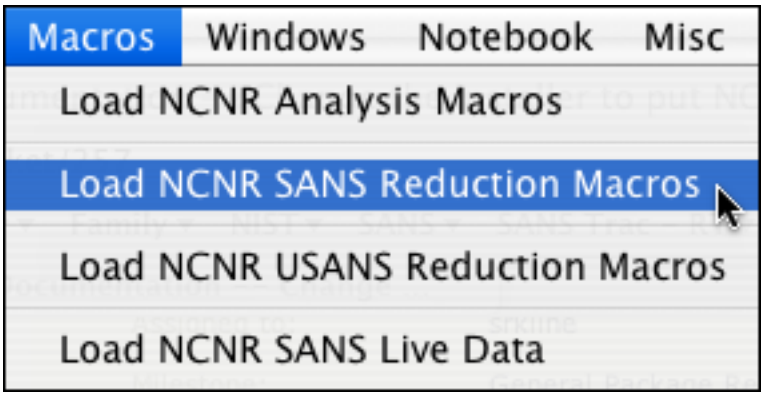
- **SANS Data Reduction Tutorial**

10/2003 Version 4.2
08/2006 Version 5
05/2008 Version 5.10
04/2010 Version 5.20 (Package 7.0)
12/2010 Version 5.20 (Package 7.04)
03/2012 Version 5.20 (Package 7.10)
06/2012 Version 5.20 (Package 7.20)
11/2014 Version 5.20 (Package 7.2+)

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



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.

If you use this software to reduce or analyze your data, please reference:
"Reduction and Analysis of SANS and USANS Data Using IGOR Pro"
S. R. Kline, *J. Appl. Cryst*. **39** (2006) 895–900.

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

SANS Experiment Planning Tools

SASCALC

Simulation of 1D SANS Data

Simulation of 2D SANS Data

General Description

SANS Overview

SANS Reduction Using the Demo Version

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 collected on the VAX or through ICE. 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 a main server and are protected from deletion. During your SANS experiment, as each data file is collected, 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 main server 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 USB drive 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, empty 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.

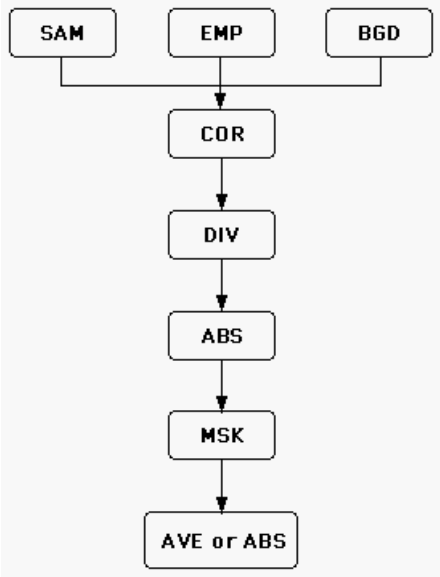
The data in work folders are processed by invoking a protocol that performs a sequence of specific operations, in some cases writing the result to a different work folder, overwriting the previous contents. Ultimately, the corrected data is saved to disk in the desired format in an "averaging" step. 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. must 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:

COR = (SAM - BGD) - [Tsam/Temp](EMP - 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_DDMMMYY_NGn.DIV** files which indicate the date the measurement was made (**DDMMMYY**) 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) -> $d\Sigma(Q)/d\Omega$ in units of 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:

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

where:

ϕ = 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,
ϵ = 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:

$$d\Sigma(Q)/\Delta\Omega = [\ I(Q)\ MONs\ ds\ Ts\ ]/[\ Is(0)\ MON\ d\ T\ ]\ [d\Sigma s(0)/\Delta\Omega]$$

where:

Is(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 Is(Q) are from radially averaged work files then MONs=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 $K= \phi\ A\ \Delta\Omega\ \epsilon\ t$ is the scaling factor, automatically calculated as follows: $\phi\ A\ \epsilon$ is the total (empty beam transmission) detector counts per unit time/attenuation factor at the used wavelength, t is the counting time $x10^8$/MCR, and $\Delta\Omega$ is equal to $(0.5\ cm/sample\text{-}to\text{-}detector\ distance\ in\ cm)^2$.

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.

The final averaging step can also be set to save the reduced data in a 2D ASCII format. The 2D ASCII format can be re-read into the SANS Reduction package for further processing. See 2-D Work File Arithmetic.

SANS System Requirements

• Macintosh or PC

• IGOR Pro installed <http://www.WaveMetrics.com> As of 2/06, v.6.0 is the current IGOR version, and these macros require IGOR Pro v. 6.0 or higher. 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 6.0x 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 Using the Demo Version

The Igor 6 Demo software is fully funcitonal for the first 30 days. After the trial period, the NCNR macros are still functional, but those using the demo version for reduction will have the obvious limitation that they will not be able to save, or copy/paste into other programs. Some specialized operations that use the clipboard will not function since saving and copy/paste is of course, not allowed. Printing also has an Igor watermark overlay. Thus the only real limitation is that reduction needs to be done in one sitting (without quitting Igor), and that publication graphics must be generated in another software package.

During the reduction process (even with the Demo version):
- All corrections to raw data headers are written directly to the files on disk.
- Reduced and averaged data files are written to disk as ASCII output that can be plotted with other software.

The ONLY special step that demo users may want to do is:
- Protocols for data reduction are usually saved with the experiment. Since this is not allowed, protocols must be exported (see Build a Data Reduction Protocol) and imported again if you quit the demo version.

• SANS Reduction, USANS Reduction, Analysis Macros, and the Tutorial data are available on our website:
<http://www.ncnr.nist.gov/programs/sans/manuals/data_red.html>
Follow the instructions on the webpage for downloading and installing the NCNR_SANS_Packge.

What's New in SANS

Changes (11/2014):

• Beta version of Automated SANS Data Reduction has been added.

• Simulation of a series of samples or a whole "experiment" can now be done as easily as a real SANS instrument, by setting up a series of simulation runs. Select Macros-> "Load Simulation Run Builder" to access these features.

• Event Mode procedures have been improved.

Changes to Version 5.2 (Package 7.20) (06/2013):

• Polarization procedures have been improved

• Full support for the new 10m SANS instrument at NGB have been added, including SASCALC

• Event mode data can now be processed through a convenient panel. Data collected in oscillatory, stream, TOF, or TISANE modes can be visualized, sliced, and processed. An XOP has been written to speed up the processing of these (often) very large files. See Event Mode Data

• A panel to allow batch fitting of a single model to a large number of data sets has been implemented. It allows full control of the input guesses, data range, and held and constrained parameters. Once the starting information is gathered, the fits run unattended and save reports of the results. See: Auto Fit (or Batch Fitting)

• Package loaders for processing data from various facilities have been consolidated onto the Macros menu rather than separate templates. Data handlers from different facilities cannot be loaded into the same experiment.

Changes to Version 5.2 (Package 7.10) (03/2012):

• Polarization reduction procedures have been added

• Full 2D error propagation has been added. It can be exported as 2D QxQy? ASCII and used for 2D analysis in the NCNR Analysis macros or SASView.

• Gravity effects have been fully included in the 2D resolution function. See Resolution Function in 2D

Changes to Version 5.2 (Package 7.04) (12/2010):

• A "Sector_PlusMinus" averaging opition has been added. It is a sector average that uses both sides of the detector, defining the left side as negative q-values.

• A Rebinning panel has been added to Re-Bin Data to improve counting statistics after it has been reduced to 1D.

• A Data Set Management panel has been added to allow re-saving and batch conversion of 1D data files into canSAS XML or NIST 6-column format.

Changes from Version 5.1 to Version 5.2 (Package 7.0) (04/2010):

• Simulation of SANS data has been added. Working with the Analysis models, you can now optimize the instrument setup for the expected scattering of your sample while also obtaining estimates of countrates and counting statistics in a simulated data set. See SASCALC , Simulation of 1D SANS Data, and Simulation of 2D SANS Data.

• Reduction and Analysis can now be carried out in the same Igor experiment. Reduction and analysis modules can be loaded as needed, and hidden when no longer in use.

• Patching of raw data files is now easier with improved filtering to locate files.

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

• General amrithmetic operations can now be performed on two 1D data sets, improving the former Subtract_1D operation.

Changes from Version 5.0 to Version 5.10 (2/2008):

• SASCALC, a tool for optimizing instrument setup is now an integral part of the Reduction package.

• NSORT - can now preview the scaling and overlap of data without writing a file. Also, a warning is displayed if the rescaling multiplier for overlap is more than allowed accuracy of absolute scaling (+/-5%).

• Added feedback button on main panel to submit bug reports and feature requests. Requires a web browser and active internet connection.

• An ASCII export format that is comaptible with GRASP software (C. Dewhurst, ILL) is now available.

• Included detector corrections to account for the variation of efficiency at large detector angles.

• ABS parameter selection now presents a more logical dialog to select the required empty beam file.

• Updated the resolution calculations to fully account for focusing lenses.

• Included updated attenuator calibration tables.

Changes from Version 4.2 to Version 5 (8/2006):

• Added string on SANS_Data display window to show the current sample label.

• (BSG) Changed Transmission.ipf to use a secondary method for calculating transmissions based on the whole detector. "Total" transmission is calculated as well as the normal transmission defined by a box. The ratio of the two transmissions may be useful for identifying multiple scattering. See Calculate Transmissions

• Added to Transmission.ipf to account for empty beam and sample transmission measurements taken with a different number of attenuators. The transmission is now rescaled by the ratio of attenuator transmissions, and is logged to the history window.

• Fixed minor bug in resolution calculation. Previous calculations were using pixel width of 1.0 cm as for Cerca detectors, rather than 0.5 cm for Ordela detectors. The error introduced in sigma_Q was less than 5%, and not a significant difference in smearing calculations.

• Additional (minor) bug fixes and speed improvements.

Changes from Version 4 (10/2001) to Version 4.2 (08/2003):

Display enhancements

• SANS Menu items will open or make visible the most commonly used panels so that they can quickly be located on screen.

Export formats

• The currently displayed SANS Data, including fully or partially corrected data can be saved as 2D ASCII. This data can be directly read in and operated on using 2-D Work File Arithmetic.

New operations

• 1-D data plots are now controlled by a Plot Manager making it easier to load and append data to graphs, and to remove old data sets from Igor's memory. See Plot Averaged Data.

• Subtraction of 1D datasets can be performed, as well as subtraction of constant backgrounds or simple rescaling of data. See Data Set Arithmetic.

• 2-D Work File Arithmetic operations are simplified, reading in and generating 2D ASCII format.

• A Marquee menu operation will graph a vertical or horizontal selection of the SANS Data display. See Marquee Operations.

• A SANS Preferences panel has been added to set parameters for non-standard experiments.

Improved functions

• Absolute scaling based on an empty beam measurement has been changed to improve accuracy.

• Protocols are now portable, and can be exported as a text file to be imported into a new experiment.

• Sort operation now allows rescaling of a single data set. See Sort and Combine Averaged Datasets.

• Detector sensitivity files can be created for the NG1 SANS which has two beam stops.

• Bin Width during 1D averaging can be adjusted from default values as a SANS preferences item.

• During the COR step, files are checked for Transmission=1. Options to temporarily override are presented. The check can be turned off/on as a preference item.

• Schematics now can be generated in either log or linear intensity scale.

• Data is rescaled to correct for attenuation when a reduction protocol is executed, even if no subtractions are performed.

• Help buttons are available on most panels that will jump to the relevant help section.

Instructions for the Impatient

1) Load the "NCNR SANS Reduction Macros" 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

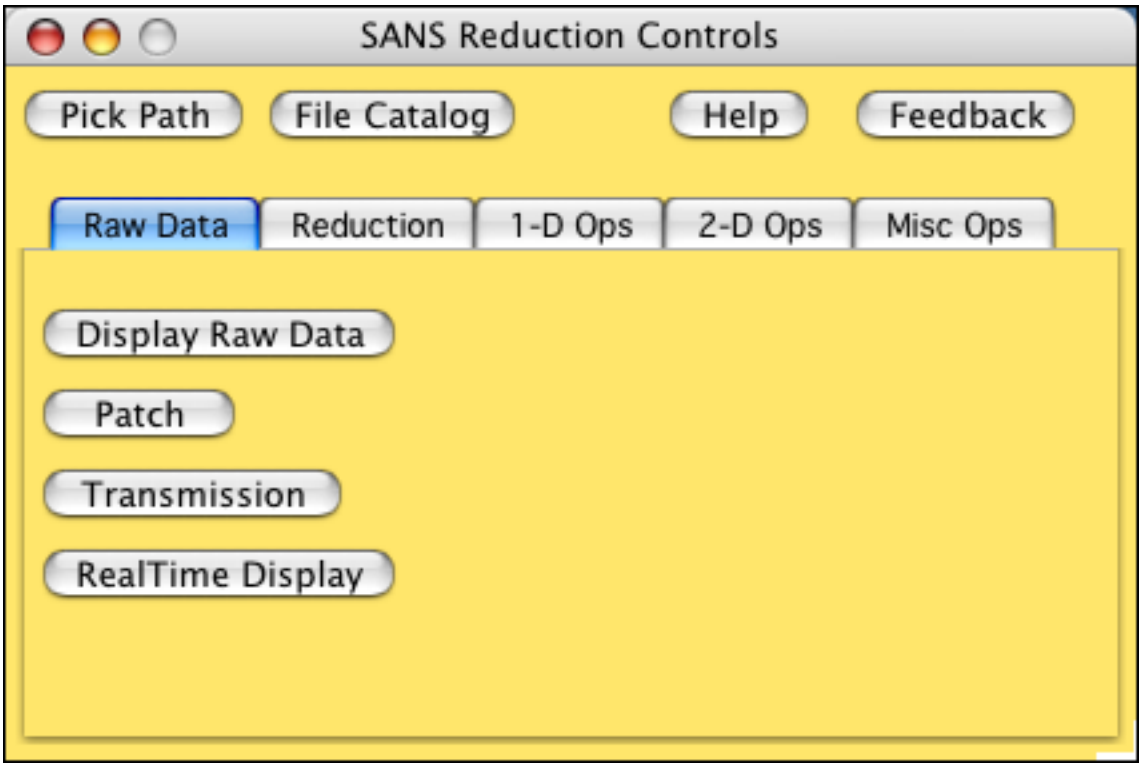
Tutorial Instructions

Main Controls

What: Upon opening a blank 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 Main Panel of SANS Reduction Controls is automatically created. If you've lost this panel on the screen, selecting SANS->Main Control Panel 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.

File Catalog: 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.

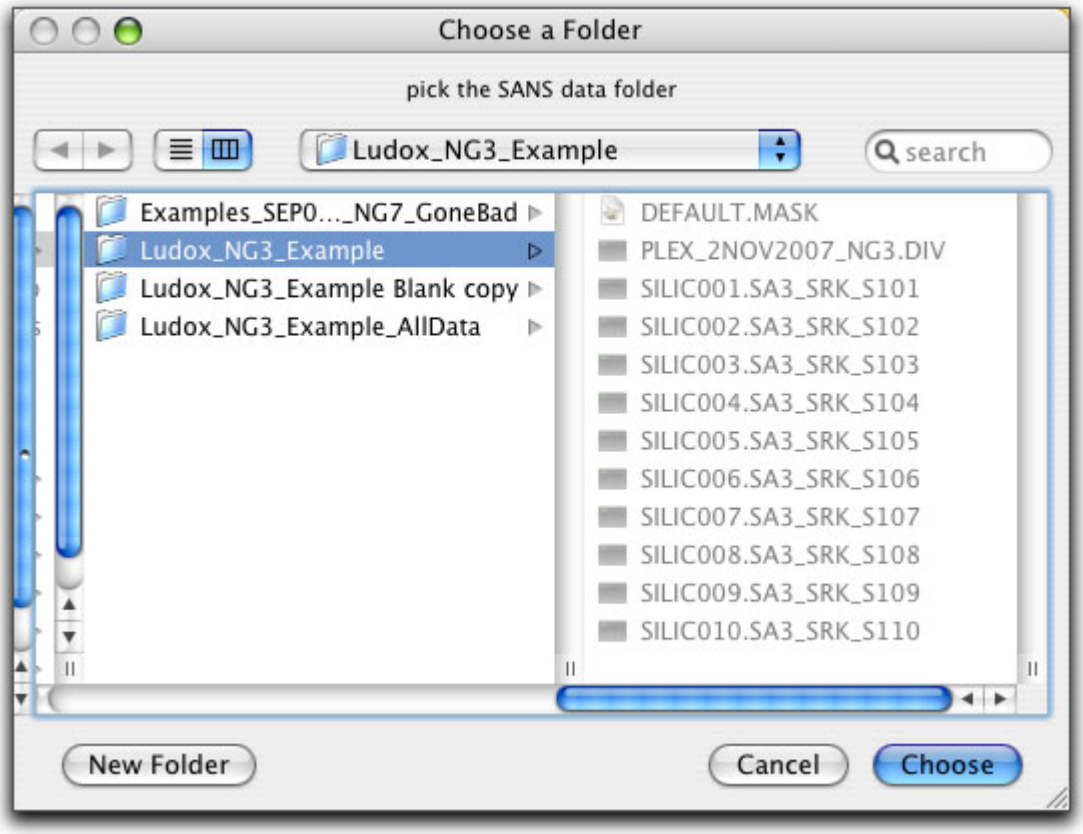
Feedback: will automatically direct you to a web page that is a form where you can submit a bug report or a feature request.

There is also a SANS Menu that is always visible on the main menu bar. Menu selections will generate the input panels as if the corresponding button had been pressed on the Main Panel, or simply bring the window to the front if it has been misplaced. The Initialize step is run automatically as the experiment is launched, but can be re-run at any time to ensure that the SANS Preference values are reset to their default values. 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

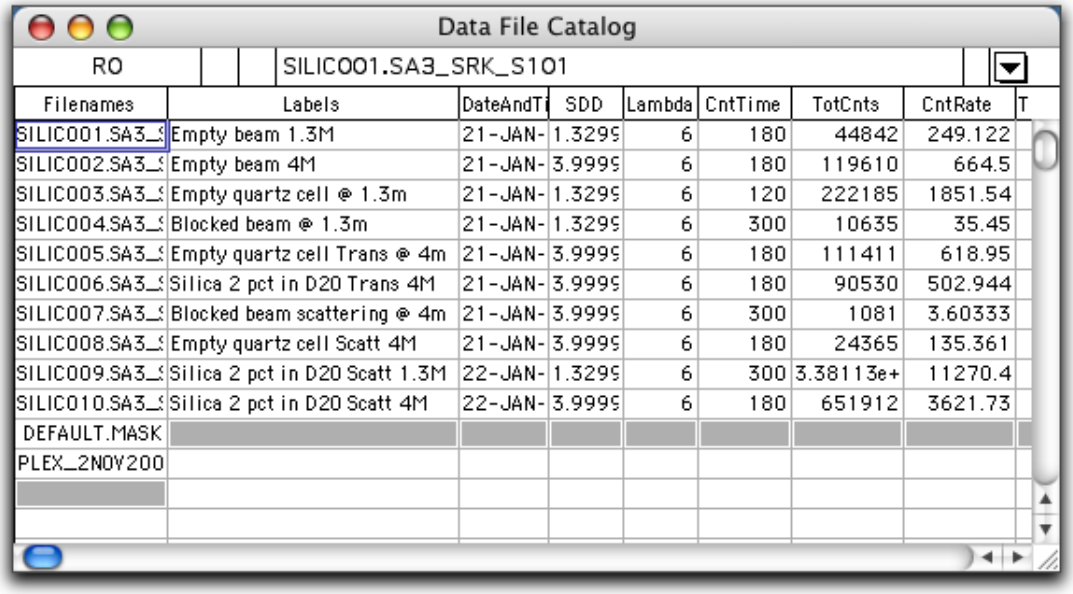
List the Data Files

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, the dialog will look slightly different.



Once the path is set, click "File Catalog" 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 "File Catalog" 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.



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^{-1}) 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 though 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.

