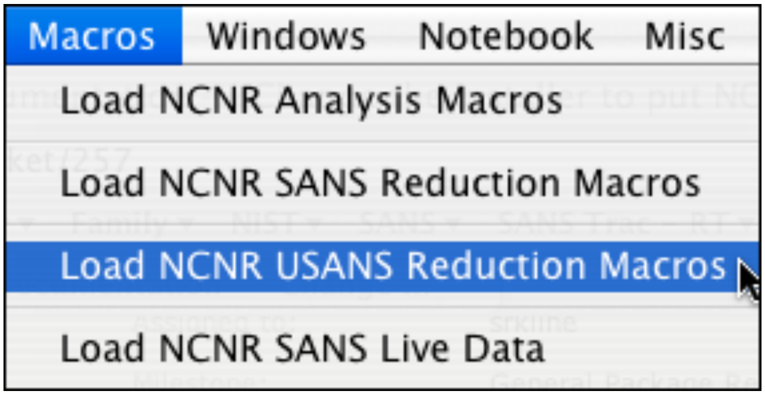
- **USANS Data Reduction**

12/2010 Vers. 2.3 (Package 7.04)
04/2010 Vers. 2.3 (Package 7.0)
03/2010 Vers. 2.3
03/2012 Vers. 2.3 (Package 7.10)

This implementation of the USANS data reduction procedures is designed to allow reduction of raw (ICP) scans from the BT5 USANS instrument into standard I(Q) format. The output corrected data is smeared with the resolution function of the USANS instrument, so called "slit-smeared" data. The USANS Reduction macros are designed to provide an easy to use, graphical interface for the reduction of raw data files into a portable ASCII format. The USANS macros and all raw ".bt5" data can be easily copied and carried to your home institution for convenient use. As of 10/2009, USANS Reduction macros require IGOR Pro v. 6.1x. As always, the macros will work with the free Demo version of IGOR.

Once the macros are installed, you can start a reduction experiment by selecting "Load NCNR USANS Reduction Macros" from the Macros menu:



If you use this software to reduce or analyze your data, please reference:

> "Reduction and Analysis of SANS and USANS Data Using IGOR Pro"
> S. R. Kline, *J. Appl. Cryst*. **39** (2006) 895-900.

Videos containing abbreviated instructions and more tips for use of the macros are available at the NCNR web site:
<http://www.ncnr.nist.gov/programs/sans/data/movies/reduction_analysis_movies.html>

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What's New (12/2010):

- Detector dead time has been updated as a result of a hardware change on 11/8/2010.

What's New (04/2010):

- Simulation of USANS data has been added. Similar to SASCALC for SANS, you can now adjust the angular ranges and steps, optimizing the instrument setup for the expected scattering of your sample. See UCALC and Simulation of USANS Data.

- Reduced 1D data is now written out in canSAS standard XML format.

- Individual raw (.bt5) files can be added together to improve statistics if a sample is re-measured at a single angular range. See Adding Raw BT5 Files.

- Two full data sets (all angular ranges) can be added together to improve statistics. See Adding Two Data Sets.

What's New (1/2007):

- Display of currently running dataset from BT-5 (when run at NCNR).

- Filtering of file list to show only files with a given prefix.

Overview of USANS

In general, a complete USANS measurement will require sample and empty cell scattering measurements as well as a background countrate. Scattering measurements are are typically broken into several files, each covering separate non-overlapping angular ranges (q-range). Since the intensity is measured across the central beam for both sample and empty cell scattering measurements, transmission information is implicitly included.

As data is collected during a USANS experiment, a copy of your data is mirrored to a central server, "Charlotte". This server is available through guest connections to PC's through the Network Neighborhood, and to Macs through AppleShare. This allows you to reduce your data from any location within the building. Your data will be located in a folder on Charlotte->ICP Data->bt5->yyyymm->month. "yyyymm" is the year and month of the beginning of the reactor cycle, and "month" is the month of data collection. The original data file remains on the instrument control computer as a backup. Raw ICP data files collected on USANS are denoted with the extension ".bt5". Data files are ASCII text containing header information followed by raw detector count values versus analyzer angle.

Data reduction procedures automatically detect the zero angle peak of the main beam, convert the angle into q (1/Å), and normalize to monitor counts and counting time. The transmission as measured by the analyzer (T_{Rock}) is determined by measuring the peak intensity with and without the sample: $T_{Rock} = I(peak)_{sample} / I(peak)_{empty}$. The transmission measured by the transmission detector is calculated again from the ratio of counts with and without the sample, this time with the analyzer detuned (angles greater than 2 °). $T_{Wide} = TRANS_{sample} / TRANS_{empty}$. Wide angles are used since the transmission detector countrate is attenuated at analyzer angles close to the main peak.

Data correction is made using the following relation:

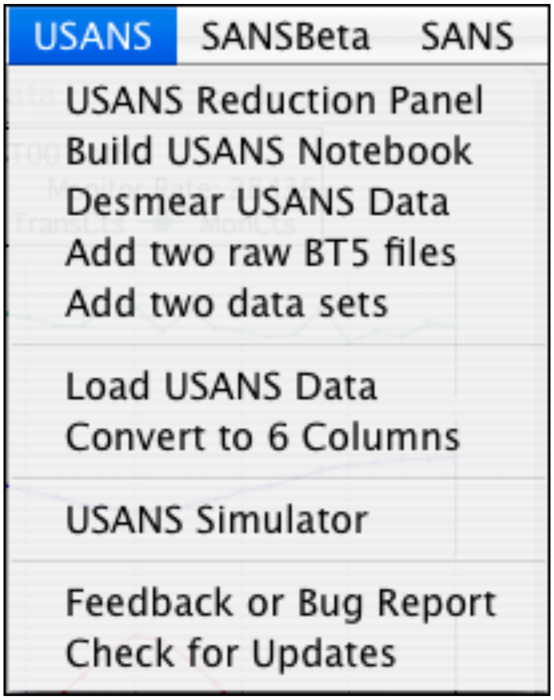
$$I_{COR}(q) = I_{SAM}(q) - T_{rock} I_{EMP}(q) - (1 - T_{rock}) I_{BGD}$$

Corrected data is converted to absolute scale by a conversion factor:

$$K = \frac{1}{I_{peak} T_{wide} d_s \Delta\Omega}$$

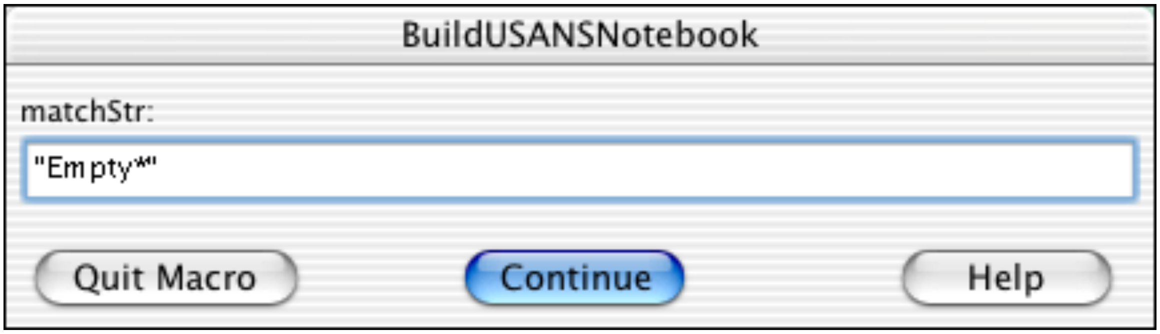
where d_s is the sample thickness in cm, and $\Delta\Omega$ = 7.1E-7 ster is the solid angle accepted by the analyzer. In general, if the ratio $T_{rock}/T_{wide} < 0.9$ this indicates a significant amount of multiple scattering. Please see your local contact.

USANS Menu



The USANS menu has only a few items:

1) USANS Reduction Panel: will call up the main reduction panel. This panel is automatically opened with a new experiment.
2) Build USANS Notebook: generates a notebook with a listing and brief description of data files in the specified data directory. Be sure to specify a match string with your file prefix and the wildcard character "*" to allow you to filter out files with a specified "prefix*", since the folder on Charlotte can be quite full.

