

## • USANS Data Reduction

02/2008 Vers. 2.21

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. Data output is smeared with the resolution function of the USANS instrument, so called "slit-smeared" data. This reduction package now includes the capability to desmear datasets.

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 04/2006, USANS Reduction macros require IGOR Pro v. 4.0x. As always, the macros will work with the free Demo version of IGOR.

If you use this software to 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.

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### **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.

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### **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 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  $q$  ( $1/\text{\AA}$ ), and normalize to monitor counts and counting time. The transmission as measured by the analyzer ( $T_{\text{Rock}}$ ) is determined by measuring the peak intensity with and without the sample:  $T_{\text{Rock}} = I(\text{peak})_{\text{sample}} / I(\text{peak})_{\text{empty}}$ . 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  $2^\circ$ ).  $T_{\text{Wide}} = \text{TRANS}_{\text{sample}} / \text{TRANS}_{\text{empty}}$ . 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:

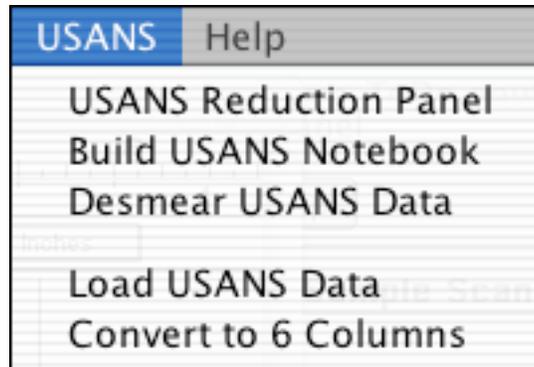
$$I_{\text{COR}}(q) = I_{\text{SAM}}(q) - T_{\text{Rock}}I_{\text{EMP}}(q) - (1-T_{\text{Rock}})I_{\text{BGD}}$$

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

$$K = 1 / [I_{\text{peak}} T_{\text{Wide}} d_s \Delta\Omega]$$

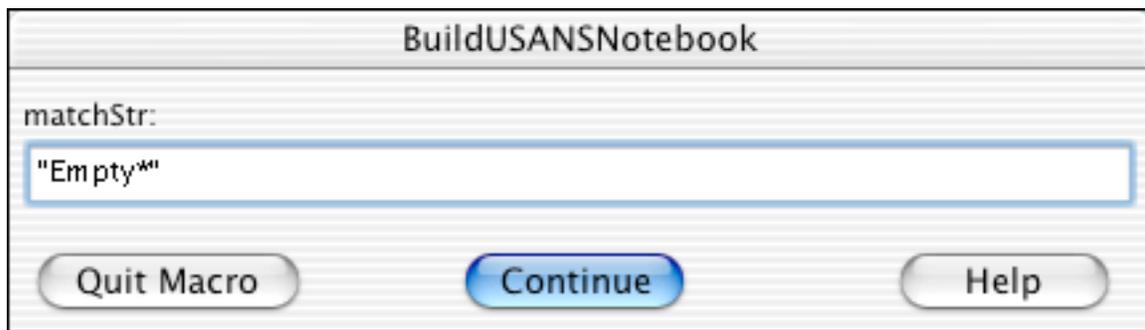
where  $d_s$  is the sample thickness in cm, and  $\Delta\Omega = 7.1\text{E-}7$  ster is the solid angle accepted by the analyzer. In general, if the ratio  $T_{\text{rock}}/T_{\text{wide}} < 0.9$  this indicates a significant amount of multiple scattering. Please see your local contact.