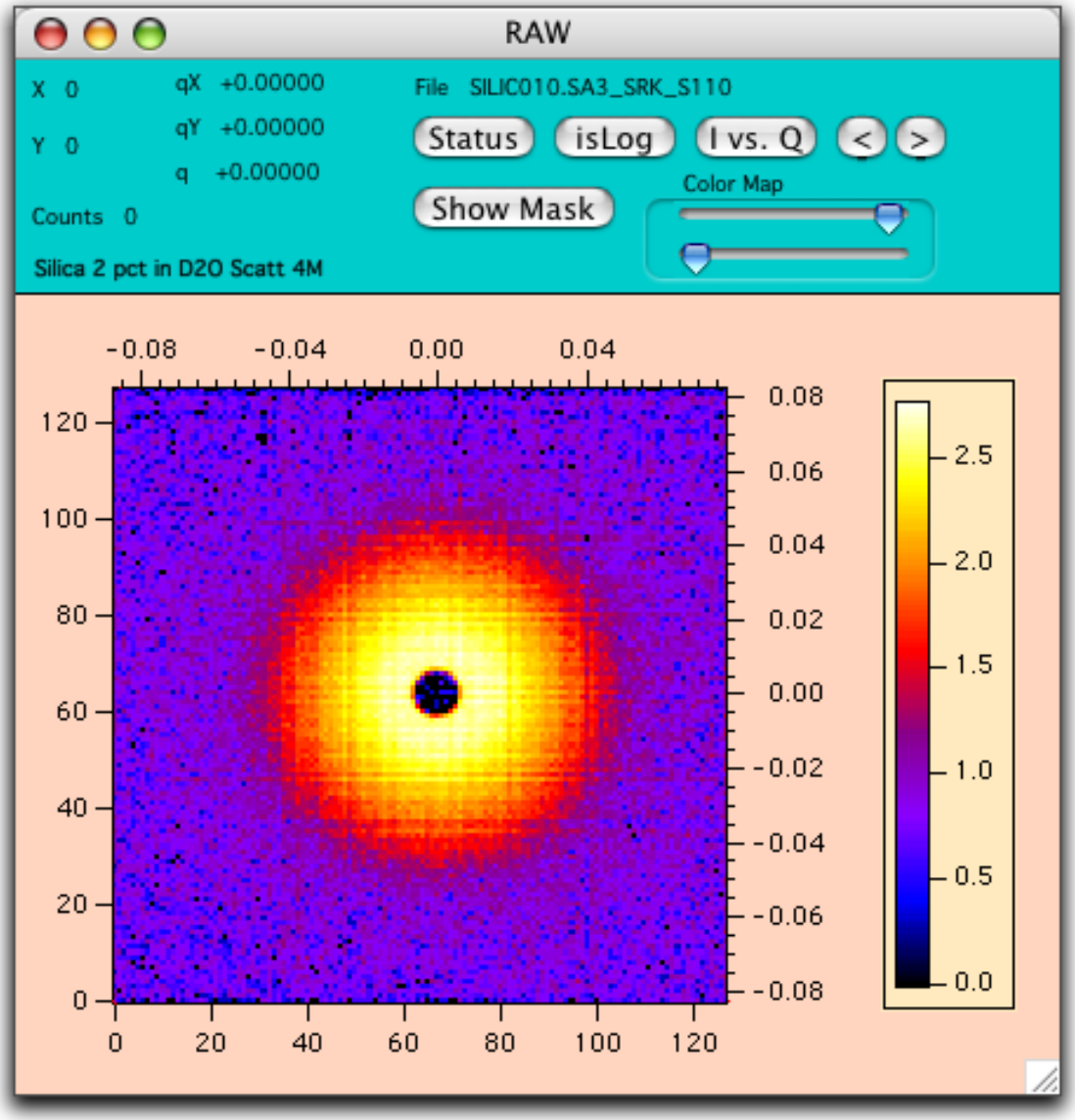
isLin: toggles the color map scaling of the detector counts from linear to logarithmic. When the data is log-scaled, the button will read "isLog".

I vs. Q: displays a new panel with averaging options to produce a 1-D averaged dataset of the 2-D data, or save the data in a 2D format. 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. It will search +/- 10 run numbers, in case some run neumers have been skipped.

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 vales 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 (+/- delta phi) each direction from the central angle (phi).

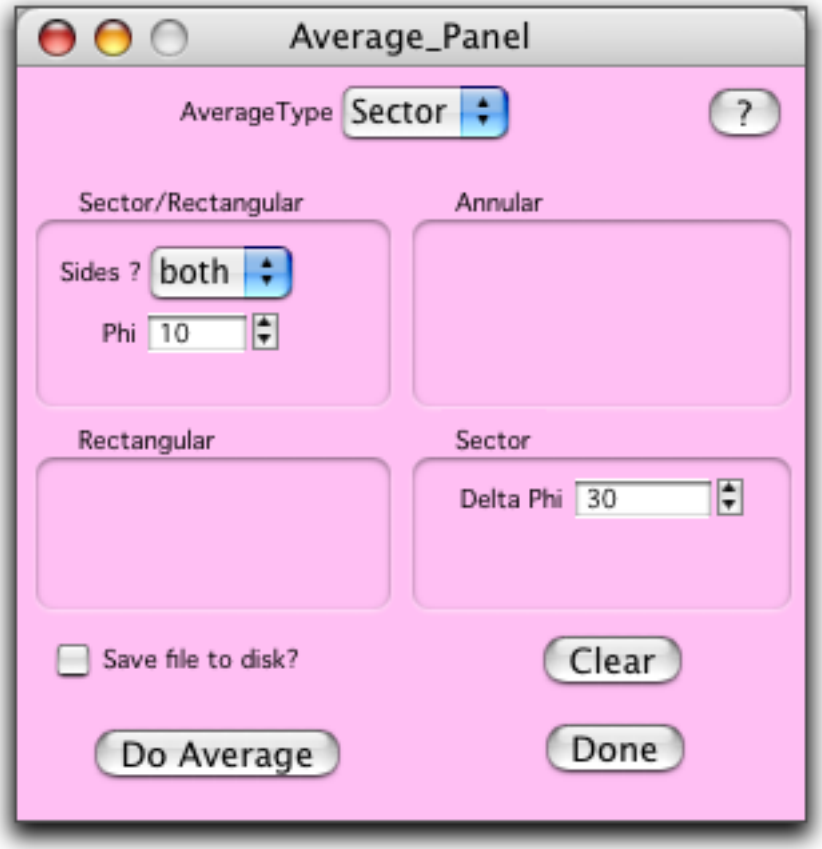
• "Sector_PlusMinus" uses both sides of the detector, defining the LEFT side as "negative" q-values. Everything else behaves as a normal sector average.

• "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.

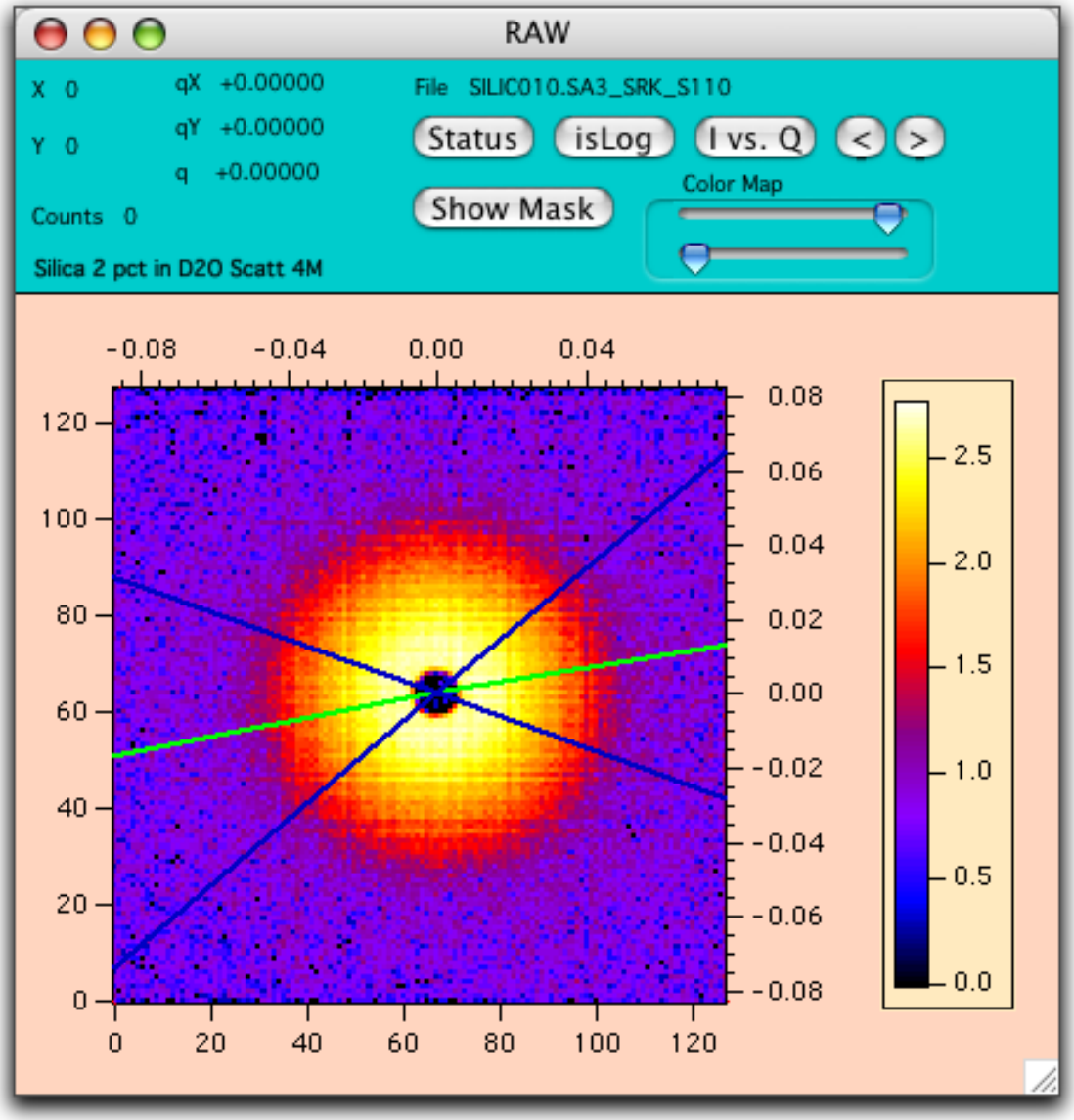
• "2D ASCII" saves the currently displayed data in 2D form in terms of intensity versus pixel coordinates. This data can be re-read using the 2-D Work File Arithmetic Panel to perform further processing steps.

• "QxQy ASCII" saves the currently displayed data in 2D form in a three column format, converting each detector pixel into Qx and Qy and its corresponding intensity. This data format cannot be re-read into the SANS macro set.

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



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), +/- 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.

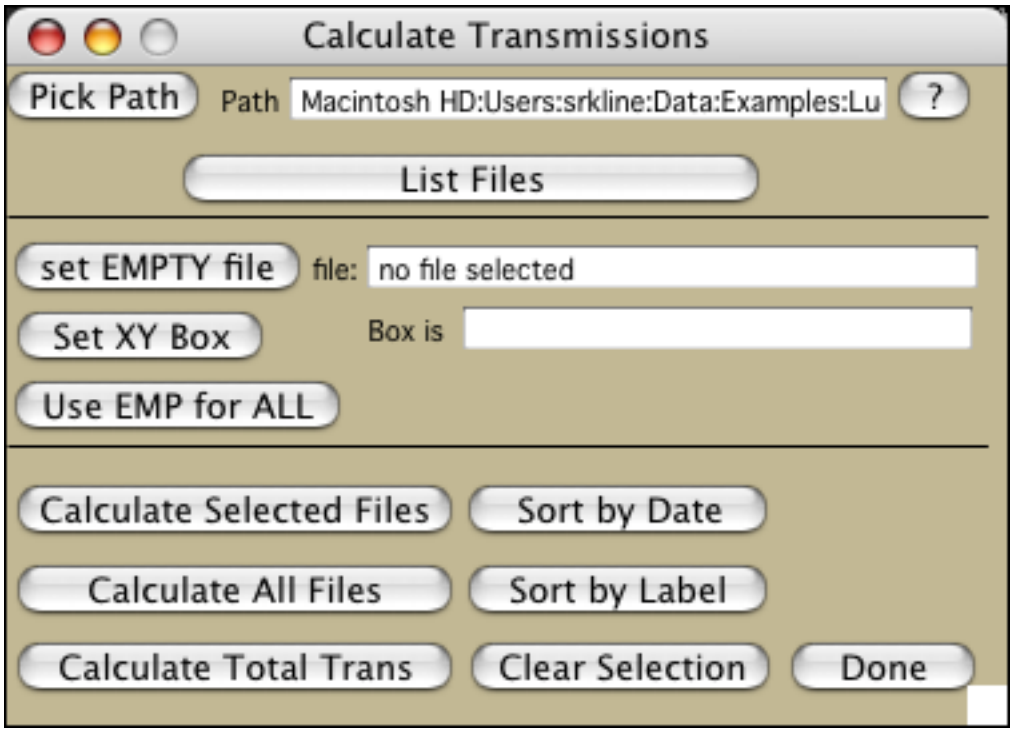
For Circular, Sector, and Rectangular averages, the data is binned in a width of one pixel as default. For Annular averages, the circle of 2π is broken into 72 bins as default. These values can be changed using the SANS Preferences panel.

Calculate Transmissions

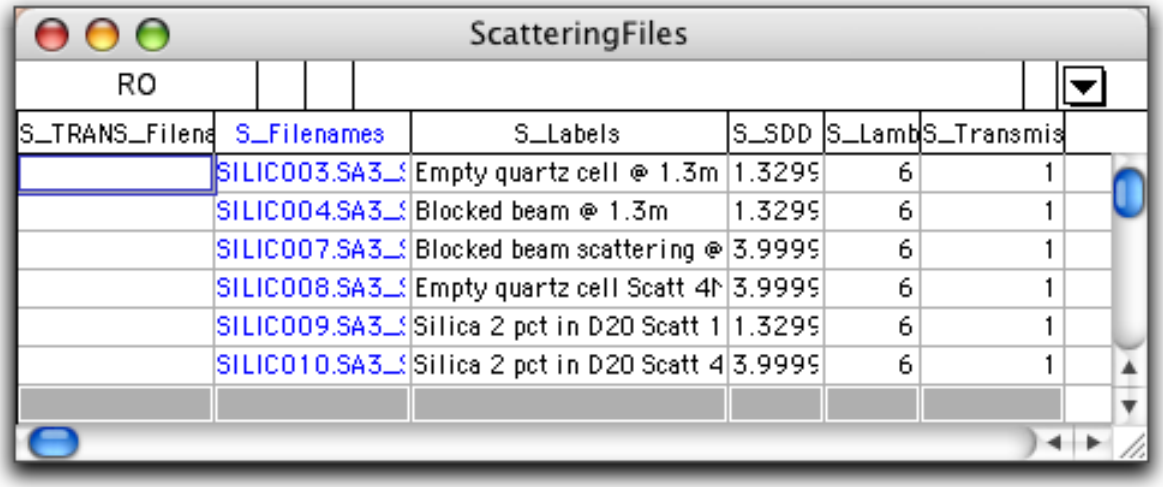
What: Transmission of samples and sample containers must be calculated and entered into the headers of the raw data files for proper subtraction of non-sample scattering during data reduction. Here we will create the "associations" between the transmission measurements and the scattering files to which they correspond. Transmissions will then be calculated and automatically patched to the file headers. Optionally, the transmission can be calculated using the whole detector (=Total Transmission) and compared to the transmission in a small box around q = 0 as a way to estimate multiple scattering.

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

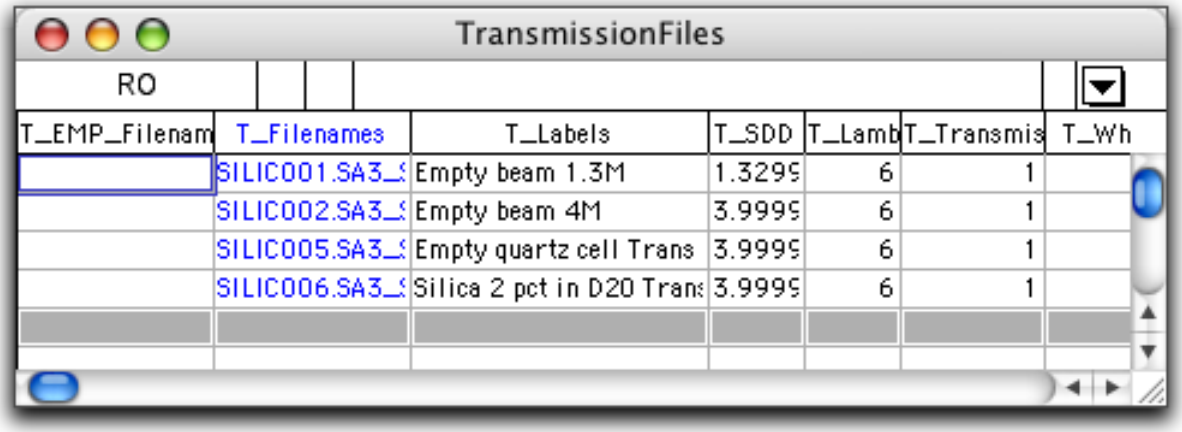
main panel. The following new panel will appear:



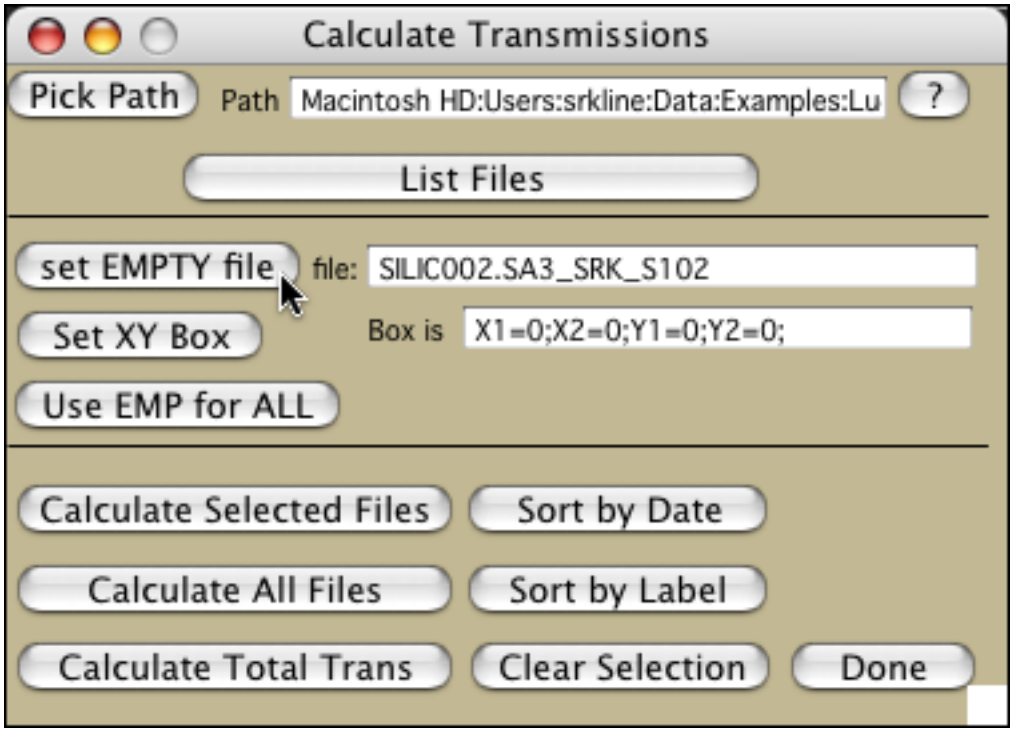
2) Click on "List Files" to build two tables - one with scattering files:



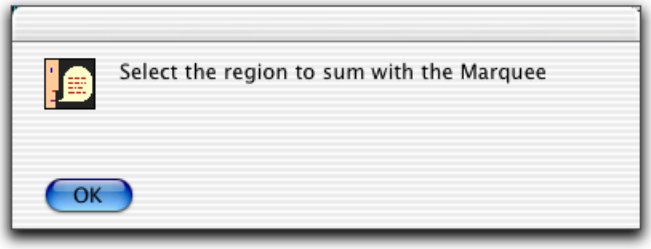
and another with transmission files. The transmission files are automatically separated from the scattering files based on the beamstop location (off-center) in the header of the raw data file.