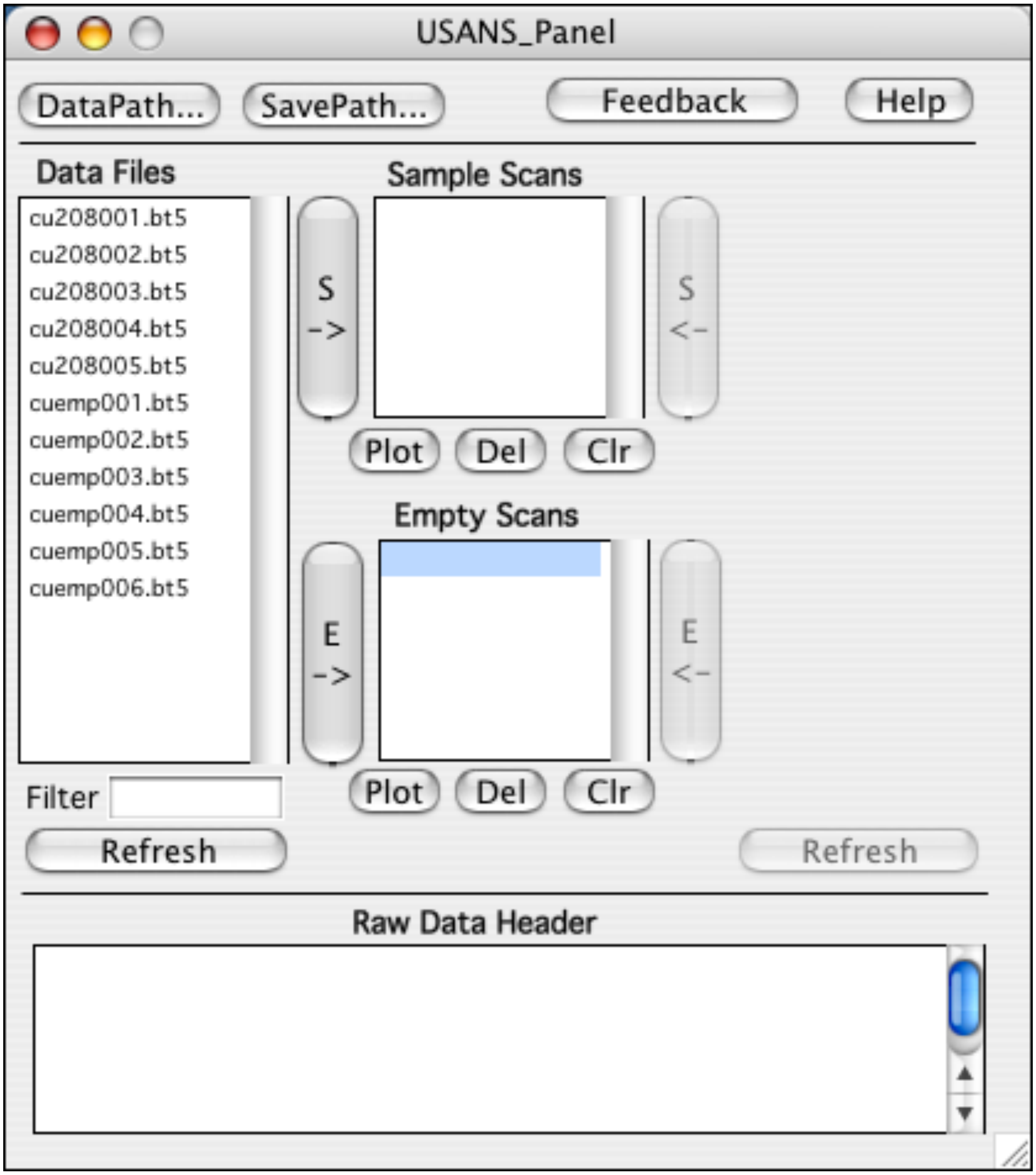


matchStr:
"Empty*"

3) Desmear USANS Data: described in detail below in Desmearing USANS Data
4) Add two raw BT5 files: for adding two .bt5 files that were collected at the same angular range. See Adding Raw BT5 Files.
5) Add two data sets: adds two full data sets. See Adding Two Data Sets.
6) Load USANS Data: Will load and plot corrected or desmeared USANS or SANS data (not for raw data).
7) Convert to 6 Columns: will take (old, pre Nov2004) 3-column USANS "COR" data set, and write out a new data file with 6-columns that is compatible with the SANS/USANS analysis package. The additional 3 columns will contain the slit height dQv = 0.037 (1/A). Data files more recent than Nov. 2004 will already be in the 6-column format with dQv = 0.117 (1/A)
8) USANS Simulator: allows comfiguration of the USANS instrument and simulation of what

scattering you can expect to measure for your sample. See Simulation of USANS Data.
9) Feedback or Bug Report: Opens a trac web page where you can report a bug or submit a feature request. You must be connected to the internet to reach the web page.
10) Check for Updates: If connected to the internet, this will check the NCNR server to see if there is an updated version of the macros. If there are, you can go to the web page and manually update.

Main USANS Controls



cu208001.bt5
cu208002.bt5
cu208003.bt5
cu208004.bt5
cu208005.bt5
cuemp001.bt5
cuemp002.bt5
cuemp003.bt5
cuemp004.bt5
cuemp005.bt5
cuemp006.bt5

The USANS_Panel will open automatically when the macros are loaded. Initially all of the list boxes will appear empty, and are waiting for data.

The controls on the panel are:

DataPath...: Use this button to select the folder containing the raw ICP data files.

This is typically the file server "Charlotte", in the correct subfolder of Charlotte:ICPData:BT5:

SavePath...: Use this button to select the folder on your local computer where corrected data is to be saved.

Help: Displays this USANS Data Reduction help file.

Refresh: Refreshes the file list from the folder chosen in "DataPath" in the case of the button below the Data Files list. In the case of the button below the Current Data list, a web page that downloads the latest data is launched using the default web browser. The system waits 20s for this to occur before updating the file list.

Filter: By entering the prefix of the data files you want to see and pressing refresh, the Data Files list will be limited to those files matching the filter string.

->S: Transfers the selected raw data files from the Data Files list to the list of Sample files. Does nothing more than copy the filenames.

->E: Same action as "->S", but adds to the list of Empty files.

<-S: Transfers the selected raw data files from the Current Data list to the list of Sample files. Does nothing more than copy the filenames.

<-E: Same action as "S<-", but adds to the list of Empty files.

Del: Deletes the selected file from the Sample (or Empty) file list, whichever list is adjacent to the button.

Clr: Clears all entries from the Sample or Empty files list, whichever list is adjacent to the button. This also clears SAM or EMP data from the COR_Graph, and clears COR data if necessary.

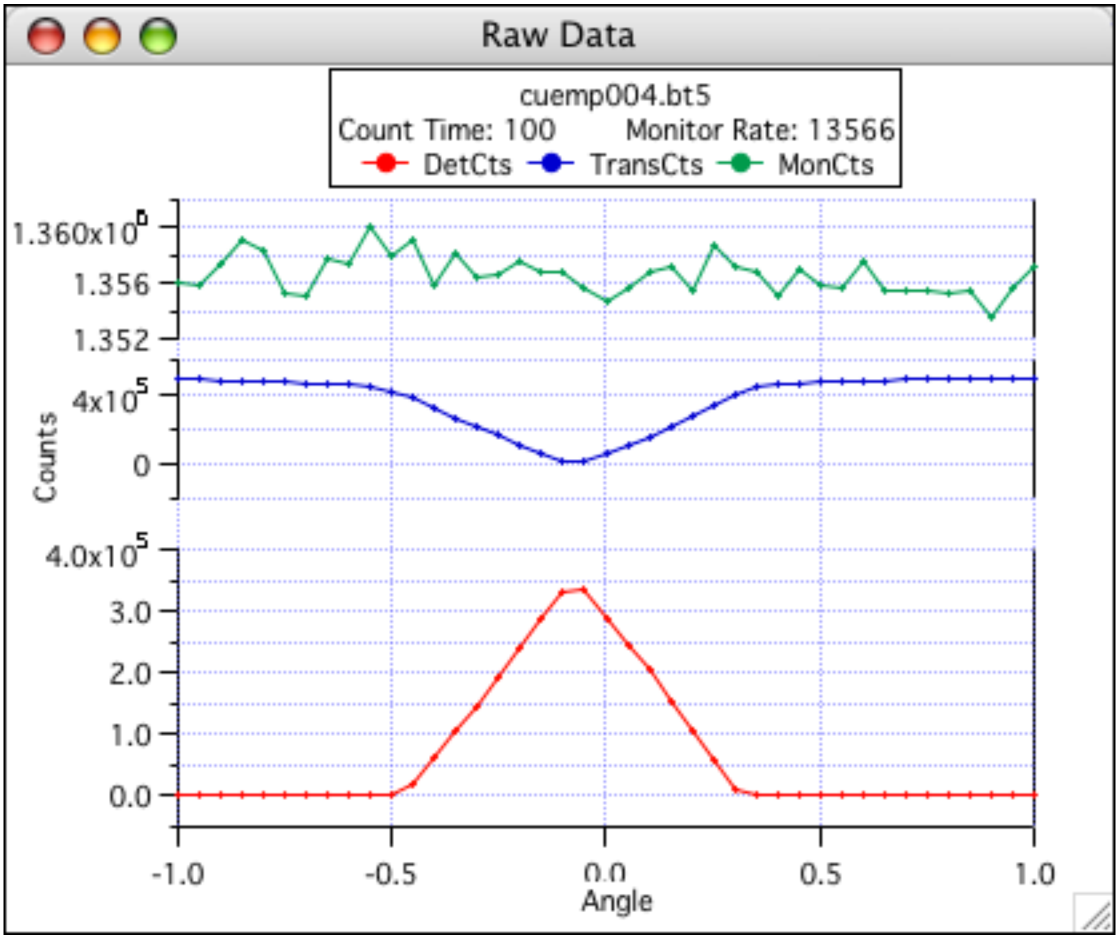
Plot: Plots the Sample or Empty files in the COR_Graph window. Before plotting the raw data, the zero angle is located, data sets are combined and normalized, and angle is converted to q-values (1/A).

- The raw data file list is limited to include only files whose name ends in ".bt5" indicating that they are raw USANS data files. Do not change the extensions of your raw data files, and do not use a ".bt5" suffix on your corrected datasets.
- The Raw Data Header automatically displays the header information of the selected raw data file. Filename, date/time of collection, sample title, counting time per point, and the angular range/step are listed. If there are multiple files selected, the header of the first file is displayed.
- A graph of the selected Raw USANS Data file is automatically plotted when a file is selected. The graph is automatically updated when a new file is selected.
- The Sample file list and the Empty file list do not need to have runs added in angular order. Files in the list will be combined and sorted by detector angle.
- There is a short sentence of help explanation associated with each button or control on the USANS_Panel and the COR_Graph. On windows, this text is displayed at the bottom of the screen when the mouse is over the control. On the Macintosh, text is displayed by balloon help,

which can momentarily be activated by holding down ctrl-opt-cmd.