## USANS Menu



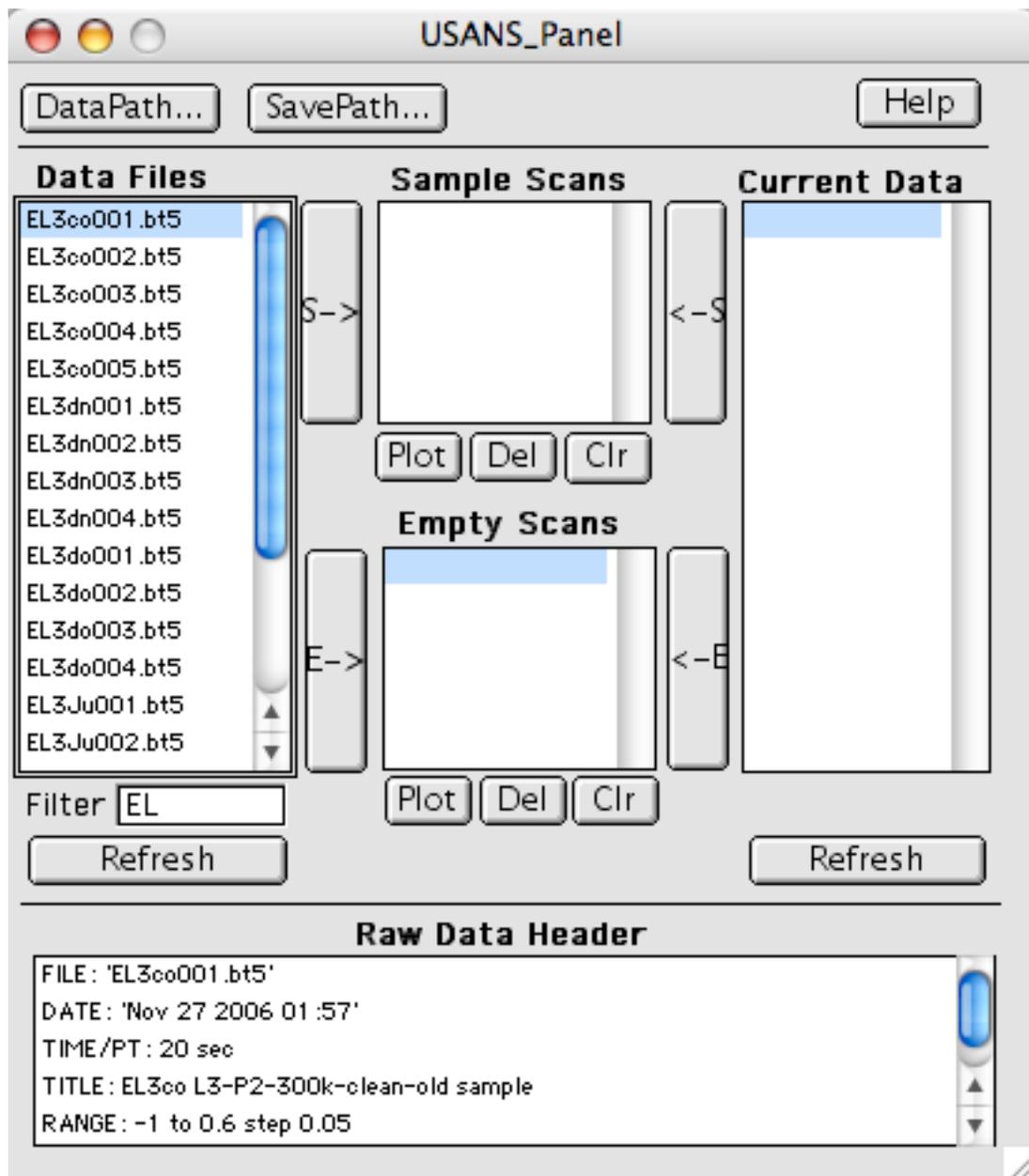
The USANS menu has only a few items:

- 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.



- 3) Desmear USANS Data: described in detail below in [Desmearing USANS Data](#)
- 4) Load USANS Data: Will load and plot corrected or desmeared USANS or SANS data (not for raw data).
- 5) 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  $dQ_v = 0.037$  (1/A). Data files more recent than Nov. 2004 will already be in the 6-column format with  $dQ_v = 0.117$  (1/A)

### Main USANS Controls



The USANS\_Panel will open automatically when a blank reduction template is opened. 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.