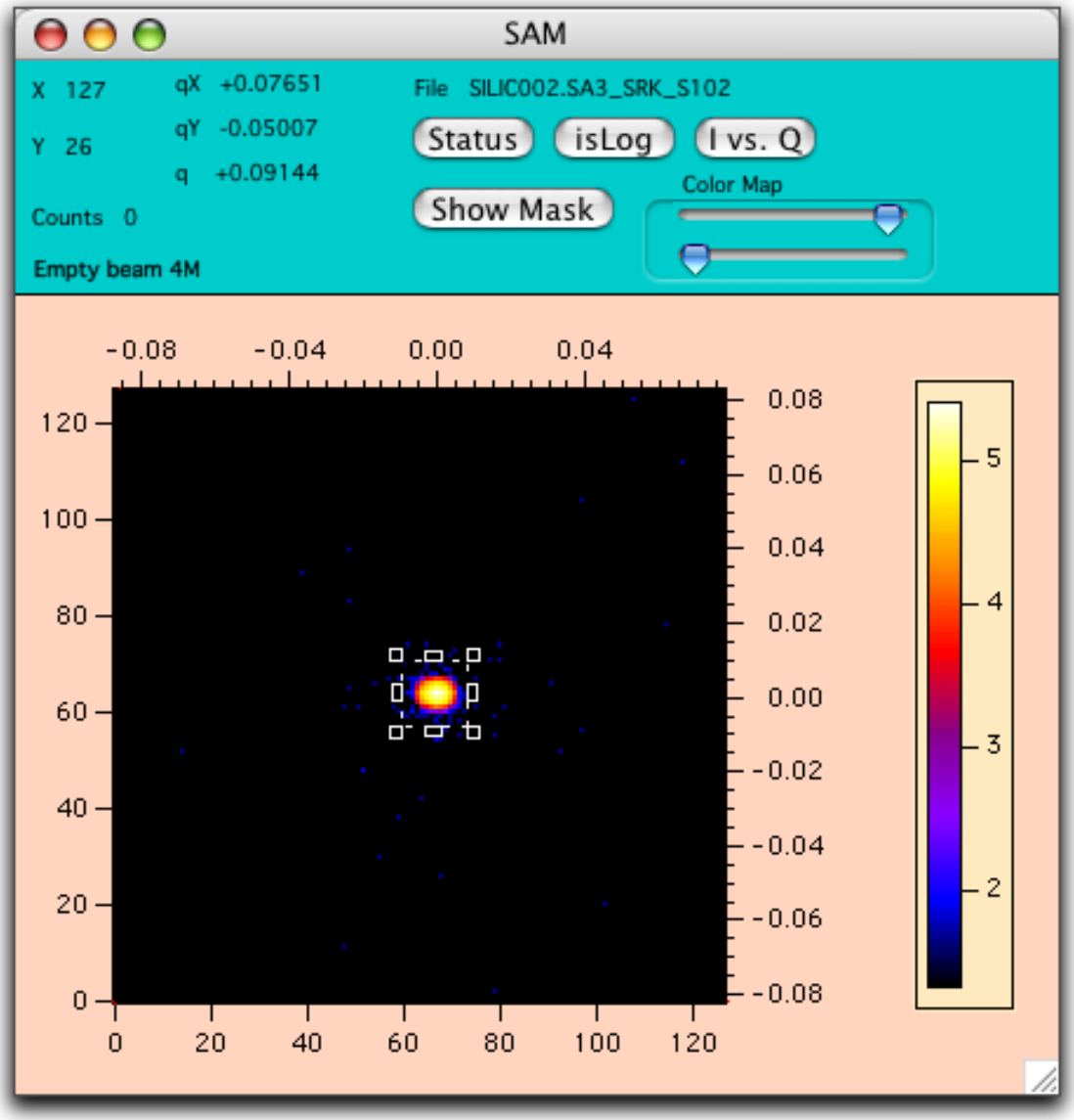
3) Find the empty beam transmission measurement in the TransmissionFiles table. It is in the blue "T_Filenames" column. For the tutorial, it is file SILIC002.SA3..... Click on this file to select it (just that cell in the table). In the Transmission Panel, click "Set EMPTY File" to set this file as the empty beam. The filename appears, as well as the box coordinates:



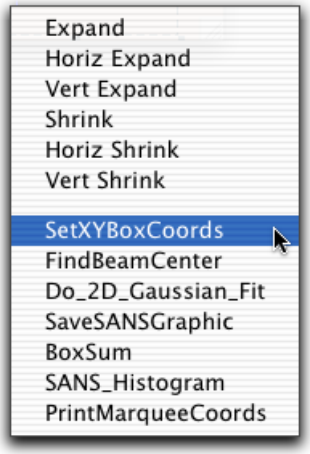
The "intensity" of the empty beam is found by summing the number of counts on the detector over a specific rectangular region of the detector. Currently the box coordinates are zeros, so we need to pick the rectangle. Do this by clicking "Set XY Box". The raw data file (SILIC002) will be displayed, and 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.

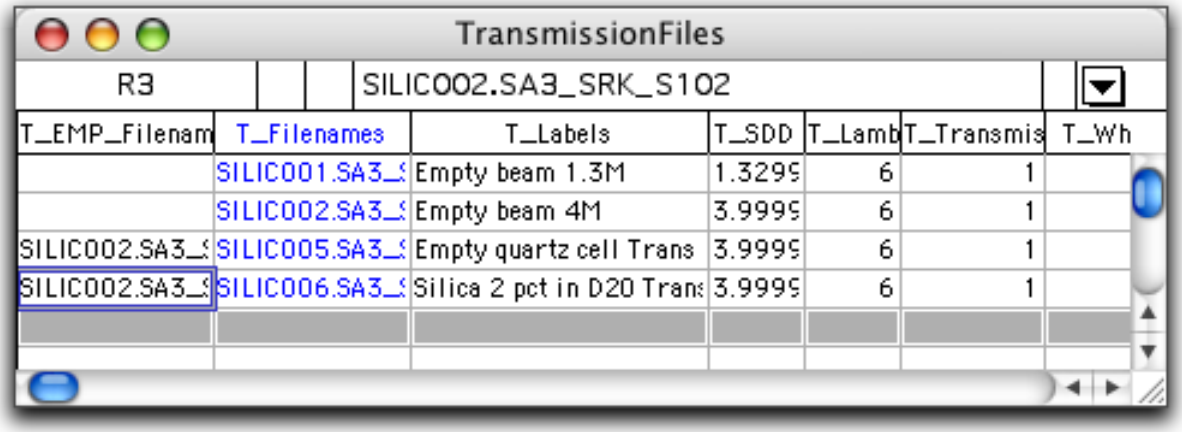


Click to get a menu, and near the middle, select "Set XY Box Coords".



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.

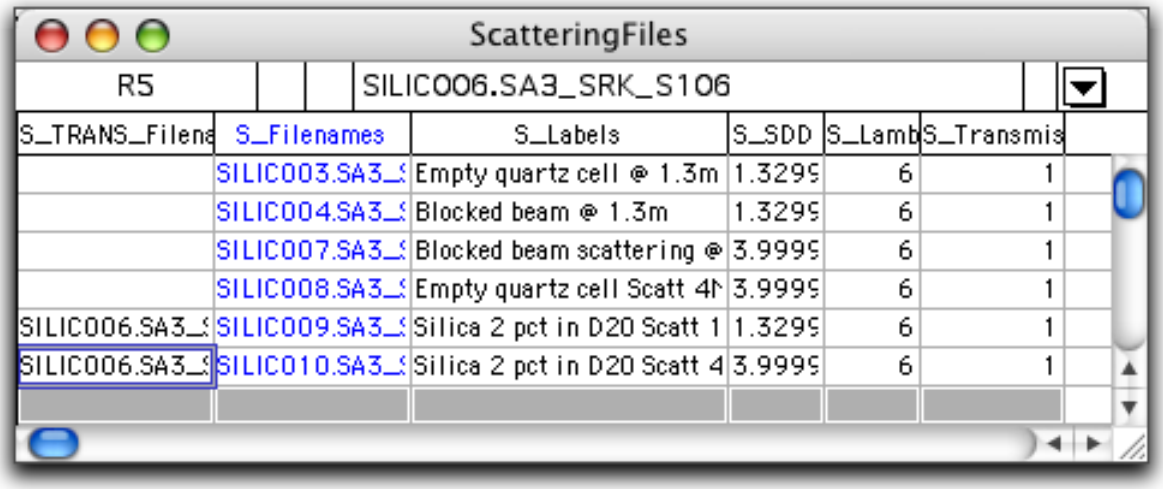
4) Now make the associations between the empty beam file and each of the transmission measurements. Each transmission measurement for a sample must be normalized relative to the empty beam transmission (and should therefore be less than unity). Make the EMPty beam association by selecting the empty beam file (in the blue column), copying it, and pasting the filename into the "T_EMP_Filename" column. Transmission was only measured of two samples: the silica (2 % by weight of colloidal silica in D2O, held in a quartz cell), and an empty quartz cell. Note the consistent sample and transmission labels (that you enter when you acquire data). Keep the "trans" or "scatter" identifiers at the end of the labels - or drop them altogether. The program already knows the difference. The TransmissionFiles Panel should look like below.



*** A faster way to make the empty beam association is to click "Use EMP for All". This will fill in the empty beam file for all of the transmission measurements. 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), but if there's a file listed there, it doesn't matter. If you have transmissions measured at multiple wavelengths, you'll need to do the assignment by hand.

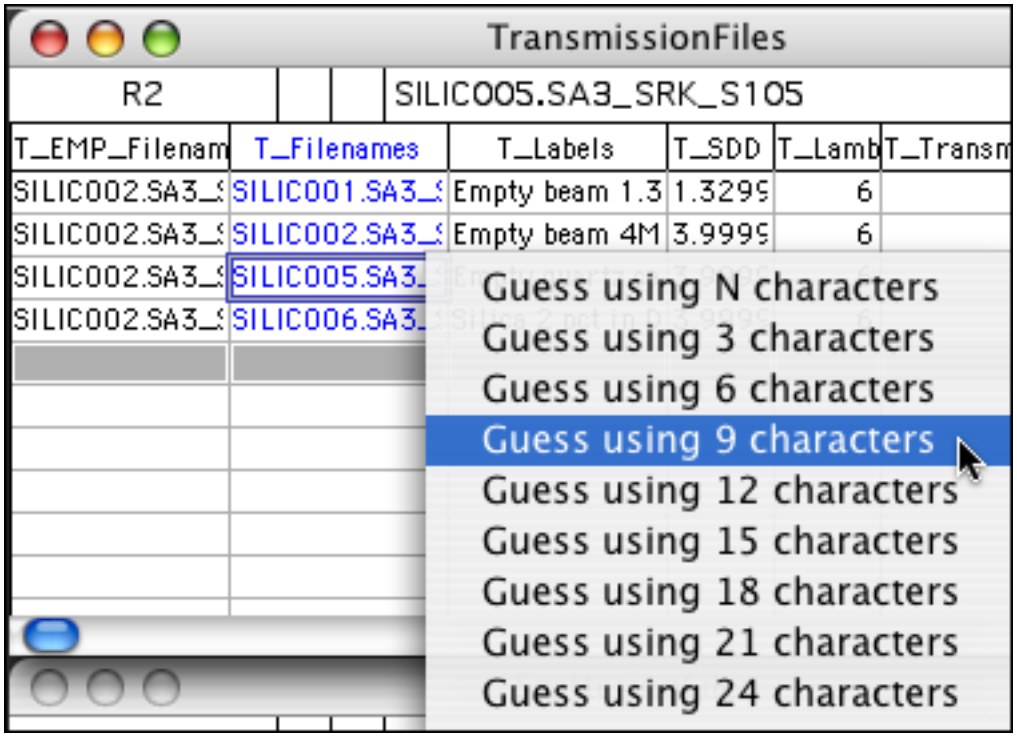
5) Now make the association between the transmission measurement of the silica (SILIC006) and the scattering file(s) for the same sample. In this case, the silica scattering was measured twice - using two different instrument configurations. The sample is the same, and so is the

transmission, so copy the filename of the silica transmission (SILIC006...) from the blue "T_Filenames" column, and paste it into the (2) proper locations in the "S_TRANS_Filenames" column in the ScatteringFiles table, like this:

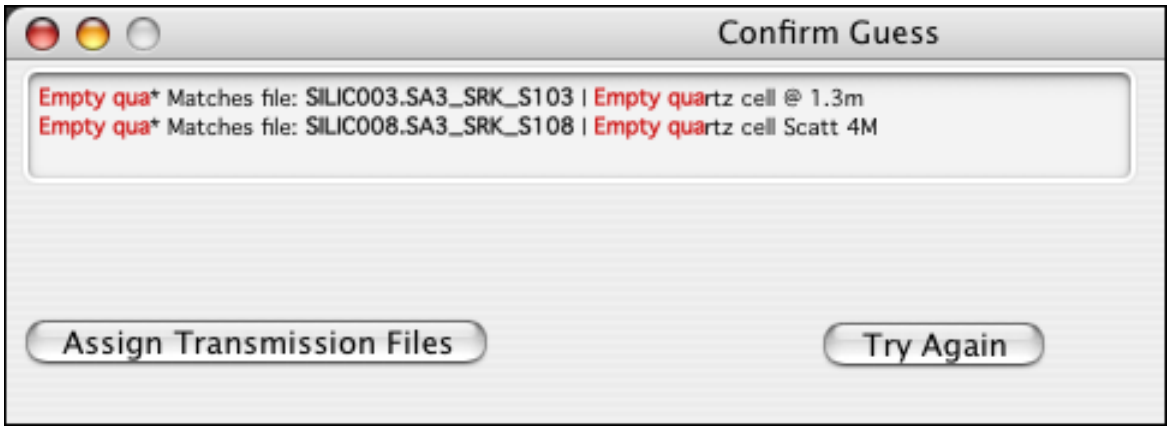


If you were consistent in your sample labels, it is often more convenient to group the same samples together, rather than a chronological listing of the scattering files. Click the "Sort by Label" button in the Transmission Panel to get the following listing - note that the previous associations are carried along, and now the scattering measurements are conveniently grouped together.

** A faster way to assign the transmissions is to have the program try to guess the assignments based on the sample labels. To do this, select a single transmission file name from the TransmissionFiles table (from the blue column), then shift-click on the cell. A contextual menu will appear (on the up-click...) Pick the number of characters you want to use to try to match. It will try to match the FIRST 'N' CHARACTERS in the transmission file label to the scattering file label. Here, I chose 9 characters to match the title of "Empty quartz cell..."



The program tries to find all of the sample scattering files that have a matching sample label, and presents the results:

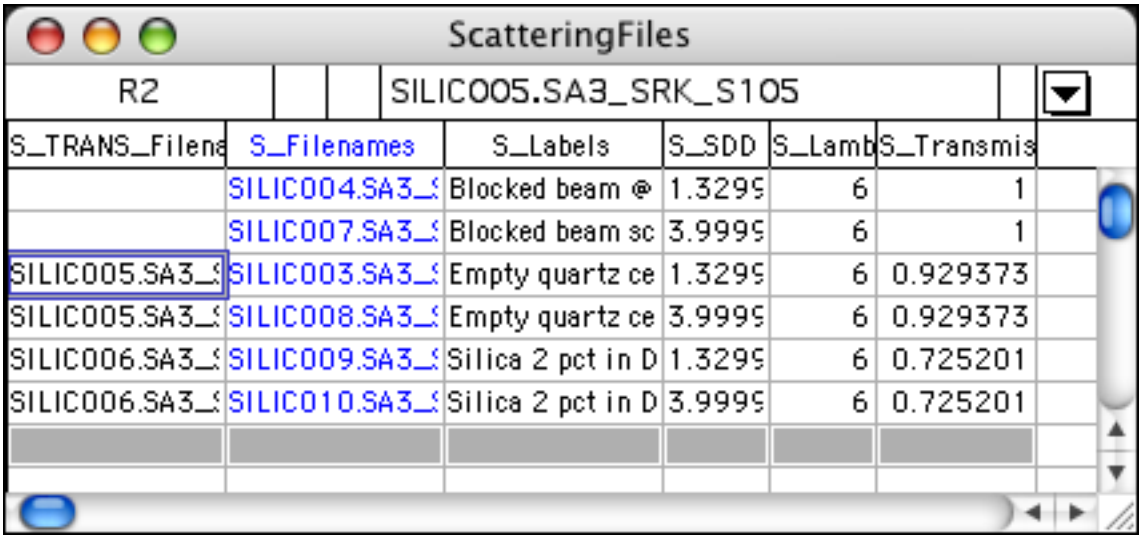


If the match correctly identified the scattering files, then "Assign Transmission Files" will do the assignment, and then immediately calculate the transmission. If not enough or too many "matches" were found, try again.

Hint #1: Get out of the habit of sample labels that start with "S. " for scattering files and "T. " for transmission files. Igor has other ways of discerning transmission vs. scattering files.

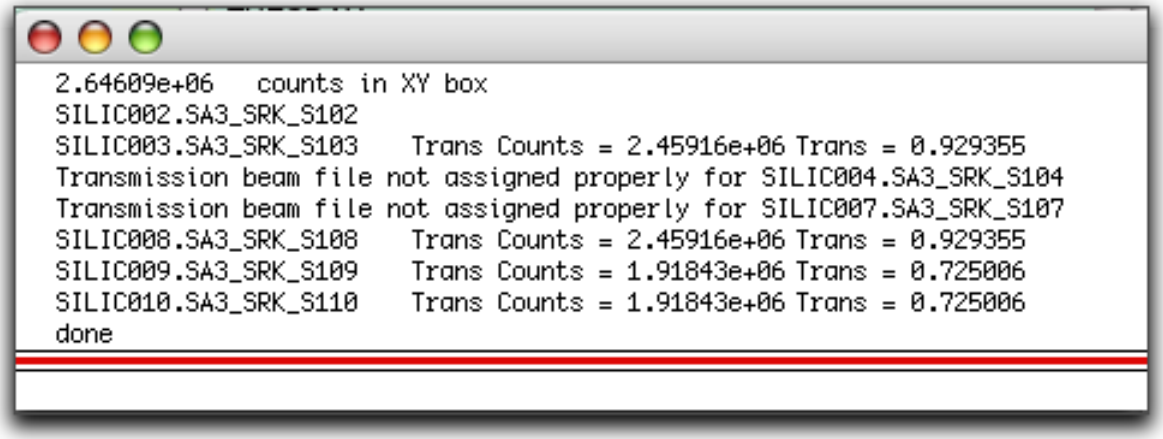
Hint #2: Use a large number of characters to match to minimize chances of a false match.

When you're all done, the scattering file table will look like this - where all of the transmissions have been calculated.



S_TRANS_Filena	S_Filenames	S_Labels	S_SDD	S_Lamb	S_Transmis
	SILIC004.SA3_S	Blocked beam @	1.3295	6	1
	SILIC007.SA3_S	Blocked beam sc	3.9995	6	1
SILIC005.SA3_S	SILIC003.SA3_S	Empty quartz ce	1.3295	6	0.929373
SILIC005.SA3_S	SILIC008.SA3_S	Empty quartz ce	3.9995	6	0.929373
SILIC006.SA3_S	SILIC009.SA3_S	Silica 2 pct in D	1.3295	6	0.725201
SILIC006.SA3_S	SILIC010.SA3_S	Silica 2 pct in D	3.9995	6	0.725201

6) If you need to calculate any of the transmissions manually, "Calculate All Files" or "Calculate Selected Files". The results of the calculation are displayed in the command window (usually at the bottom of the screen, cmd-J or ctrl-J will bring it to the front). The transmission files were not assigned properly for SILIC004... and SILIC007... 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 File Catalog table, however, is not updated (unless you force it to update by clicking File Catalog on the main panel again).



7) If you have made incorrect assignments, you can either copy/paste the correct files and then recalculate the transmissions (they will simply overwrite the old, incorrect value), or you can select the "wrong" files, and click "Clear Selection" to remove the assignment and reset the transmission to one.

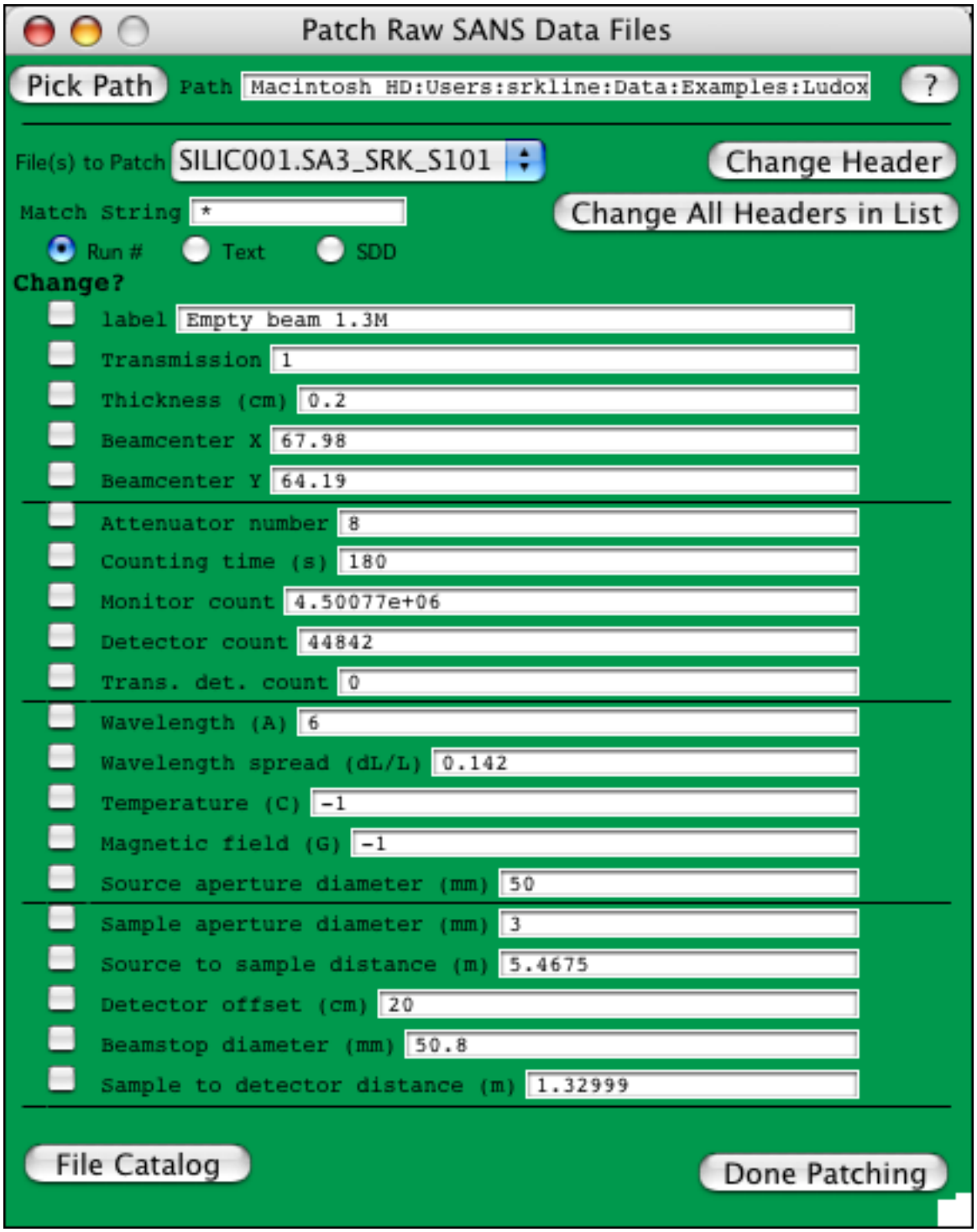
8) Transmission calculations are done. Clicking done will remove the panel and both tables. All of the tables and associations are regenerated by starting again from the "Transmission" button on the main panel. The previous associations are retained, and newly collected data files will have no associations. 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.

