

## • **SANS Data Reduction Tutorial**

11/2001 Vers. 4

This tutorial guides you through the basic features of data reduction using IGOR Pro.

For a "hands-on" experience, you may download the set of Tutorial Data, or use your own data, although there are some specific references to the Tutorial set. To work through the tutorial on your own, you must already have IGOR Pro and the SANS Reduction procedures installed. Once installed, open a blank data reduction experiment "SANS\_Reduction\_v4d.pxt", or a similar version. In addition to this help file, all SANS panels include balloon help (Mac) or command-line help (PC) that describes the action of each button or field in a panel.

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## General Description

### SANS Overview

The SANS Data Reduction using IGOR Pro is an implementation of the VAX data reduction procedures in an easier to use, graphical interface. It is designed to work on Macintosh or PC, and works directly on raw binary data files as they were collected on the VAX. All Raw SANS data files and reduction software can be carried to your home institution.

The procedures and software that are available for displaying and processing 2D SANS data (subtracting background, converting to an absolute scale, averaging, etc.) to produce reduced 1D or 2D data in intensity versus wavenumber (I vs. Q) form are described in the following sections. This section describes the underlying concepts of data reduction and the organization of the reduction program.

The raw, 2D (128 rows x 128 columns) data collected at the instruments resides in SANS user accounts in the form of individually named binary files. The format of the data file names is:

**XXXXXNNN.SAn\_INI\_AMMM**

where **XXXXX** is a 5-character sample prefix, **NNN** is an automatically incremented 3-digit run number, and **SAn** denotes the SANS instrument where the data was collected (**n**=1 for the NG1 SANS instrument, **n**=3 for NG3, and **n**=2 for NG7 SANS). **INI** denotes the user's initials, and **AMMM** is a 4-digit alphanumeric run identifier for archiving purposes. Raw data files are stored on the VAX and are protected from deletion. In addition, during your SANS experiment, as each data file is collected on the VAX, the raw data files are mirrored to a central server, "Charlotte". If your SANS account is NG3SANS41, your data will be located in the "NG3SANS41" folder on Charlotte. Charlotte is visible to Macs through Appleshare (connect as a guest), and to Windows through the Network Neighborhood (NCNR group, Map the "SANS Data" folder as a network drive). This central server allows you to (within the building) work directly with the data on Charlotte. The data on the VAX remains untouched, as a backup. You can see and reduce the data while at the instrument, in the computer room, or in the user offices. Once your experiment is finished, all of your data - raw data files, averaged data, IGOR Demo version (if needed), SANS Reduction Macros... can be copied from Charlotte onto a Zip disk or CD and carried home (a typical SANS session will produce between 2-6 MB of raw data). Data reduction can be completed (if necessary) at your home institution, without having to work around the NIST Firewall. FTP'ing of raw binary data from the NCNR to your home institution is not recommended, as the binary data structure is not always preserved even in a "binary" transfer.

The 128x128 data values in the raw data files are never altered; only the file header, which contains parameters such as the beam center coordinates, transmission, detector distance, etc. can be modified (using a Patch operation). For analysis, the data are loaded into

a working folder "**EXT**", where **EXT** is a 3-letter mnemonic of the data "type" that represents the logical function of the data in the reduction sequence or the result of a processing step. For example, **SAM**, **EMP**, and **BGD** represent sample data, empy cell data, and background data, respectively. The data type **COR** identifies the results of combining the **SAM**, **EMP**, and **BGD** data to produce sample data that has been corrected for background and empty cell scattering.

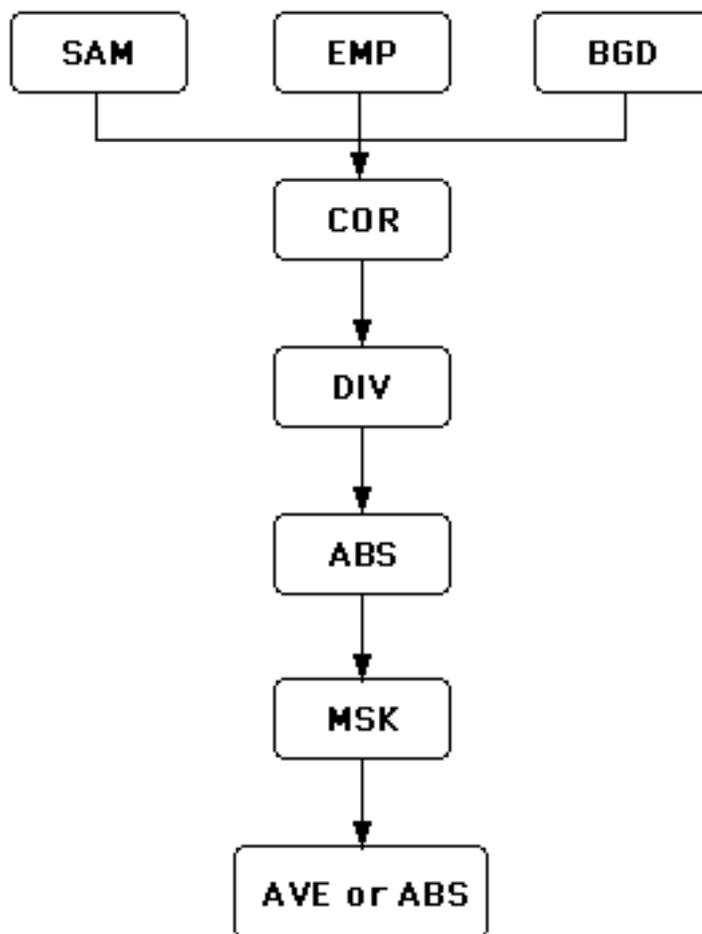
The data in work folders are processed by invoking a protocol that performs a sequence of specific operations, in some cases writing the result to a different work folder, overwriting the previous contents. Ultimately, the corrected data is saved to disk in the desired format in an "averaging" step. Typically the 2D data is circularly averaged to produce 1D (I vs. Q) ASCII data files. These 1D data files contain instrumental resolution information in addition to the intensity data. The "averaging" step can be configured to save a variety of 1D formats, including 2D ASCII files or PNG graphics images. See [Average Options](#) for details.

Once data are reduced to I vs. Q form, various types of linearized fits can be performed. See [Fit Lines to Your Data](#) for details.

### **Data Reduction Overview**

Many of the data reduction programs make use of information recorded in the raw data header at the time the data were taken. Therefore, the correct values of parameters such as the X-Y coordinates of the beam center, the detector offset, the sample transmission, etc. should be in the raw data header before proceeding with the data reduction. Parameter values can be viewed and edited using the [Patch File Headers](#) operation which operates on one file at a time, or can operate on multiple files. Only the raw data headers are modified, leaving the data unaffected. Be sure to patch file headers with the correct values before proceeding with data correction.

The most commonly used sequence (or protocol) of data reduction steps is shown schematically in the figure below.



### Initial correction

As data is loaded for use as SAM, EMP or BGD data types, each dataset is normalized to a fixed number of incident neutrons (corresponding to a monitor count of  $10^8$  counts) to facilitate comparisons between data sets. Sample data is corrected for background and empty cell scattering according to the algorithm:

$$\text{COR} = (\text{SAM} - \text{BGD}) - [\text{Tsam}/\text{Temp}](\text{EMP} - \text{BGD})$$

where Tsam is the transmission of the sample and Temp is that of the empty cell. Note that Tsam and Temp are taken with respect to the empty beam. Thus, if no cell is used (i.e., empty beam condition), Temp = 1.0. The results of this operation are stored in another work folder, COR.

### Detector Efficiency Corrections

An important step in the data reduction process involves correcting for the detector response. A data set can be corrected for non-uniformities in the detector efficiency by dividing the data, pixel-by-pixel, by the measured scattering from an isotropic scatterer such as plexiglass or water. Plexiglass runs are measured periodically by the instrument scientists for this purpose and saved as **PLEX\_DDMMYY\_NGn.DIV** files which indicate the date the measurement was made (**DDMMYY**) and the instrument used (**NGn**). These files are stored on Charlotte in a folder named **NGn\_FILES**. The DIV file for the current

cycle should be copied to your directory before reducing your data.

Subsequently the corrected data, COR, is divided, pixel-by-pixel, by the contents of DIV. This calibrated result is written to a separate work folder, CAL.

### **Absolute Scaling (optional)**

At this point the CAL data may be converted to an absolute intensity scale ( $I(Q) \rightarrow d\Sigma/d\Omega$  in units of  $\text{cm}^{-1}$ ) by specifying an absolute scaling factor. In order to find the scaling factor, the scattering from a standard sample or an attenuated empty beam must have been measured under the same experimental conditions. The scattered intensity  $I(Q)$  produced by the averaging operation is related to the absolute cross-section  $d\Sigma(Q)/d\Omega$  by the expression:

$$I(Q) = \phi A d T (d\Sigma(Q)/d\Omega) \Delta\Omega \varepsilon t,$$

where:

$\phi$  = flux on the sample,

$A$  = sample area,

$d$  = sample thickness,

$T$  = measured sample transmission,

$\Delta\Omega$  = solid angle subtended by one pixel of the detector,

$\varepsilon$  = detector efficiency, and

$t$  = effective counting time, which was renormalized to give  $10^8$  monitor counts (MON).

By dividing this expression for the data by a similar expression for the standard sample, ABS calculates the absolute cross-section for the data from:

$$d\Sigma(Q)/\Delta\Omega = [ I(Q) \text{ MONs } ds Ts ] / [ I_s(0) \text{ MON } d T ] [ d\Sigma_s(0)/\Delta\Omega ]$$

where:

$I_s(0)$  = measured intensity of the standard sample at  $Q=0$ ,

$ds$  = thickness of the standard sample and

$Ts$  = measured transmission of the standard sample (which is wavelength dependent).

Note that if  $I(Q)$  and  $I_s(Q)$  are from radially averaged work files then  $\text{MONs}=\text{MON}$ .

Another, often simpler method for rescaling data to an absolute intensity consists in a direct measurement of the beam flux at the sample using the area detector. This measurement is similar to the empty beam measurement when measuring transmissions (move attenuators in and the beam stop out). The quantity  $K = \phi A \Delta\Omega \varepsilon t$  is the scaling factor, automatically calculated as follows:  $\phi A \varepsilon$  is the total (empty beam transmission) detector counts per unit time/attenuation factor at the used wavelength,  $t$  is the counting time  $\times 10^8/\text{MCR}$ , and  $\Delta\Omega$  is equal to  $(0.5 \text{ cm/sample-to-detector distance in cm})^2$ .

In some cases, it is not necessary to convert your data to absolute scale.

### **Masking the dataset**

The last step before averaging the data to reduce it to  $I$  vs  $Q$  form is to mask the dataset. This operation has the effect of marking, or masking, specific pixels in the 2D data field that are to be ignored in the subsequent averaging process.

## Averaging the dataset

At this point the corrected data can be reduced to I vs Q or saved in another format. Typically, the averaging operation is used to perform either a radial, angular sector or rectangular average (ignoring all masked pixels) of the 2D data field to reduce it to I vs Q. The averaged data are stored in individually named ASCII (text) files. Data that have been converted to an absolute scale are, after averaging, stored in a file with the extension .ABS; otherwise, the results are stored in a file with the extension .AVE.

## SANS System Requirements

- Macintosh or PC
- IGOR Pro installed <http://www.WaveMetrics.com> (v. 4.0 is the current version). As of 10/2001, SANS Reduction macros require IGOR Pro v. 4.0x. As always, the macros will work with free Demo versions of IGOR.

**NOTE:** You DO NOT need to purchase IGOR Pro to reduce your data. You can use either the (free) Demo version of IGOR Pro, or the full version. IGOR 4.0x or higher is required. Some features are, however, unavailable in the Demo version. (The use of certain trade names or commercial products does not imply any endorsement of a particular product, nor does it imply that the named product is necessarily the best product for the stated purpose.)

- SANS Reduction Macros and the Tutorial data are available on our website: [http://www.ncnr.nist.gov/programs/sans/manuals/data\\_red.html](http://www.ncnr.nist.gov/programs/sans/manuals/data_red.html)  
Follow the instructions on the webpage for downloading and installing the SANS Reduction Macros.
- The output ASCII (I(q) vs. q) files are also compatible with a collection of models that can be fitted to your SANS data. These models are available at: [http://www.ncnr.nist.gov/programs/sans/manuals/data\\_anal.html](http://www.ncnr.nist.gov/programs/sans/manuals/data_anal.html), and use IGOR Pro's curve fitting features.

## What's New in SANS

Changes from Version 3 (11/2000) to Version 4 (10/2001):

### Display enhancements

- Added Qx and Qy scales to the detector image.
- The 1-D plot window allows simple rescaling of X or Y axes for popular views such as logarithmic, Guinier, Zimm, or power laws.
- Color Mapping can now be adjusted using familiar slider bar controls.

### Export formats

- In data reduction protocols, "Average" options now include 2D\_ASCII (detector coordinates), I(Qx,Qy) as three columns, or as a PNG graphics image.
- A Marquee menu operation allows the current detector image (with the color scale) to be saved in a variety of graphics formats. See [Marquee Operations](#).

### New operations

- NG1 transmission files can now easily be converted so that they will be automatically recognized as such, allowing transmissions to be calculated through the transmission panel.

See the [Misc Ops Tab](#).

- A "Tile RAW 2D" operation allows tiling of PNG images of raw data files in a layout window that can be annotated and printed. See [Tile 2-D Images](#).
- A Marquee menu operation allows a selected region of the detector image to be fitted with a 2-D Gaussian function. Results are reported in terms of Qx and Qy rather than pixel values. See [Marquee Operations](#).
- A [Detector Sensitivity File](#) (DIV) can be created from within IGOR, and is written out as a VAX-formatted file.
- Data in work sub-folders can be copied to new folders, such as STO or SUB.
- A "Work File Math" panel is available that will perform simple arithmetic operations on workfile (2-D) data. See [2-D Work File Arithmetic](#).
- Raw 2-D data files can be batch exported as ASCII files in two formats, either versus pixel (x,y) or q-value (Qx, Qy). See [2-D ASCII Export](#).
- A Marquee menu operation will perform a box sum over a selected region, for a list of data files. Data files are added to SAM to normalize before summing the region. See [Marquee Operations](#).
- Data reduction protocols can now include DRK files (collected with the beam shutter closed) for proper data correction in certain specialized situations.

### Improved functions

- Files can be entered into protocols or multiple reduction panels as comma-delimited lists of run numbers instead of "Set" selections from the CAT/VShort Table. Run number lists may be non-consecutive and include dashes to cover inclusive file ranges.
- Protocols are now portable, requiring only that the data path is properly set.
- Sample data collected with attenuators present is automatically corrected and rescaled using attenuator calibration tables.
- Fit and Fit/RPA panels now have consistent behavior and do all required file loading and plotting.
- Mask drawing is simplified and allows editing of previously saved masks.
- Sort operation now warns if there are no overlapping data points.
- NG1 SANS data now uses the attenuator calibration table from NG7 for intensity calibration and data correction steps.

### **Instructions for the Impatient**

- 1) Open the "SANS\_Reduction..." experiment and pick the data path
- 2) [List the Data Files](#)
- 3) [Calculate Transmissions](#)
- 3) [Build a Data Reduction Protocol](#)
- 4) [Reduce a File](#)
- 5) [Sort and Combine Averaged Datasets](#)
- 6) Write journal article

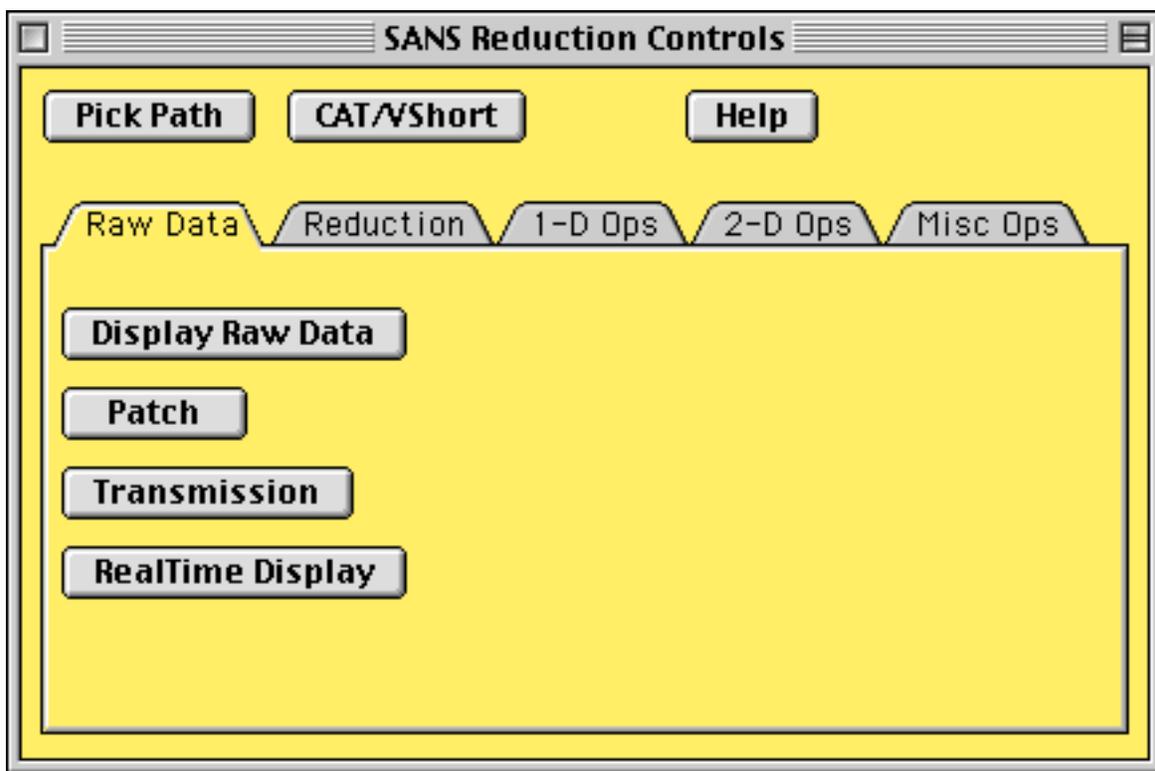
## **Tutorial Instructions**

### **Main Controls**

**What:** Upon opening a blank template experiment for SANS data reduction, this main control panel is the starting point for viewing your data, performing the data reduction, plotting the

averaged data, and performing some simple analysis. It organizes the essential controls for SANS data reduction in one location.

**How:** The SANS Reduction macros are loaded and compiled automatically upon opening the "SANS\_Reduction..." experiment. After successfully compiling, the Main Panel of SANS Reduction Controls is automatically created. If you've lost this panel on the screen, selecting SANS->Initialize from the main menu bar will bring this window to the front. Clutter can be minimized by closing auxiliary panels when not in use. Panels are automatically re-created on demand.