Raw USANS Data

Selecting a raw data file produces a graph similar to the following:



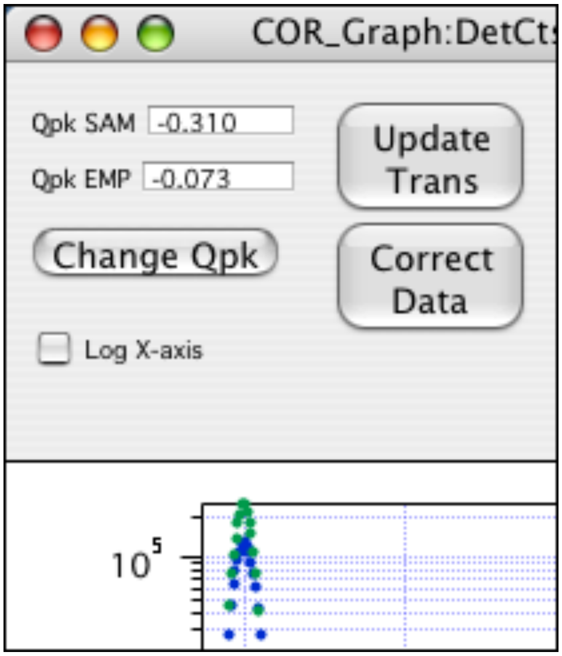
The three traces displayed are (top-to-bottom): Monitor Counts, Transmission detector counts, and Main Detector counts. Count values are not normalized and the error bar shown is due to counting statistics. Counts are plotted against the angle of the analyzer. This plot is useful for inspecting the contents and quality of a raw data file. It is automatically updated when a new raw data file is selected.

USANS Data Correction

Once you have identified the correct datasets for sample and empty scans by inspecting the file headers and the raw data, the following steps will guide you through the basics of reducing USANS data to a final I(q) format.

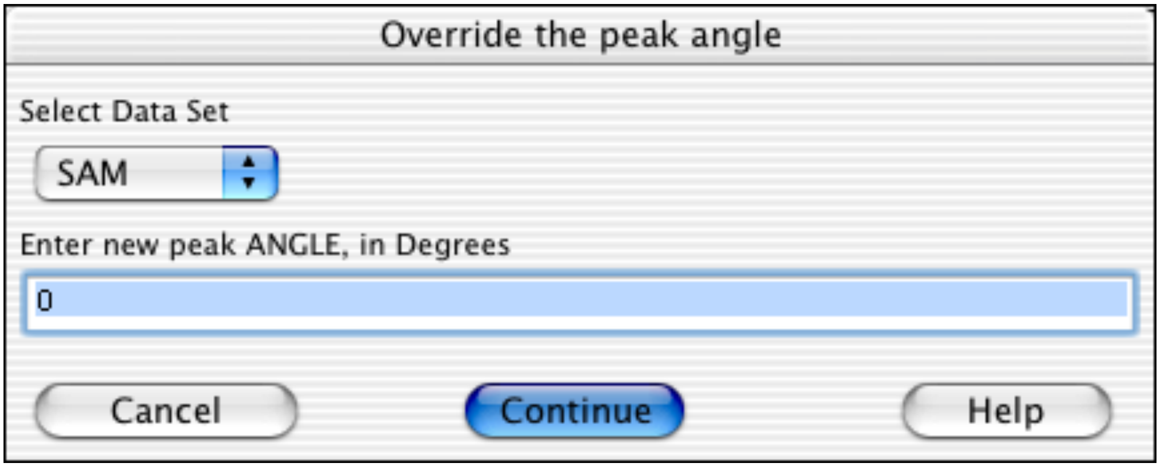
1) "Plot"-ing sample scans or empty scans will generate a "COR_Graph" window. During this step, the data is normalized to 1.0E6 monitor counts, shifted to zero angle, and converted to Q-values. The zero angle value for each dataset is found automatically, and is reported in the upper left of the control bar. Confirm that these values make sense, and that the peaks of the scattering data are correctly at zero Q on the graph. Tha automatically determined peak values

rarely need to be adjusted.



Qpk SAM -0.310
Qpk EMP -0.073

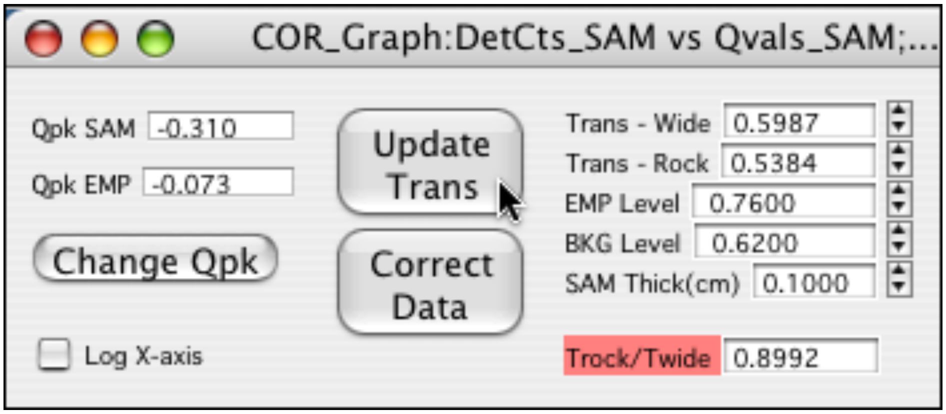
If peak of either file is not correct, inspect the raw data (See Raw USANS Data) to manually find a better peak position, and enter it manually by selecting "Change Qpk". You will be presented with the following dialog to change one of the peak angles. If both are incorrect, you will have to perform this operation twice.



Select Data Set SAM

Enter new peak ANGLE, in Degrees 0

2) Once the peak locations are satisfactory, calculate both the wide angle and peak transmissions by selecting "Update Trans". The calculated values are displayed to the right of the button. Make sure that the values are as expected. Updating the transmissions has no effect on the appearance of the graph.



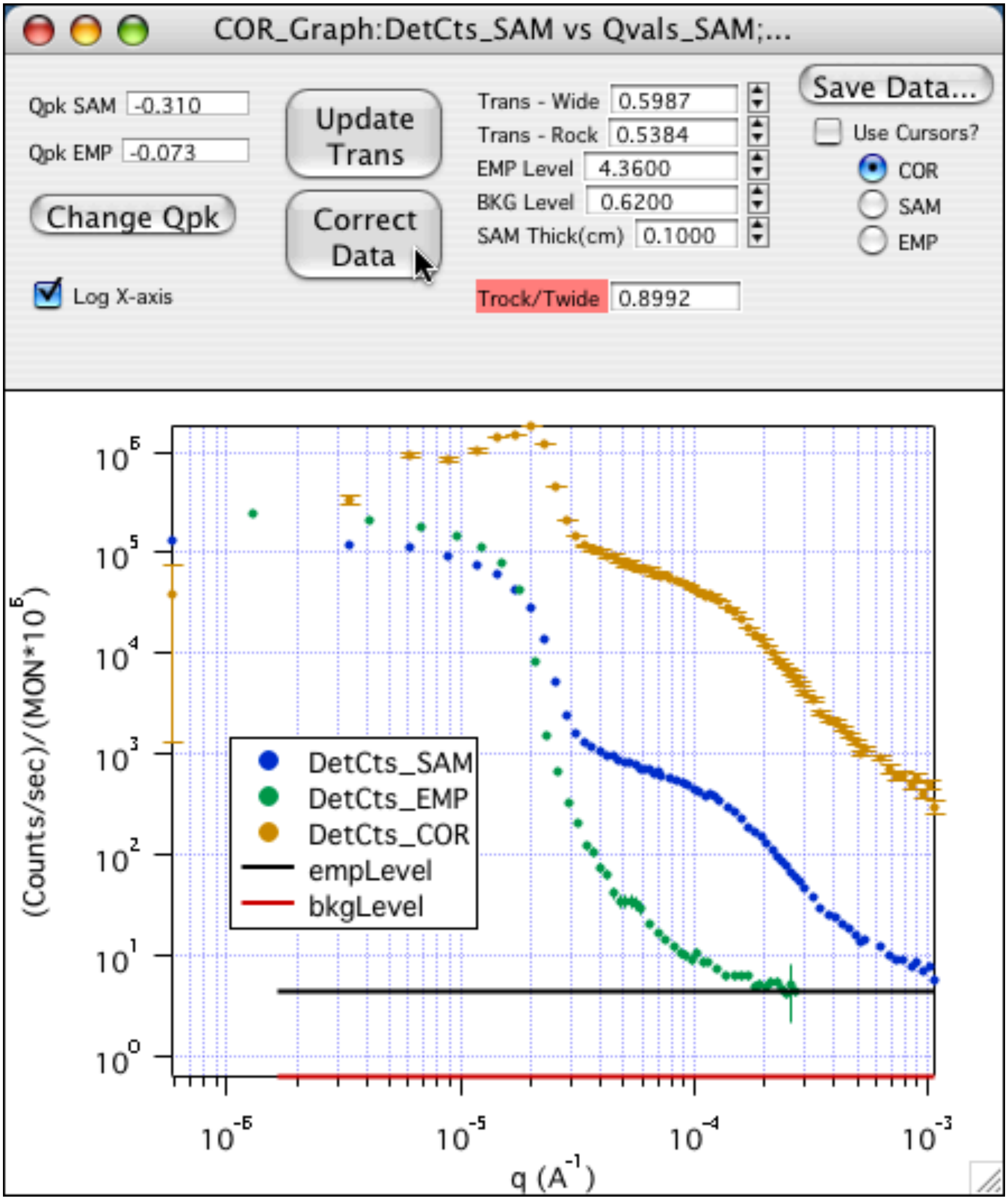
Qpk SAM -0.310
Qpk EMP -0.073
☐ Log X-axis
Trans - Wide 0.5987
Trans - Rock 0.5384
EMP Level 0.7600
BKG Level 0.6200
SAM Thick(cm) 0.1000
Trock/Twide 0.8992

Pay special attention to the Trock/Twide ratio. For this sample, it is highlighted in red, since the ratio is less than 0.9. This may be an indication that there is too much multiple coherent scattering present in your sample. Talk to your local contact if this is the case. You may be able to modify your sample to improve your data.

3) A high-Q empty cell level and constant background level will be subtracted from your data. Both levels are in detector counts per 1.0E6 monitor counts. New values can be entered directly into the fields or incremented using the arrows. The empty level will be used as an extension of the empty cell scattering data, which falls quickly to a constant level and so is typically not measured over the full q-range. The EMP level that you set will only be used where there is no experimental data. The background (BKG) level is constant throughout the entire q-range. See your local contact for the appropriate background level to use.