9) To check your sample for multiple scattering, use the Calculate Total Trans button. Make the association between trans files and empty beam, as described above. Select the trans files you wish to calculate and click Calculate Total Trans. The transmission is calculated using the actual “box” method (as above) and then using the counts on the entire detector. If these numbers differ by more than 10% you should talk to your local contact because there may be significant multiple scattering in your sample.

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.

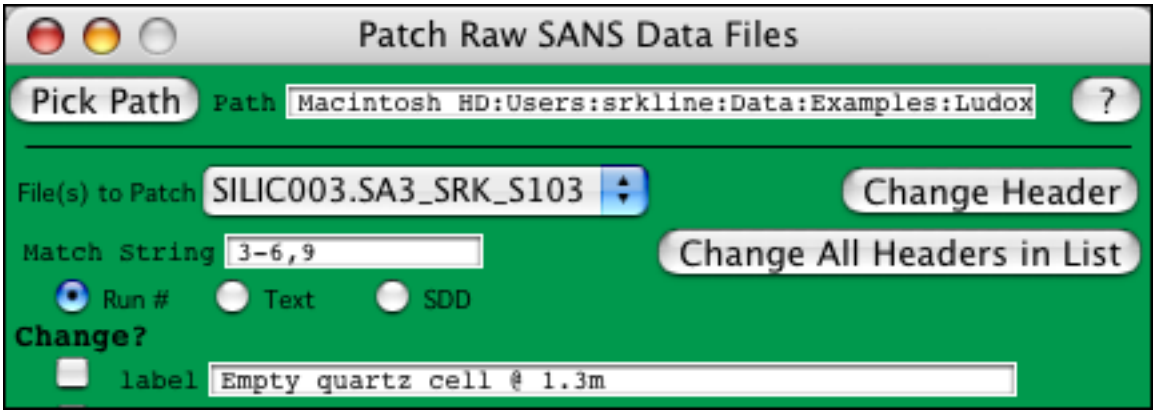


Click in the "Match String" box and hit return to refresh the list. Since the Match String is "*", all data files will be shown. The header information in the displayed file in the popup is shown below it in the text fields. If, for example, you want to change the sample label, you simply enter the new 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

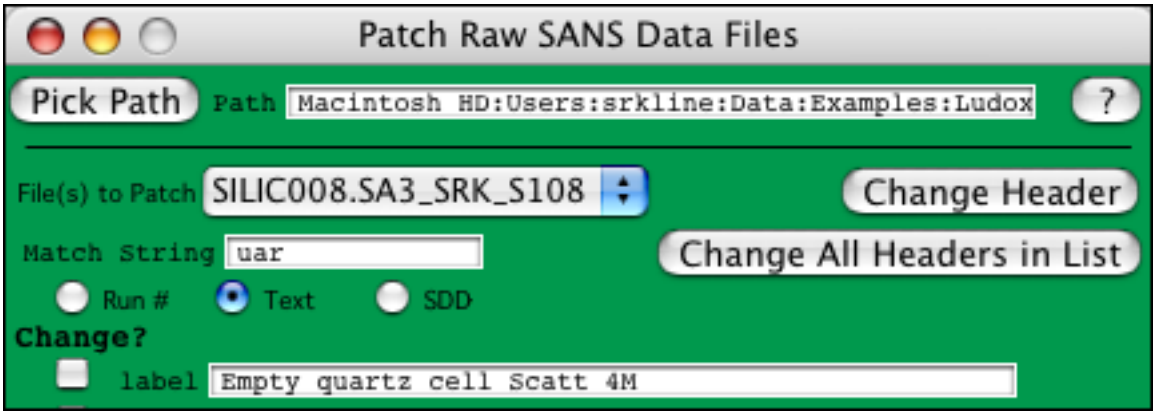
the ones you want). Then click "change all headers in list". You will be warned that it will change more than just the top file, and say "yes" to change all the files in the list. Transmissions were calculated previously using the Transmission panel, and should all be correct here.

For more efficient filtering of the files:

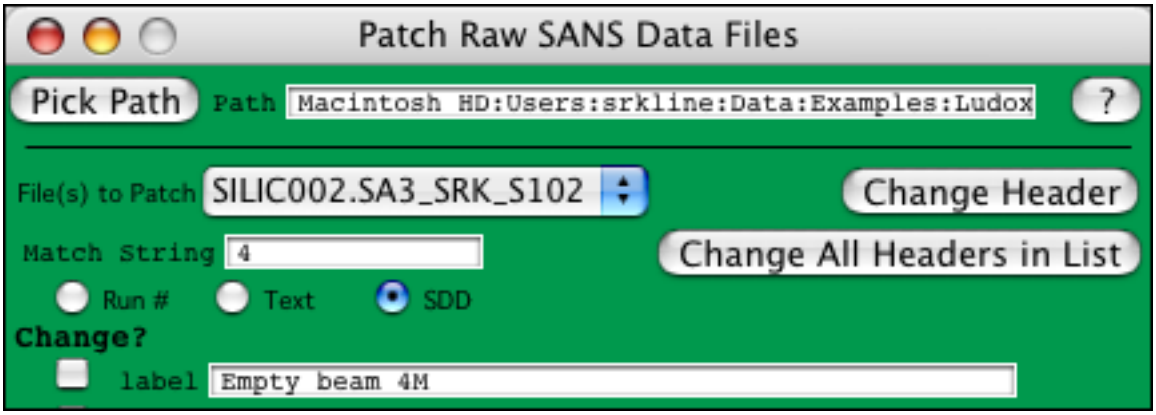
By Run#:
- Enter a list of run numbers (comma delimited) or a range of run numbers specified by a dash.



By Text:
- Enter some text (no wild card needed) and grep will search the entire file for the text match. Here "uar" returns matches for qUARtz cell. The file name is also in the file header, so these are searched too.



By SDD (Sample to detector distance):
- Enter the sample to detector distance (in meters). You can use a wild card at the end of the distance, so for example 13* will find 13.17m, and 4* will find 3.9995m, so it's easier to find a match.

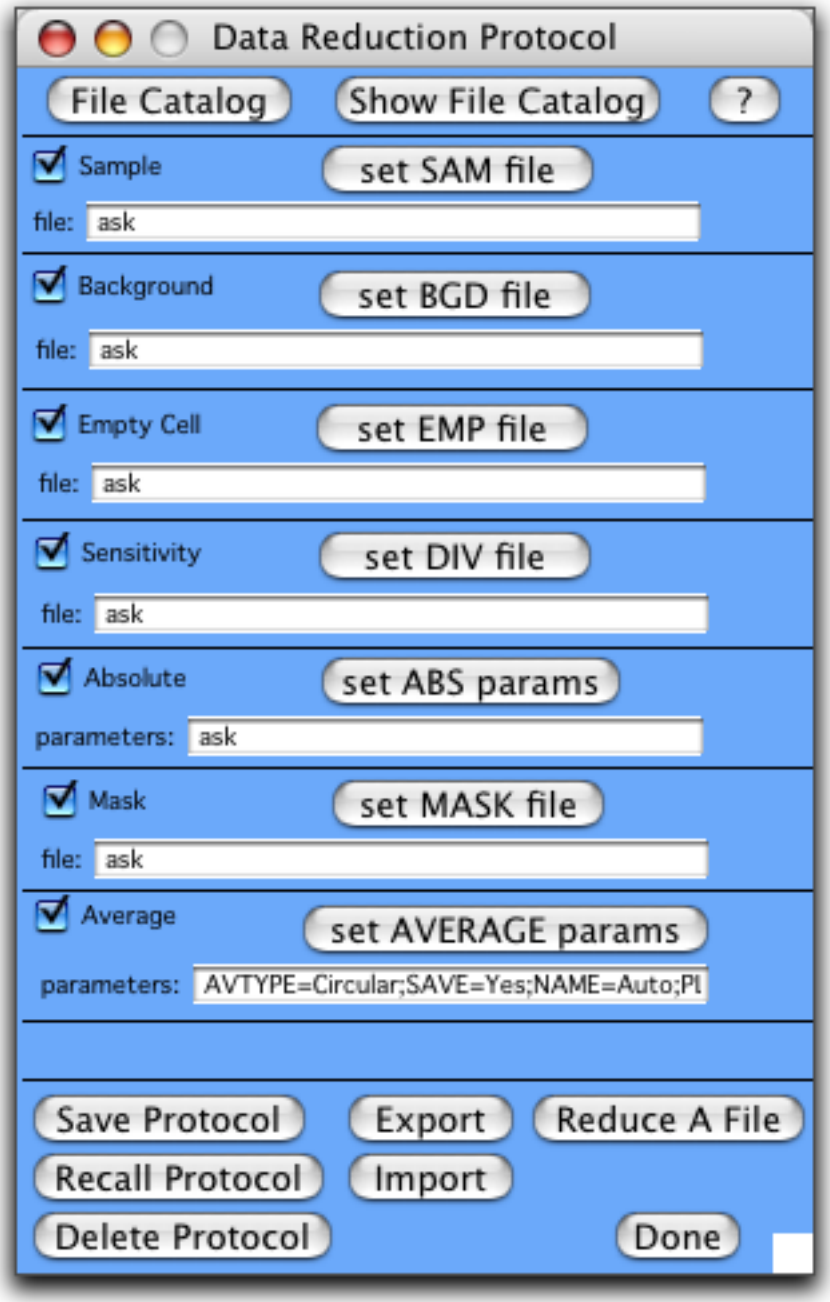


Build a Data Reduction Protocol

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 4 meter sample to detector configuration and use absolute scaling from an empty beam measurement. Click "Show File Catalog" 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.



2) Fill in the background file by finding it in the listing (run SILIC007), clicking to select the filename, and then clicking "Set BGD file" on the panel. The following dialog appears:

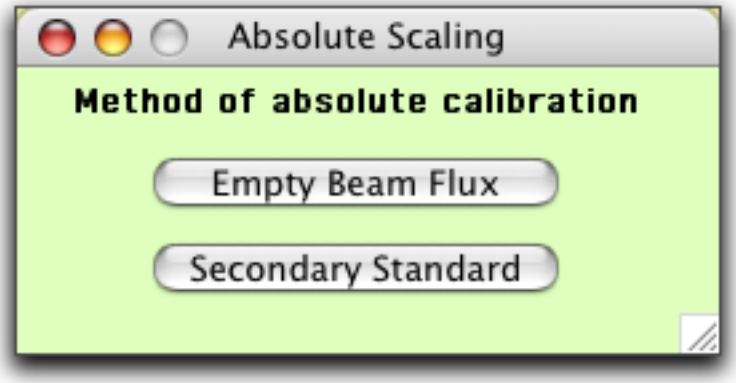
Say "Yes" to reset the list of files. This will set this single file (the selected text) as the background file. If several background files were collected and it is desired to add them

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.

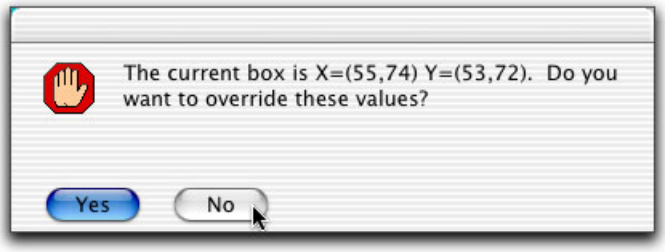
3) Fill in the EMPty cell file in the same way that the BGD file was set. It is run SILIC008.

4) Set the detector sensitivity (DIV) file. The file is PLEX_2NOV2007_NG3.DIV (at the bottom of the Data File Catalog 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:

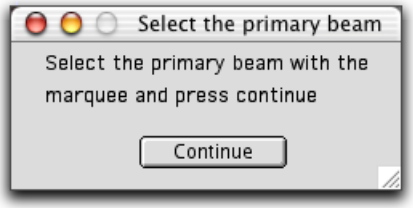


If you are using a measured secondary standard for calibration, "Secondary Standard" will allow you to enter your own values (i.e. the standard thickness, transmission, I(q=0), and the tabulated cross-section of the standard sample). In this case, select "Empty Beam Flux" and you will be prompted for an empty beam measurement (at 4 meters) to use for absolute intensity calibration. When the dialog appears, select run SILIC002..., which is the empty beam measurement. The file will be opened, and you will be prompted to keep or override XY coordinates. This is the box encompassing the direct beam that you set during the calculation of the transmission. This is exactly the same region you want to sum over for absolute scaling, so click "no" to accept these values.



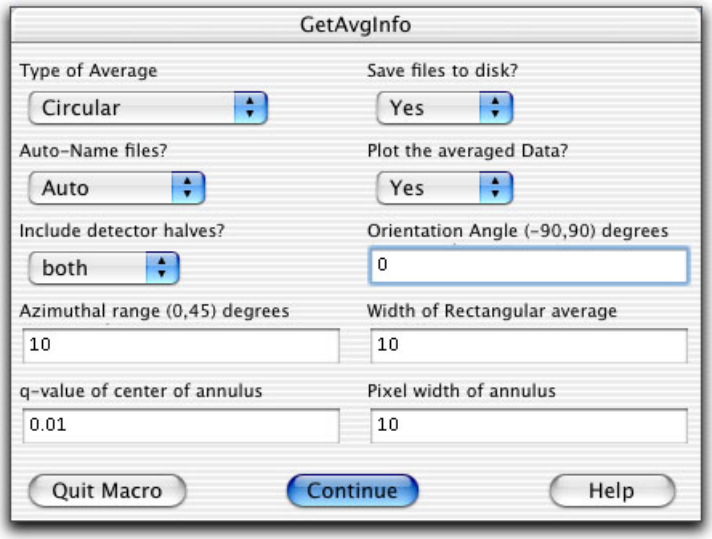
You will (may) next be prompted with a dialog to open a file. It is asking for the detector sensitivity file (DIV), as stated in the title of the dialog. The DIV file is needed for the calculation of the absolute scaling factor, so select PLEX_2NOV2007_NG3.DIV from the dialog, and open it. Now, with all information at hand, the scaling factor, kappa, is calculated and written both to the command window and to the text field in the Protocol Panel.

If you had not selected an XY box in the empty beam file, you would be presented with the following dialog (this will happen when you set up the protocol for the 1.33 meter configuration). Simply drag a box encompassing the primary beam, and click continue to dismiss the panel. Do not set the XY box using the marquee menu - it is not necessary for this step. Simply click Continue. The value of kappa and your box coordinates will be written to the command window.

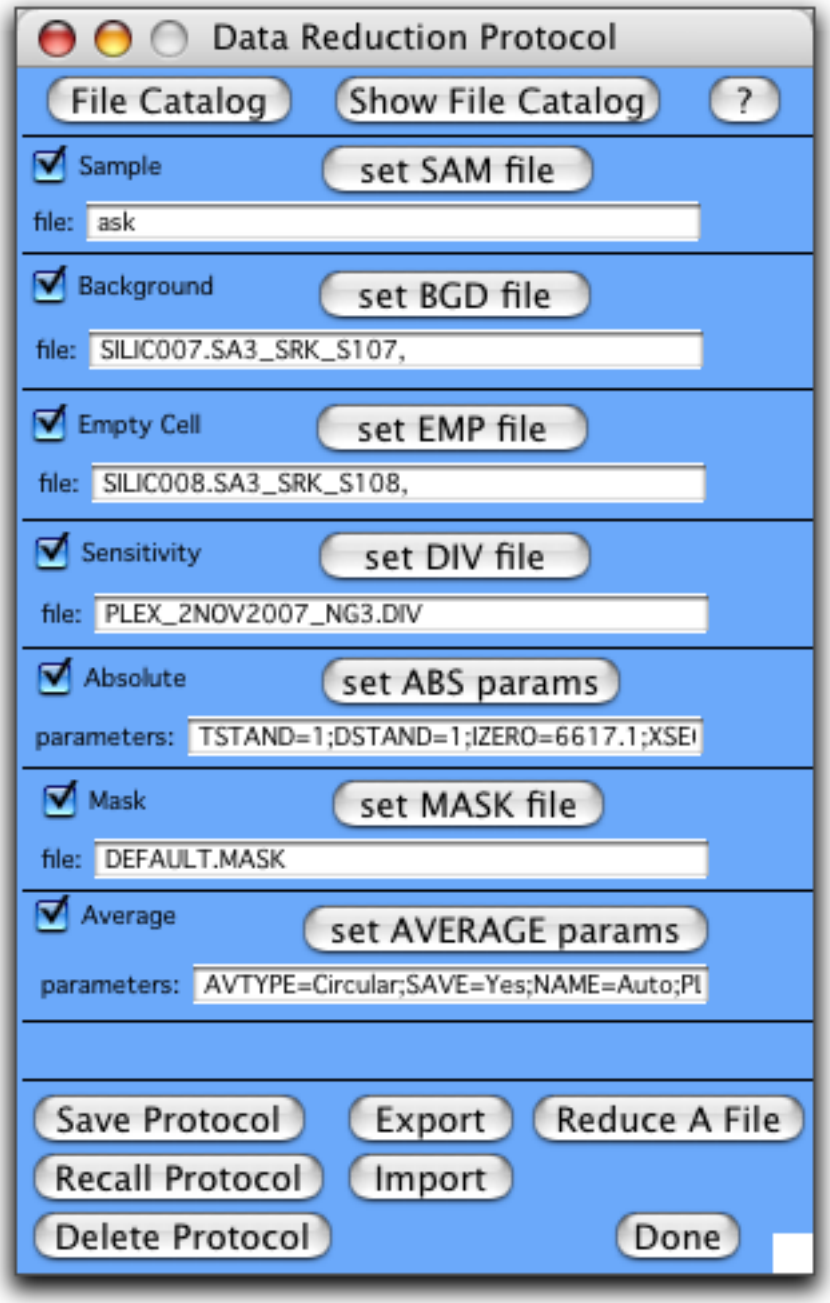


6) Returning to the Protocol Panel, click on the "DEFAULT.MASK" filename in the listing, which is a simple mask to exclude the edges of the detector. Click "set MASK" to set the filename. The mask file was created either in IGOR Pro or in SANS Image. Note that this is NOT the same format as a "WORK.MSK" 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. If you are saving as a PNG graphics file, the log or linear color scaling will be based on the setting in the preferences panel: SANS Preferences

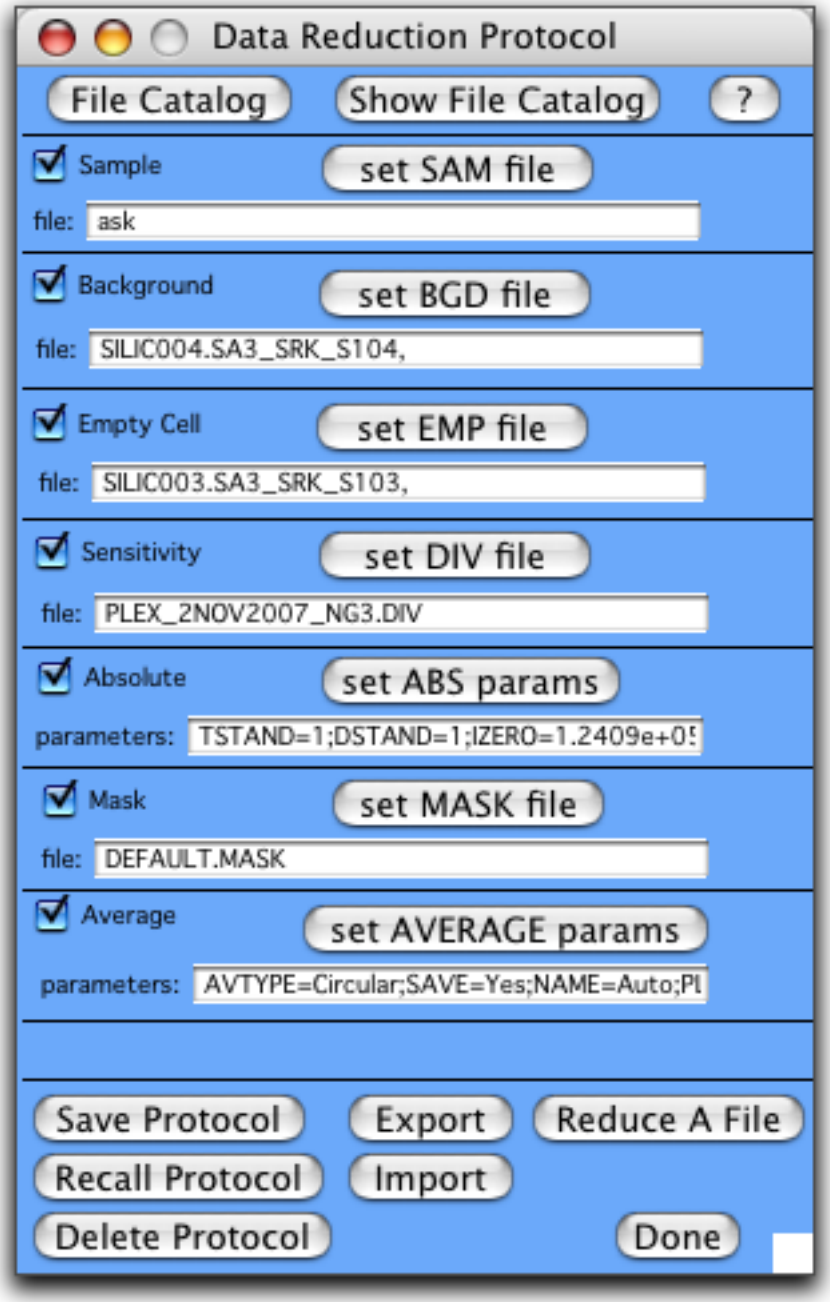


8) Once all fields are set to their correct files / parameters, click "Save Protocol" to save these settings for later recall, using a descriptive name for the protocol. "sdd_4meters" is a good choice for this protocol. Your Protocol Panel should look like this:



9) Set up another protocol to reduce the data at the 1.33 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 1.33 meters is SILIC004. Simply highlight the filename field in the panel, and type the run number, 4 (leading zeros are not needed). You do not need to click the "set" button, simply enter the number. Run SILIC003 is the empty quartz cell scattering, so enter 3 for the EMP file. Then set new ABS parameters in the same way as you did previously in step 5, but using the empty beam flux measurement at 1.33 meters. Save this protocol as "sdd_1_3meters" 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.