The buttons are:  
(always visible)

Pick Path: presents a dialog to select the folder that contains your data. This only needs to be set once, at the beginning of a data reduction session.

CAT/VShort: after the data path has been set, this will generate a table of information about each file in the data folder. The table is very useful to identify each file and for building reduction protocols.

Help: will display this help file.

For a detailed description of the buttons contained on all of the tabs, see:

[Raw Data Tab](#)

[Reduction Tab](#)

[1-D Ops Tab](#)

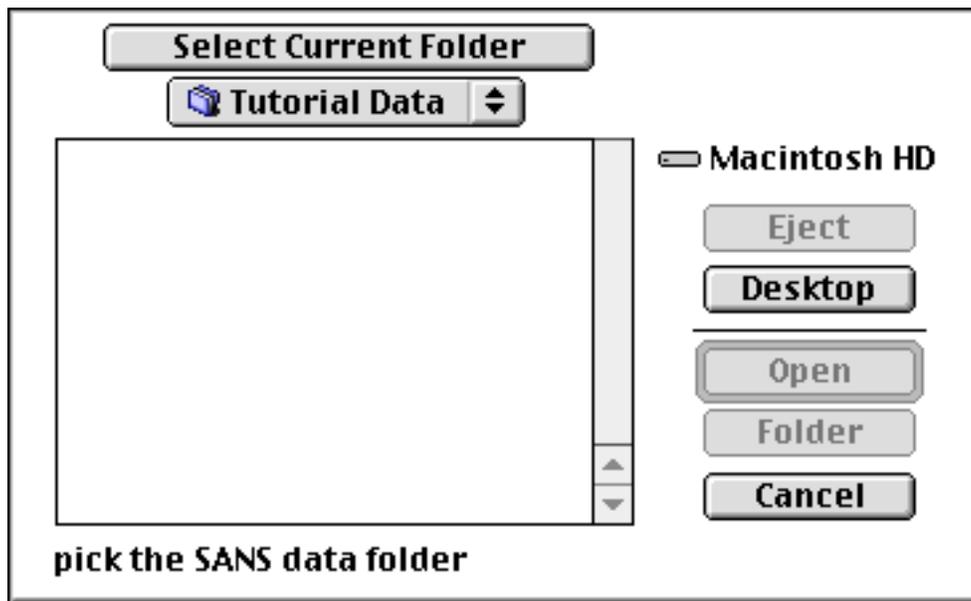
[2-D Ops Tab](#)

[Misc Ops Tab](#)

**List the Data Files**

**What:** Set a path to your data folder. Then create a "Catalog" table with information about your data files, available for use in building data reduction protocols.

**How:** All of the raw data files, detector sensitivity files, mask files, etc. must be kept in a single folder for IGOR to access them. From the main panel, click "Pick Path" to set the path to this folder. On a Mac, if your data is inside "Tutorial Data", the dialog should look like this. On Windows it will look slightly different.



Once the path is set, click "CAT/VShort" to create a catalog table listing of all of the files in the selected folder. Raw SANS data files will show descriptive header information like the label, counting times, and thickness and transmission. The columns can be resized to see the whole label, etc., or delete columns of information you don't want to see. This table is also used interactively for building data reduction protocols, and is detailed later. Clicking "CAT/VShort" again will rebuild the list of files, and should be done if files were added to the folder or to confirm that header information was updated correctly. The table will list all of the files in the data folder, displaying information about raw SANS data files only. Files that are not recognized as raw SANS data are appended to the bottom of the "FileNames" column. Note that in the "FileNames" column, there are two important files listed that are not raw SANS data - these are the mask and detector sensitivity files.

R7C0		SSY2K009.SA2_CJG_L462			
FileNames	Labels	DateAndTime	SDD	Lambda	CntTin
SSY2K002.SA2.	beam center 6m and 6A	7-JUN-2000	6	6	
SSY2K003.SA2.	T. APOFERRITIN 6m and 6A	7-JUN-2000	6	6	
SSY2K004.SA2.	S. APOFERRITIN 6m and 6A	7-JUN-2000	6	6	9
SSY2K005.SA2.	blocked beam 6m and 6A	7-JUN-2000	6	6	3
SSY2K006.SA2.	buffer Sample 6m and 6A	7-JUN-2000	6	6	3
SSY2K007.SA2.	T.empty 6m and 6A DL/D	7-JUN-2000	6	6	
SSY2K008.SA2.	T.beamcenter 1.6m and 6A	7-JUN-2000	1.6	6	
SSY2K009.SA2.	s.apoferritin 1.6m and 6A	7-JUN-2000	1.6	6	9
SSY2K010.SA2.	blocked beam 1.6m and 6A	7-JUN-2000	1.6	6	9
SSY2K011.SA2.	buffer 1.6m and 6A DL/D	7-JUN-2000	1.6	6	9
DEFAULT.MASK					
PLEX_03MAY00					

## The Display Window

**What:** Display a raw 2-D SANS data file and get some simple information about the data.

**How:** 2-D SANS data is displayed by clicking "Display Raw Data" under the Raw Data Tab on the Main Panel. A standard dialog is presented to select the raw data file. The data is displayed versus detector pixel (left and bottom axes) and versus Qx and Qy (top and right axes), along with a color scale. Important information about the data is displayed at the top of the graph, including the filename, the (X, Y) position of the cursor, and the count value. If the display type is "RAW" then this is the actual neutron counts for that pixel. If the displayed data is one of the correction steps, it may not be an integer neutron count value. The horizontal, vertical, and total q-values (in Angstroms<sup>-1</sup>) are also displayed. Further information about the file can be displayed by clicking the "Status" button, and the information is printed to the command window at the bottom of the screen. The color mapping of the detector counts can be toggled between logarithmic and linear scale by clicking the "isLin" button. The current label on the button, either "isLog" or "isLin" gives the current scaling. The displayed data can be averaged (without doing any reduction steps) by clicking the "I vs. q" button. This will present a new panel with the [Average Options](#). For averages of sectors or slices of the 2D dataset, the region to be averaged is marked on the dataset in response to the angles and widths chosen in the panel. The defaults are for a standard circular average of the full dataset.

If the data displayed is "RAW" data, and a path to the data has been chosen, left and right arrow buttons will also be present on the graph. This will display the next (or previous) run number in the data folder, if available, without having to proceed from the main panel through an open file dialog to select the file. The Color Map sliders can be adjusted as desired to alter the color display of the data.

The controls are:

Status: prints selected information about the displayed file to the command window at the bottom of the screen.

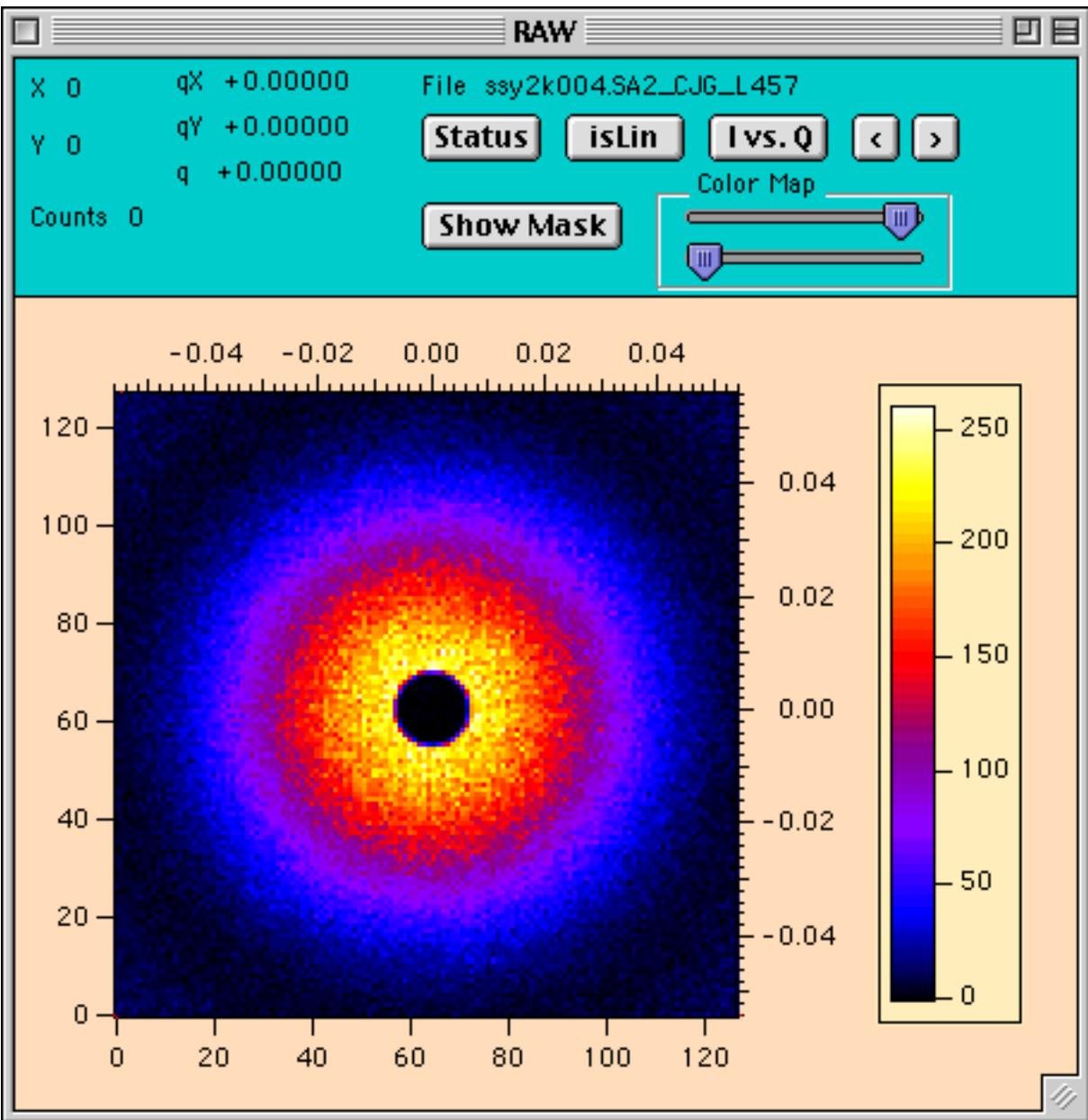
isLin: toggles the color map scaling of the detector counts from linear to logarithmic. When the data is log-scaled, the button will read "isLog".

I vs. Q: displays a new panel with averaging options to produce a 1-D averaged dataset of the 2-D data. No reduction steps are performed.

Left/Right Arrows: are only visible if the displayed data is "RAW" data. If the data path has been set, these buttons will increment the display to the next (or previous) run number, bypassing the open file dialog.

Show Mask: toggles the currently loaded mask file (if present) on/off the dataset in a bright green color, indicating which data points are to be excluded from the 1-D average.

Color Map Sliders: adjust the upper and lower threshold limits for the color scale to highlight features in the 2-D detector image.



### **Average Options**

**What:** This feature allows you to perform different types of averages on your data, and allows you to see what regions of the detector will contribute to the average. Open the Average Panel, and try out some different types of averages. The regions to be averaged are clearly shown on the data, and can be easily adjusted. The numerical values of pixels, angles, etc. can be used later in reduction protocols.

**How:** Open the Average Panel either using the "I vs Q" button on the Display window, or the "Average" button on the Misc Ops tab of the main panel. You will then be able to average whatever data is currently in the display.

- "Circular" is the default average type. It will perform and average in constant q-rings around the (x,y) pixel location of the beam center. The default pixel width is fixed at one, and there are no other options to set when doing a circular average.
- "Rectangular" will average in constant q-arcs, but limited to a rectangular swath of a specified width of pixels. This rectangular swath can be oriented at any angle, and include either side or both sides of the detector.
- "Sector" is very similar to Rectangular, except that the width of the sector is specified in degrees ( $\pm$  delta phi) each direction from the central angle (phi).
- "Annular" will perform an average centered at a single q-value (q-center), and averaged over a width of a specified number of pixels. The data is returned as a function of angle (phi) in degrees. If a normal x-y coordinate system is drawn through the beamcenter, zero angle corresponds to the positive x-axis and proceeds counter-clockwise. Therefore 270 degrees corresponds to the negative y-axis.

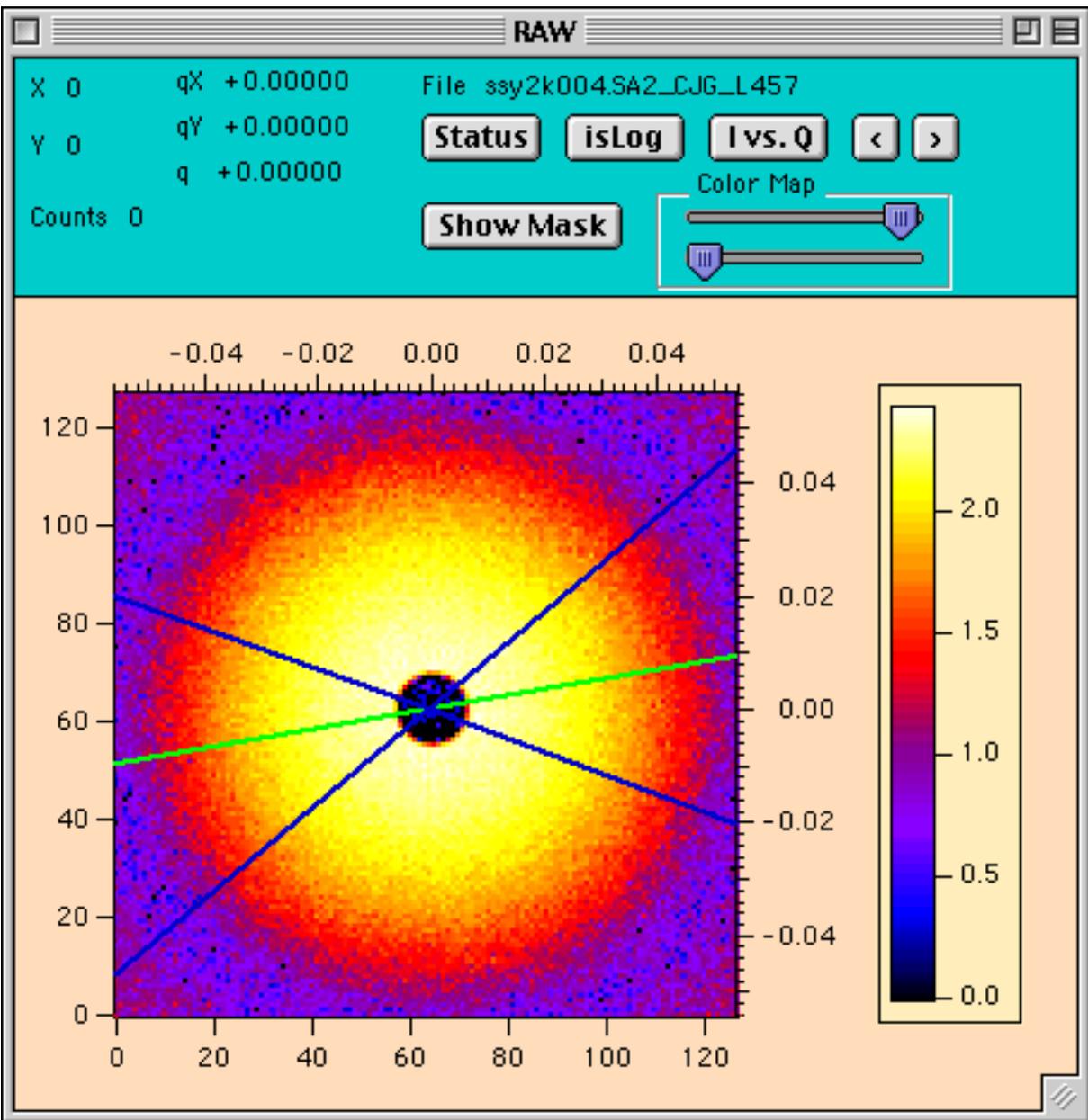
For this selection of sector average, and the angles phi and delta phi:

The screenshot shows a dialog box titled "Average\_Panel" with a pink background. At the top, "AverageType" is set to "Sector". The dialog is divided into four sections:

- Sector/Rectangular:** "Sides ?" is set to "both", and "Phi" is set to 10.
- Annular:** "Q-center" is set to 0, and "Q Delta" is set to 1 (pixels).
- Rectangular:** "Width" is set to 1 (pixels).
- Sector:** "Delta Phi" is set to 30.

At the bottom, there is a checkbox for "Save file to disk?" which is unchecked. There are three buttons: "Do Average", "Clear", and "Done".

The corresponding Display shows what data will be included. The green line is the center of the average (phi) and the blue lines are maximum extent of the sector (Delta Phi),  $\pm$  30 deg = 60 degrees total angle.



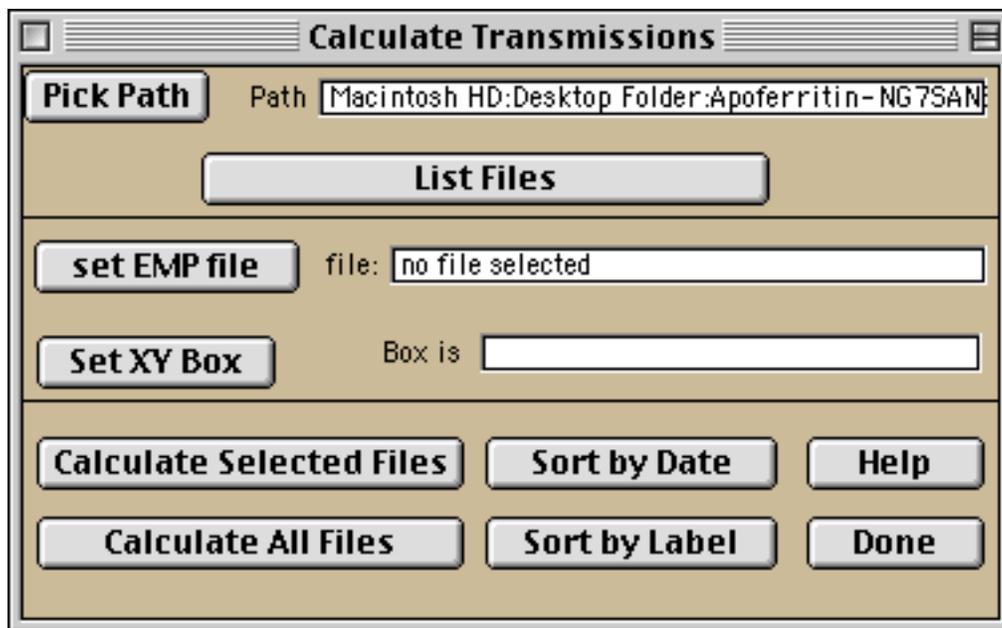
Averaged data that has been saved from this panel (only if "Save File to disk?" is checked) will have "unknown" files listed as its protocol, since there's no way of knowing what steps have been performed on the 2-D data. If you know what you've done to the data, you're ok - it's just there as a warning.