4) Enter the correct sample thickness in the field provided. This value will be used when placing your corrected data on absolute scale.

5) Now correct your data by selecting "Correct Data". A new "DetCts_COR" dataset will be generated and added to the graph. The "COR" data is on absolute scale. The EMP and SAM data have only been rescaled for time and monitor counts.

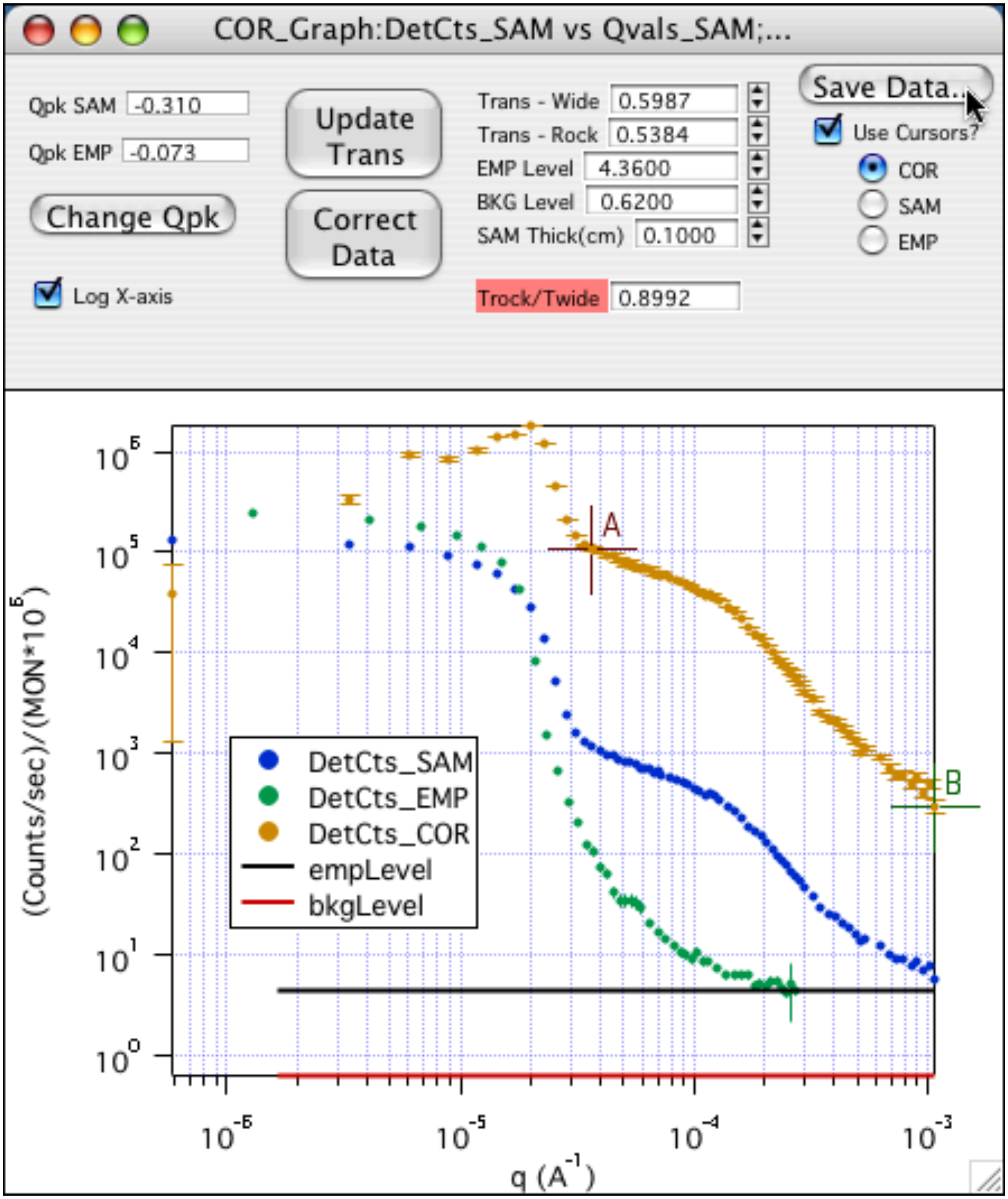


Qpk SAM -0.310
Qpk EMP -0.073
Trans - Wide 0.5987
Trans - Rock 0.5384
EMP Level 4.3600
BKG Level 0.6200
SAM Thick(cm) 0.1000
Trock/Twide 0.8992

Saving USANS Data

Any of the three datasets can be saved in ASCII format by selecting the set using the radio buttons, and then "Save Data..." Sub-ranges can be selected by using the cursors (A<B) on the selected set. The active cursor can be moved L-R using the arrow keys. The active cursor is filled black in the information panel at the bottom of the graph. Clicking the circle or the square will toggle the cursor state active/fixed. The data point number, x, and y values are also

shown here.



COR_Graph:DetCts_SAM vs Qvals_SAM;...

Qpk SAM -0.310

Qpk EMP -0.073

☑ Log X-axis

Trans - Wide 0.5987

Trans - Rock 0.5384

EMP Level 4.3600

BKG Level 0.6200

SAM Thick(cm) 0.1000

Trock/Twide 0.8992

☑ Use Cursors?

● COR
○ SAM
○ EMP

Saved data files can be loaded and plotted using the "Load USANS Data" under the USANS menu. This macro will also load standard SANS data files for comparison.

Desmearing USANS Data

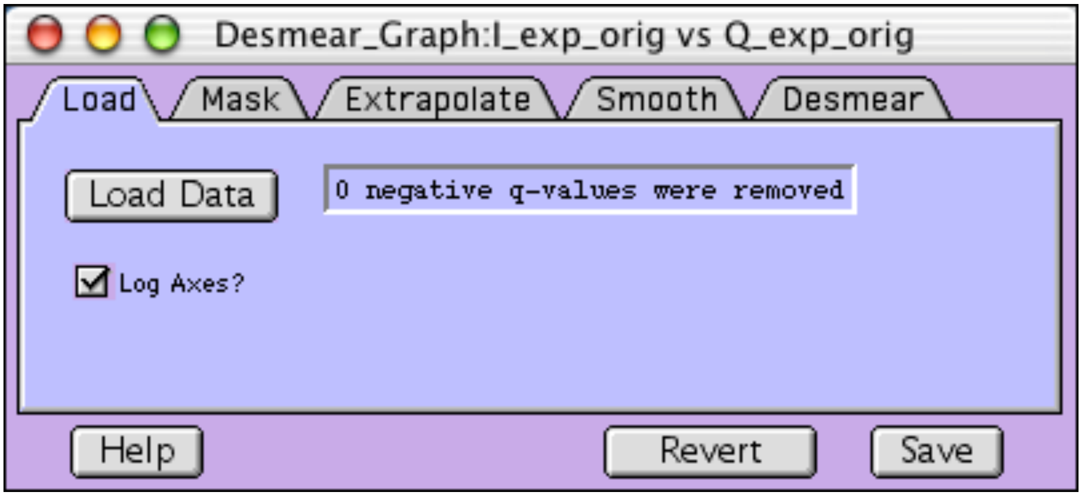
This implementation of Lake's method for desmearing slit-smeared data is a direct conversion of FORTRAN code supplied by John Barker. The smoothing routines use Igor's built-in box smoothing and spline interpolation routines.

Input: Either 3-column (q/i/s) or 6-column (q/i/s/-dqv/-dqv/-dqv) slit-smeared USANS data sets (ASCII, ".COR" extension is typical).
Output: 6-column (q/i/s/sq/qbar/fs) desmeared data sets where sq is set to a small value, "faking" a perfect resolution function for use later in analysis.

To Use:

Choose "Desmear" from the Macros menu to start. The panel opens with a slate of tabs to choose from. **Work left-to-right to complete the steps to desmear your data.** You can skip any or all of the mask/extrapolate/smooth steps.

Load Tab:

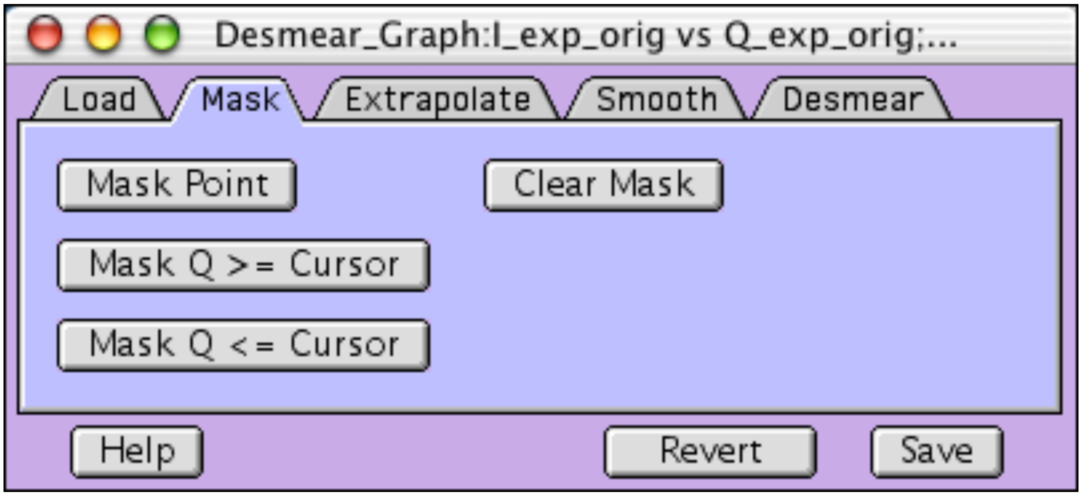


0 negative q-values were removed

☑ Log Axes?

"Load data" will read and plot the data, reporting the dQv value for slit height, if it found one in the data file. If none found, 0.117 (1/A) is used (found under the Desmear Tab). The dQv value can be overridden before the desmear step. Data that has been previously loaded will not require a repeat extraplation of the high-q slope.
- The total number of negative q-values removed from the data set is reported. Negative q-values are fatal to Lake's algorithm.
-The checkbox will toggle the scaling of both the X and Y-axes.