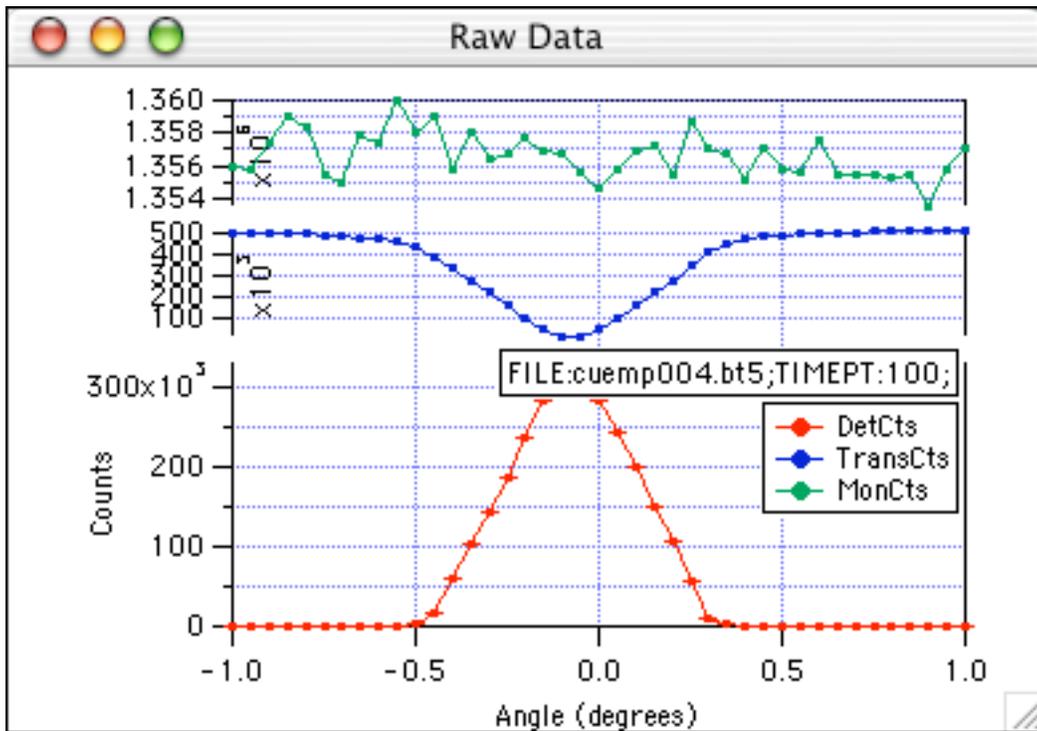
Clr: Clears all entries from the Sample or Empty files list, whichever list is adjacent to the button. This also clears SAM or EMP data from the COR\_Graph, and clears COR data if necessary.

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 ( $1/\lambda$ ).

- 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:

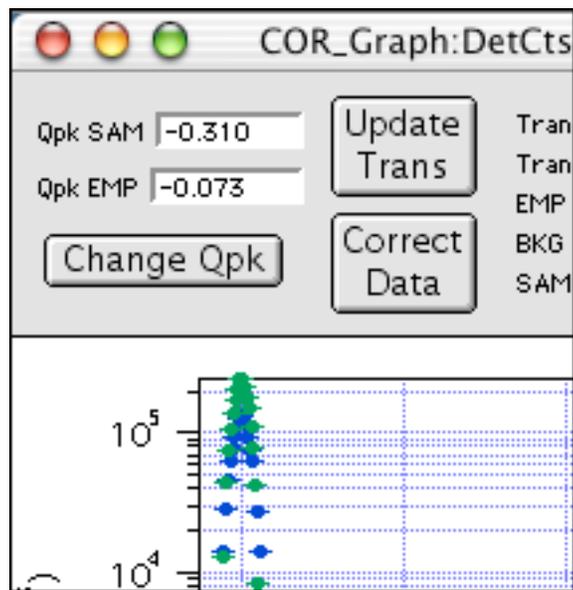


The three traces displayed are (top-to-bottom): Monitor Counts, Transmission detector counts, and Main Detector counts. Count values are not normalized and the error bar shown is due to counting statistics. Counts are plotted against the angle of the analyzer. This plot is useful for inspecting the contents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

### USANS Data Correction

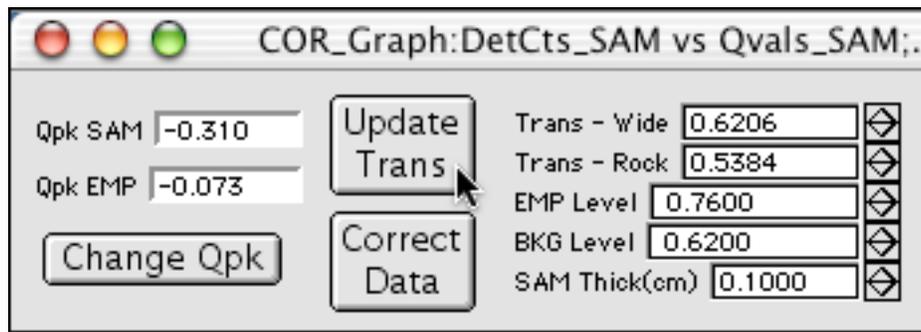
Once you have identified the correct datasets for sample and empty scans by inspecting the file headers and the raw data, the following steps will guide you through the basics of reducing USANS data to a final  $I(q)$  format.