### **Calculate Transmissions**

**What:** Transmission of samples and sample containers must be calculated and entered into the headers of the raw data files for proper subtraction of non-sample scattering during data reduction. Here we will create the "associations" between the transmission measurements and the scattering files to which they correspond. Transmissions will then be calculated and automatically patched to the file headers.

**How:** 1) Open the Transmission panel by clicking "Transmission" on the Raw Data tab of the

main panel. The following new panel will appear:



2) Click on "List Files" to build two tables - one with scattering files:

ScatteringFiles

ROCO

S_TRANS_Filena	S_Filenames	S_Labels	S_SDD	S_Lamb	S_Transn
	<a href="#">SSY2K004.SA2</a>	S. APOFERRITIN 6m	6	6	1
	<a href="#">SSY2K005.SA2</a>	blocked beam 6m an	6	6	1
	<a href="#">SSY2K006.SA2</a>	buffer Sample 6m a	6	6	1
	<a href="#">SSY2K009.SA2</a>	s.apoferitin 1.6m :	1.6	6	1
	<a href="#">SSY2K010.SA2</a>	blocked beam 1.6m	1.6	6	1
	<a href="#">SSY2K011.SA2</a>	buffer 1.6m and 6A	1.6	6	1

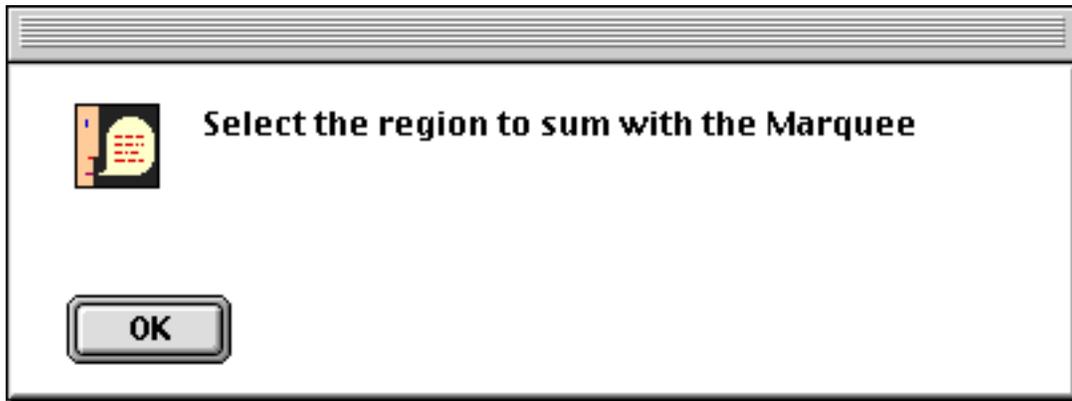
and another with transmission files. The transmission files are automatically separated from the scattering files using the beamstop location (off-center) in the header of the raw data file.

TransmissionFiles				
ROCO				
T_EMP_Filenam	T_Filenames	T_Labels	T_SDD	T_Lamb
	SSY2K002.SA2	beam center 6m	6	6
	SSY2K003.SA2	T. APOFERRITIN	6	6
	SSY2K007.SA2	T.empty 6m and	6	6
	SSY2K008.SA2	T.beamcenter 1.	1.6	6

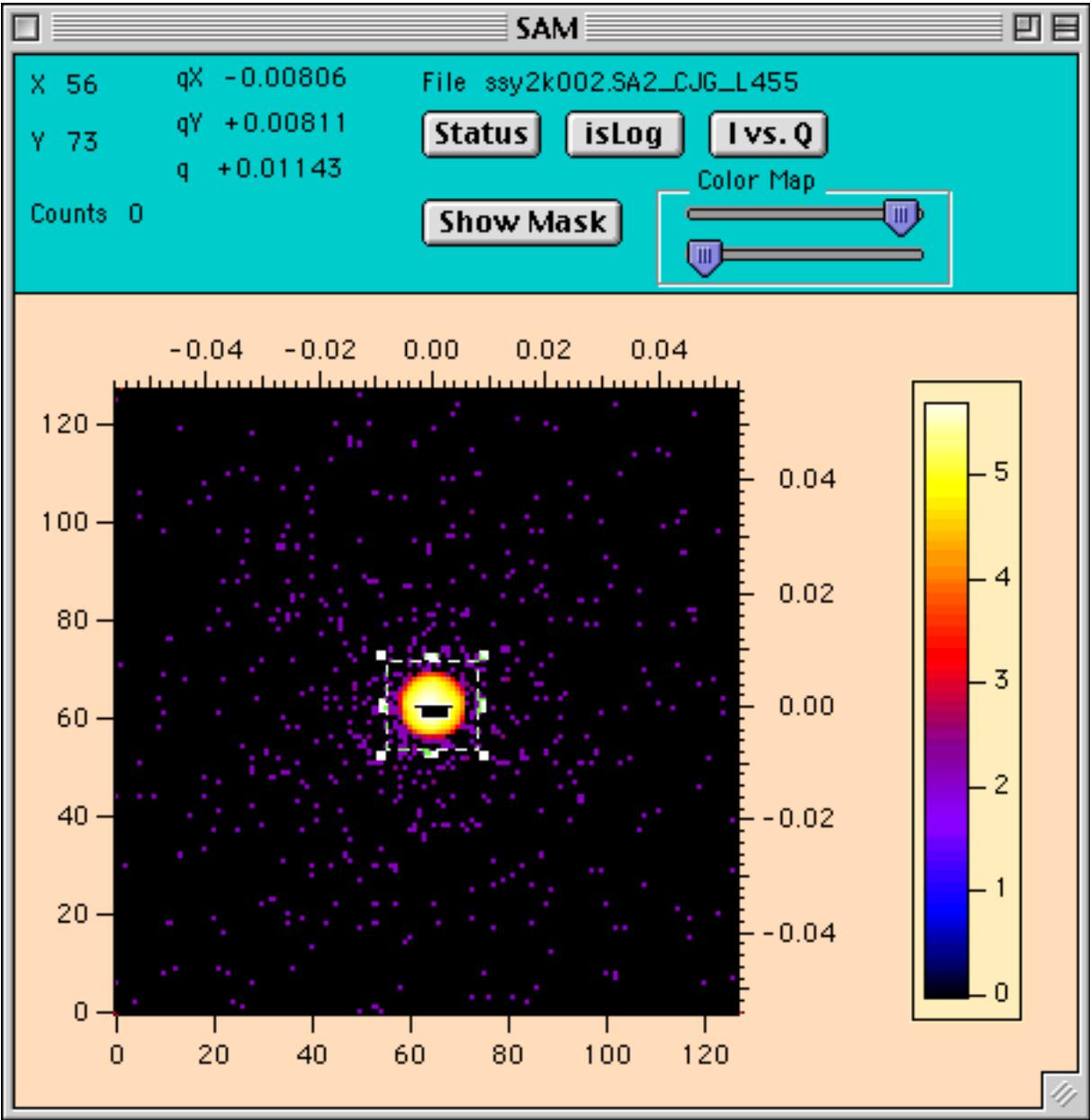
3) Find the empty beam transmission measurement in the TransmissionFiles table. It is in the blue "T\_Filenames" column. For the tutorial, it is file SSY2K002.SA2..... Click on this file to select it (just that cell in the table). In the Transmission Panel, click "Set EMP File" to set this file as the empty beam. The filename appears, as well as the box coordinates:

Calculate Transmissions	
<b>Pick Path</b>	Path <input type="text" value="Macintosh HD:Desktop Folder:Apoferitin-NG7SANE"/>
<b>List Files</b>	
<b>set EMP file</b>	file: <input type="text" value="SSY2K002.SA2_CJG_L455"/>
<b>Set XY Box</b>	Box is <input type="text" value="X1=0;X2=0;Y1=0;Y2=0;"/>
<b>Calculate Selected Files</b>	<b>Sort by Date</b> <b>Help</b>
<b>Calculate All Files</b>	<b>Sort by Label</b> <b>Done</b>

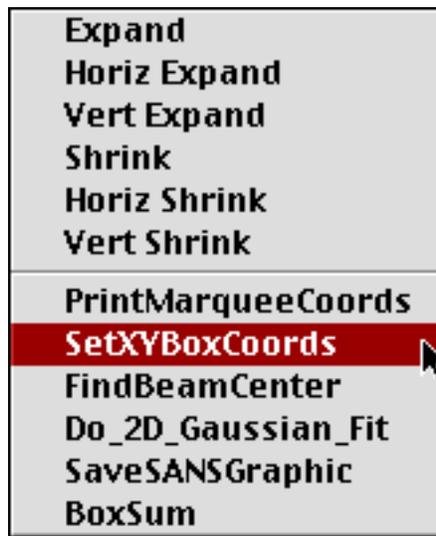
The "intensity" of the empty beam is found by summing the number of counts on the detector over a specific rectangular region of the detector. Currently the box coordinates are zeros, so we need to pick the rectangle. Do this by clicking "Set XY Box". The raw data file (SSY2K002) will be displayed, and you will be presented with the following dialog:



In the data display, click and drag a marquee that encompasses the primary beam. You may find it easier to see the full extent of the beam if you switch the display to log scale. Move the cursor inside the marquee, to get an "upside-down hat" cursor.



Click to get a menu, and near the bottom, select "Set XY Box Coords".



The pixel values for the box will be updated to the Transmission panel, and are written to the empty beam file header for future calculations. You won't need to do this again. Note that the marquee selection can also be used to measure the beam center, or centroid of any selected region. See [Marquee Operations](#) for more details.

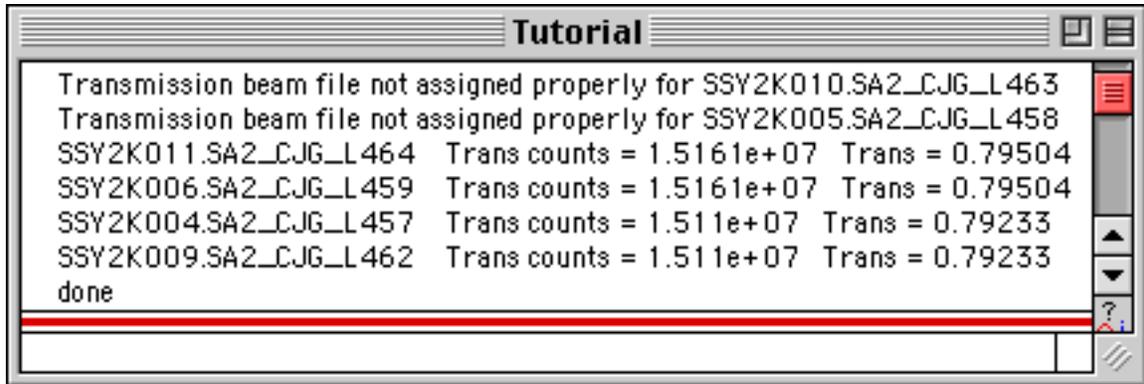
4) Now make the associations between the empty beam file and each of the transmission measurements. Each transmission measurement for a sample must be normalized relative to the empty beam transmission (and should therefore be less than unity). Make the EMPTY beam association by selecting the empty beam file (in the blue column), copying it, and pasting the filename into the "T\_EMP\_Filename" column. You obviously don't need to associate the empty with itself, or with the beamcenter measurement that was taken at a different sample-to-detector distance (T\_SDD). Transmission was only measured of two samples: the apoferritin (a protein in an aqueous buffer, held in a quartz cell), and the buffer alone in the same cell. Note that the sample label says "T. empty...", but it's really the buffer. You should try to do better with your sample labels. The TransmissionFiles Panel should look like this:

T_EMP_Filename	T_FileNames	T_Labels	T_SDD	T_Lambda
	SSY2K002.SA2	beam center 6m	6	6
SSY2K002.SA2	SSY2K003.SA2	T. APOFERRITIN	6	6
SSY2K002.SA2	SSY2K007.SA2	T.empty 6m and	6	6
	SSY2K008.SA2	T.beamcenter 1.	1.6	6

5) Now make the association between the transmission measurement of the apoferritin (SSY2K003) and the scattering file(s) for the same sample. In this case, the apoferritin scattering was measured twice - using two different instrument configurations. The sample is the same, and so is the transmission, so copy the filename of the apoferritin transmission



SSY2K010... and SSY2K005... which is not a problem, since these are our blocked beam files and we don't calculate the transmission of these files anyways. The other four transmissions are calculated correctly, and these transmission values are automatically patched to the raw file headers, and updated to the ScatteringFiles table. The CAT/VShort table, however, is not updated (unless you force it to update by clicking CAT/VShort on the main panel again).



7) Transmission calculations are done. Clicking done will remove the panel and both tables. All of the tables and associations are regenerated by starting again from the "Transmission" button on the main panel. The previous associations are retained, and newly collected data files will have no associations. If the empty beam file had been previously set, it does not need to be set again, no matter what the panel indicates. Re-"setting" the EMPTy file as in step 3 will show that the box coordinates are not zeros, but are the coordinates that you previously selected with the marquee. In addition, if you only want to calculate the "new" files, select them in the blue "S\_Filenames" column, and "Calculate Selected Files". It won't hurt to calculate all of the files, but it is a waste of time.

### **Patch File Headers**

**What:** Some of the information in the file header may have been incorrectly set at the time of data collection, and must be updated before data can be correctly reduced. Here we can change header values in the raw data files. Typically, no information needs to be changed here, since transmission values were automatically "patched" by the Calculate Transmission step.

**How:** From the Raw Data tab on the main panel, click "Patch". This will display a new panel that can be used to verify and change certain fields in the raw data headers. If the data path is not set, do it now using the "Pick Path" button. Click (and release) the popup menu of files to refresh the list. Since the Match String is "\*", all data files will be shown. The "\*" has the usual wild-card meaning. Only a single wildcard can be used to trim the list of files displayed in the popup. The header information in the displayed file in the popup is shown below it in the text fields. If, for example, you want to change the sample label, you simply enter the new text into the box, check the "change" box next to it, and click "change header". If the "change" box is not checked, that field cannot be changed in the file header. This feature prevents accidentally changing values you don't intend to change. To patch the same information to a series of data files (like the beam center X and Y) enter the new values and check the "change" boxes. You can use the match string to trim the file popup to include the files that you want to change (you may have to change the files in a few batches to change just the ones you want). Then click "change all headers in list". You will be warned that it will change more than just the top file, and say "yes" to change all the files in the list.

Transmissions were calculated previously using the Transmission panel, and should all be correct here.

**Patch Raw SANS Data Files**

**Pick Path** Path

File(s) to Patch

Match String

**Change?**

label

Transmission

Thickness (cm)

Beamcenter X

Beamcenter Y

Attenuator number

Counting time (s)

Monitor count

Detector count

Trans. det. count

Wavelength (A)

Wavelength spread

Temperature (C)

Magnetic field (G)

Source aperture (mm)

Sample aperture (mm)

Source to sample distance (m)

Detector offset (cm)

Beamstop diameter (mm)

Sample to detector distance (m)

### **Build a Data Reduction Protocol**

**What:** Building and saving a protocol allows you to repeatedly reduce raw data files for a given configuration using the same exact sequence of corrections. Here, you can identify the

files and steps necessary to correct your data for non-sample scattering, detector sensitivity, convert to absolute scaling, eliminate "bad" detector pixels, and produce output in a variety of formats. Once a protocol is constructed for a specific instrument configuration, it can be saved and recalled for later use.

**How:** Click "Build Protocol" on the Data Reduction tab of the main panel. This will present a new panel with a list of reduction steps that can be used. Steps that are checked will be performed, steps that are not checked will be skipped (except that you will always supply a sample file, or be prompted for one). For this example, we will use nearly all of the data reduction steps, and first build a protocol to reduce data taken at a 6 meter sample to detector configuration and use absolute scaling from an empty beam measurement. Click "Show CAT/VShort" to bring the listing of files to the top, and arrange the windows so the list and the panel are visible.

1) Leave the sample field as "ask" so that the program will prompt us for the sample data file(s) when they are needed. We could specify a file to bypass the dialog, if desired.

**Data Reduction Protocol**

**CAT/VShort**      **Show CAT/VShort**

**Sample**      **set SAM file**  
file: ask

**Background**      **set BGD file**  
file: ask

**Empty Cell**      **set EMP file**  
file: ask

**Sensitivity**      **set DIV file**  
file: ask

**Absolute**      **set ABS params**  
parameters: ask

**Mask**      **set MASK file**  
file: ask

**Average**      **set AVERAGE params**  
parameters: AVTYPE=Circular;SAVE=Yes;NAME=A

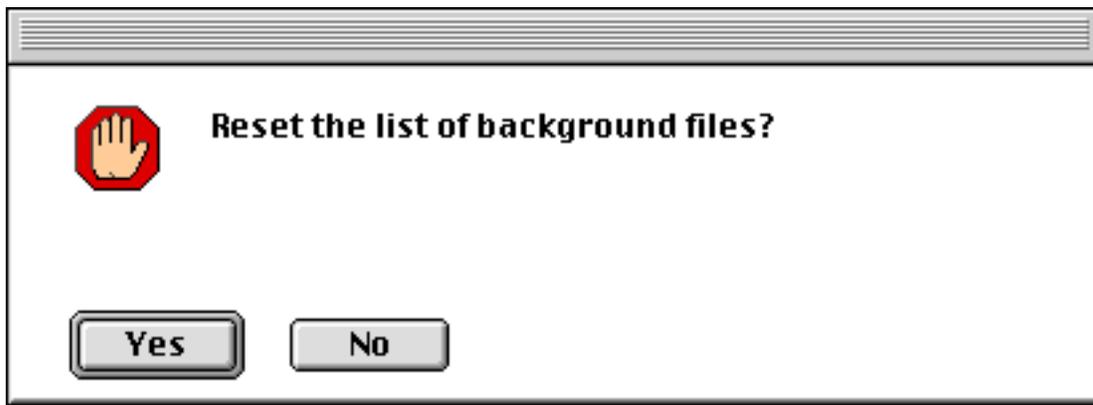
**Use DRK correction.**      DRK=none,DRKMODE=0,

**Save Protocol**      **Reduce A File**

**Recall Protocol**

**Delete Protocol**      **Done**

2) Fill in the background file by finding it in the listing (run SSY2K005), clicking to select the filename, and then clicking "Set BGD file" on the panel. The following dialog appears:

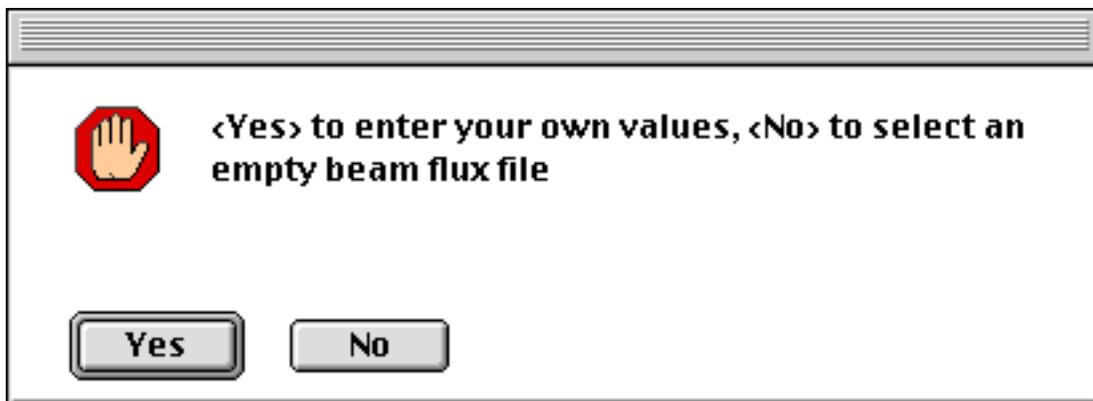


Say "Yes" to reset the list of files. This will set this single file (the selected text) as the background file. If several background files were collected and it is desired to add them together, reset the list for the first file, and then select "No" (don't reset) for additional files to add together. These additional files will be listed in the field as well and added together during the data reduction. The EMP (and SAM) file fields are set in an identical fashion.