Two additional items:

- 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... just go ask your local contact if this correction is necessary for your experiment.
- Protocols can be "Exported" as a text file that can be "Imported" into a new reduction experiment. This is most useful for users with the Demo Version of IGOR, where a save of the whole experiment is not possible.

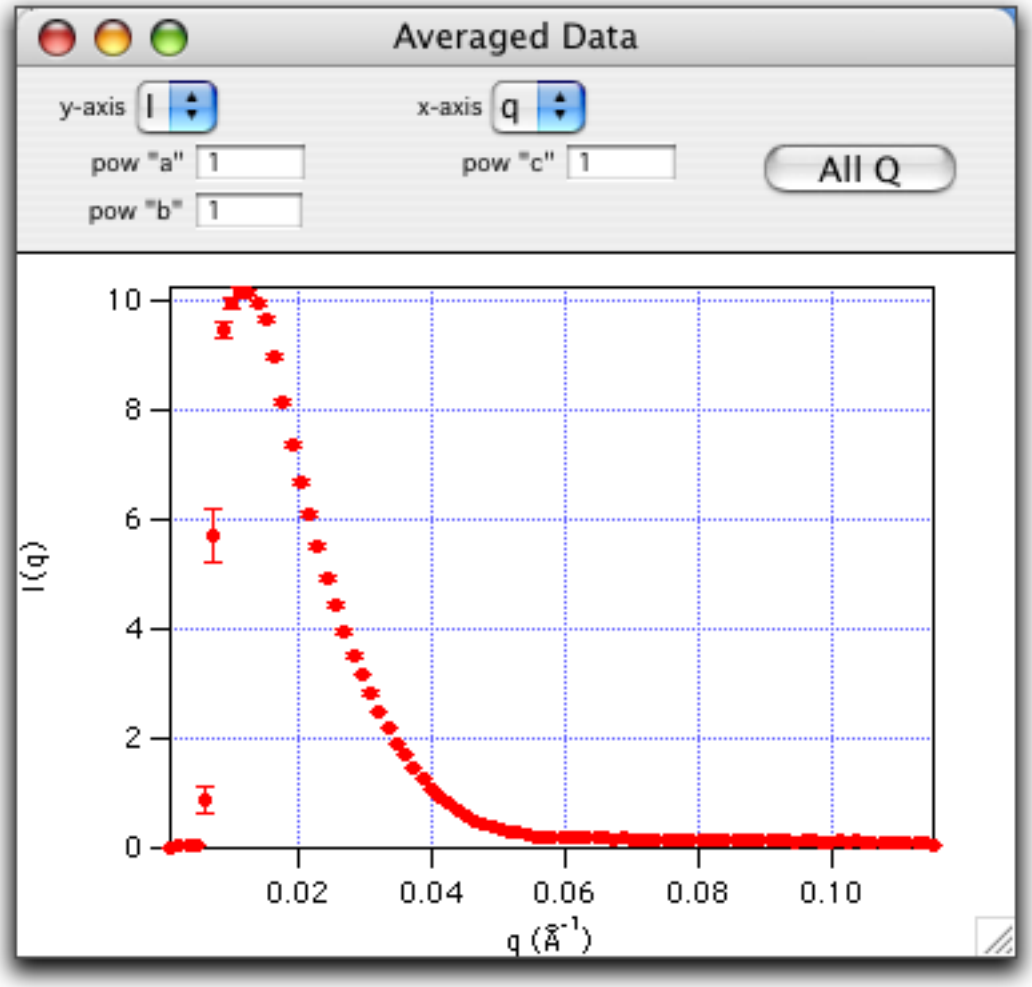
Reduce a File

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.

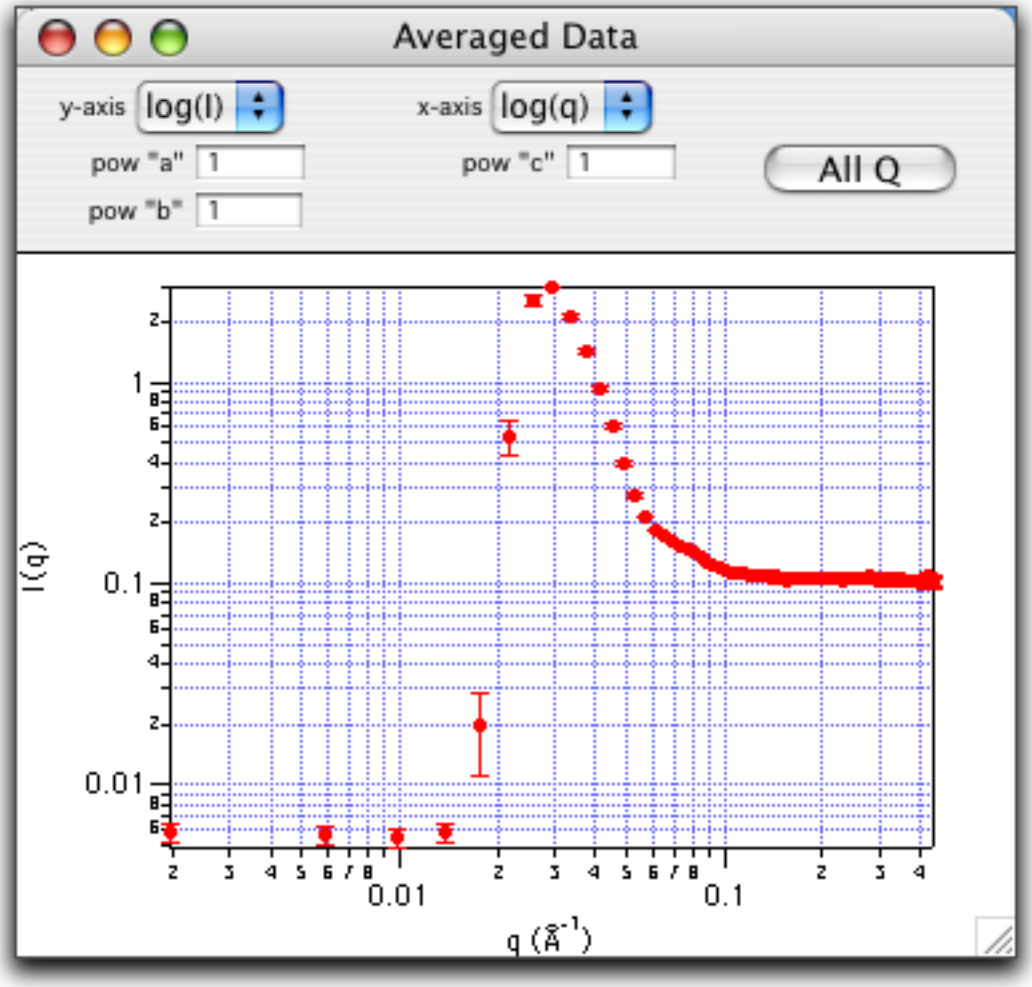
How: Since we just created and saved our two protocols, we'll use them directly from the Protocol Panel. Start with the 4-meter protocol. To make sure it's in place, click "Recall Protocol" on the panel, and pick "sdd_4meter", or whatever you named it from the list. Your protocol choices are updated in the panel. At this point, you can choose the 4-meter silica scattering file from the Data File Catalog 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 SILIC010...). 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 1.33 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 SILIC009...) 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:



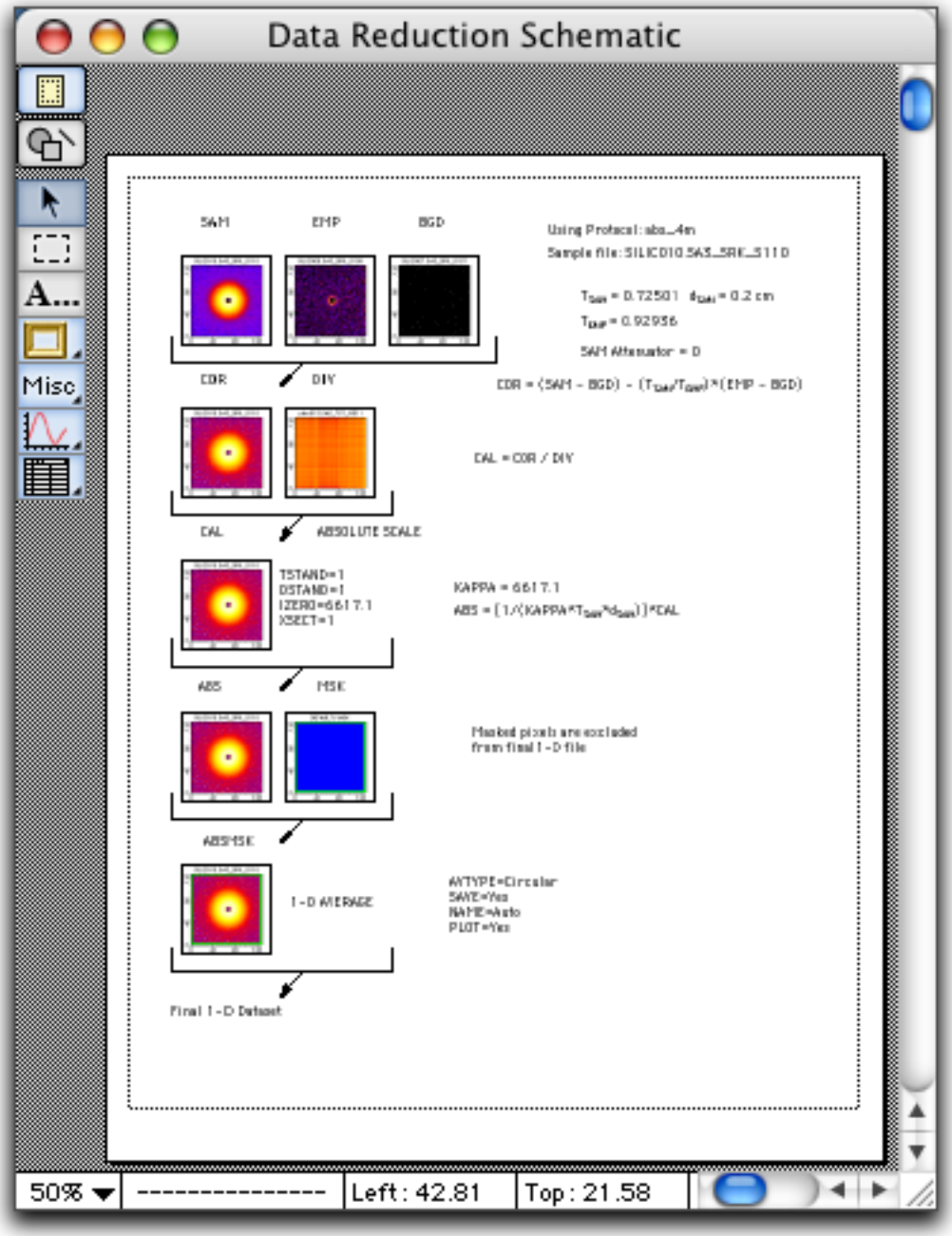
Instead of building a protocol, one could use either the "Base" protocol - which does only minimal corrections, or "DoAll" which will perform all of the data reduction steps. To see exactly which steps each of these would perform, "Recall" these blank protocols into the Protocol Panel. Unchecked steps 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. You will be prompted for either log or linear scaling of the intensity data. Make your choice and click continue. You will then be 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). The example below used log-scaling and the 4 meter silica data set.

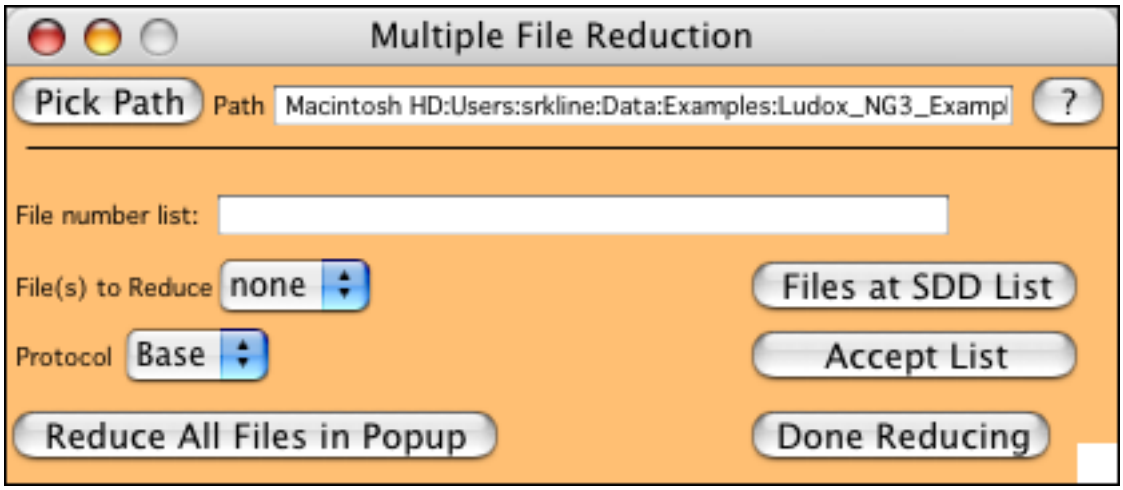


Reduce Multiple Files

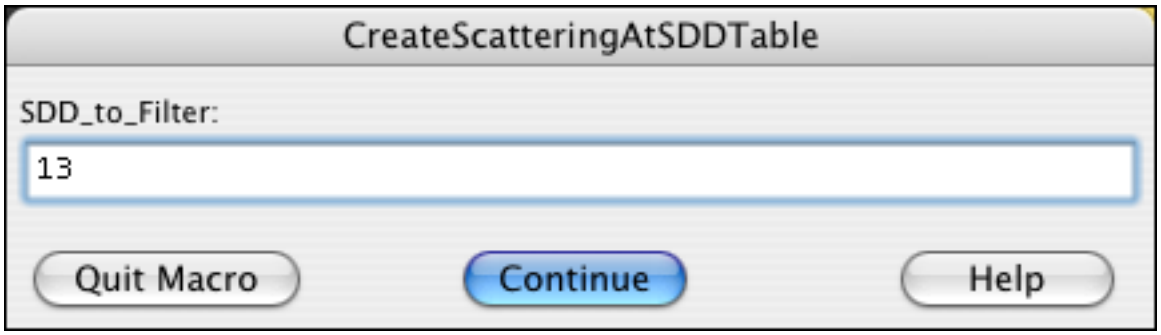
What: In a typical SANS experiment, many scattering files are collected at the same instrument configuration, and must be reduced using the same protocol. This operation allows you to reduce SANS data in a batch mode using a previously saved protocol. It also provides a filter to aid selection of scattering files taken at a particular configuration.

How: Since this tutorial only works with one file at each instrument configuration, the example is from a larger folder of data. Click "Reduce Multiple Files" on the Data Reduction tab

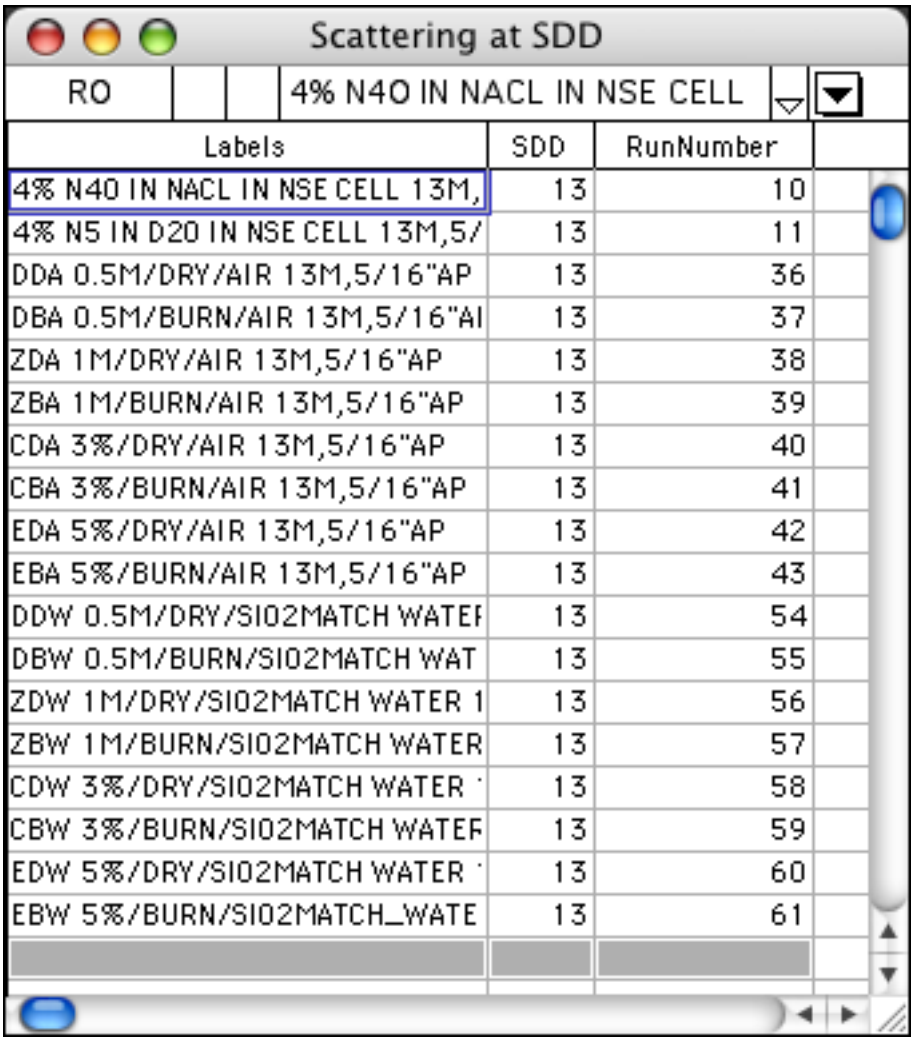
of the Main Panel. This will display a new panel with a simple interface, used as follows:



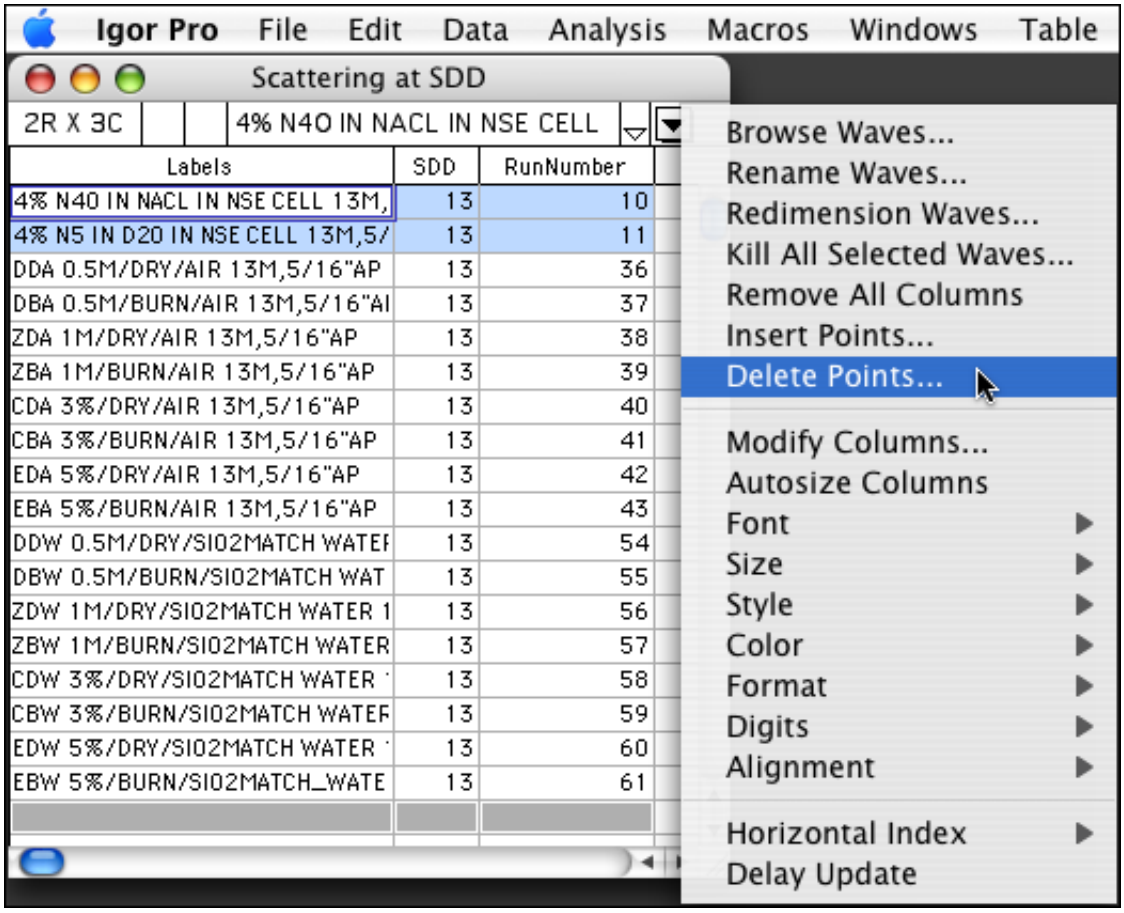
1) Enter a comma-delimited list of run numbers to be reduced (leading zeros are not needed). Note that a 'dash' can be used to indicate an inclusive range of file numbers. Hit enter or return when finished, and this list of raw data files will be displayed in the popup list. If any of the data files 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.
-OR-
You can click "Files at SDD List" to automatically filter out a list of scattering files at the sample to detector distance (SDD) that you enter:



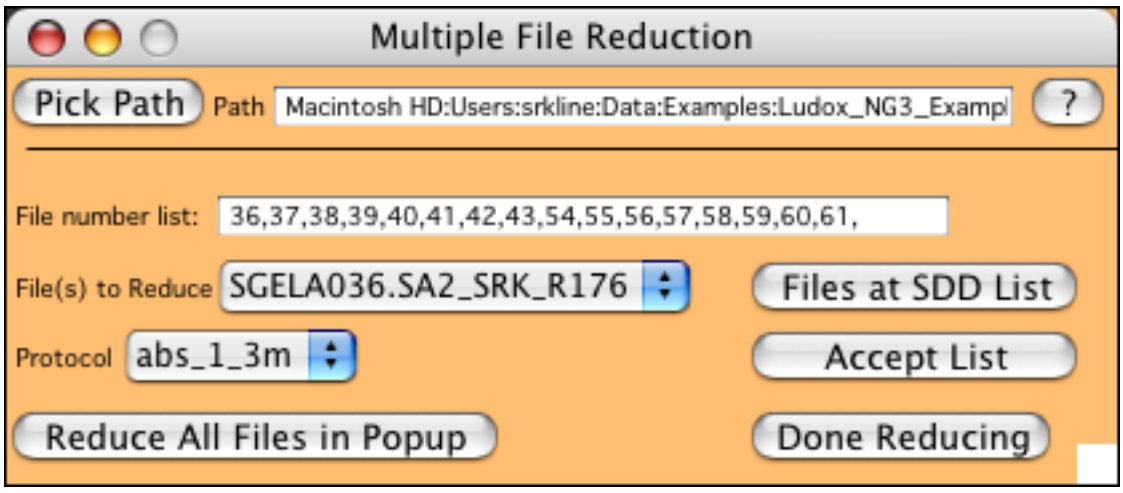
Enter the SDD in meters. If you don't get any files, check the SDD that is listed in the file catalog, and be sure you're entering enough digits (you need to be within 0.1 m to be considered a match). You will end up with a table like this:



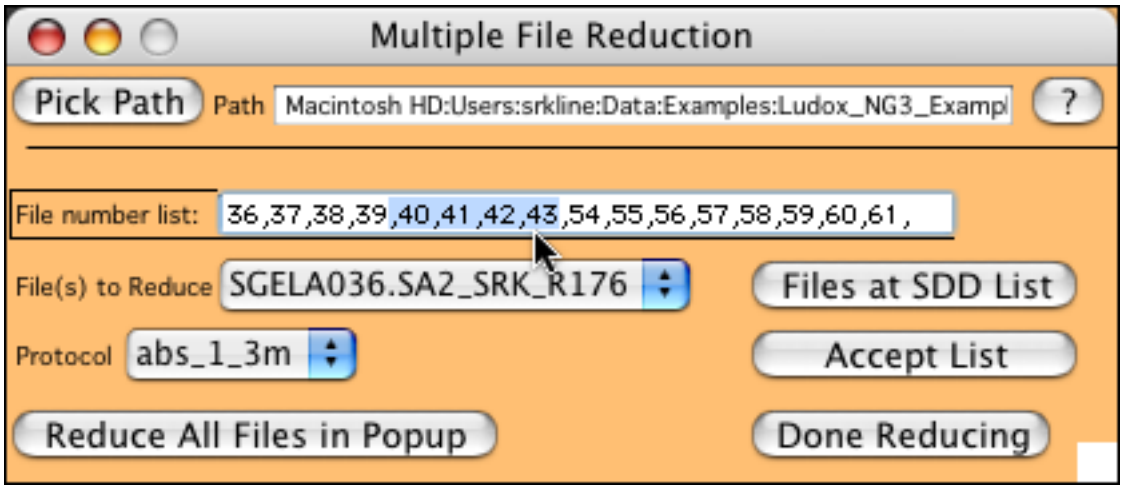
The scattering files for the empty cell and the blocked beam are automatically removed from the list. If there are additional files that you want to remove from the list, click and drag to select them, being sure to select all three columns, then click on the small triangle at the top right of the table, and select "Delete Points...". A dialog is presented - just hit return to delete the selected points.



If you're happy with the list of files as filtered, you can click "Accept List". This will enter the list, and put the files in the popup list:



If you want to remove more files from the list of files to reduce, you can simply delete these run numbers from the list, and then be sure to hit enter to update the list. Then, you'll see the updated file list in the popup.



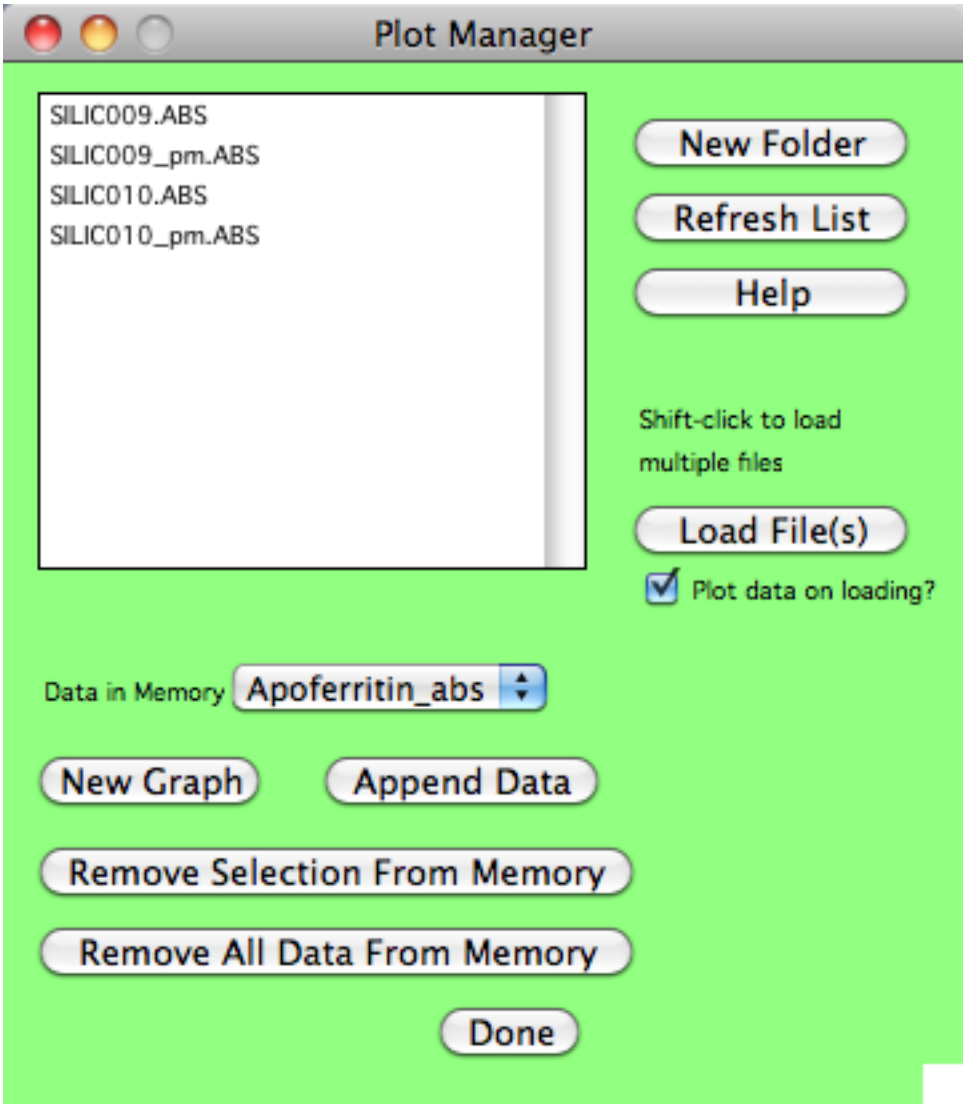
2) Once the file selection is set, select the appropriate protocol from the popup (you must have already created / tested / saved it from the Protocol Panel) to be used to reduce the selected files.

3) At this point you can 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.

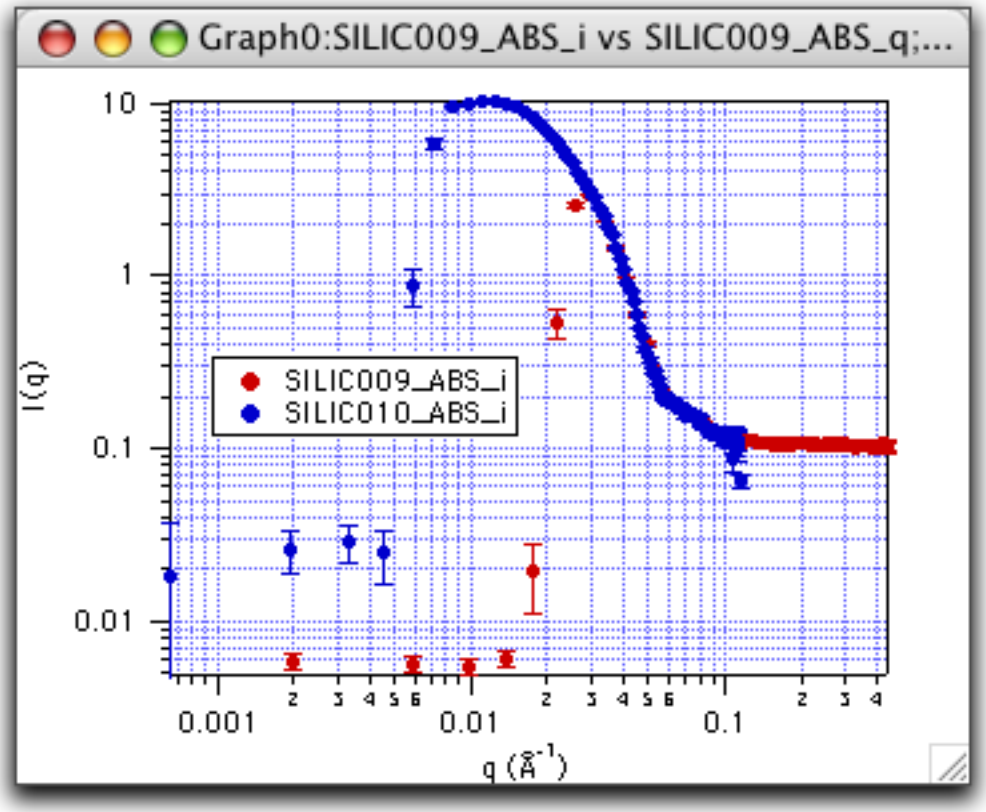
Plot Averaged Data

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

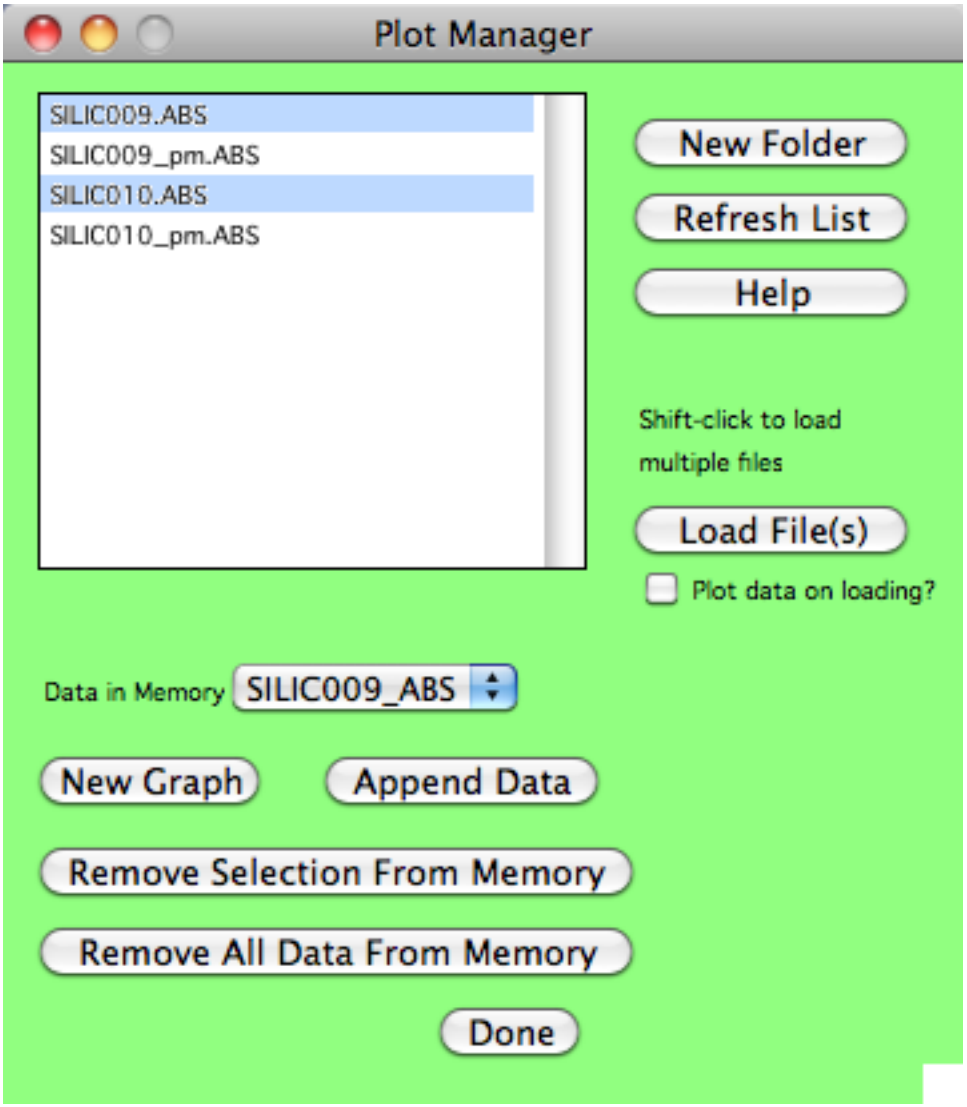
How: Click "Plot" on the 1-D Ops tab on the main panel, and the Plot Manager panel will appear.



Initially, there is no data loaded in memory, so use "Load File(s)" to load and plot the data from both detector distances, files SILIC009.ABS and SILIC010.ABS. The listing of data files is from the same data path that you set from the Main Panel. Leave the checkbox selected to automatically graph all of the selected files on the same, new graph. Shift-click to select both data files, then "Load Files" to load and graph both data sets on the same plot:

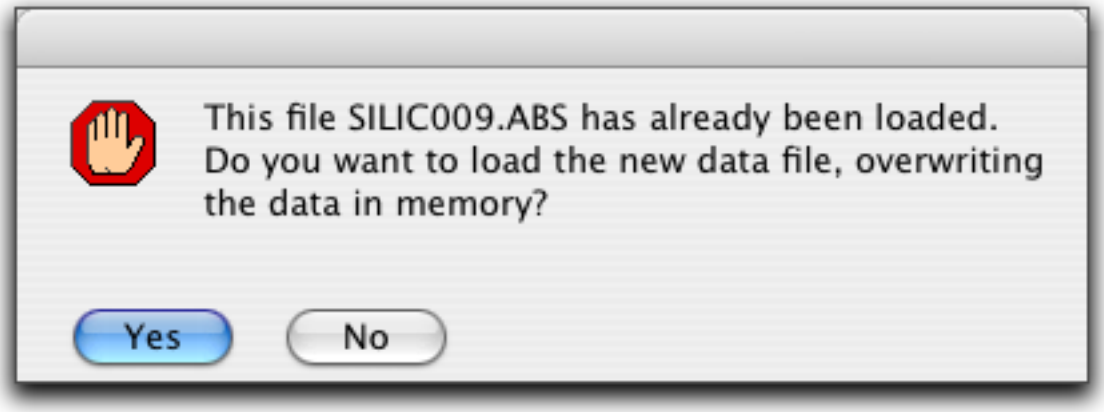


If you don't want all the data on the same graph, uncheck the box, and you will be able to graph and append data as you choose from the Plot Manager Panel. "New Graph" will create a new graph using the data set selected in the popup menu. "Append Data" will do just that to the topmost graph. Unwanted data files in the popup list can be removed from memory (the data on disk is NOT removed!) by either removing the selected file, or all files. Any data that is "in use" in a table or a graph won't be removed, and will remain in the popup list. You will have to close (and Kill) any open graphs to then be able to remove the data from memory.



NOTES:

• If you try to load a data set that is already in memory, you will see the dialog below. Clicking yes will load a fresh copy from disk into IGOR's memory. Clicking no will leave the data in memory unchanged. If you know that the data sets are the same, there is no harm in overwriting the data set in memory.