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. The automatically determined peak values rarely need to be adjusted.



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.

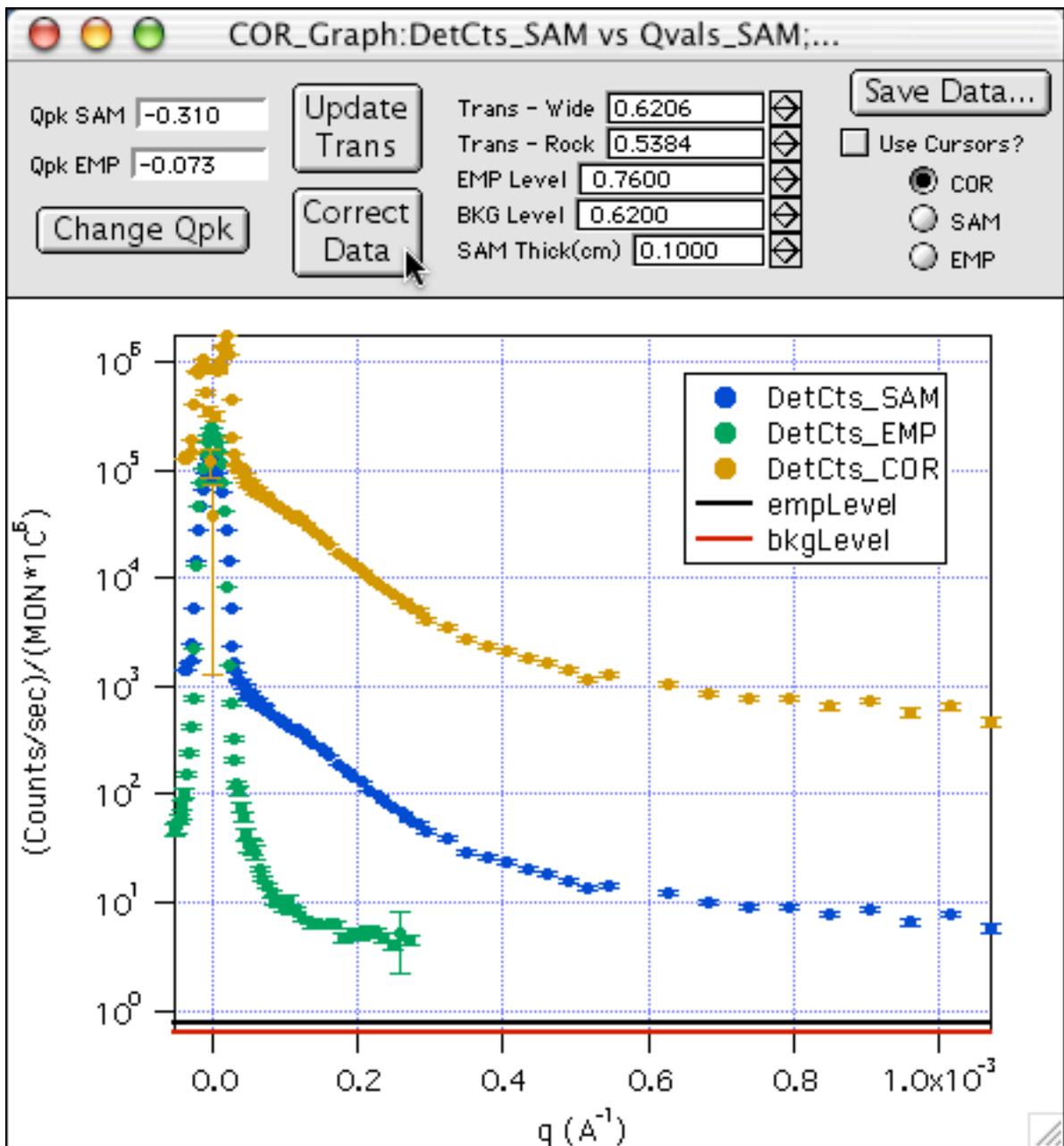
2) Once the peak locations are satisfactory, calculate both the wide angle and peak transmissions by selecting "Update Trans". The calculated values are displayed to the right of the button. Make sure that the values are as expected. Updating the transmissions has no effect on the appearance of the graph.