3) Fill in the EMPty cell file (actually the buffer solution, in this example) in the same way that the BGD file was set. It is run SSY2K006.

4) Set the detector sensitivity (DIV) file. The file is PLEX\_03MAY00\_NG7.DIV (at the bottom of the CAT/VShort table). Note that it is not a raw SANS data file, and is not recognized as such by the listing. There can only be one detector sensitivity file assigned to a protocol.

5) Set the absolute scaling parameters. Click the "set ABS params" button, and the following dialog appears:



Select "No" and you will be prompted for an empty beam measurement (at 6 meters) to use for absolute intensity calibration. When the dialog appears, select run SSY2K002..., which is the empty beam measurement. The file will be opened, and the absolute scaling parameters will be calculated and listed in the field on the Protocol Panel. If you are using a measured secondary standard for calibration, "Yes" will allow you to enter your own values (i.e. the standard thickness, transmission,  $I(q=0)$ , and the tabulated cross-section of the standard sample).

6) Click on the "DEFAULT.MASK" filename in the listing, which is a simple mask to exclude the edges of the detector. Click "set MASK" to set the filename. The mask file was created either in IGOR Pro or in SANS Image. Note that this is NOT the same format as a "WORK.MSK" file from the VAX.

7) Default values for a circular average of the data (annulus width is always one pixel) should already be in the field. If not, or a different average is desired, click "set Average

Params", and set the desired values in the dialog. Note that 2-D ASCII export formats or a save of the SANS graphic are regarded as "Average Types" since this is the protocol step where reduced data is written to disk. Of course, some of the fields do not apply for a given type of average, and their values are ignored.

**GetAvgInfo**

Type of Average	Save files to disk?
<b>Circular</b> ▼	<b>Yes</b> ▼
Auto-Name files?	Plot the averaged Data?
<b>Auto</b> ▼	<b>Yes</b> ▼
Include detector halves?	Orientation Angle (-90,90) degrees
<b>both</b> ▼	0
Azimuthal range (0,45) degrees (Sector)	Width of Rectangular average (1,128)
10	10
q-value of center of annulus	Pixel width of annulus
0.01	10

**Quit Macro**      **Continue**      **Help**

8) Most experiments do not need to use a DRK correction file, which is measured with the main shutter closed. This measurement is typically only necessary when... go ask your local contact if this correction is necessary for your experiment.

9) Once all fields are set to their correct files / parameters, click "Save Protocol" to save these settings for later recall, using a descriptive name for the protocol. "sdd\_6meters" is a good choice for this protocol. Your Protocol Panel should look like this:

**Data Reduction Protocol**

**CAT/VShort**      **Show CAT/VShort**

**Sample**      **set SAM file**  
file: ask

**Background**      **set BGD file**  
file: SSY2K005.SA2\_CJG\_L458,

**Empty Cell**      **set EMP file**  
file: SSY2K006.SA2\_CJG\_L459,

**Sensitivity**      **set DIV file**  
file: PLEX\_03MAY00\_NG7.DIV,

**Absolute**      **set ABS params**  
parameters: TSTAND=1;DSTAND=1;IZERO=3239;

**Mask**      **set MASK file**  
file: DEFAULT.MASK,

**Average**      **set AVERAGE params**  
parameters: AVTYPE=Circular;SAVE=Yes;NAME=A

**Use DRK correction.**      DRK=none,DRKMODE=0,

**Save Protocol**      **Reduce A File**

**Recall Protocol**

**Delete Protocol**      **Done**

10) Set up another protocol to reduce the data at the 1.6 meter configuration. This involves selecting a different background file, empty cell (buffer) file, and empty beam file for absolute scaling. The mask and detector sensitivity files do not need to be changed, nor do the averaging options. This time, we will use a (faster) method for "setting" the files for each step. The BKG file for 1.6 meters is SSY2K010. Simply highlight the filename field in the panel, and type the run number, 10 (leading zeros are not needed). You do not need to click the "set" button, simply enter the number. Run SSY2K011 is the buffer scattering, so enter 11 for the EMP file. Then set new ABS parameters in the same way as you did previously in step 5. Save this protocol as "sdd\_1\_6meters" or something else descriptive. Before saving the protocol, the run numbers are parsed into filenames, and the Protocol Panel should now have the following information. If a file could not be parsed, you would be informed of the offending number. Note also that multiple (and non-consecutive) runs can be added together by simply typing a comma-delimited list of run numbers. Dashes can be used to represent

inclusive ranges. See [Reduce Multiple Files](#) for an example.

**Data Reduction Protocol**

CAT/VShort    **Show CAT/VShort**

Sample    **set SAM file**  
file: ask

Background    **set BGD file**  
file: SSY2K010.SA2\_CJG\_L463,

Empty Cell    **set EMP file**  
file: SSY2K011.SA2\_CJG\_L464,

Sensitivity    **set DIV file**  
file: PLEX\_03MAY00\_NG7.DIV,

Absolute    **set ABS params**  
parameters: TSTAND=1;DSTAND=1;IZERO=1.181

Mask    **set MASK file**  
file: DEFAULT.MASK,

Average    **set AVERAGE params**  
parameters: AVTYPE=Circular;SAVE=Yes;NAME=A

Use DRK correction.    DRK=none,DRKMODE=0,

**Save Protocol**    **Reduce A File**

**Recall Protocol**

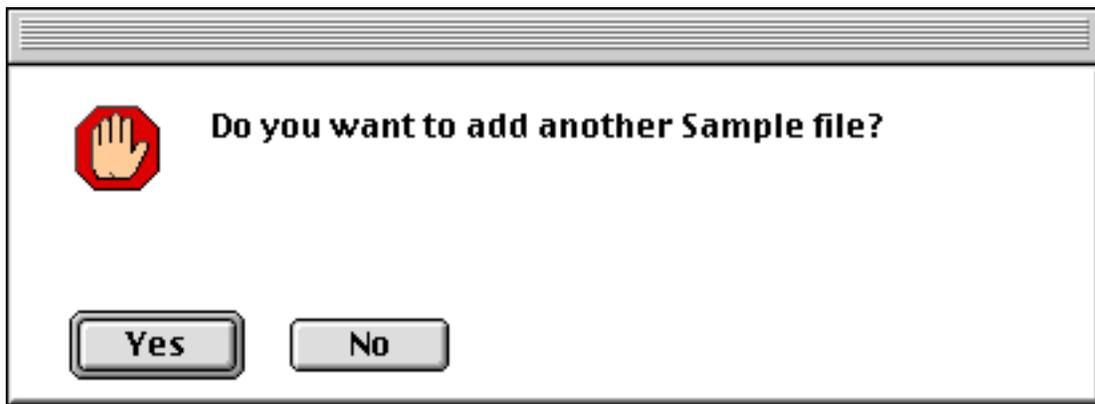
**Delete Protocol**    **Done**

### **Reduce a File**

**What:** Process a raw SANS data file to a 1-D average using a previously saved protocol, or use a blank protocol where you will be prompted for each data file as needed.

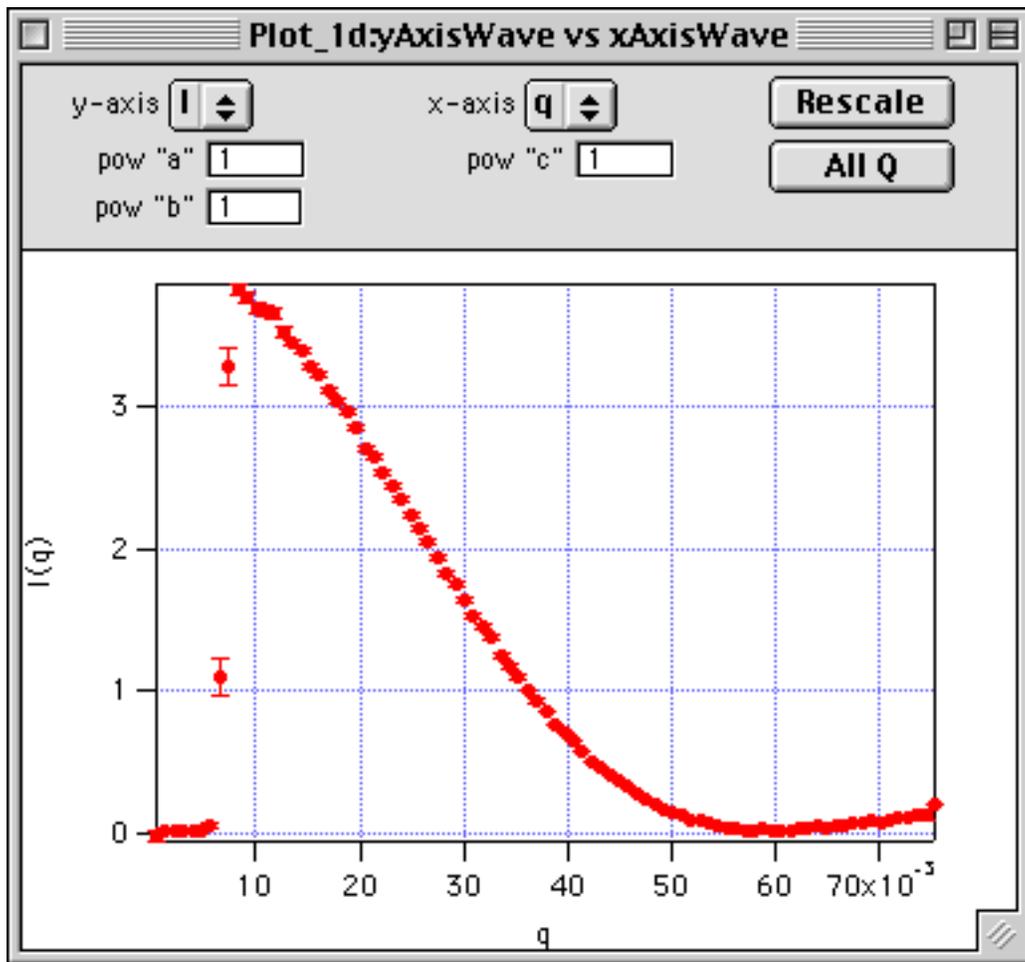
**How:** Since we just created and saved our two protocols, we'll use them directly from the Protocol Panel. Start with the 6-meter protocol. To make sure it's in place, click "Recall Protocol" on the panel, and pick "sdd\_6meter", or whatever you named it from the list. Your protocol choices are updated in the panel. At this point, you can choose the 6-meter apoferritin scattering file from the CAT/Short window, and "Set SAM File", or since the

protocol says "ask", just let it prompt you with a file dialog. You could also enter a list of run numbers. When done, click "Reduce A File" on the Protocol Panel. Pick the scattering file from the dialog if prompted (it's run SSY2K004...). The file will be displayed, and you will be prompted to add another sample file, if desired:

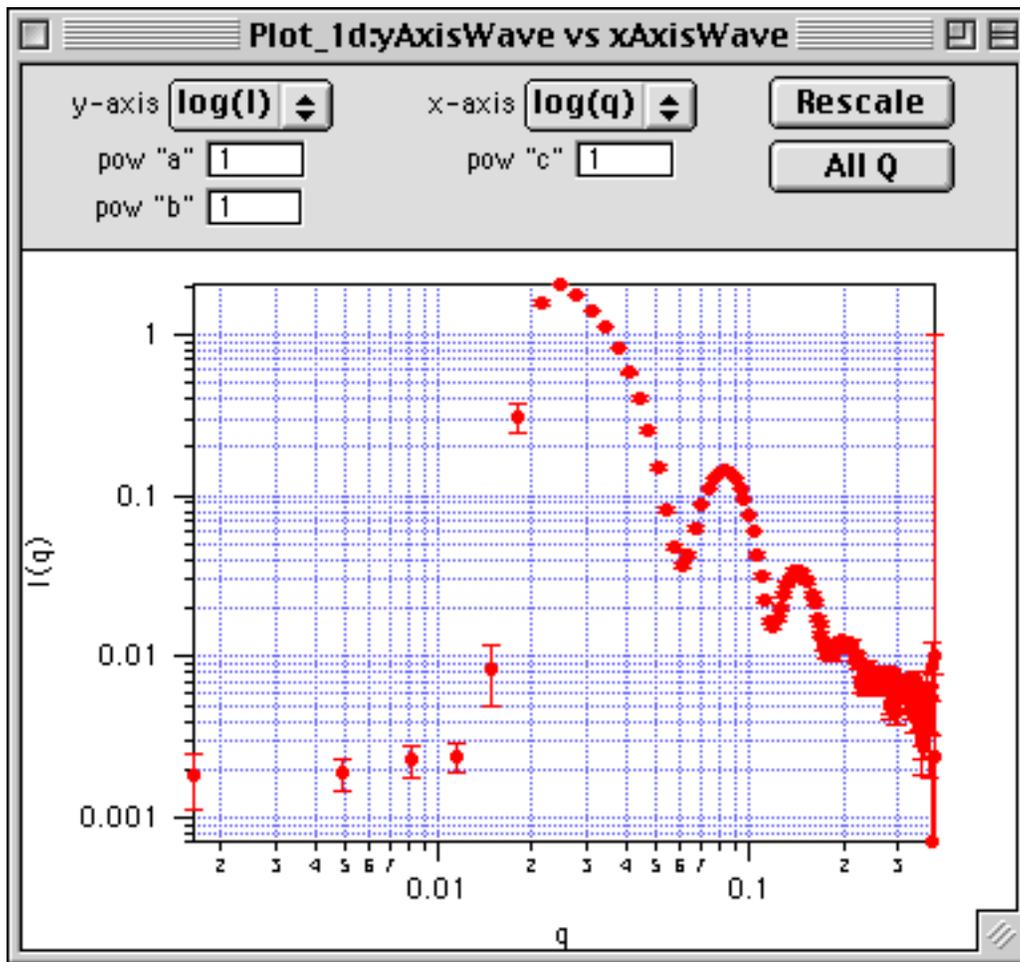


If you re-measure a sample at the identical configuration, you can add these raw data files together to improve the counting statistics. In this case, we only have one file, so (No) we don't want to add another data file.

The data reduction will proceed through the protocol, showing each intermediate step along the way. Watch closely - if something doesn't look right, go back and check it out after the reduction is done. If something is grossly in error, the reduction can be aborted (cmd-. on Macintosh, or the Abort button at the lower left in Windows). This example will proceed smoothly, of course. The final result should look like this, and the command window should indicate that a data file was written, and what filename was used.



Reduce the scattering data for the 1.6 meter configuration in the same way. "Recall" the protocol that you saved, and click "Reduce A File". You will be prompted for the sample scattering file (it's SSY2K009...) and the reduction will complete as before, using the files specified in the protocol. The final result for the high q data should look like this, once you've rescaled the X and Y-axes to log-scaling:



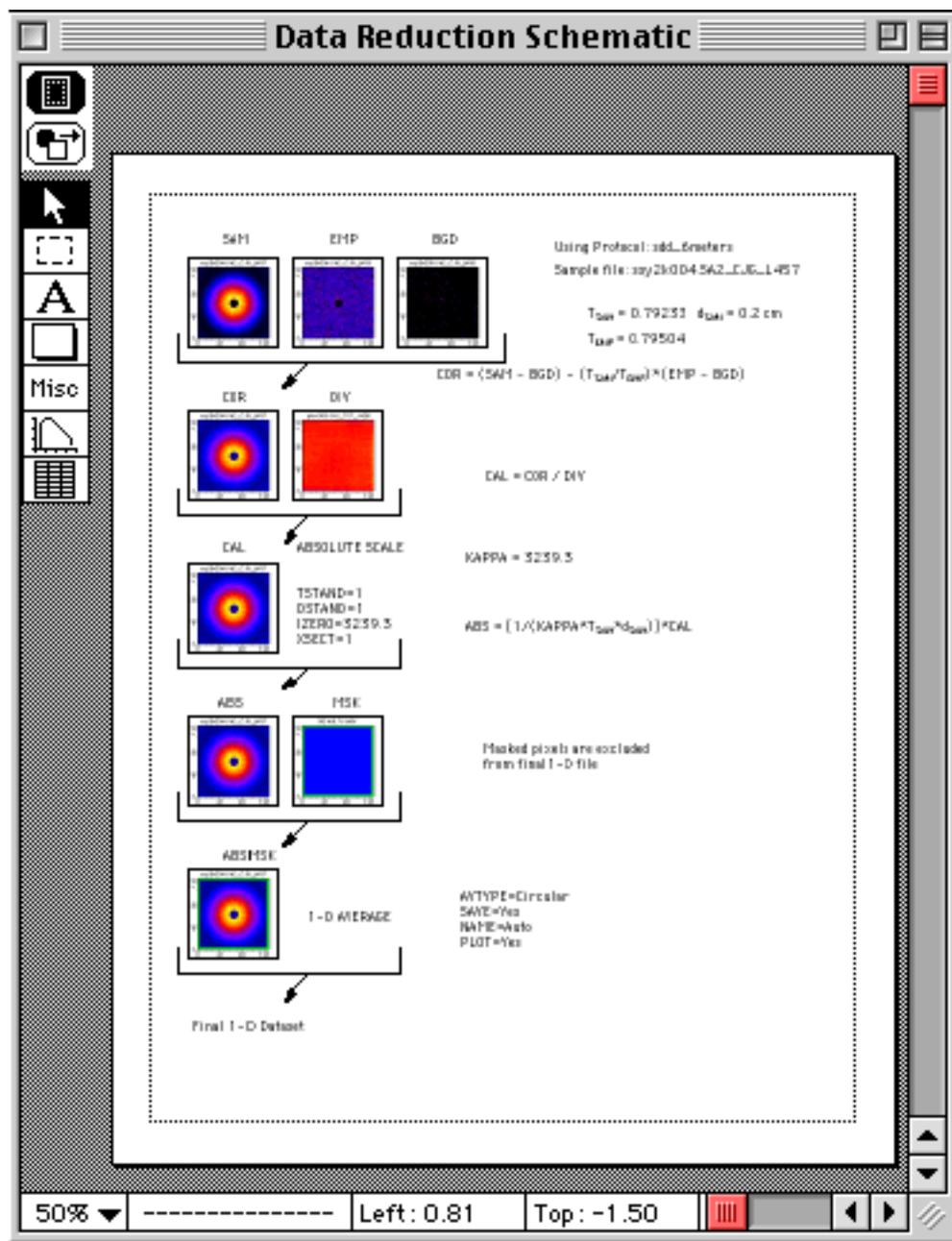
Instead of building a protocol, one could use either the "Base" protocol - which does only minimal corrections, or "DoAll" which will perform all of the data reduction steps. To see exactly which steps each of these would perform, "Recall" these blank protocols into the Protocol Panel. Unchecked steps in the protocol will be skipped, and "ask" will prompt you to pick the required files from a standard open file dialog.