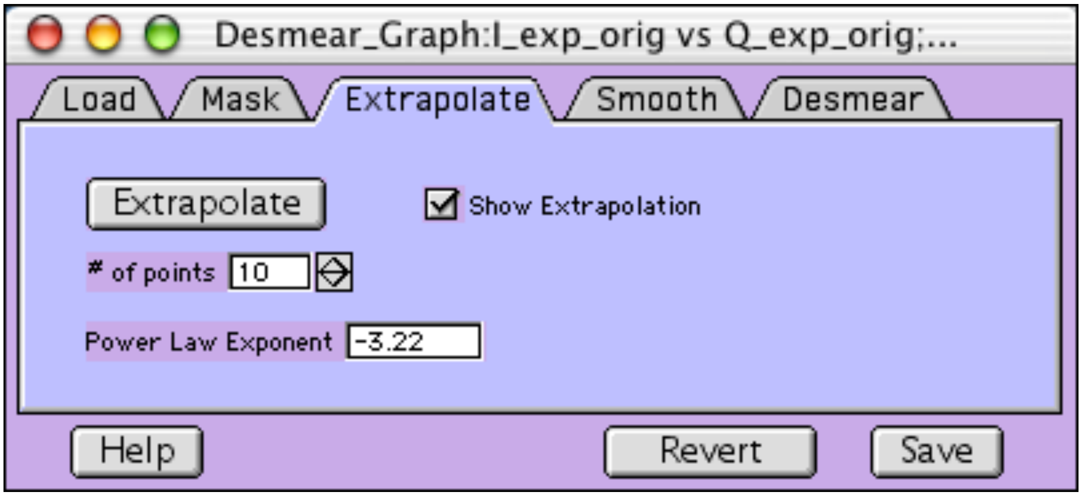
Mask Tab:



It may be necessary to mask some of the very low q-values before desmearing. (Sometimes these points can have negative intensities and are not visible on a log(I) axis !)

- Clicking on the "Mask" tab will automatically initiate masking. The cursor is drawn on the graph.
- Right/Left arrows move the cursor
- Click "Mask Point" to toggle mask/unmask of the data point at the cursor. Masked points are shown as a larger red and white circle.
- You can also mask a range of data either greater than or less than (and including!) the current cursor position by using the appropriately named button. Like the pointwise button, these TOGGLE the mask state.
- Clear mask will unmask all of the data so you can start over.
- When finished, click on any other tab to proceed with desmearing using the masked data set.

Extrapolate Tab:



☑ Show Extrapolation

# of points 10

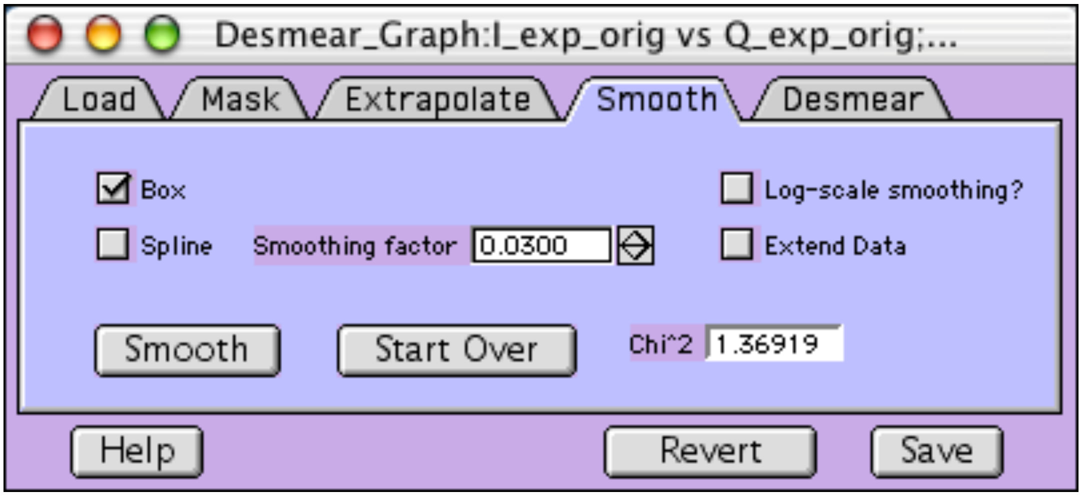
Power Law Exponent -3.22

"Extrapolate" will find the power law scaling that is needed for the desmearing algorithm. If the data was extrapolated on loading, then that slope is automatically used here. So you can in general, skip this step if the extrapolation on loading the data file was acceptable.

- N points of the high Q end of the smeared data are fitted. The slope reported is (fitted

slope - 1), as the desmearing requests the slope of the desmeared curve.
- The fitted value can be overridden by entering a (negative!) value for the slope in the box.
- The checkbox toggles the display of the extrapolation.

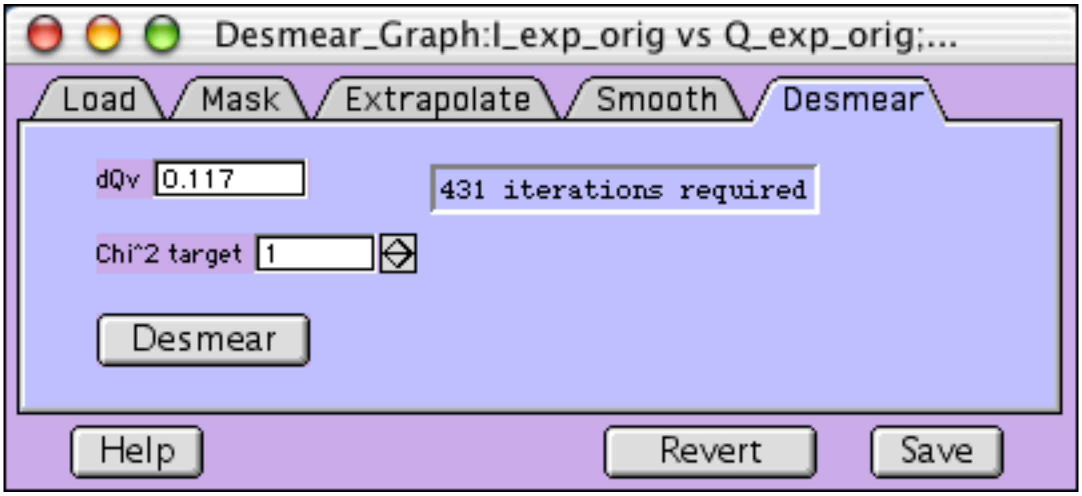
Smooth Tab:



☑ Box
☐ Spline
Smoothing factor 0.0300
☐ Log-scale smoothing?
☐ Extend Data
Chi^2 1.36919

Smoothing is the trickiest and most subjective operation. It is best to avoid any smoothing of the data if at all possible. Smoothing, by definition, alters your experimental data. If abused, smoothing can introduce artifacts that will look very appealing for interpretation in the desmeared data. You have been warned.
- "Box" will do one pass of 3-point box smoothing.
- "Spline" will do a Smoothing Spline fit to the data.
- If both methods are checked, the box smooth is done first. Both methods pad with values equal to the end points.
- The "Smooth" button will do one pass of the checked type of smoothing.
- If end effects create a poor result, "Extend Data" will linearly extend the data to low Q (Qmin=0.5*lowest q) and do a power law at high Q (Qmax=1.5*highest q) to (maybe) do a better job at minimizing end effects during smoothing.
- Repeatedly clicking "Smooth" will repeat one pass of the checked operations. I have found reasonable results after several passes of box smoothing with one final pass of spline smoothing. Multiple passes of spline smoothing are usually too severe and introduce artifacts at low q.
- The Chi^2 reported is between the smoothed data and the original data. Hence a value of Chi^2=1 is "optimal" and values greater than one are "over-smoothed".
- Log scale smoothing will smooth the data based on a logarithmic rescaling of the intensity data. I have had limited success with this.
- "Start Over" will trash all of the smoothing so that you can start over. Quite useful if you've gone too far with the smoothing and want something less severe.

Desmear Tab:



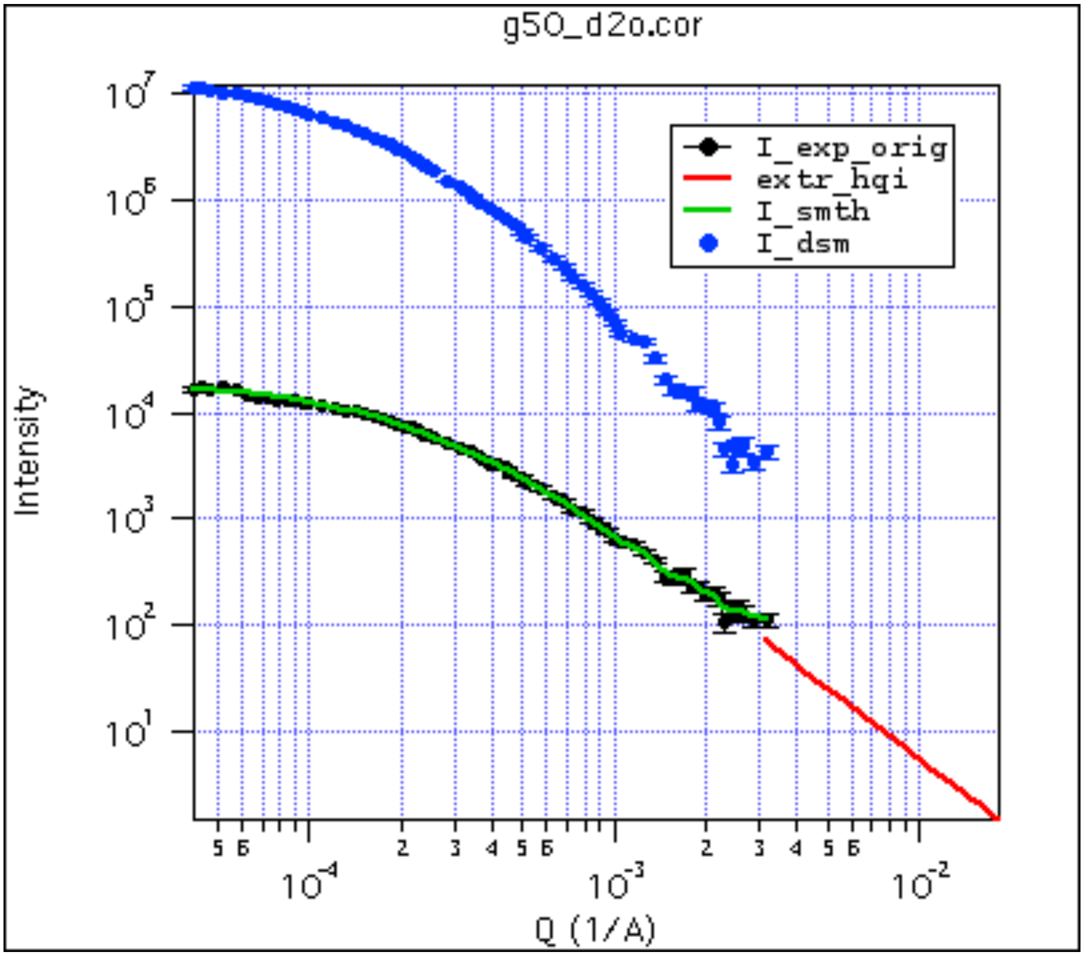
dQv 0.117

Chi^2 target 1

431 iterations required

"Desmear" will desmear the data as loaded, masked, or smoothed if it exists.
- It will use the power law exponent from the Extrapolate Tab
- dQv is loaded with the original data. 0.117 is the value for data taken at USANS since November 2004.
- The desmearing will proceed to reach the Chi^2 target as entered on the panel. Chi^2=1 is a good choice.
- Clicking "Desmear" will initiate the desmearing. Progress of the iterations is reported in the command window, and the final number of iterations required is reported in the panel. The desmeared data is automatically added to the plot.
- Clicking "Desmear" again will give you the same thing back - but "Smooth" again, or change the exponent, dQv, or Chi^2, and you'll need to desmear again to get the new result.

Be sure to save your desmeared data...



Always Visible Controls:

"Help" will show this help file.

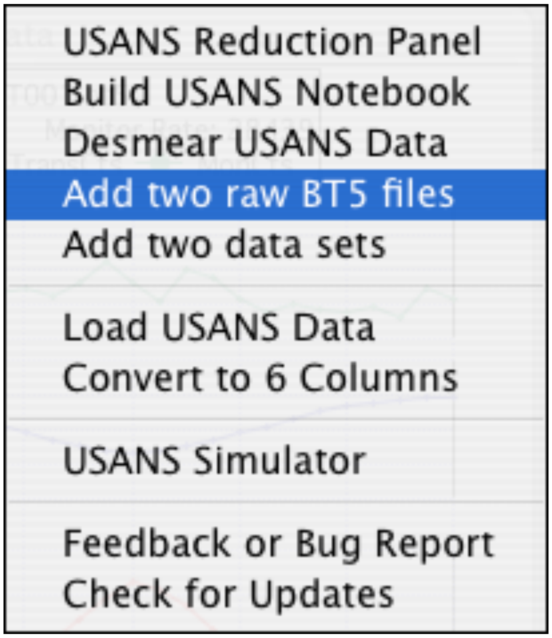
"Save" will write the desmeared data in a 6-column format. The header will have the file name, chi^2, power law slope, number of iterations, number/type of smoothing passes, and the date.

"Revert" will discard all of the desmearing and smoothing that has been done and starts you with a fresh copy of the original data set. "Load Data" will also clear all of the old data, and allow you to start fresh on a new data set.

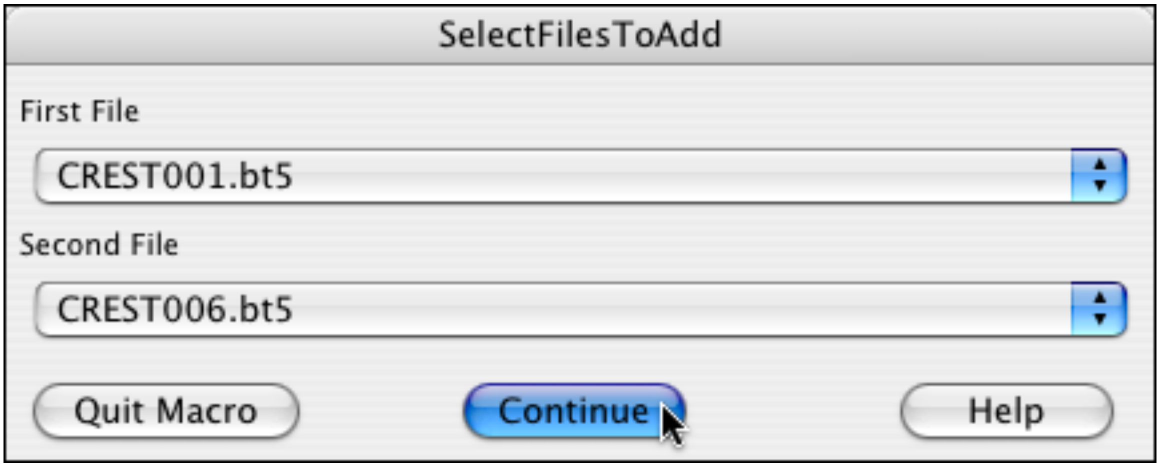
Adding Raw BT5 Files

Adding two raw .bt5 files can be done when a sample has been measured two or more times in order to get better counting statistics. Only files with the same angle range and the same number of points can be added. Files that do not strictly meet these criteria cannot be added. Since these are raw data files, the zero angle shift is not known, so NO shifting is done - the two files are added together, point-by-point and the counting time is summed. The file names of the two added files are listed in the new title of the summed file. The sum can be repeated with a summed file as one of the inputs files to add more than two files together. The output file is in raw .bt5 format, and is to be treated as any other raw data file.

To sum two raw data files together, choose "Add two raw bt5 files" from the USANS menu:



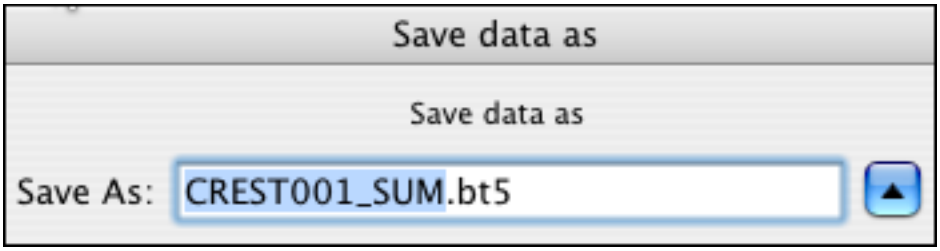
Then select the two files from the popup menus:



First File: CREST001.bt5

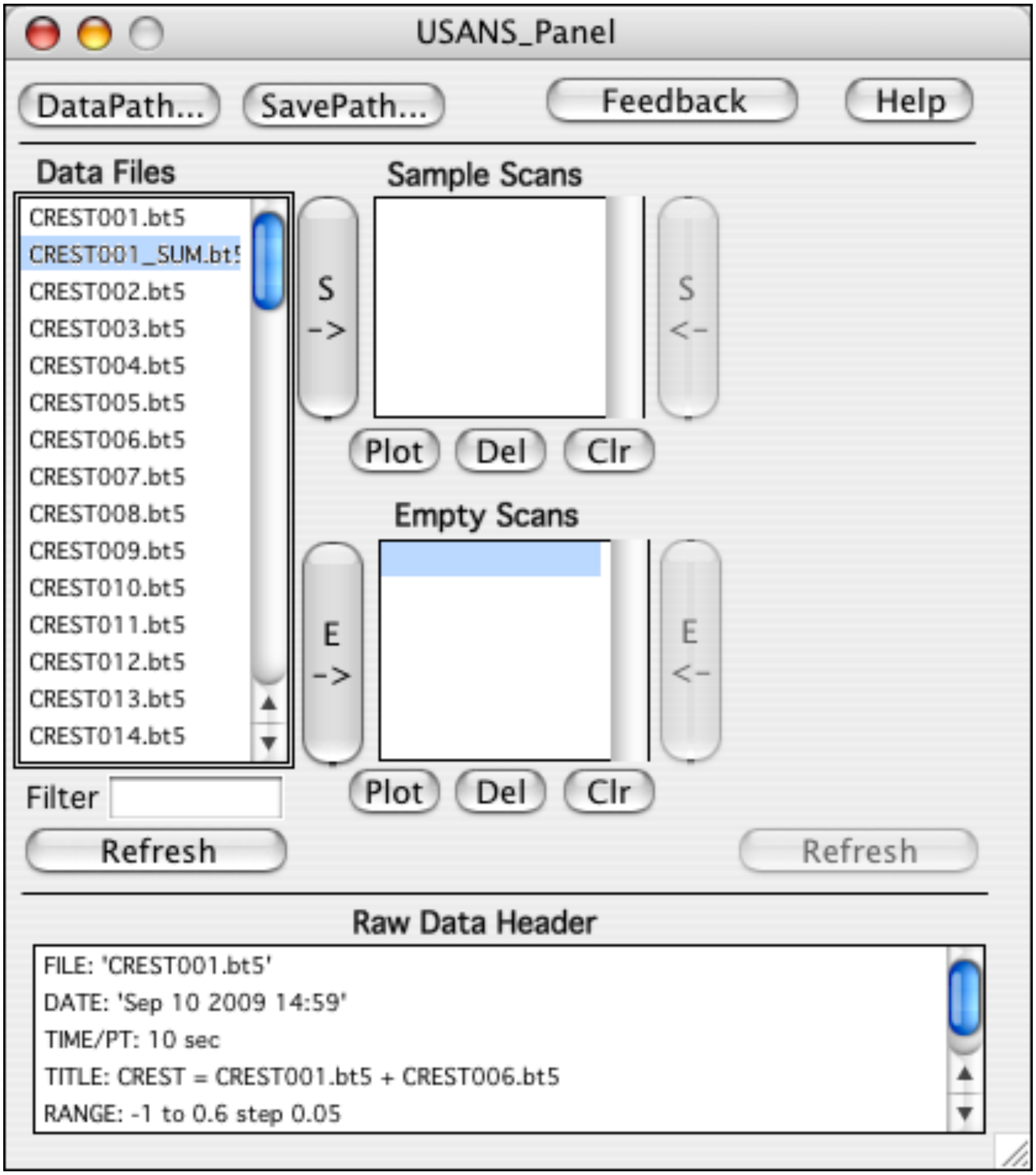
Second File: CREST006.bt5

You'll be prompted to save the output file. "_SUM" is automatically tagged on the suggested file name.