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.

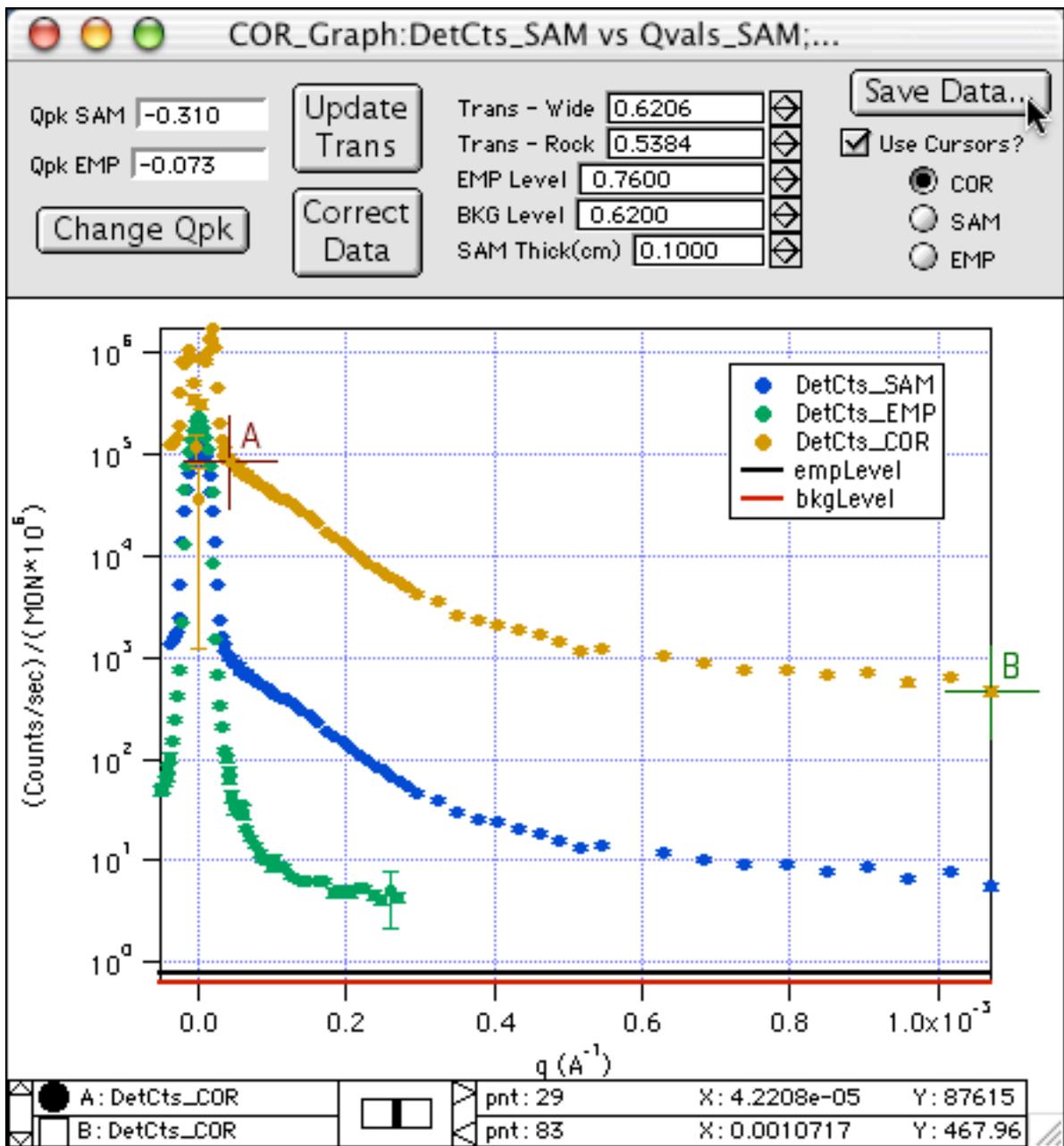
4) Enter the correct sample thickness in the field provided. This value will be used when placing your corrected data on absolute scale.

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.



### 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.



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-smear 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.