### **Schematic of Data Reduction Operation**

**What:** The Schematic operation reduces a data file using a previously saved protocol and creates a printable layout showing all the details. This helps you see what happened at each step of the way during the data reduction. It is very useful for diagnosing problems in data reduction. NOTE: if you are using a demo version of IGOR Pro, you will not be able to do this step (sorry), but you will be able to view the intermediate files individually, by using the "Display 2D" button on the [2-D Ops Tab](#) on the main panel.

**How:** To see what steps were used and what the files looked like, click "Show Schematic" on the Misc Ops tab of the main panel. When prompted for the protocol, choose one that you just created and saved. You will then be prompted for a "Sample Data file" - choose the appropriate scattering run again, and it will be reduced again in exactly the same way. Once the reduction is complete, small images of the intermediate steps will be created, and placed in a layout window. This can be inspected (or printed in color) to see exactly what data files were used at each step, what numerical constants were used and what file was saved. A

placeholder box titled "Not Used" is in place of steps that were not used (at your request) in the reduction protocol. A placeholder box titled "No Data" means that you wanted to use that step, but an error occurred, and no data could be found (usually a file has been improperly specified).



### Reduce Multiple Files

**What:** In a typical SANS experiment, many scattering files are collected at the same instrument configuration, and must be reduced using the same protocol. This operation allows you to reduce SANS data in a batch mode using a previously saved protocol.

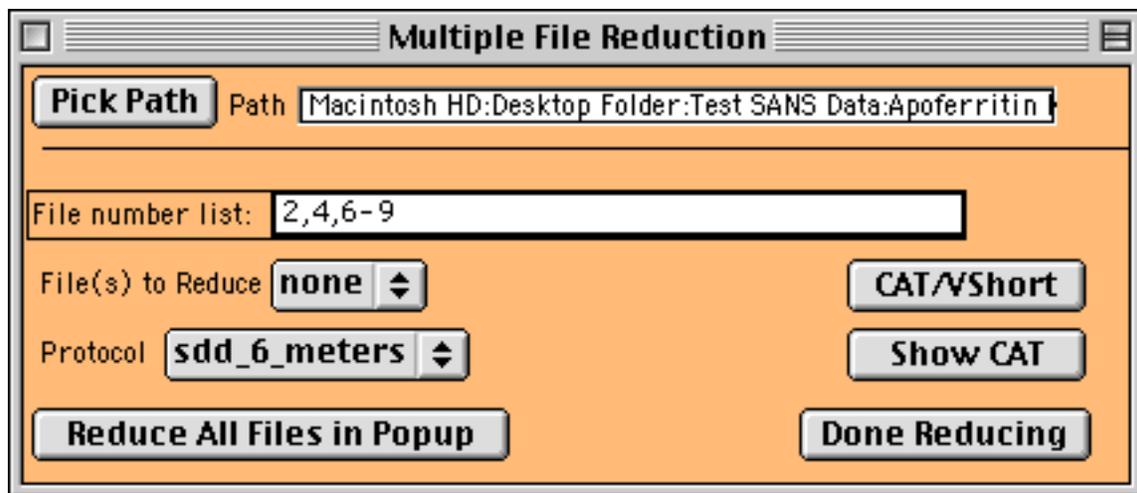
**How:** Since this tutorial only works with one file at each instrument configuration, no data will actually be processed here. Click "Reduce Multiple Files" on the Data Reduction tab

of the Main Panel. This will display a new panel with a simple interface, used as follows:

1) Enter a comma-delimited list of run numbers to be reduced (leading zeros are not needed). Note that a 'dash' can be used to indicate an inclusive range of file numbers. Hit enter or return when finished, and this list of raw data files will be displayed in the popup list. If any of the data files cannot be found, you will be alerted to the offending file number. Check the popup list to confirm that these are indeed the file(s) that you want to reduce.

2) Select the appropriate protocol from the popup (you must have already created / tested / saved it from the Protocol Panel) to be used to reduce the selected files.

3) At this point you would click "Reduce All in Popup" to reduce all of the files in the list with the chosen protocol. Of course, don't do it with the tutorial data - the files in the list are not all at the same configuration - it's just an example. As each file is reduced, all of the intermediate steps are shown. Automatic naming is the best choice in a protocol when reducing multiple files, since no input is required from the user.

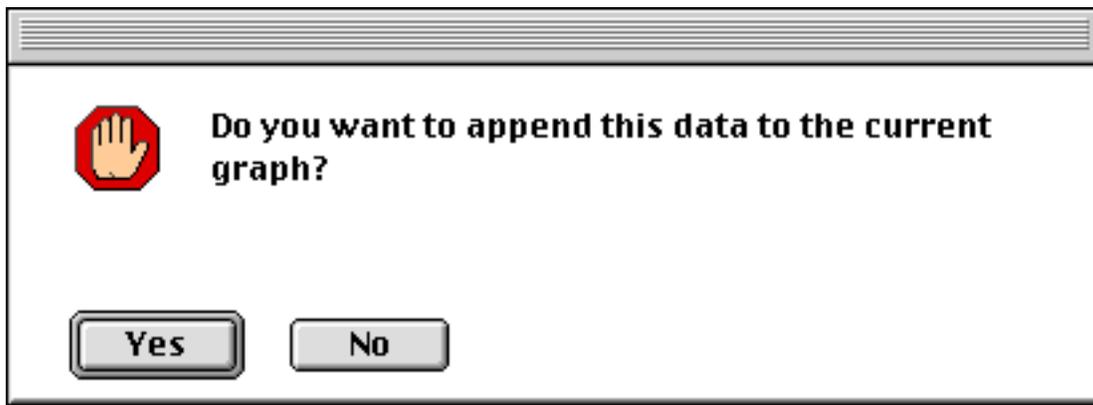


### Plot Averaged Data

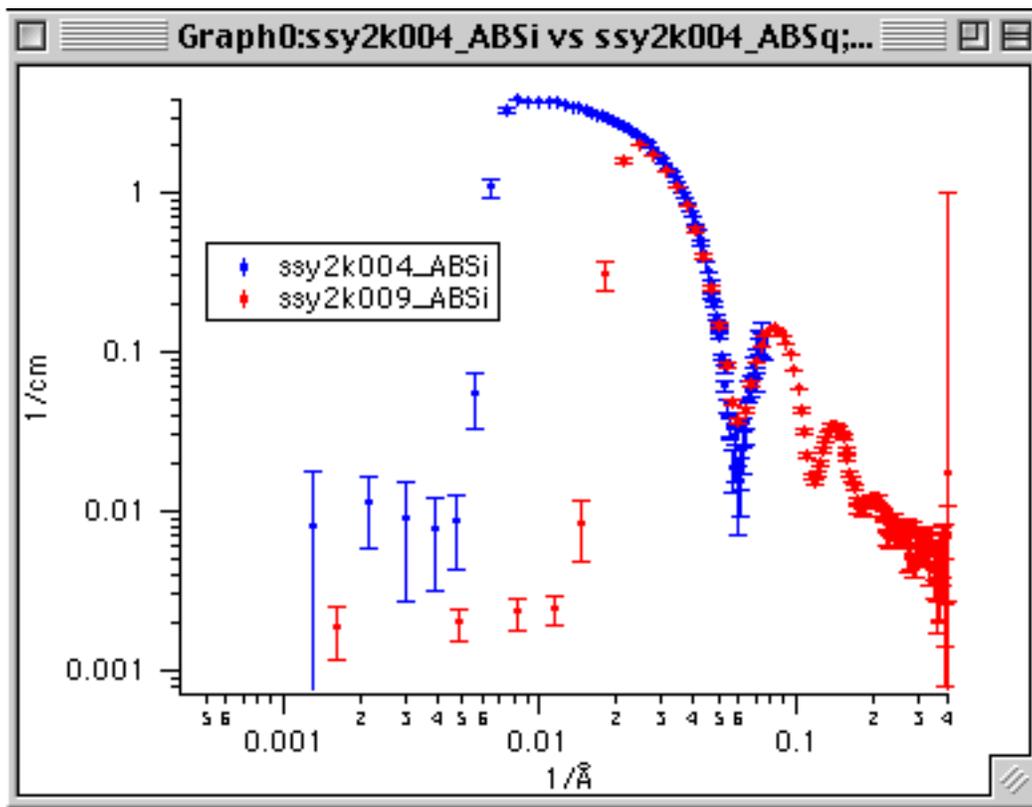
**What:** Plots 1-D averaged data files in a nice graph, allowing you to plot multiple datasets on the same graph.

**How:** Click "Plot" on the 1-D Ops tab on the main panel, and a dialog will be presented for you to select the file to load. If the file has not already been loaded, it will load and automatically be graphed. To change the graph appearance, click on what you want to change, and a dialog will appear. The Graph menu also allows for a wide variety of customization of the graph appearance.

- If the top window is a graph, you will be presented with the option to add the data to the "top" graph:



PLOTting both of the apoferritin files (either order) will generate a graph like this:



**NOTE:** The 2-D Display window is also a graph. If the Display window is on top, you don't want to overlay a 1-D dataset on top. If you do, the display will look garbled - just close the 2-D display and it will redisplay correctly the next time it is drawn.

- If you see a message that "This file has already been loaded..." then you will need to use "Append Traces to Graph..." from the Graph menu. From the lists, select the y-data (the intensity, ends in "i") and the x-data (q-values, ends in "q") and append to the graph.

### **Sort and Combine Averaged Datasets**

**What:** After collecting data at 2 or 3 instrument configurations, it is convenient to combine these data files into a single file, eliminate "bad" data points, and scale the data sets to

overlap. Plot the individual data files at the two different q-ranges, trim off the "bad" data points (behind the beamstop and at the corners of the detector), automatically adjust the scaling to get perfect overlap between datasets, and write out the combined data file.

**How:** Click "Sort" on the 1-D Ops tab on the Main Panel. This will display a new panel.

**NSORT - Rescale and combine 1-D files**

**Pick Path** Path: Macintosh HD:Desktop Folder:Apoferritin-

**Low Q:**  
ssy2k004.ABS  
 Normalize to this file  
Delete Points?  
Beg Pts 0  
End Pts 0  
Plot  
 Update ?

**Medium Q:**  
DEFAULT.MASK  
 Normalize to this file  
Delete Points?  
Beg Pts 0  
End Pts 0  
Plot  
 Update ?

**High Q: (or none)**  
none  
 Normalize to this file  
Delete Points?  
Beg Pts 0  
End Pts 0  
Plot  
 Update ?

Auto Scale  
Mult factor 1-2 1  
Mult factor 2-3 1  
To Manually scale data, enter scale factors above

**Write Combined File** **Done**

Select the data set with the lowest q-values (the 6-meter data set, ssy2k004.abs) as the "Low Q" data file. Plot it, and remove points from the beginning and end of the set that were behind the beamstop or at the edges with large error bars (the omitted points will be displayed as open circles, and are a copy of the original data set). Do the same for the higher q-range (the 1.6-meter set) as the "Medium Q" dataset. If you had a third, still higher q-range, you would plot that set as "High Q", but we have none. Note that if you only have data from two instrument configurations, treat them as "Low" and "Medium" and set the "High Q" set to "none".

**NSORT - Rescale and combine 1-D files**

**Pick Path** Path:

---

**Low Q:**   Normalize to this file

Delete Points? Beg Pts  End Pts   Update ? **Plot**

---

**Medium Q:**   Normalize to this file

Delete Points? Beg Pts  End Pts   Update ? **Plot**

---

**High Q: (or none)**   Normalize to this file

Delete Points? Beg Pts  End Pts   Update ? **Plot**

---

Auto Scale      Mult factor 1-2

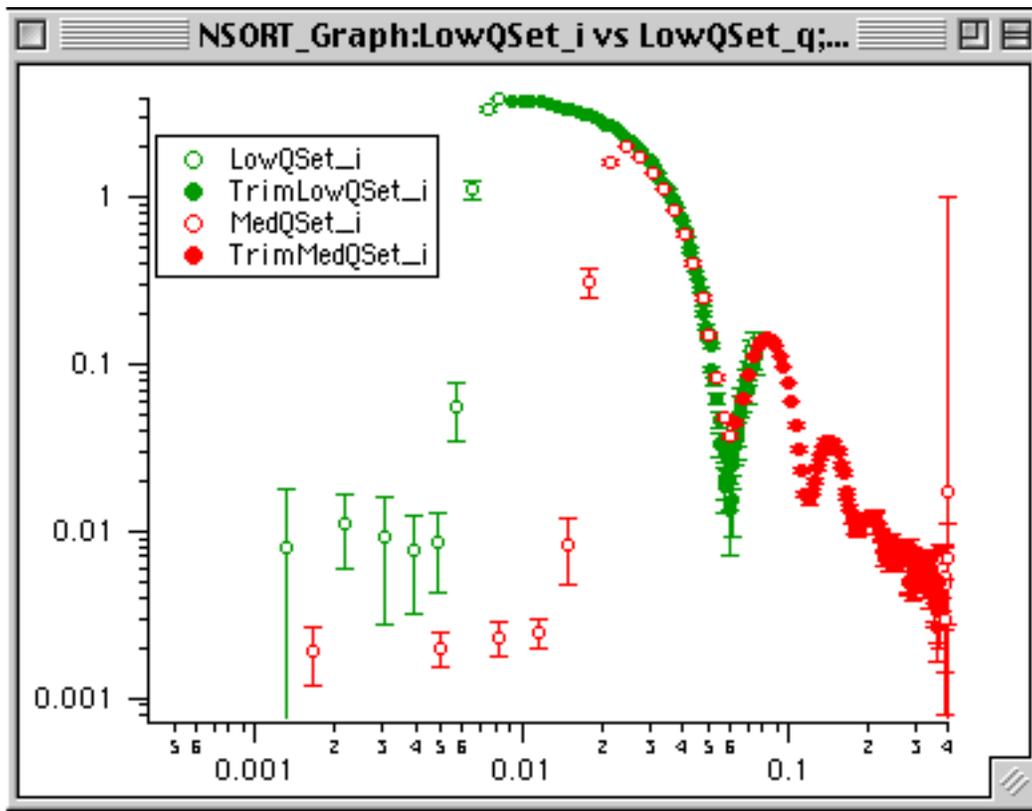
                                 Mult factor 2-3

To Manually scale data, enter scale factors above

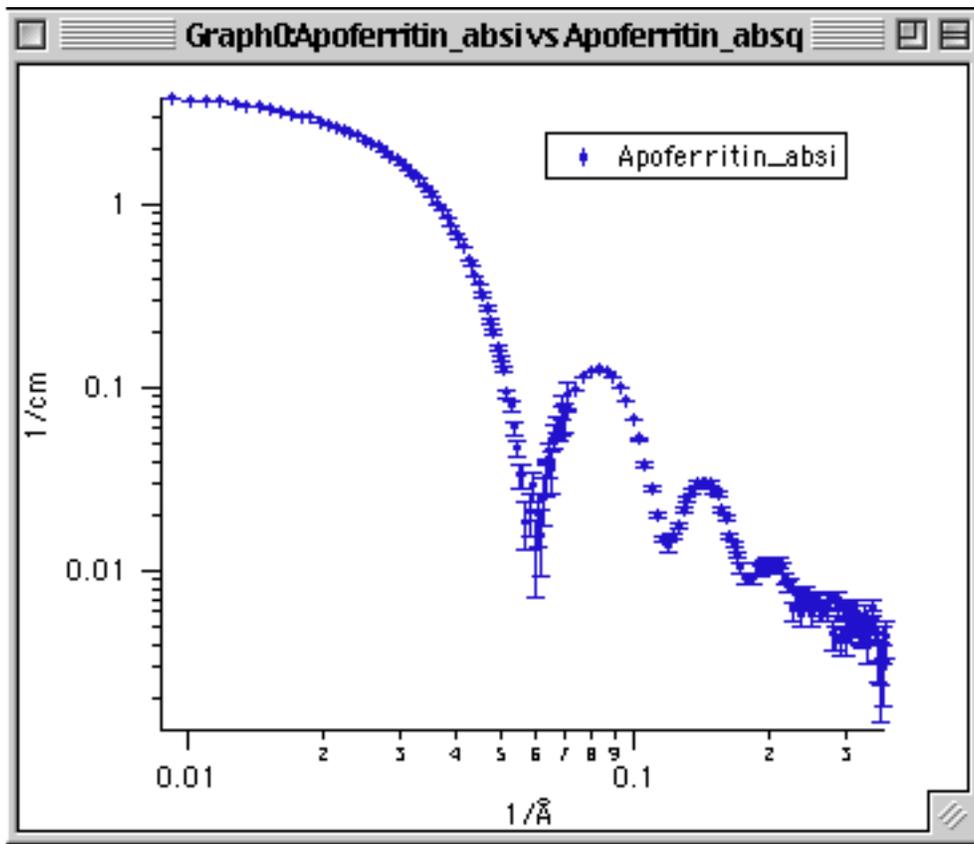
---

**Write Combined File** **Done**

The NSORT graph should look something like this. Be sure "auto scale" is selected for automatic calculation of the overlap constant (or you can enter your own if you wish). Also check the set that you want the combined set to be normalized relative to (you can only choose one). Click "Write Combined File" to create a new file. You will always be prompted for a new name for the combined data set. The header of this file will indicate which files were combined, and the scaling factors used. The automatic scale factor(s) are reported to the panel. For datasets already on absolute scale, the scaling factor should not be far from unity.