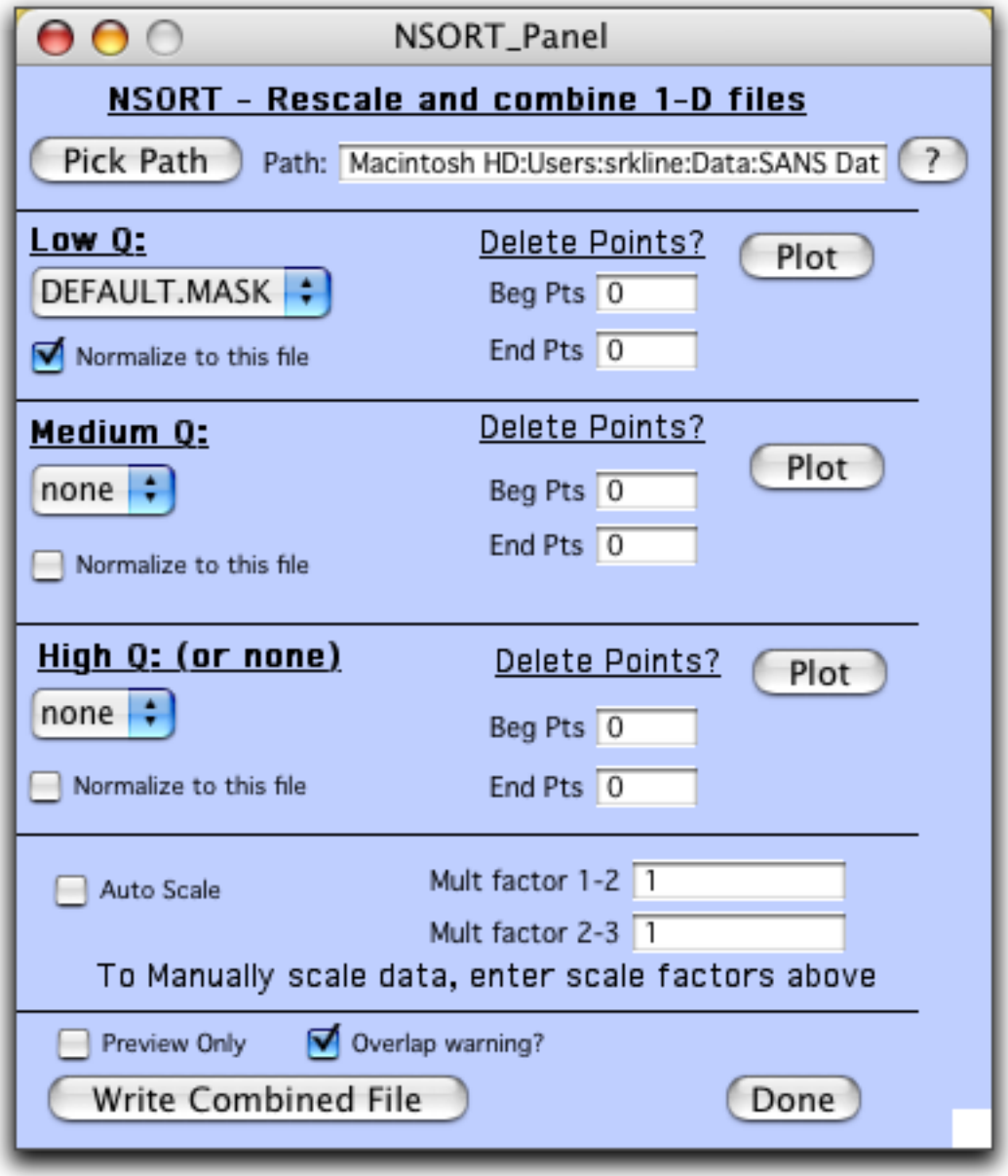
• To change the graph appearance, click on what you want to change, and a dialog will appear. The Graph menu also allows for a wide variety of customization of the graph appearance.

• 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.

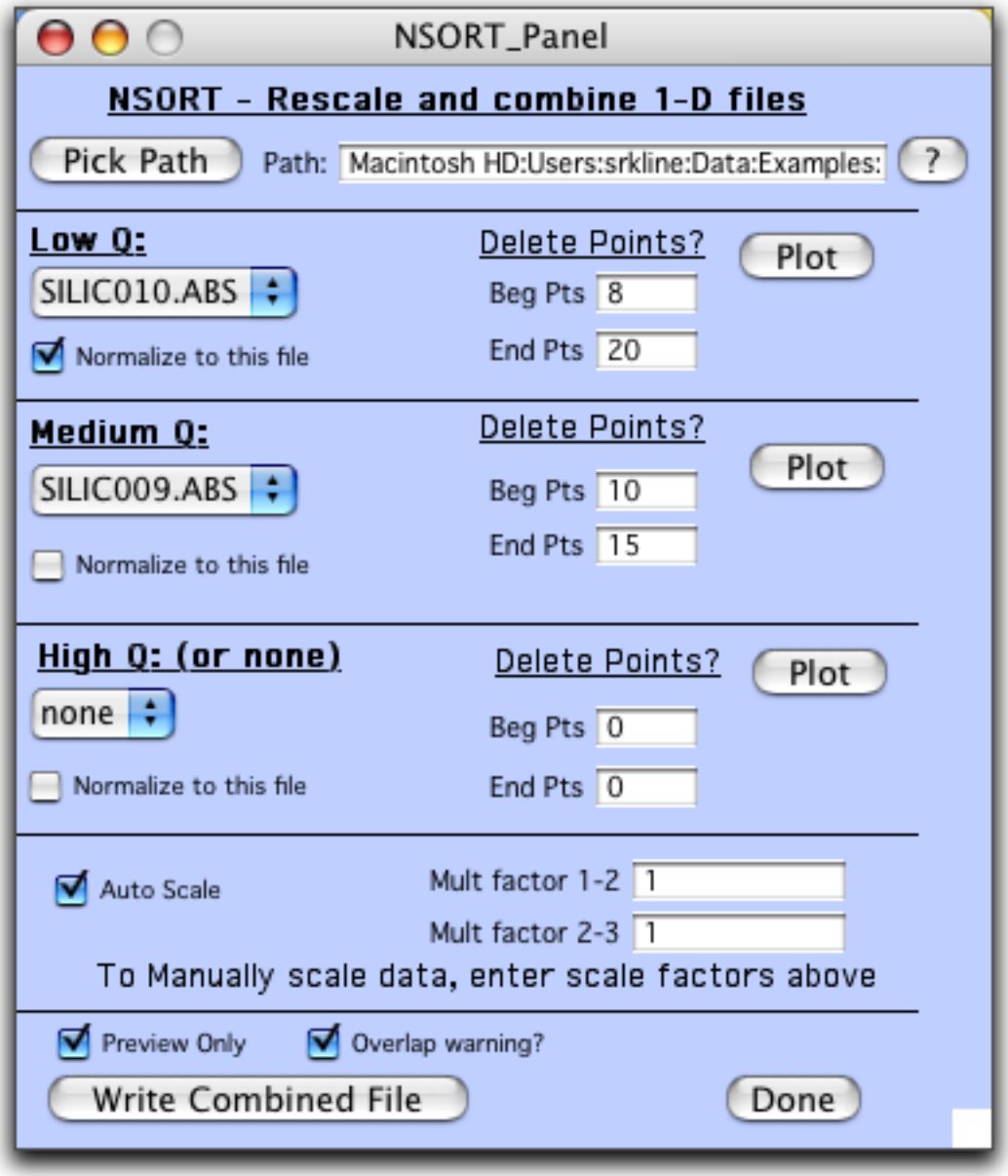
Sort and Combine Averaged Datasets

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. In addition, a single data set can be trimmed and rescaled

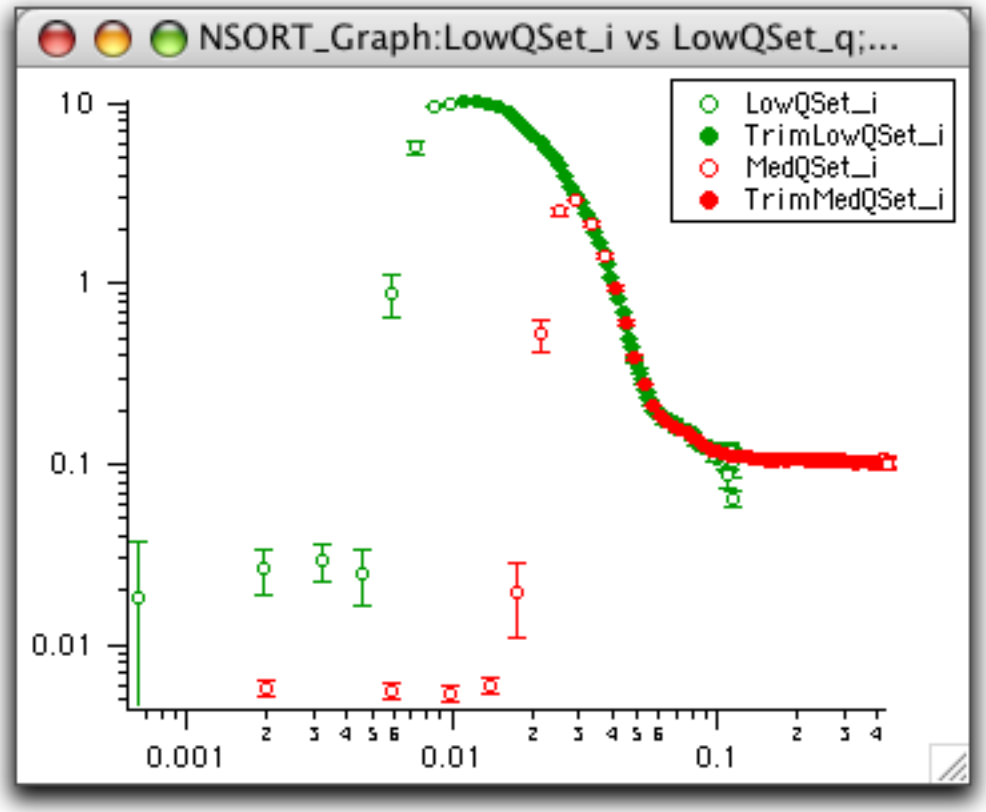
How: Click "Sort" on the 1-D Ops tab on the Main Panel. This will display a new panel.



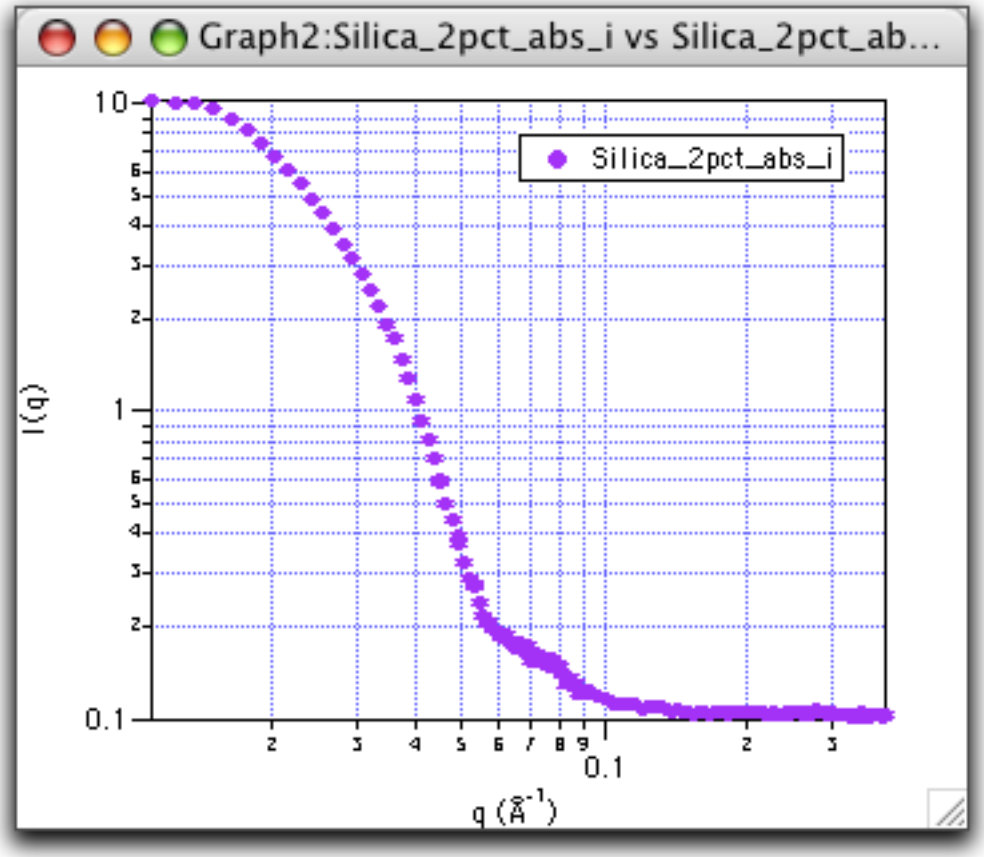
Select the data set with the lowest q-values (the 4-meter data set, SILIC010.ABS) as the "Low Q" data file. Plot it, and remove points from the beginning and end of the set that were behind the beamstop or at the edges with large error bars (the omitted points will be displayed as open circles, and are a copy of the original data set). Do the same for the higher q-range (the 1.33-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". If you have only one data set, it is the "Low Q" set, and both Medium and High Q popups should be set to "none".



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). If you select "Auto Scale" and "Preview Only", and then Click "Write Combined File", the medium Q data set will be rescaled to match the low Q, and the overlap constant is displayed. If the overlap multiplier is out of the accepted tolerances, you will be warned, and it may be a good idea to talk with your local contact about why this happened. At this point, no combined file has actually been written. To create a new file, uncheck the "Preview Only" box, then click "Write Combined 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 Silica_2pct.abs), once plotted should look something like this:



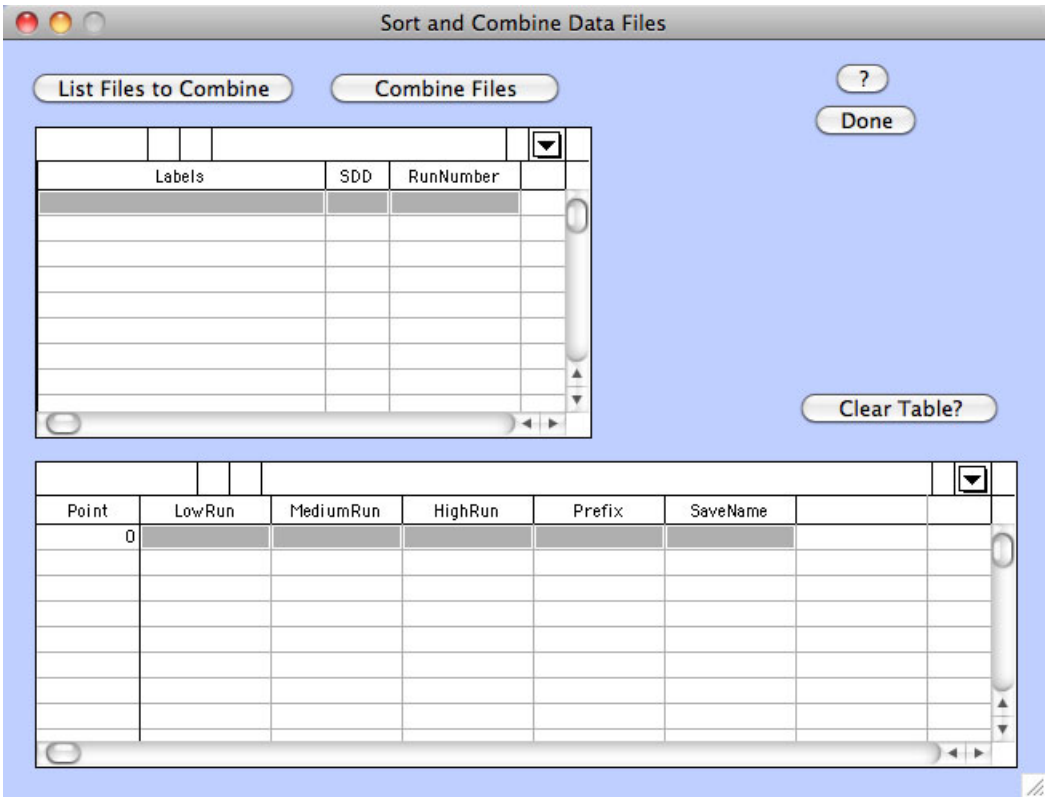
Batch Combine Data Files

If you have many data files to combine at the same conditions, set up the NSORT panel with the number of points and scaling that is best for your data, and then try batch combining the files. Either two or three data files can be combined. **BEFORE USING THIS FEATURE:**

(1) reduce all of your data to 1D (MUST be ".ABS" or ".ABSx")

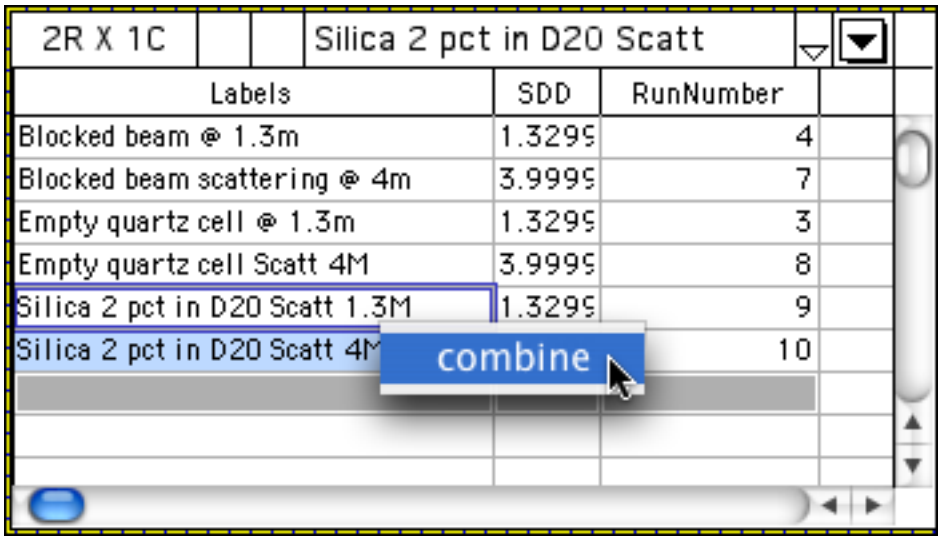
(2) open the NSORT panel, and test out the combination of one set of scattering files. These numbers of points to trim will be used for all data files.

From the 1D Ops Tab, click on "Combine 1D Files". A panel appears, and you are prompted to "Clear Table?". Answering "Yes" will clear everything you have typed in both tables so you can start fresh. If are continuing to combine files or wish to re-combine files, "no" will leave your tables untouched.



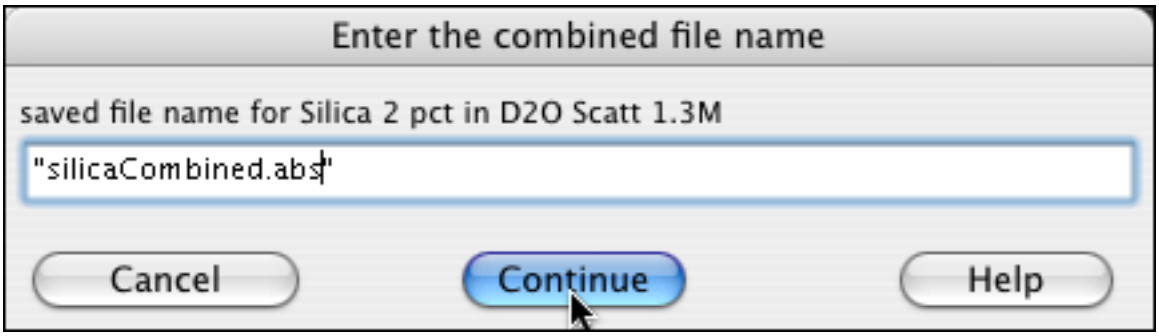
1) Click on "List Files to Combine". Two tables are generated. The top table is a table is of scattering files, sorted by sample label so that the files that need to be combined are grouped together, speeding up the search through the File Catalog. The other table is one that is a listing (row-wise) of the 2 or 3 run numbers to combine, their file prefix, and the name you want to use for the combined file (include whatever extension you want).

2) In the top "Files To Combine" table, select a group of (2 or 3) files to combine. You can shift-click to select, or drag and shift-click on the selection. Either way, on the shift-click(up), a contextual menu appears with one item: "combine" (yes, do this).



You will be prompted for the file name of the combined file. Be sure to include the .abs extension on the file name. The run numbers are automatically entered in the bottom "Run numbers to combine"

table. "LowRun" means the lowest q-values, "HighRun" is the highest q-values. In this example, there are only TWO detector distances, so they are in Low and Medium, and the run number for High is set to zero (so no file is used). The prefix is automatically determined from your .ABS files as they were generated from your data reduction protocol.



RO 10

Point	LowRun	MediumRun	HighRun	Prefix	SaveName
0	10	9	0	SILIC	silicaCombined.abs
1	8	3	0	SILIC	emptyCell.abs
2					

3) If you enter the wrong file name, or if a run number is incorrect in the table, simply edit the table before combining the files.