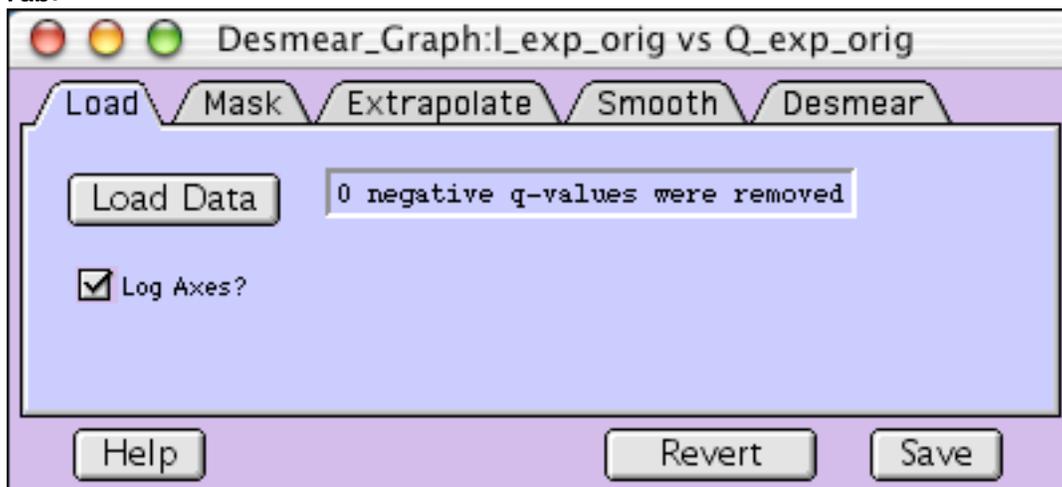
Input: Either 3-column (q/i/s) or 6-column (q/i/s/-dqV/-dqV/-dqV) slit-smearred USANS data sets (ASCII, ".COR" extension is typical).

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:



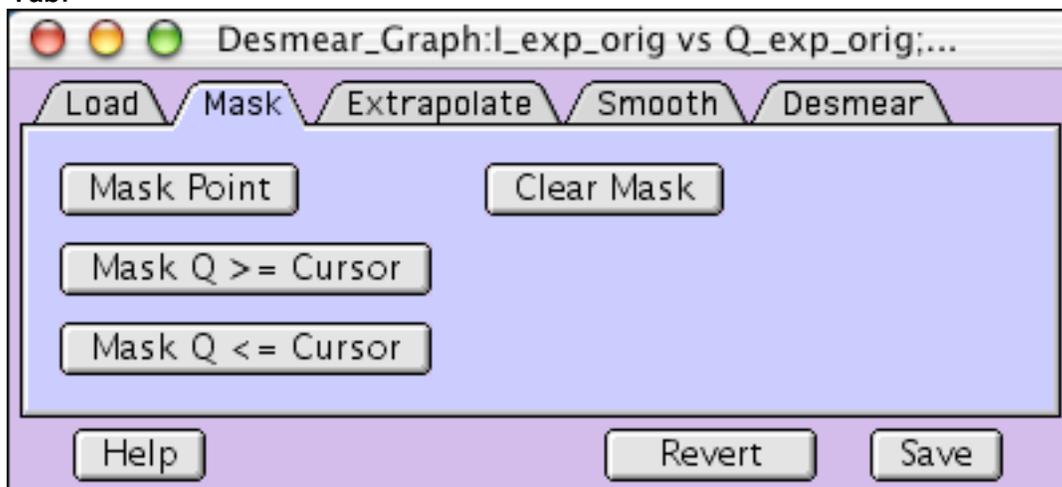
"Load data" will read and plot the data, reporting the dqV value for slit height, if it found one in the data file. If none found, 0.117 (1/A) is used (found under the Desmear Tab).

The dqV value can be overridden before the desmear step.

- 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.