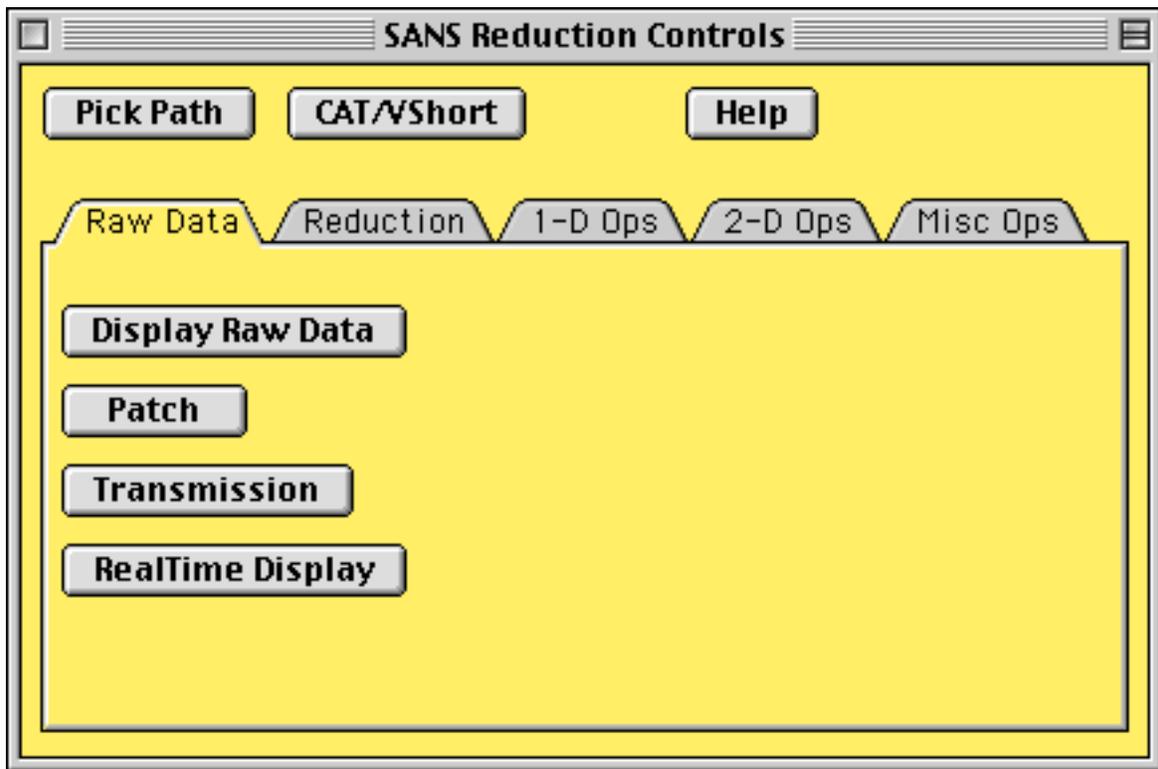
The final, combined and overlapped dataset (I named it Apoferritin.abs), once plotted should look something like this:



## Additional Operations

Main Panel Tabs

Raw Data Tab



The buttons are:

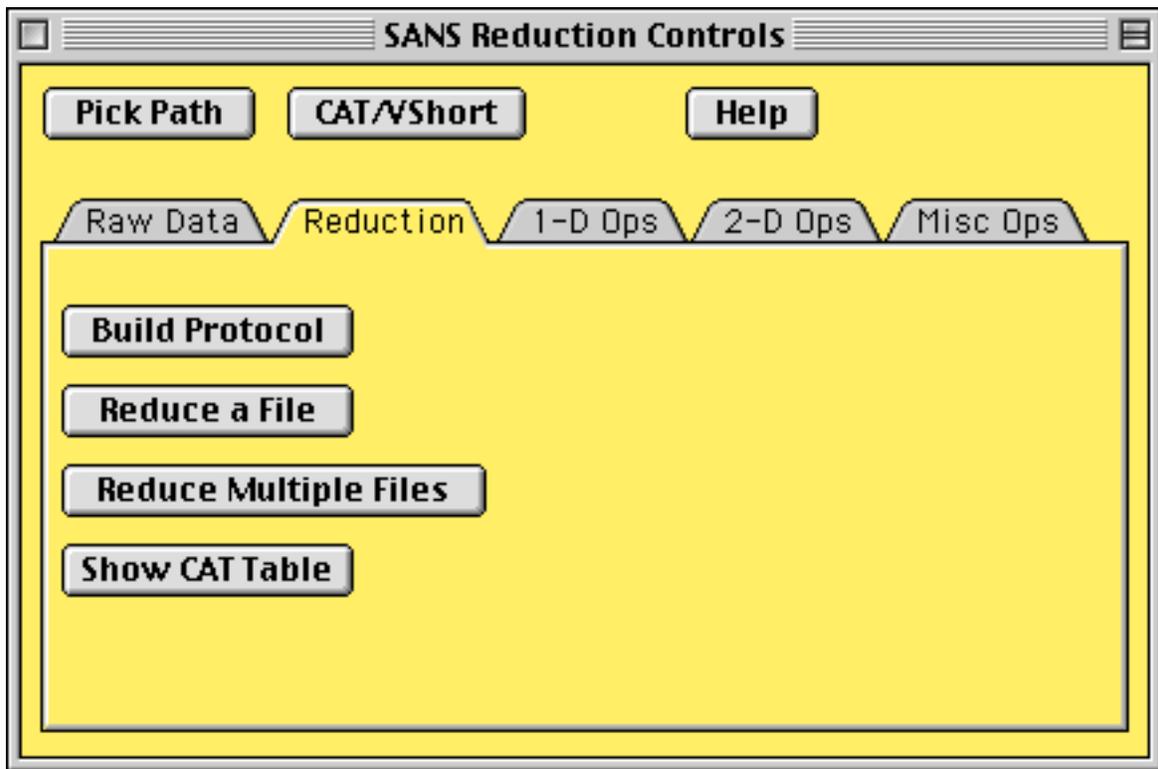
Display Raw Data: presents an open file dialog to select a raw SANS data file for display, then graphs it as a 2-D image with lots of helpful information.

Patch: generates a separate panel where you can change a selected number of parameters that are stored in the header of the raw (binary) SANS data files.

Transmission: generates a separate panel with controls to allow you to set the relations between transmission files and scattering files, then to finally calculate the sample transmissions.

RealTime Display: generates a separate panel with controls for display of the live detector image. This operation is only useful during data collection at NIST and is discussed in a separate manual.

### **Reduction Tab**



The buttons are:

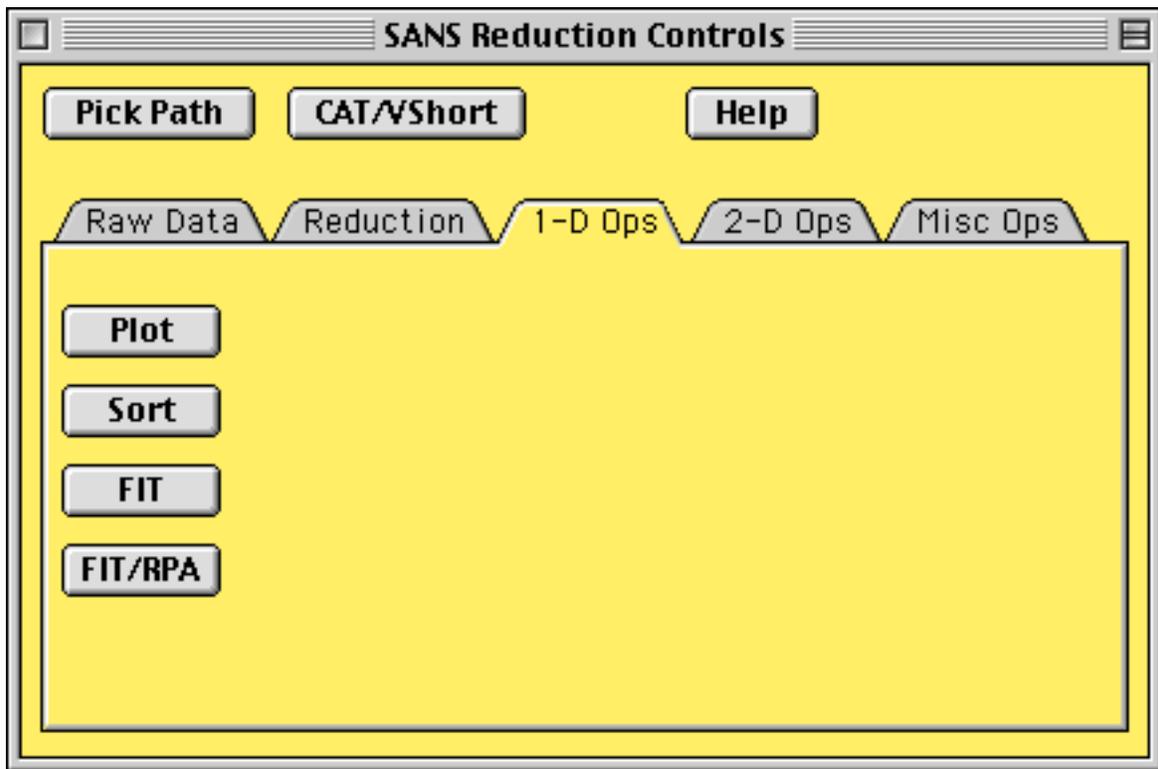
Build Protocol: generates a separate panel with controls to allow you to sequentially build the desired steps of a reduction protocol. The CAT/VShort table is used interactively to build protocols, so have the table handy.

Reduce A File: will prompt you to select a protocol, then for a sample file, followed by each of the reduction steps specified by the protocol.

Reduce Multiple Files: generates a separate panel with controls to allow you to reduce files in batch mode, using a protocol that you have previously created and saved using the Build Protocol panel.

Show CAT Table: simply brings the CAT/VShort table to the front, if it is open. It does not re-build the table from a directory listing.

### 1-D Ops Tab



The buttons are:

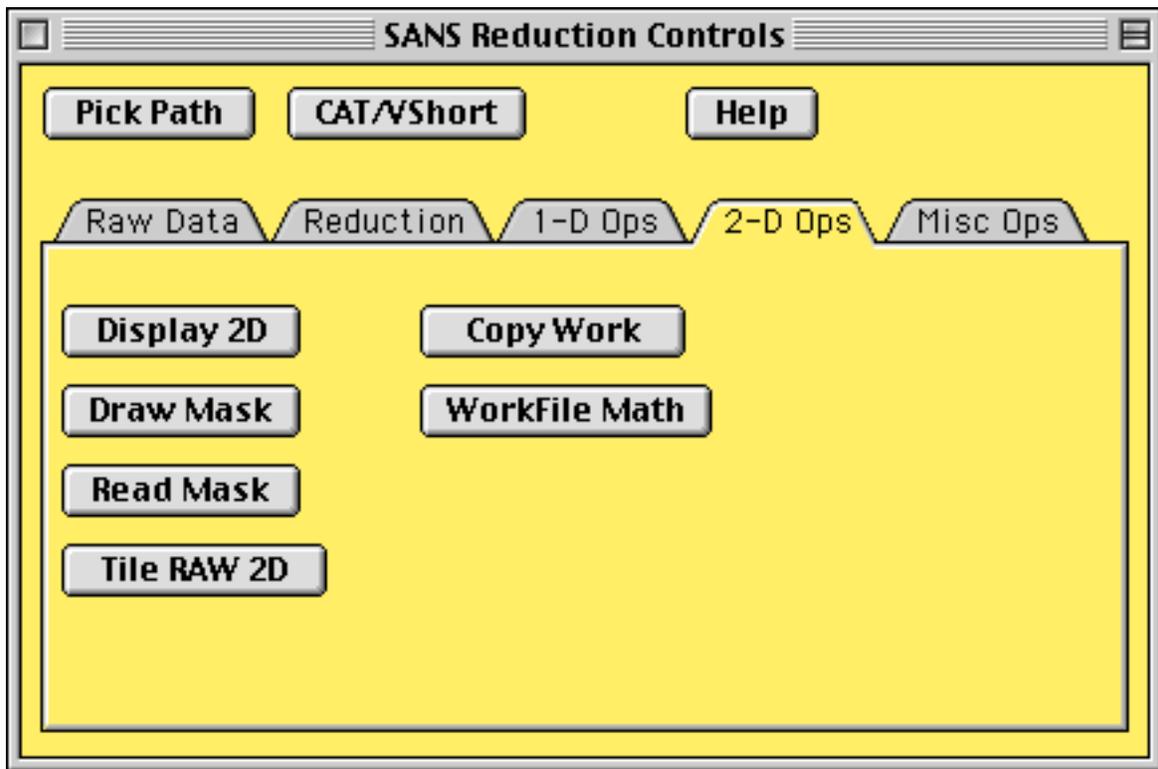
Plot: presents an open file dialog to select an averaged (1-D) dataset, and then graphs it. Multiple datasets can be plotted on a single graph.

Sort: generates a separate panel with controls to sort, internormalize, delete "bad" points, and finally combine averaged datasets from different instrument configurations into a single file.

Fit: generates a separate panel with controls to perform linearized fits to 1-D datasets. Fits can be interactively refined. Often used during the reduction of secondary intensity calibration standards.

Fit/RPA: generates a separate panel with controls to perform an RPA fit to 1-D data generated from a polymer sample used as a secondary intensity standard.

## **2-D Ops Tab**



The buttons are:

Display 2D: presents a dialog to select and display one of the intermediate work file types.

Draw Mask: generates a separate graph (of the currently displayed 2-D dataset) with controls to draw and save a mask to eliminate "bad" detector pixels from the final averaged (1-D) dataset.

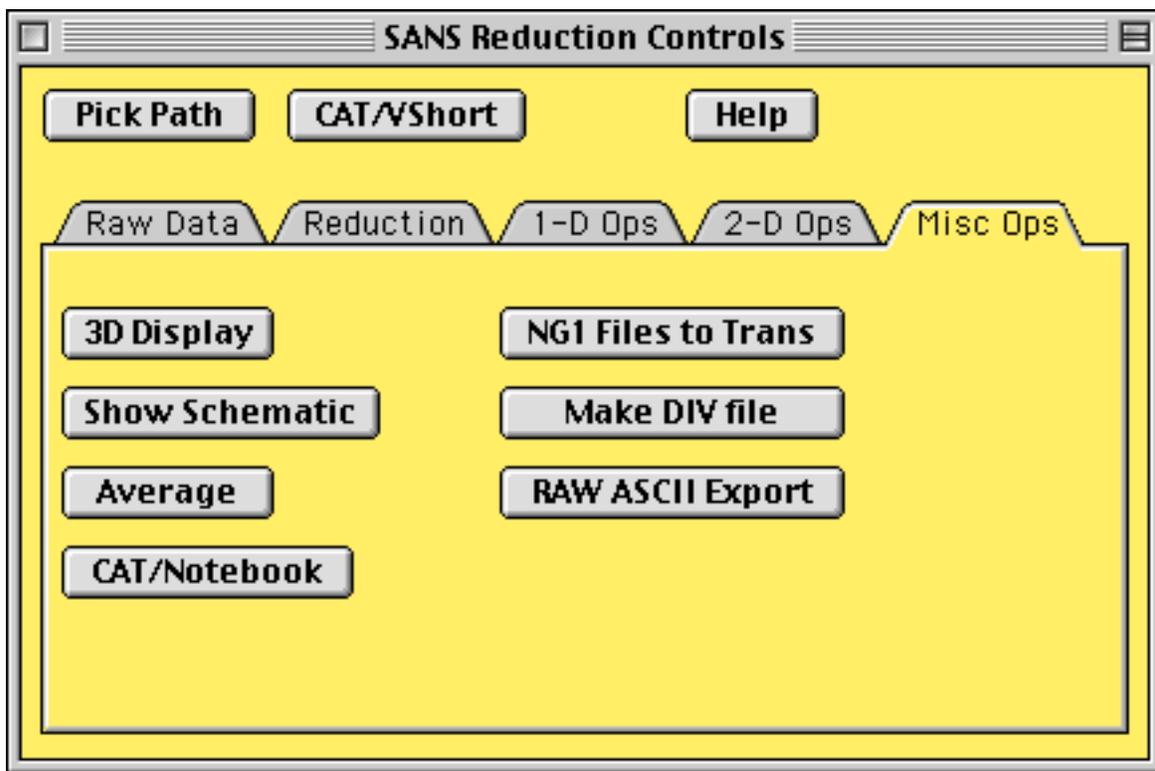
Read Mask: presents an open file dialog to read in a previously saved mask file and generates a small image of the mask.

Tile RAW 2D: generates a separate panel with controls to select any number of raw SANS files, then append images of these files to a Layout window. Images can be arranged in the layout, annotated, and printed.

Copy Work: copies the entire contents of a selected folder to a target folder.

WorkFile Math: generates a separate panel with controls to perform simple arithmetic operations on two (2-D) workfiles.

### **Misc Ops Tab**



The buttons are:

3D Display: displays the selected work file type as a 3-D wireframe plot.

Show Schematic: generates a layout showing all of the intermediate steps and files used during the reduction of a selected file and its protocol. Very useful for diagnosing data reduction errors.

Average: presents the panel with 1-D averaging options, to be applied to the currently displayed data only (not associated with protocols).

CAT/Notebook: generates a notebook with information about each file in the selected data path. Somewhat less information than CAT/VSTable, but in a notebook (text) format.

NG1 Files to Trans: generates a separate panel with controls to convert RAW transmission data files collected at NG1 SANS into raw data files that can be interpreted as such during transmission calculation.

Make DIV File: to be used only by NIST local contacts to generate detector sensitivity files for general use.

RAW ASCII Export: generates a separate panel with controls to export selected RAW SANS data files in ASCII format, either as detector pixels, or in I(Q<sub>x</sub>,Q<sub>y</sub>) triples.

### **Fit Lines to Your Data**

**What:** To obtain some quantitative information about your sample, a variety of linearized fits can be performed such as: Guinier fits, Zimm plots, Kratky plots, power laws, and other

forms. Linearized fits are also used to extract absolute scaling parameters from secondary standards (Al-7, water, silica A/B).

**How:** The reduced data file Apoferritin.abs is scattering from some sort of protein, and appears to have a Guinier region at low  $q$ . From the 1-D Ops tab on the Main Panel, click "FIT". The following panel will appear.