Save As: CREST001_SUM.bt5

Be sure to "Refresh" the Data File listing on the Main USANS panel so that you can use the summed data file. Note the new sample title of the summed data.

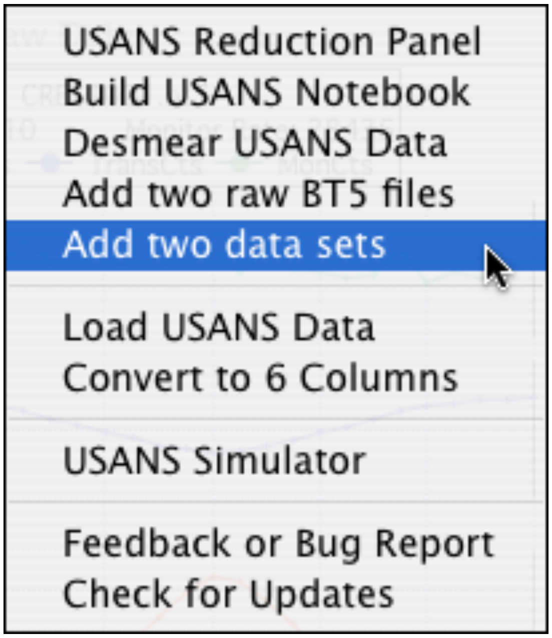


FILE: 'CREST001.bt5'
DATE: 'Sep 10 2009 14:59'
TIME/PT: 10 sec
TITLE: CREST = CREST001.bt5 + CREST006.bt5
RANGE: -1 to 0.6 step 0.05

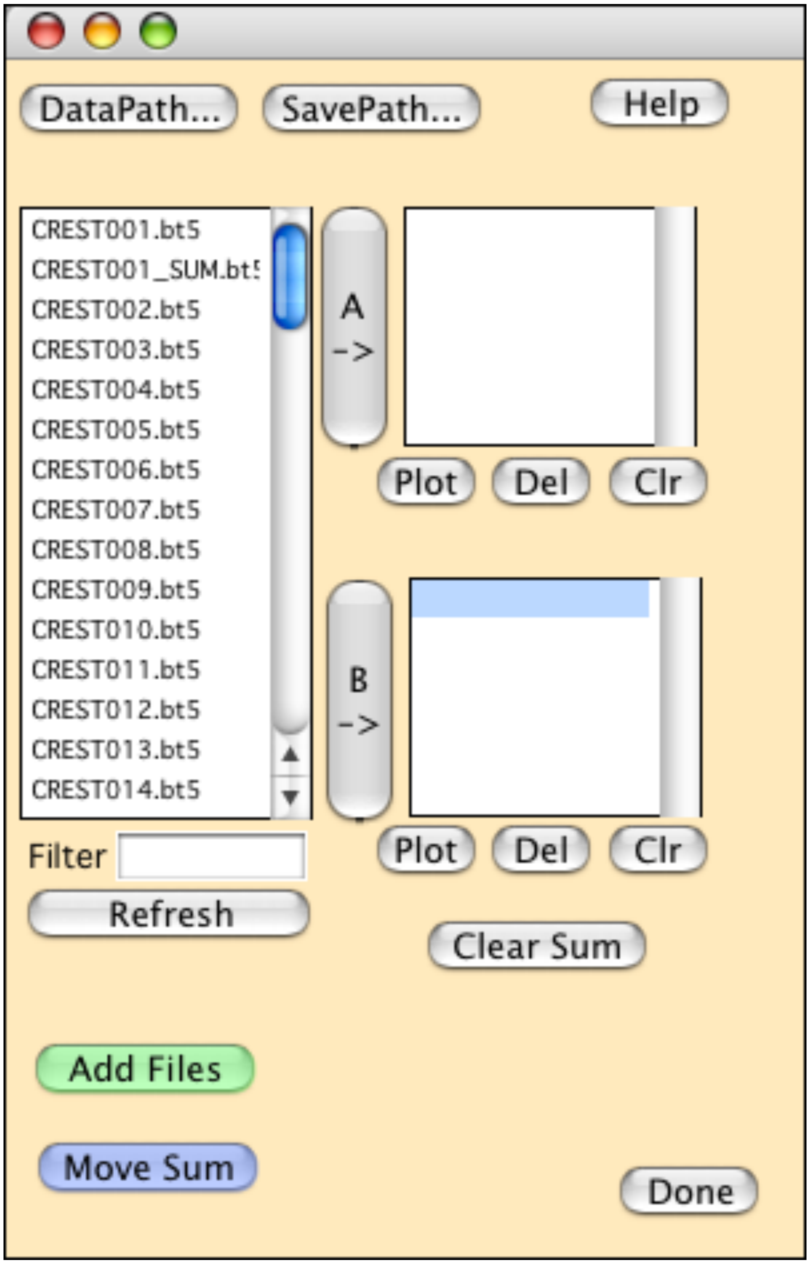
Adding Two Data Sets

Here, two complete data sets (including the main beam) are added together after loading and normalizing, and converting to Q. To use the summed data set, data is first added in a separate panel, then transferred to either the active "SAM" or "EMP" data, then used in the correction as usual. Since each data set will have a different zero offset, the q-values will be out of registry. Only those within a certain tolerance (1% by default) are actually added. Points that cannot be added are still kept in the final data set with their original error. The data file is NOT saved, because it is not a format that can be re-read in for reduction.

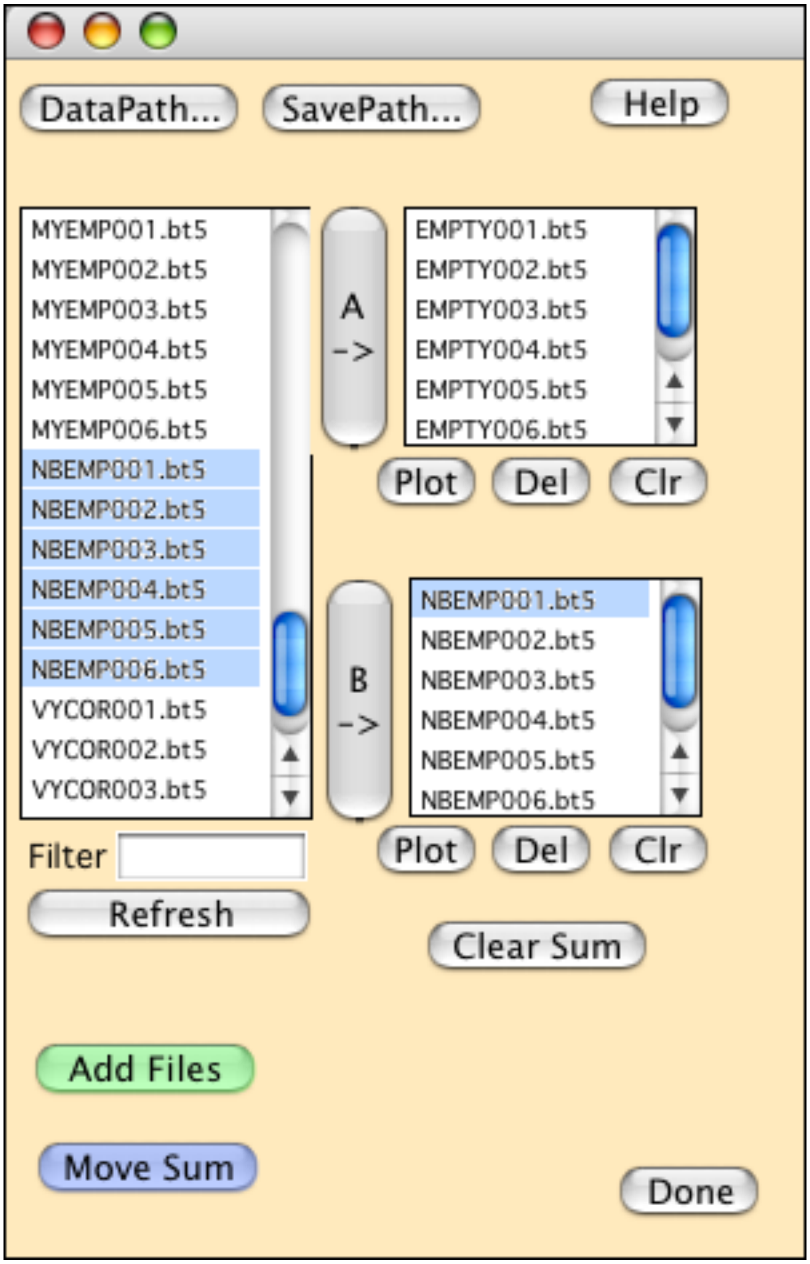
To add two data sets together, choose "Add two data sets" from the USANS menu:



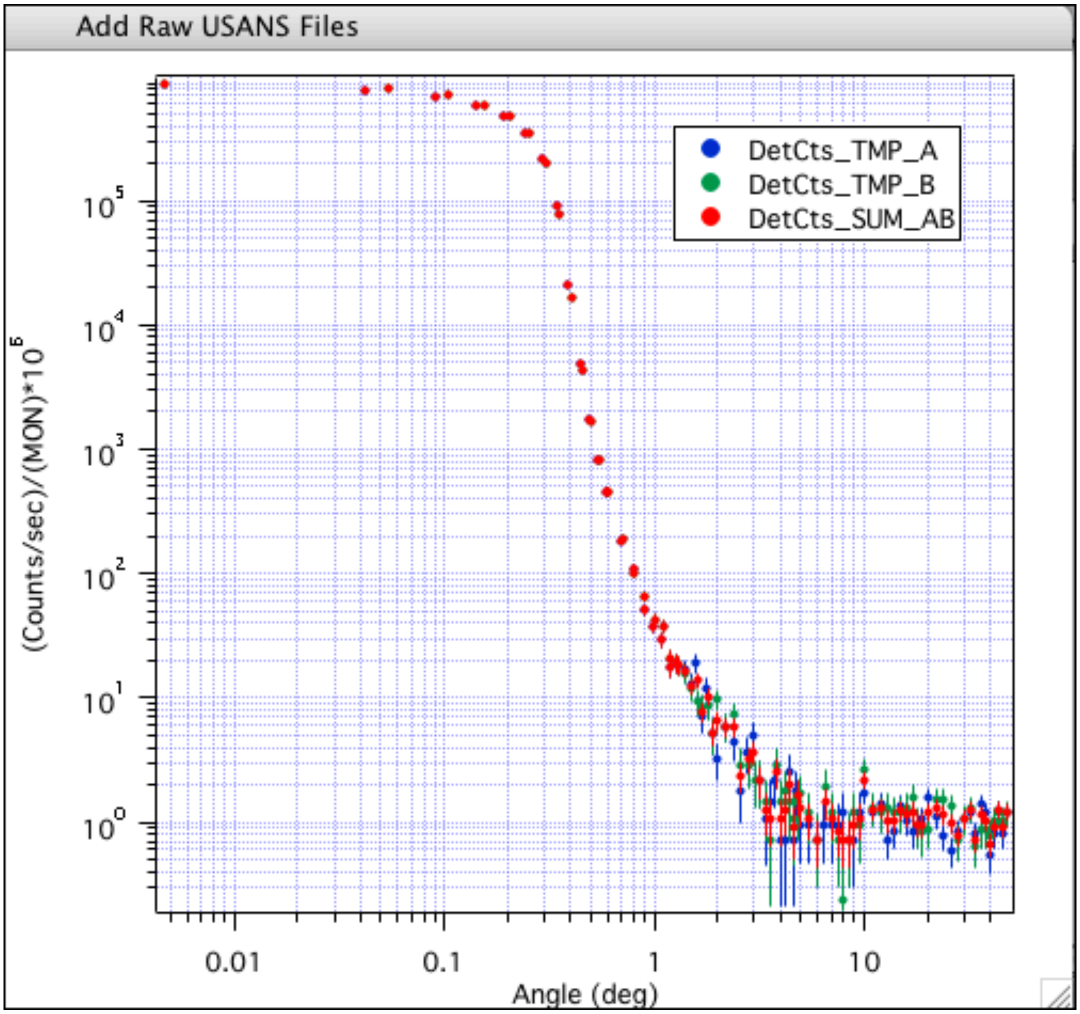
A panel appears. The left-hand side looks similar to the main USANS panel:



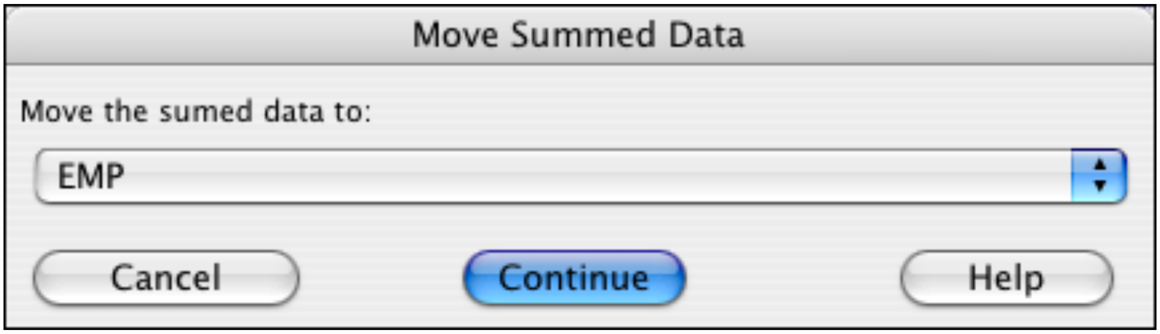
If you have already set the DataPath and the SavePath, these do not need to be reset. "Refresh" to get a list of the files. Then select the sets of data "A" and "B". The data sets are plotted within the panel, but not yet part of the normal data correction graph. Data files can be added, deleted, and cleared from sets A and B as in the Main USANS panel. Once the sets have been selected and plotted (in this case, I've chosen empty beam data that was re-measured):



Then clicking "Add Files" sums what data is in sets A and B:



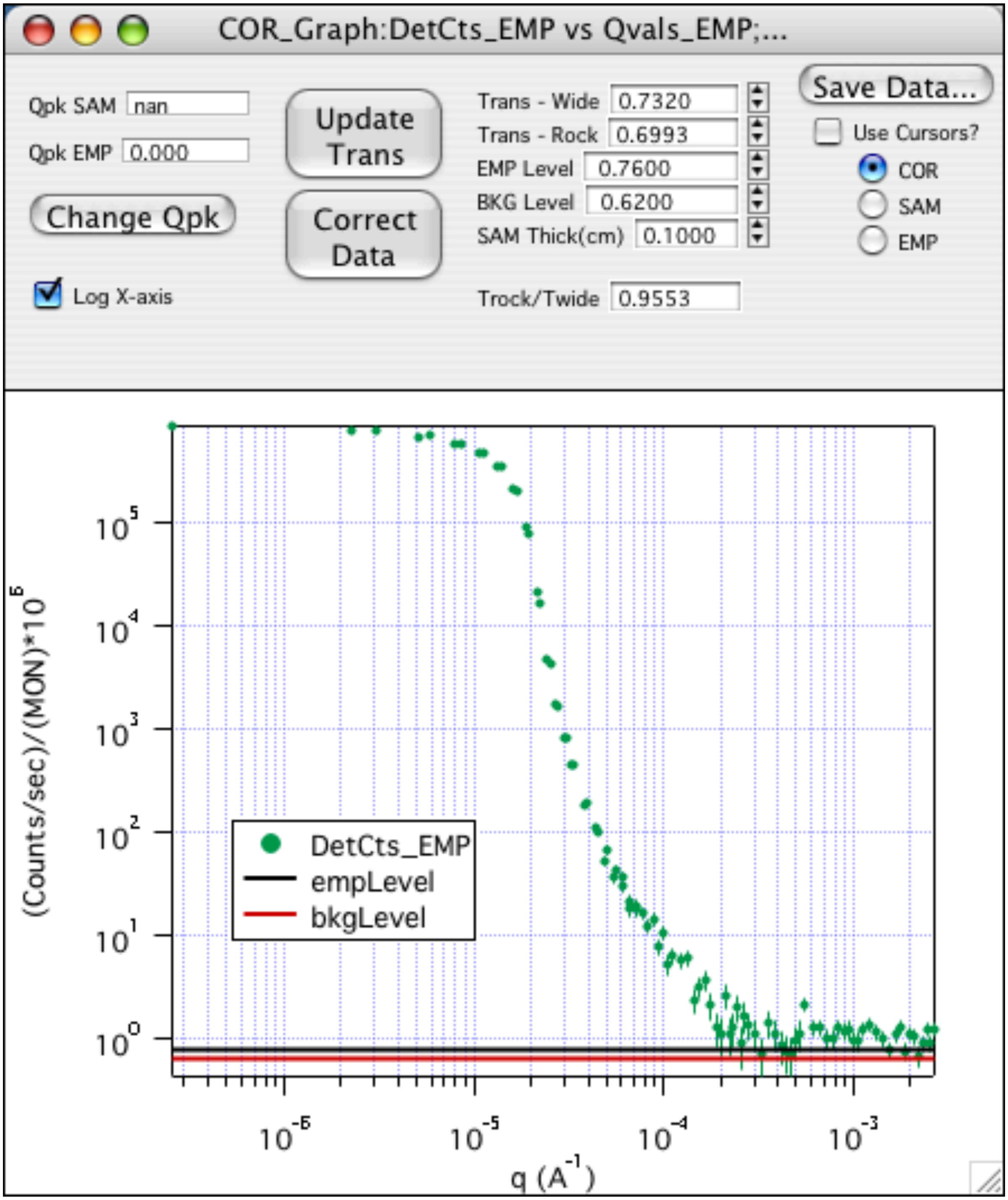
The summed data (red) has smaller error bars where the data points are close enough in q to be added (within 1%). Where the data can't be added - usually only at the lowest angles - the original data is retained in the summed set. If you don't like the result, "Clear Sum" will remove the summed data from the plot, and you can start over again. If you are happy with the sum, then you can click on "Move Sum". This will move this summed data set to the main data correction graph. You can move the summed data to either the EMP or SAM data sets.



Move the sumed data to:

EMP

The summed data that is moved appears just as if it was plotted from the main USANS panel. Note that the Qpk EMP is identically zero, since the A and B data sets were already shifted to zero angle. To remove the summed data from the data correction graph, click on "Clr" in the Main USANS panel for either the Sample or Empty data.



COR_Graph:DetCts_EMP vs Qvals_EMP;...

Qpk SAM nan

Qpk EMP 0.000

☑ Log X-axis

Trans - Wide 0.7320

Trans - Rock 0.6993

EMP Level 0.7600

BKG Level 0.6200

SAM Thick(cm) 0.1000

Trock/Twide 0.9553

☐ Use Cursors?

● COR

○ SAM

○ EMP