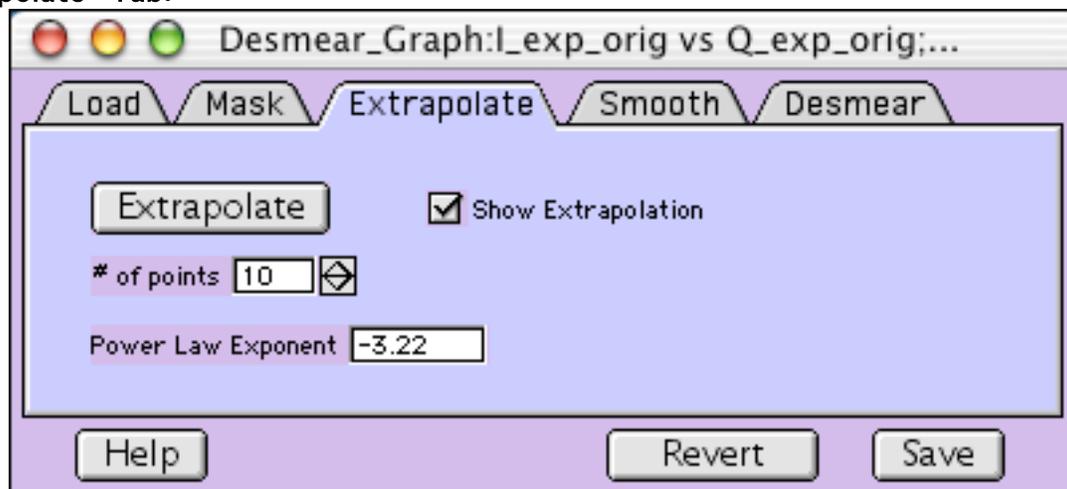
### Mask Tab:



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.

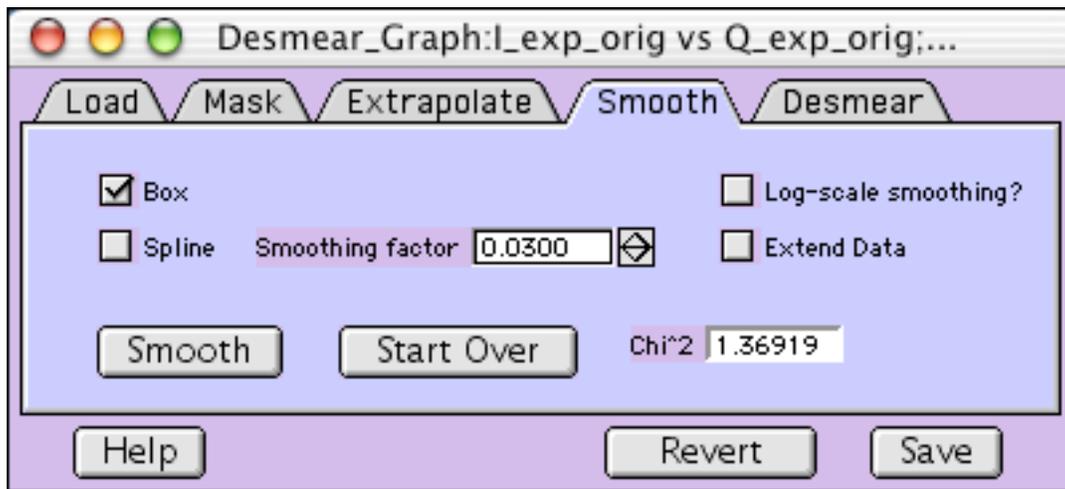
#### Extrapolate Tab:



"Extrapolate" will find the power law scaling that is needed for the desmearing algorithm.

- 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.

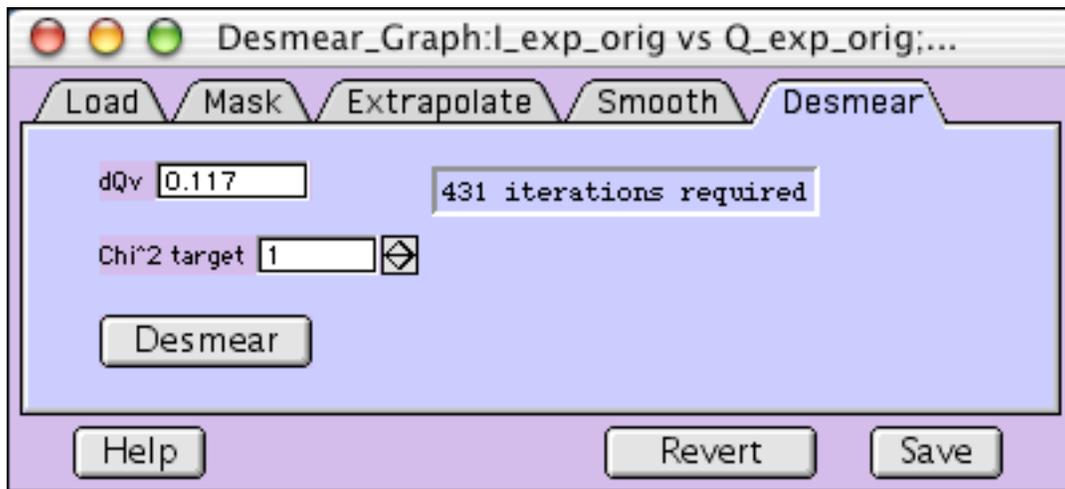
#### Smooth Tab:



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 ( $Q_{min}=0.5 \times \text{lowest } q$ ) and do a power law at high Q ( $Q_{max}=1.5 \times \text{highest } q$ ) 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  $\text{Chi}^2$  reported is between the smoothed data and the original data. Hence a value of  $\text{Chi}^2=1$  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.

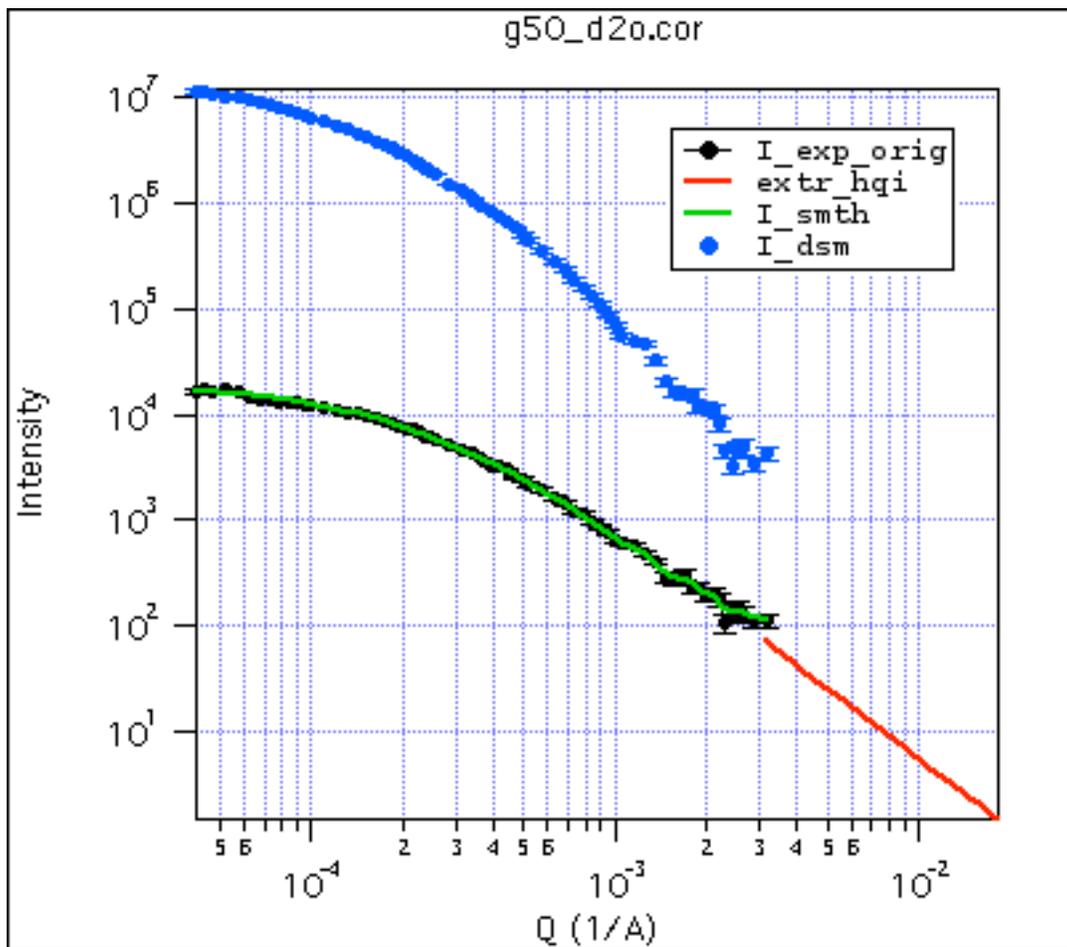
**Desmear Tab:**



"Desmear" will desmear the data as loaded, masked, or smoothed if it exists.

- It will use the power law exponent from the Extrapolate Tab
- $dQ_v$  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  $\text{Chi}^2$  target as entered on the panel.  $\text{Chi}^2=1$  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,  $dQ_v$ , or  $\text{Chi}^2$ , 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.

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