FitPanel

Select Experimental Data

Data File **Apoferritin.abs**

**Load and Plot File**

q-range to fit ( $\text{\AA}^{-1}$ )

Lower Limit 0.02

Upper Limit 0.04

**Show Full q-range**

Use cursor range from FitWindow

Select the y and x-axis scaling

y-axis **I** x-axis **q**

pow "a" 1 pow "b" 1 pow "c" 1

background 0

**Do the Fit**

Choose the apoferritin.abs data file in the first popup list. We want to fit this data over the range (0.01 - 0.03) [1/Angstroms]. Enter these values if they are not already there. To fit the data to a Guinier plot, select a y-axis scaling of "ln (I)" and an x-axis scaling of "q<sup>2</sup>". The powers a, b, and c apply to different axis scalings, and we do not need to subtract any background before doing the fit. Click "Do the Fit", and the data is scaled and fitted, with all the statistics on the graph. One standard deviation is reported along with the radius of gyration and range of  $q \cdot R_g$ .

Select Experimental Data

Data File Apoferritin.abs ⬇

Load and Plot File

q-range to fit ( $\text{\AA}^{-1}$ )

Lower Limit 0.01

Upper Limit 0.03

Show Full q-range

Use cursor range from FitWindow

Select the y and x-axis scaling

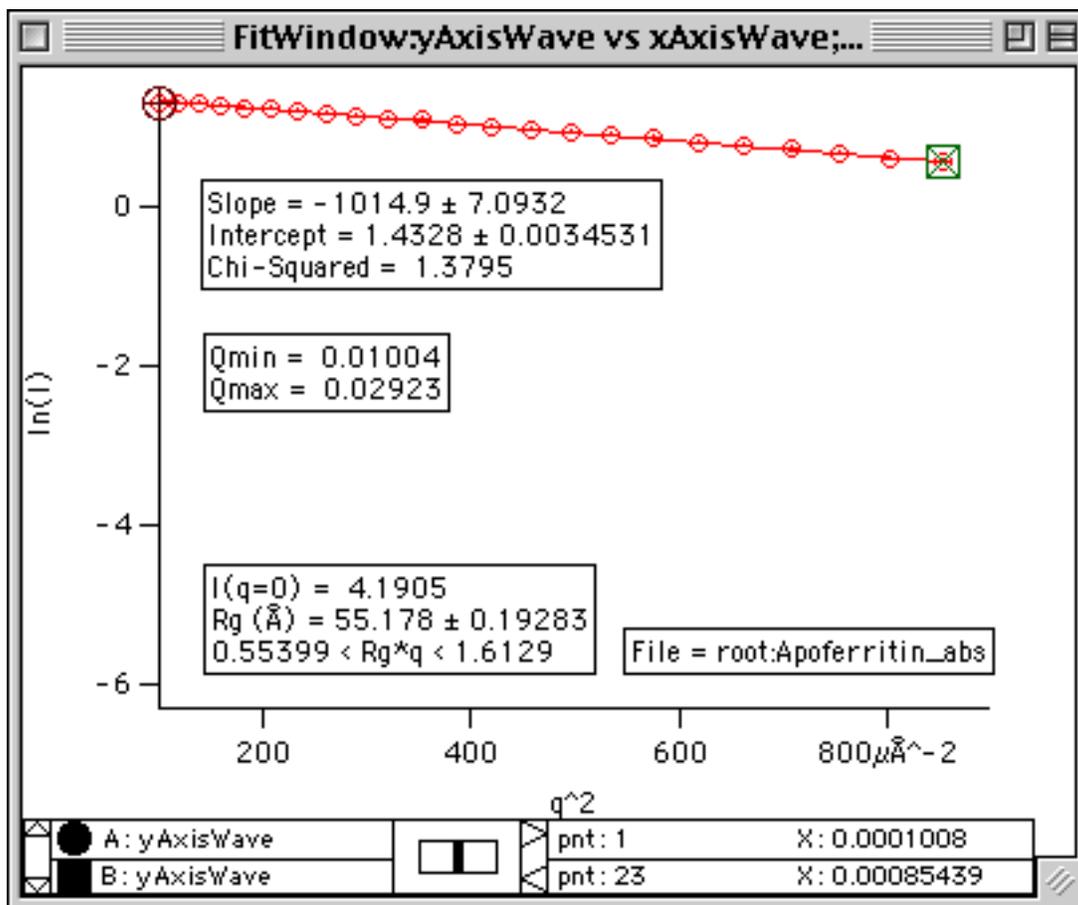
y-axis ln(I) ⬇      x-axis q<sup>2</sup> ⬇

pow "a" 1    pow "b" 1    pow "c" 1

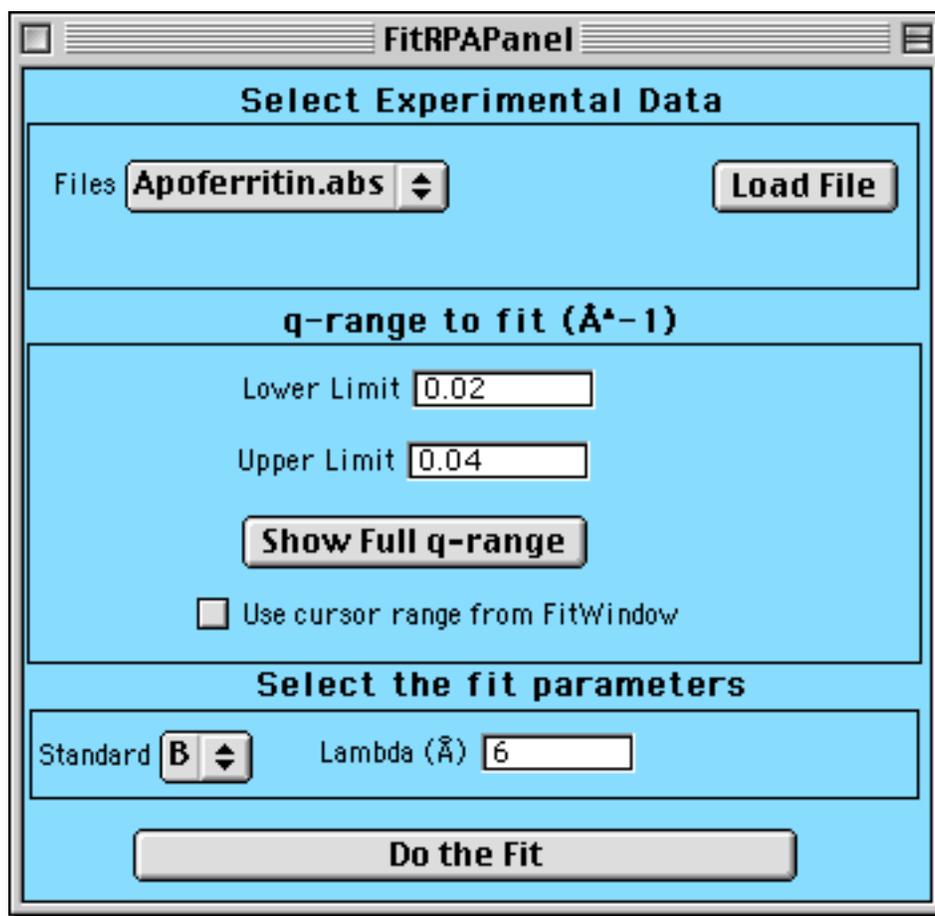
background 0

Do the Fit

This looks like a good fit, but the fit can be adjusted by either entering new q-values, moving the cursors on the graph to "better" data points, or subtracting a background value before the linearized fit is performed. Clicking "Show Full q-range" does just as stated. The data range that was fitted is marked by the cursors (and is hopefully linear for a Guinier plot).



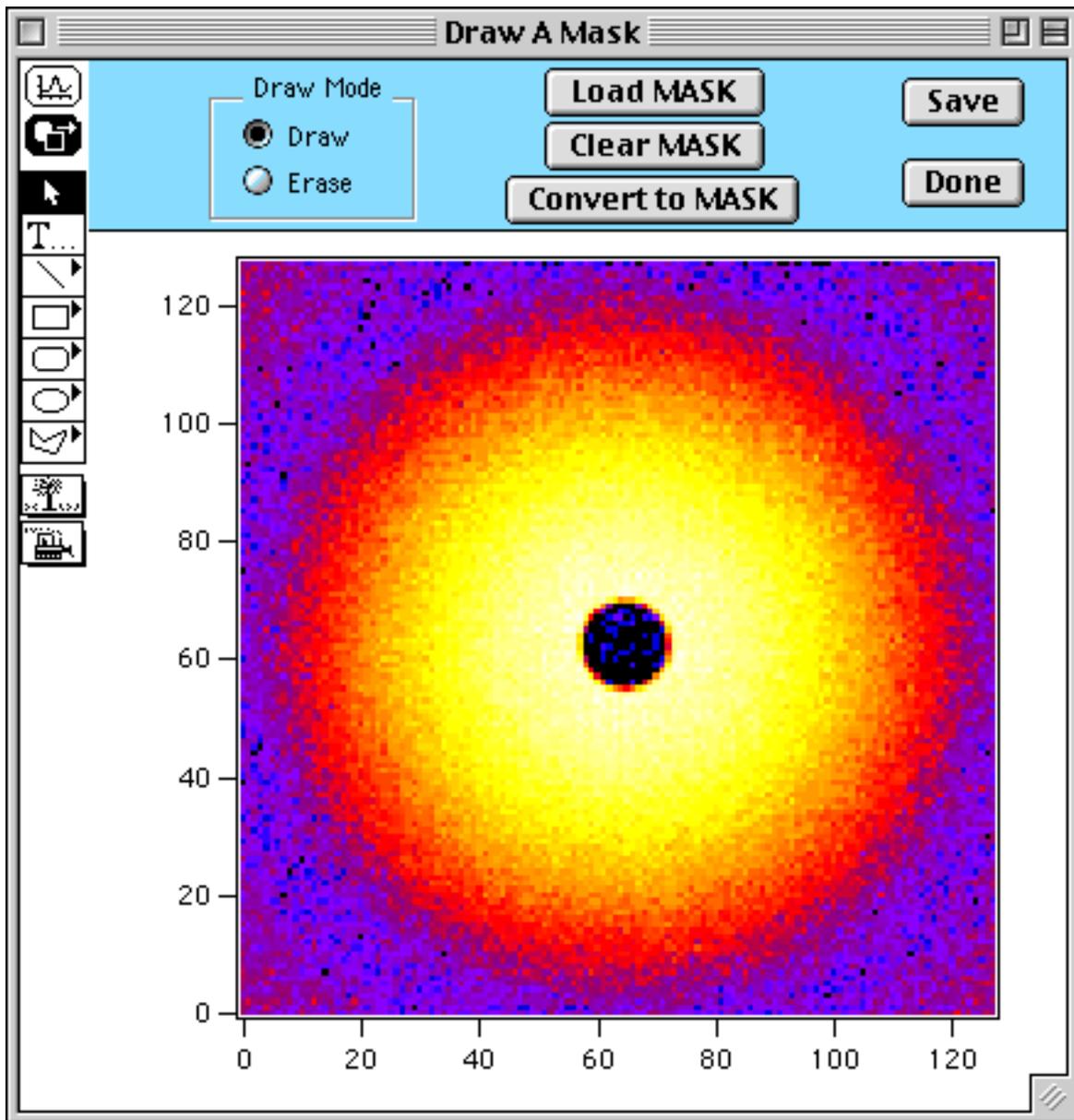
The secondary polymer standards are fitted with an RPA model (Random Phase Approximation) in order to extract the absolute scaling parameters. This panel "Fit/RPA", also from the 1-D Ops tab on the main panel, behaves much like the FIT panel. The model is specific for the polymer standards, so you need to be sure to choose the proper standard.



### **Draw a Mask**

**What:** The edges of the detector, typically 1 or 2 channels, do not count as reliably as the remainder of the detector, and should not be averaged into 1-D data. This is the usual case, and the "default.mask" should be used. Occasionally, localized regions of the detector image may need to be masked. Then a custom mask must be drawn, so that the MASKed pixels will be ignored during the averaging step.

**How:** Display a representative raw data file, then click "Draw Mask" on the main panel. The following window appears.



The control bar allows:

Draw and Erase: modes are set by the radio buttons. In Draw mode, draw objects are added to the mask file. In Erase mode, draw objects are erased from the mask.

Load Mask: loads a specified mask and puts it into the current draw layer, allowing you to "edit" a previously created mask file.

Clear Mask: clears ALL of the mask that is currently being drawn, giving you a clean slate to work from.

Convert to Mask: takes the current draw objects and converts them to the current mask (cumulatively), drawing or erasing pixels depending on the mode setting **\*\*when the objects were drawn\*\***.

Save: saves the current mask to disk, also copies the saved mask to the MSK

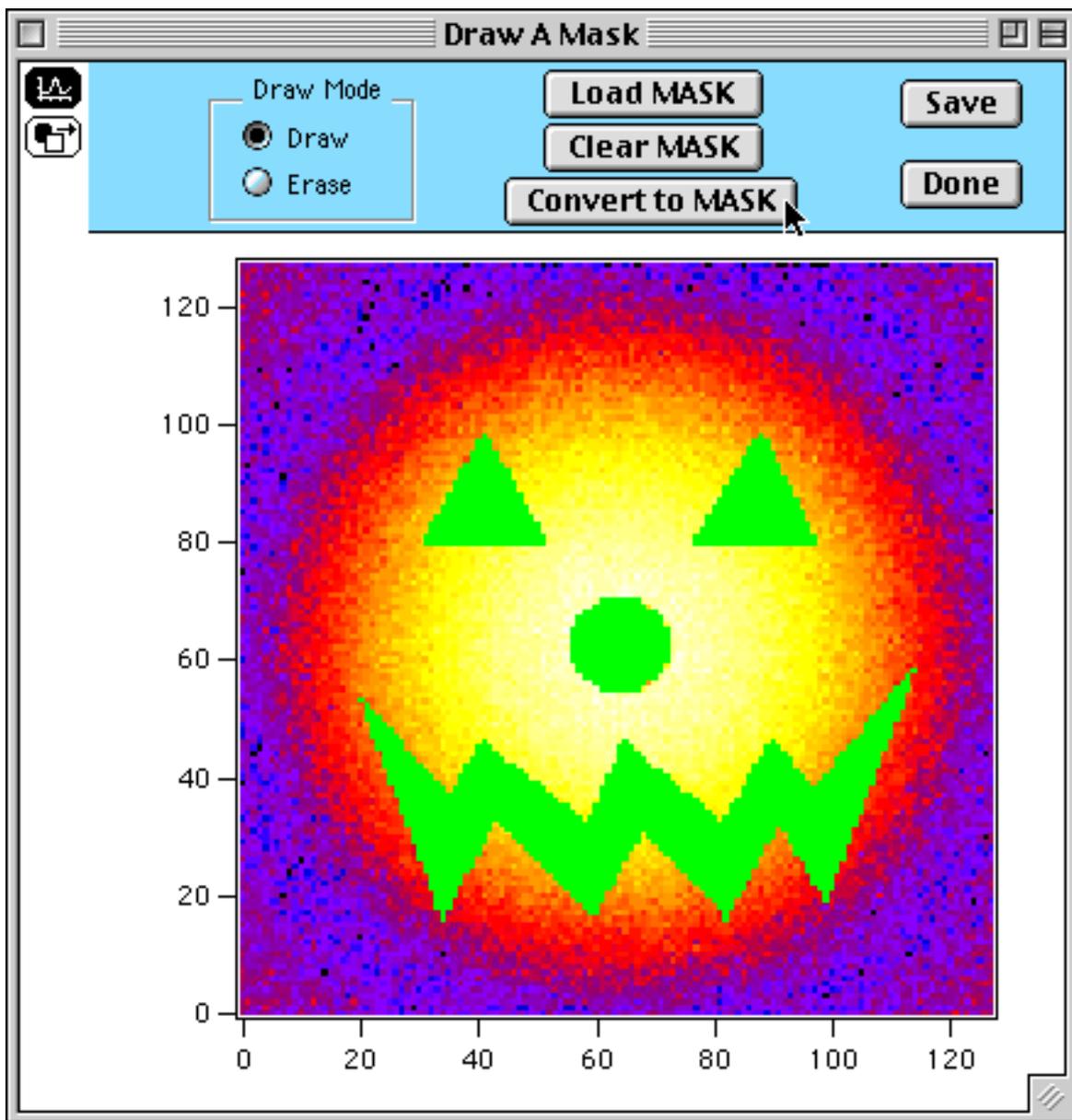
folder for immediate use.

Done: closes the window, first prompting you to save your newly drawn mask.

Tools/Graph Toggle: switches between modes where the Tool Bar is visible (below, left) or hidden (below, right). When the Tool Bar is visible, the buttons in the top control bar are inactive. When the Tool Bar is hidden, the control buttons are activated.



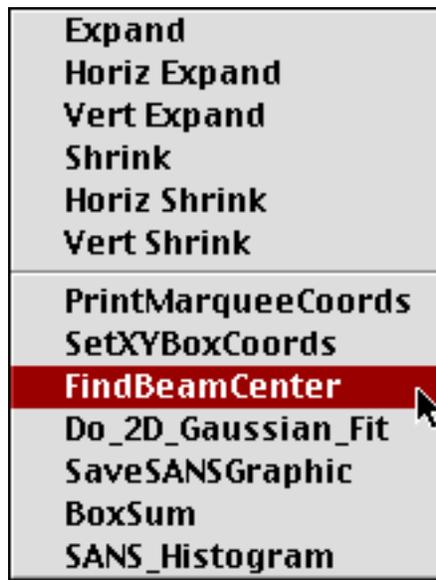
To draw a simple mask, hide the tool bar and set the mode to "Draw" using the radio buttons. Make the tool bar visible again, and select any of the polygon or circle drawing tools. Lines or text drawn will not be added to the mask. Draw the desired objects, and hide the tools. Click "Convert To MASK", and the (white) draw objects will be replaced with a green mask image. Mistakes can be "Erased", or "Clear MASK" will start fresh again. Be sure to save your mask before leaving. Once saved, the mask is pre-loaded, and can be immediately viewed on your data by clicking "Show Mask" in the Display window.



### **Marquee Operations**

**What:** The marquee menu, invoked from a marquee selection on the SANS Data Display provides several new operations.

**How:** Click and drag a marquee region in the SANS Data Display window. Then move the cursor inside the selection (to get an upside-down hat cursor) and click to get a new menu like this:



The operations are:

PrintMarqueeCoordinates: simply prints the (X,Y) extent of the selection in terms of pixel coordinates.

SetXYBoxCoords: is used (only) by the Calculate Transmission operation for setting the box range of the empty beam transmission file.

FindBeamCenter: reports the centroid (intensity-weighted) of the selected region. Results are reported in detector coordinates (1,128) and can be directly used to Patch beamcenter values in raw SANS file headers.

Do\_2D\_Gaussian\_Fit: performs a 2-D Gaussian fit over the selected region. The results for the fit are reported to the command window and displayed as a new contour plot of the fit with an image of the data behind. The details of the coefficients of the 2D Gaussian model can be found in Igor's on-line help files. Note that if the region is sufficiently non-Gaussian, the fit may not converge and report an error.

SaveSANSGraphic: presents Igor's save graphics dialog to allow you to save the 2D image (with the color scale, but not the control bar). The image can be saved in a variety of formats. PNG (2x screen) is a good cross-platform choice with a reasonable (33KB) file size.

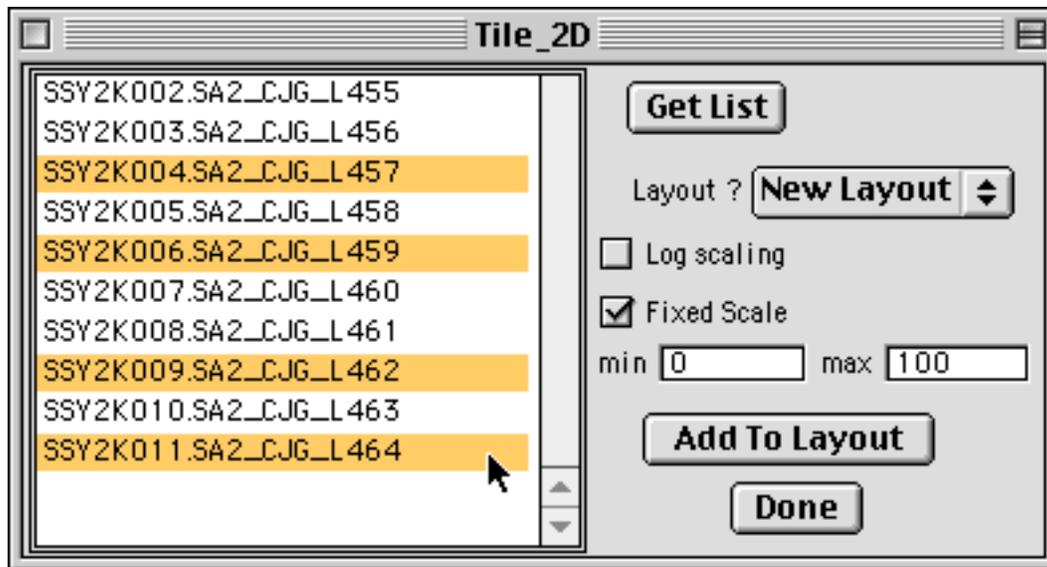
BoxSum: takes the selected XY region, then prompts you for a comma-delimited list of file numbers over which you would like to sum the selected region. Each file is then normalized by "adding" to SAM, then the Box Sum for each file is computed and reported to the command window.

SANS\_Histogram: generates a histogram of counts vs. pixel location in the selected region. Positive values are displayed in red, negative values in blue. Very useful to check the balance of counts around the beamstop for alignment.

## **Tile 2-D Images**

**What:** Allows you to create a layout of small images of a group of raw SANS data files. Often this is useful for viewing systematic trends in sample behavior, for example a sample under an applied shear field.

**How:** Click the "Tile RAW 2D" button on the 2-D Ops button on the main panel. You will be presented with the following panel:

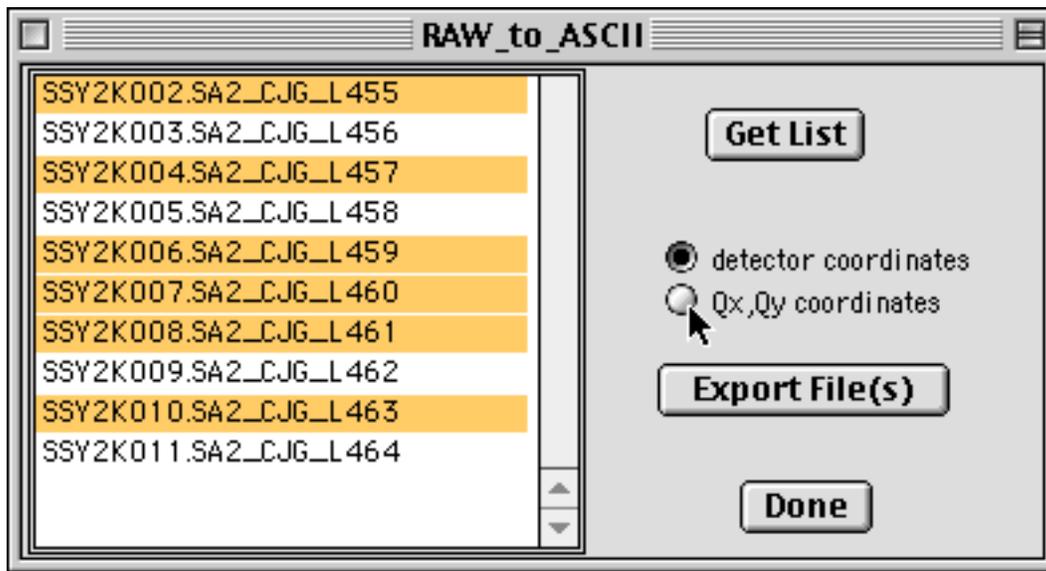


Click "Get List" to see a list of available raw SANS data files. Shift-click to select the desired files. You can choose log or linear scaling of the colors. To better compare a series of data, you can also "Fix" the minimum and maximum values of the color mapping to be the same for all of the selected files. If fixed scale is not selected, each file will be scaled to its own data range. Click "Add To Layout" to append graphics images of each of the selected files to the layout named in the popup list. The images can be arranged as desired, and annotations can be added to the layout using the drawing and text tools. Clicking "Done" will close the panel, first warning that agreeing to close the panel will delete the layouts that you have created and remove the images from memory. There is no harm in keeping the layouts open.

## **2-D ASCII Export**

**What:** Allows the export of RAW (uncorrected) data files as ASCII text, readable by other graphics packages. Two export types are available, either intensity (neutron counts) versus detector pixel (x,y), or neutron counts versus (Qx,Qy).

**How:** Open the panel by clicking "RAW ASCII Export" on the Misc Ops tab on the main panel. Click "Get List" to see a list of the raw SANS data files in your data folder. Shift-click to select the files you would like to export. Set the export type using the radio buttons, then click "Export Files" to write the ASCII files to disk. Data files will be automatically named using default names of the form "SSY2K002.ASC".

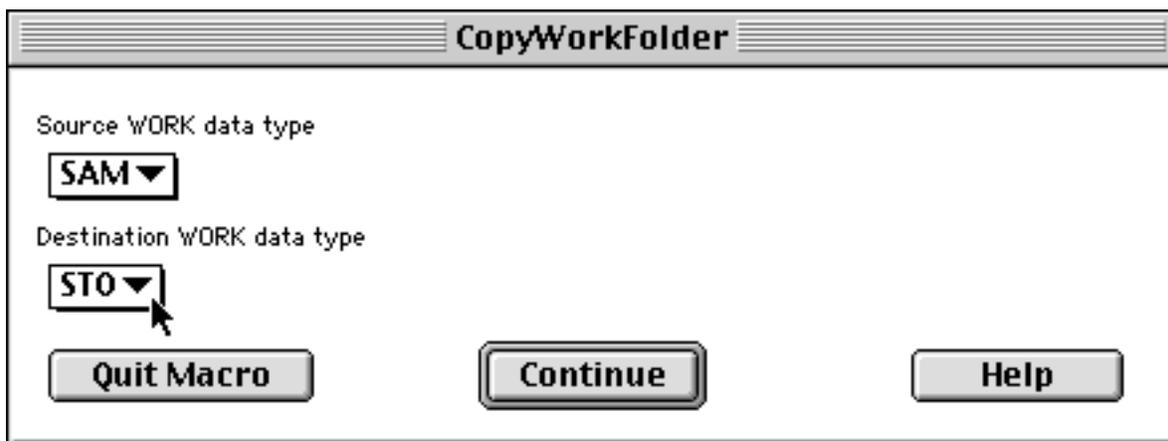


Data exported in detector coordinates is written with a header followed by a single column of data, containing  $128 \times 128 = 16384$  elements. Data exported as Qx, Qy coordinates are written as three columns: Qx, Qy, I(Qx,Qy).

### Copy Work Folder Contents

**What:** This operation duplicates the contents of any data folder into another folder. It is often useful to keep a fresh copy of a 2-D dataset when performing math operations on 2-D data.

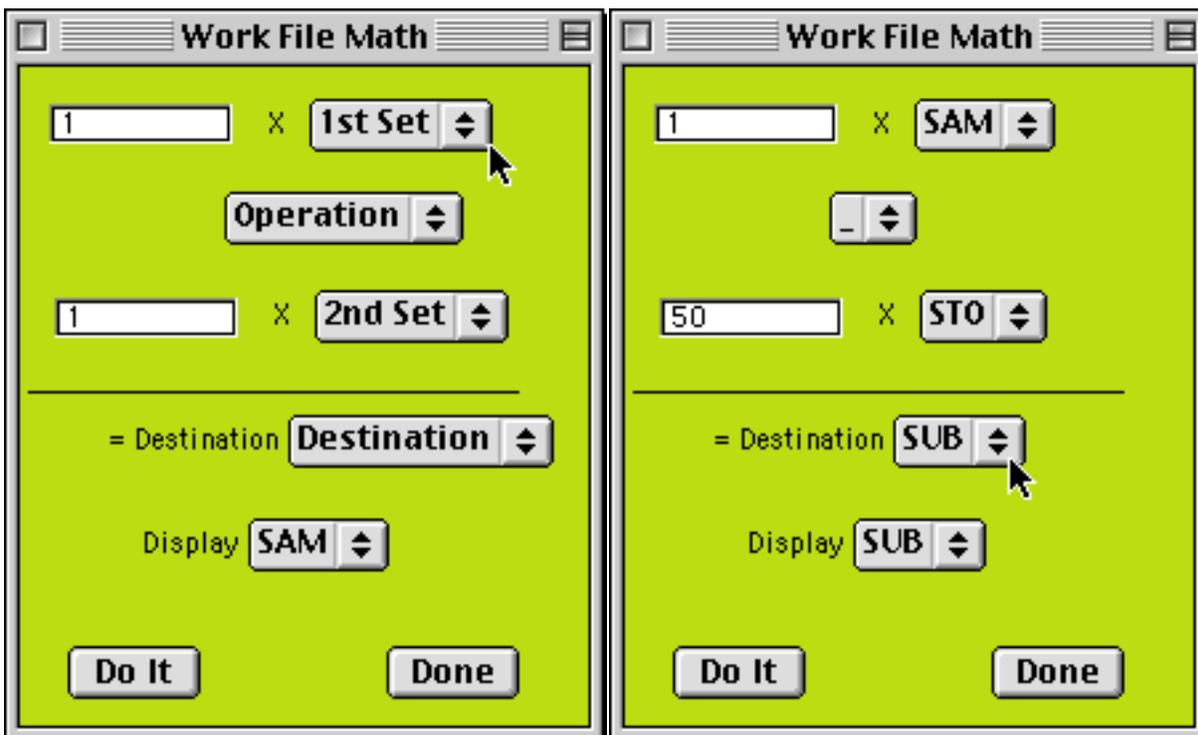
**How:** Click the "Copy Work" button on the 2-D Ops button on the main panel. You will be presented with the following dialog, prompting you for the source and destination data folders. Data in the destination folder will be overwritten, and you will not be warned. You can view the new contents of the destination folder by choosing "2D Display" on the same tab of the main panel.



### 2-D Work File Arithmetic

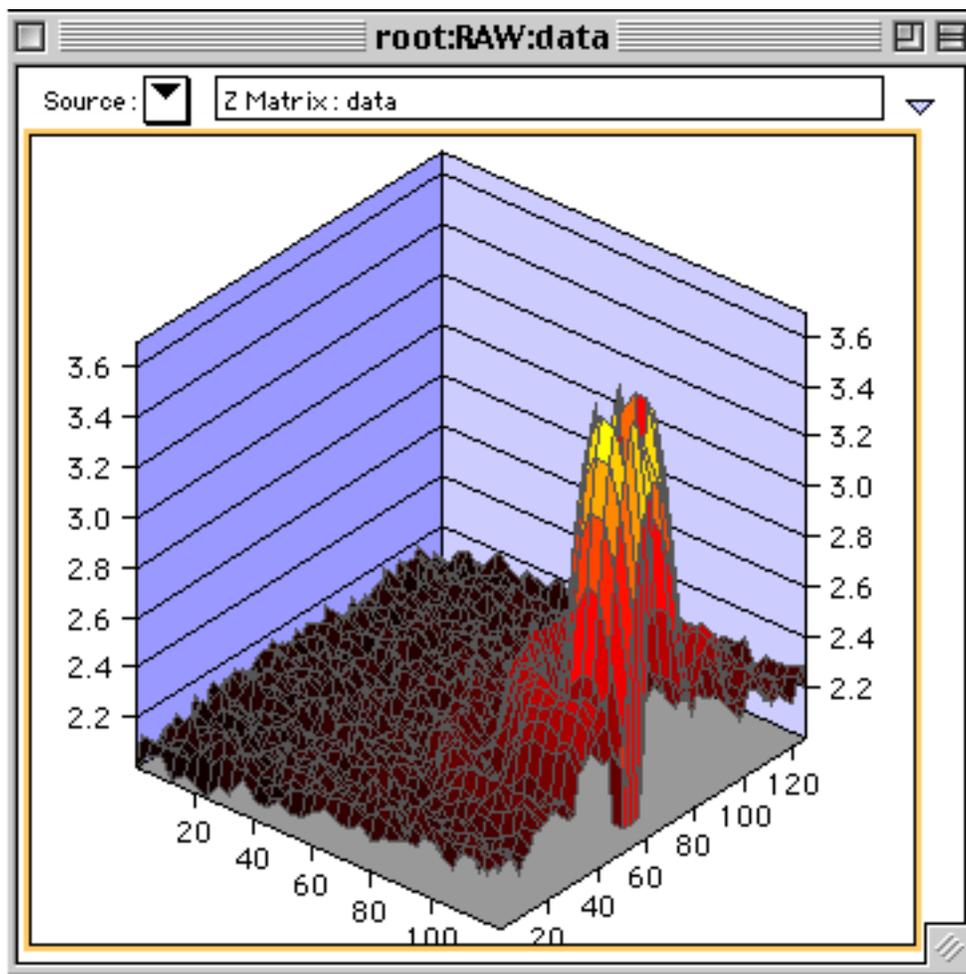
**What:** Allows simple arithmetic operations on 2-D data files, and is particularly useful for fine-tuning background corrections or rescaling of 2-D datasets. Results of the operation can be written to any work folder, viewed, and directly averaged to save the results to disk.

**How:** Click the "WorkFile Math" button on the 2-D Ops button on the main panel. You will be presented with the following panel (below, left), prompting you for the operand files, the operation, and the destination. An option for the second operand to be a unit matrix is available. In the example on the right (below), 50\*STO will be subtracted from SAM. the result will be deposited in SUB, which will also be displayed. The calculation performed will also be echoed to the command window at the bottom of the screen. The result can be averaged or saved directly using the controls on the SANS data display window. These arithmetic operations, however, cannot be incorporated into a data reduction protocol.



### **3-D Display**

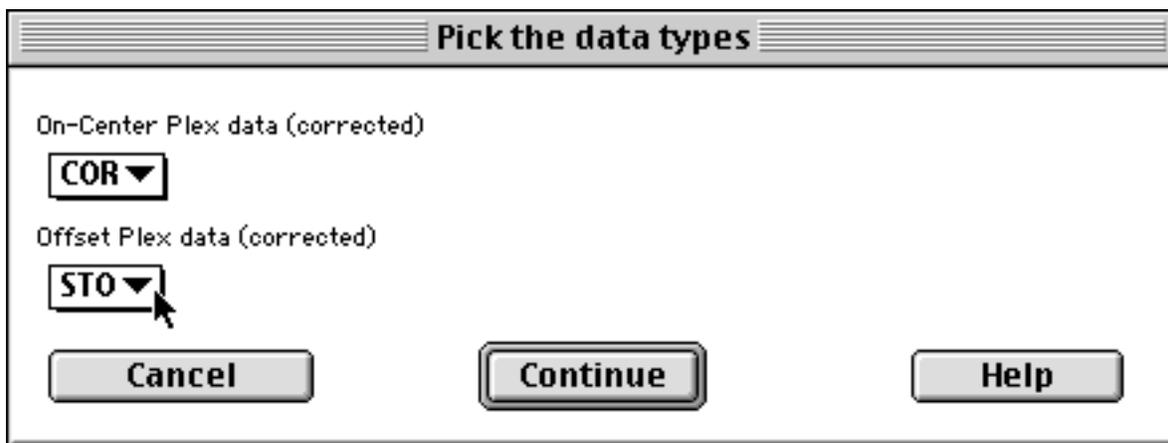
3-D display of a dataset can be done by clicking "3D Display" on the main panel. Any of the intermediate or raw data files can be displayed, in either log or linear format. To change the scaling, make a 2D display of the same data file, and change its scaling to log or linear as desired - the data in the 3D display will update as well, since it is the same data.



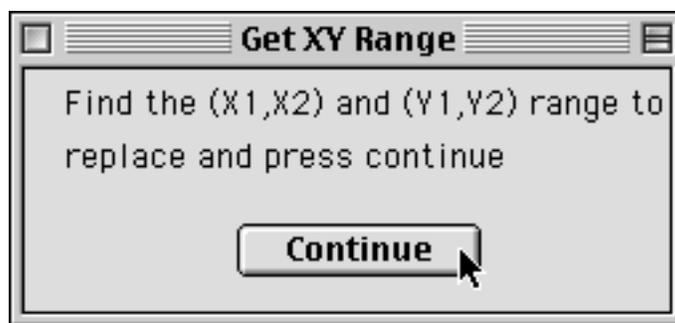
### **Detector Sensitivity File**

**What:** Allows a NIST instrument scientist to create a detector sensitivity (DIV) file from within the Igor macros. The work.div file structure created mimics the VAX-generated file and can be used directly in the SANS reduction macros. General users need not perform these steps, as sensitivity files will be provided.

**How:** At this point, the plexiglass or water files must already be reduced to the COR-level data. In this example, the data with a detector offset was reduced first, then copied into STO, then data with no offset was reduced, ending in COR. Click the "Make DIV File" button on the Misc Ops button on the main panel. You will be presented with the following dialog, prompting you for the "on-center" and "off-center" data folders.



Click "Continue", and the On-center (no offset) data will be displayed. You will be presented with the following instruction panel:



At this point, identify the XY range encompassing the beamstop, the rectangular region that is to be replaced. The region can be identified either by simply moving the cursor and noting the pixel values, or by dragging a marquee region and printing the marquee coordinates from the marquee menu. Once you have selected the XY region, click continue, and you will be presented with a simple dialog where you will enter the actual values. The rectangular region of the on-center dataset will be replaced with the same section of the offset data. After this, you will be prompted to save the final, normalized DIV file.