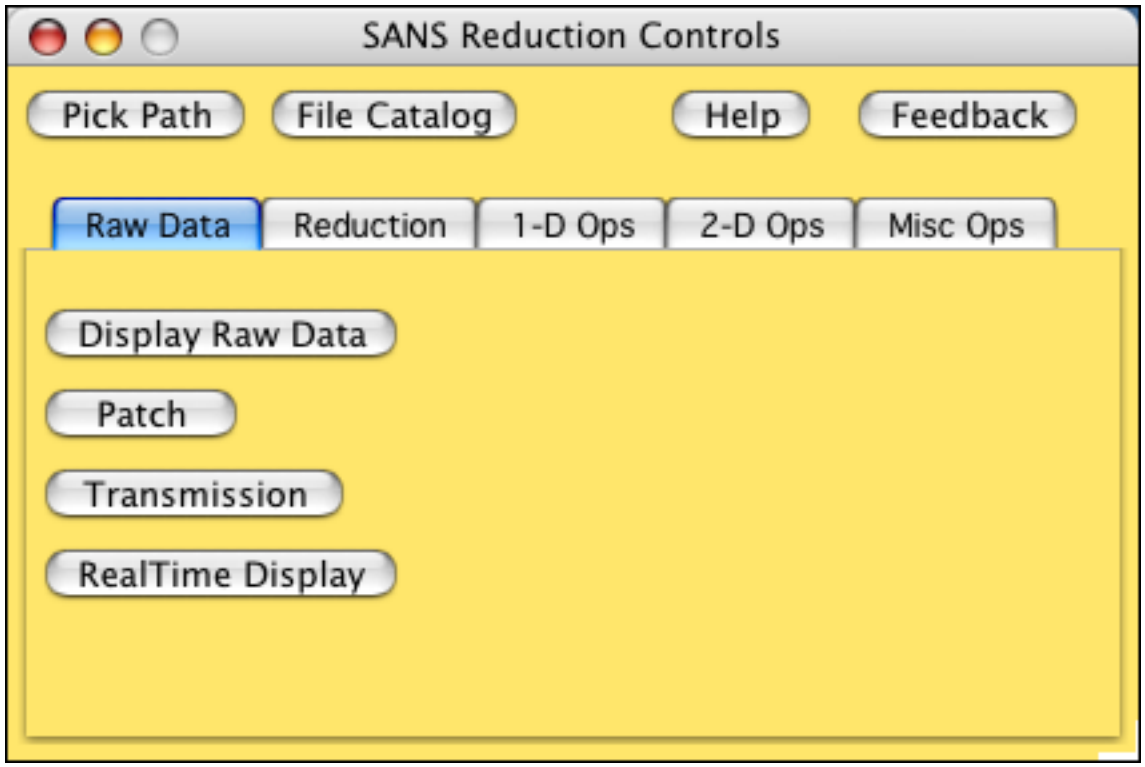
8) Once all of the files are set, click on "Combine Files". You will be prompted for file names if any of the entries in the table are blank. Otherwise, the command will silently combine all of the data files. If you have the "Overlap Warning" checked on the NSORT panel, you will see this warning, but you will not know which file is affected. You'll have to check out the headers of each file (in a text editor) to see what the scaling factors were for each file.

There are more possibilities for automatically combining files in conjunction with the NSORT panel. Any ideas would be appreciated. The feedback button is on the Main Panel.

Additional Operations

Main Panel Tabs

Raw Data Tab



The buttons are:

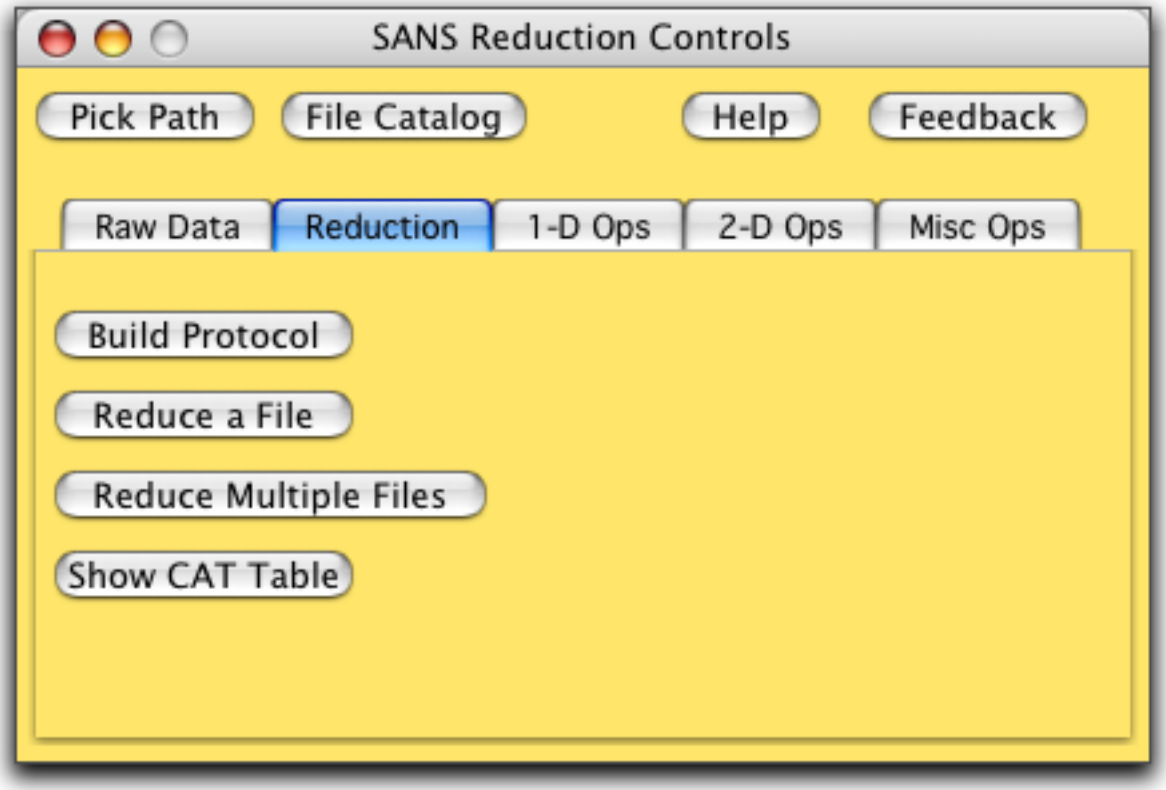
Display Raw Data: presents an open file dialog to select a raw SANS data file for display, then graphs it as a 2-D image with lots of helpful information.

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: opens the RealTime display controls. Ony useful during data acquisition.

Reduction Tab



The buttons are:

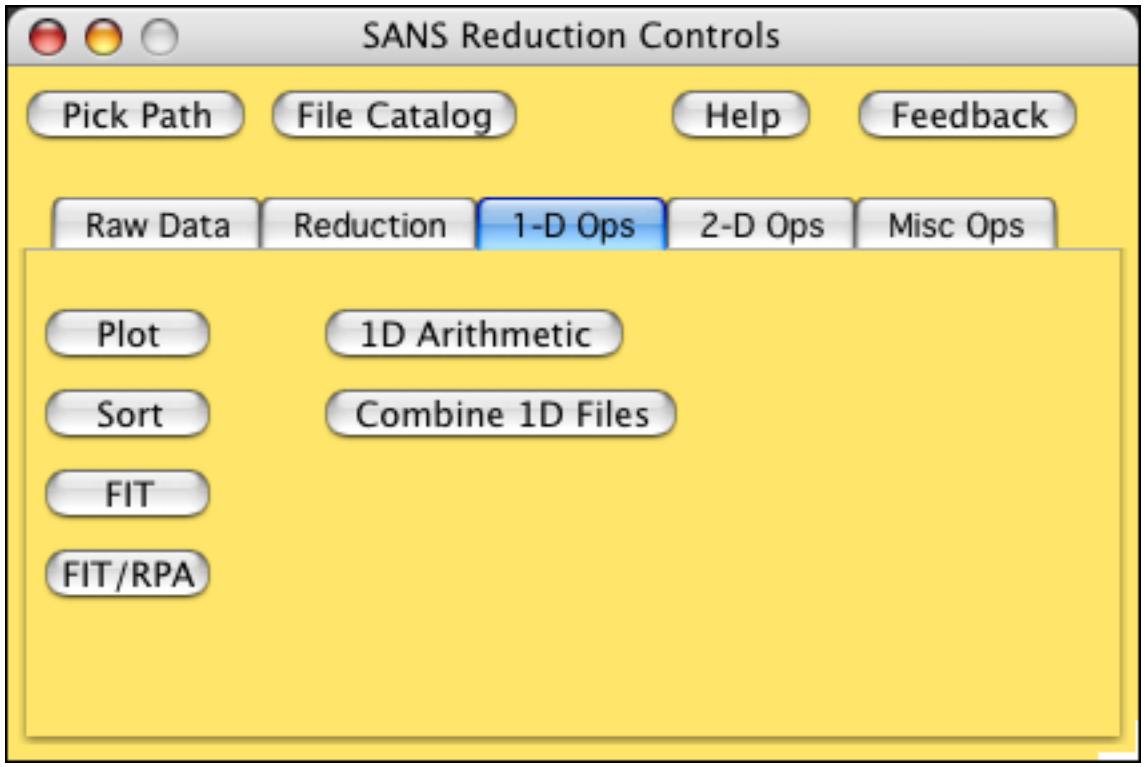
Build Protocol: generates a separate panel with controls to allow you to sequentially build the desired steps of a reduction protocol. The File Catalog table is used interactively to build protocols, so have the table handy.

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 File Catalog 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.

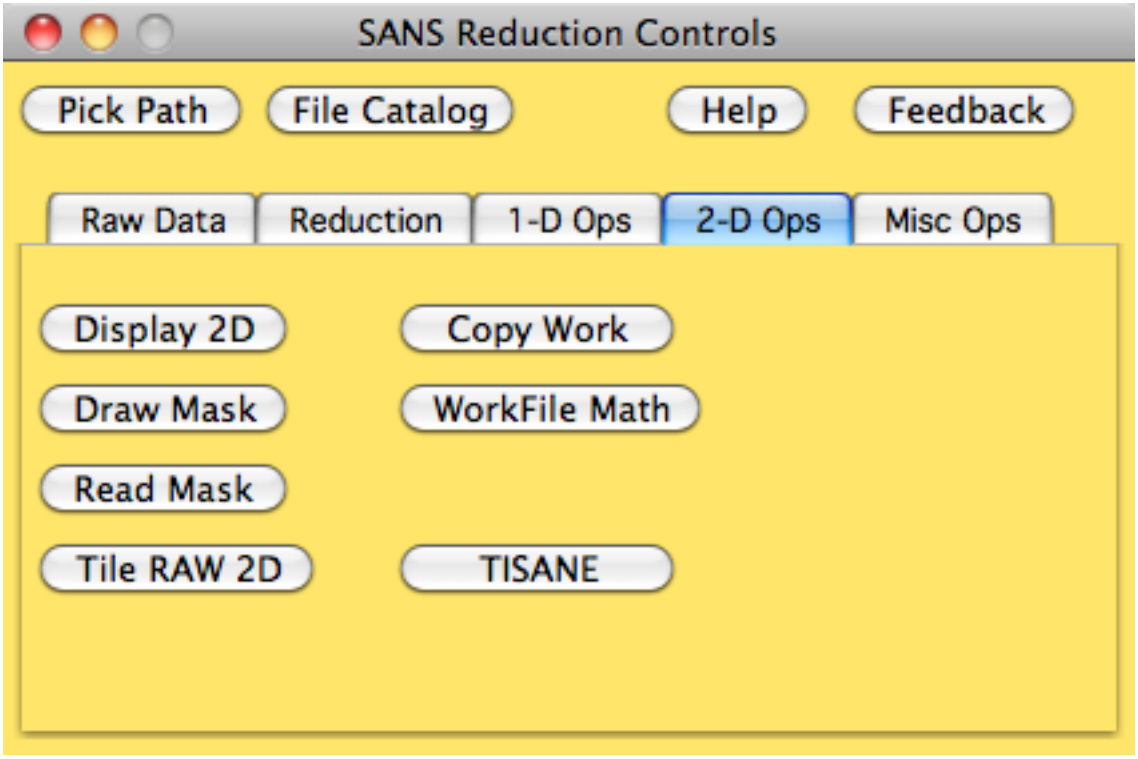
Fit: generates a separate panel with controls to perform linearized fits to 1-D datasets. Fits can be interactively refined. Often used during the reduction of secondary intensity calibration standards.

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.

1D Arithmetic: generates a separate panel with controls to perform subtraction, addition, multiplication, or addition of 1D data sets. Very useful for subtracting buffer or constant background scattering from sample scattering, and for rescaling of data sets.

Combine 1D Files: generates a separate panel to set up a tables of information to batchwise sort and combine previously reduced files. See Batch Combine Data Files.

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.

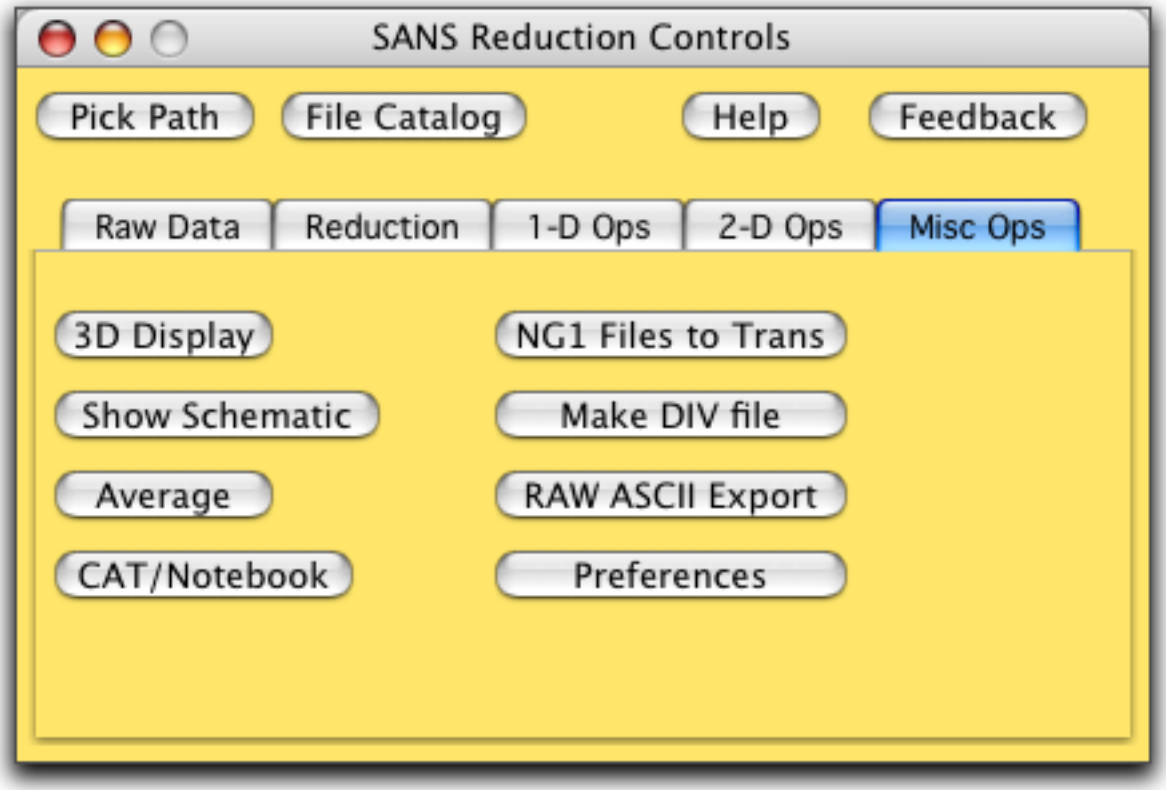
Tile RAW 2D: generates a separate panel with controls to select any number of raw SANS files, then append images of these files to a Layout window. Images can be arranged in the layout, annotated, and printed.

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) ASCII files that have been previously saved.

TISANE: currently is a placeholder for upcoming functionality to process TISANE data files.

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.

CAT/Notebook: generates a notebook with information about each file in the selected data path. Somewhat less information than File Catalog, 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 instrument scientists 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(Qx,Qy) triples.

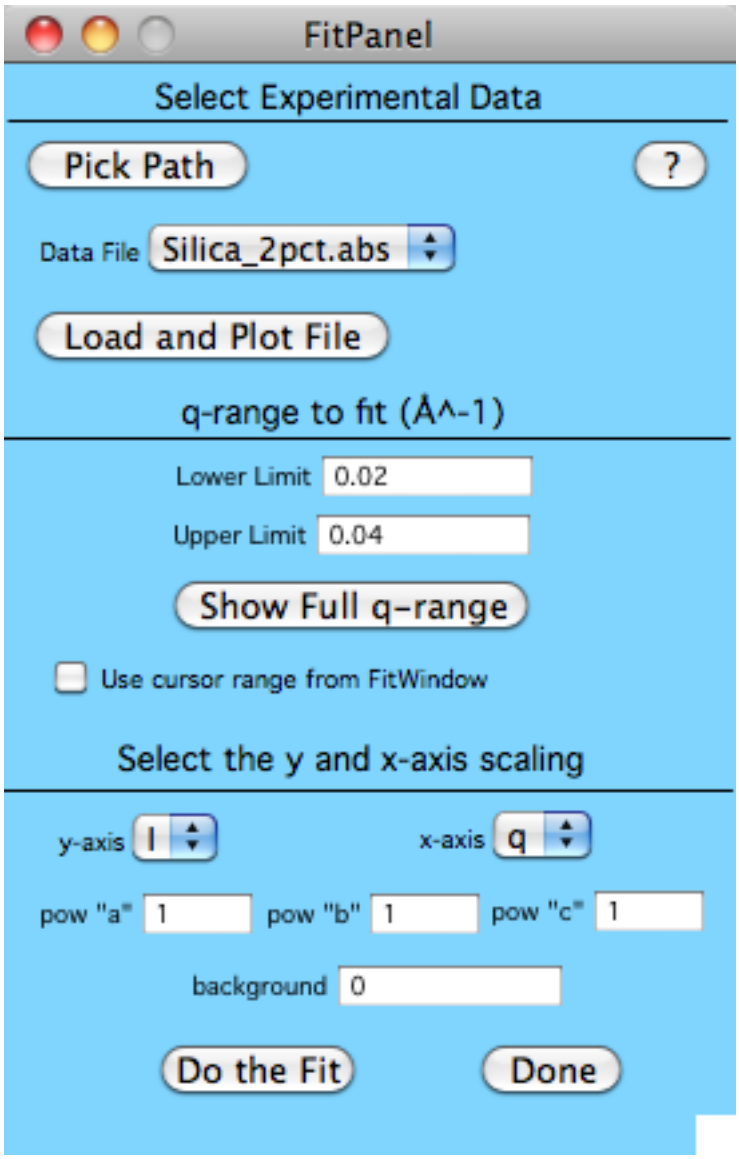
Preferences: generates a separate panel used to set several specific parameters as desired by the user. Running "Initialize" from the SANS menu will return values to their default state.

Fit Lines to Your Data

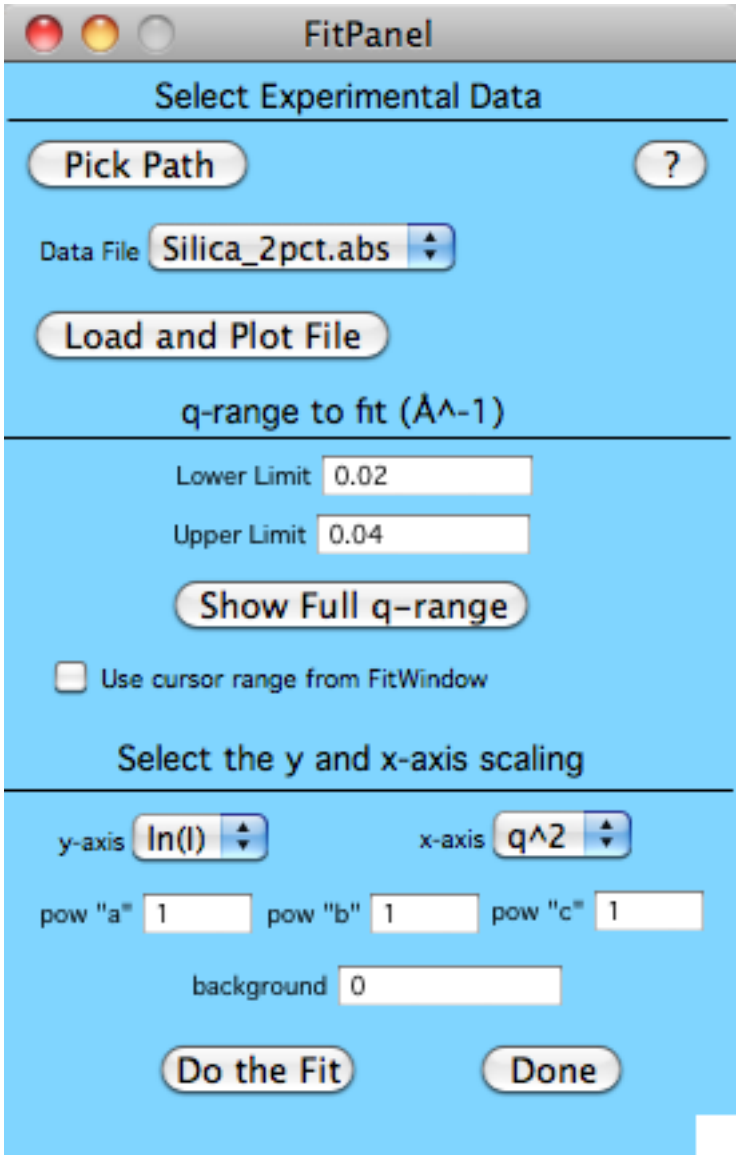
What: To obtain some quantitative information about your sample, a variety of linearized fits

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).

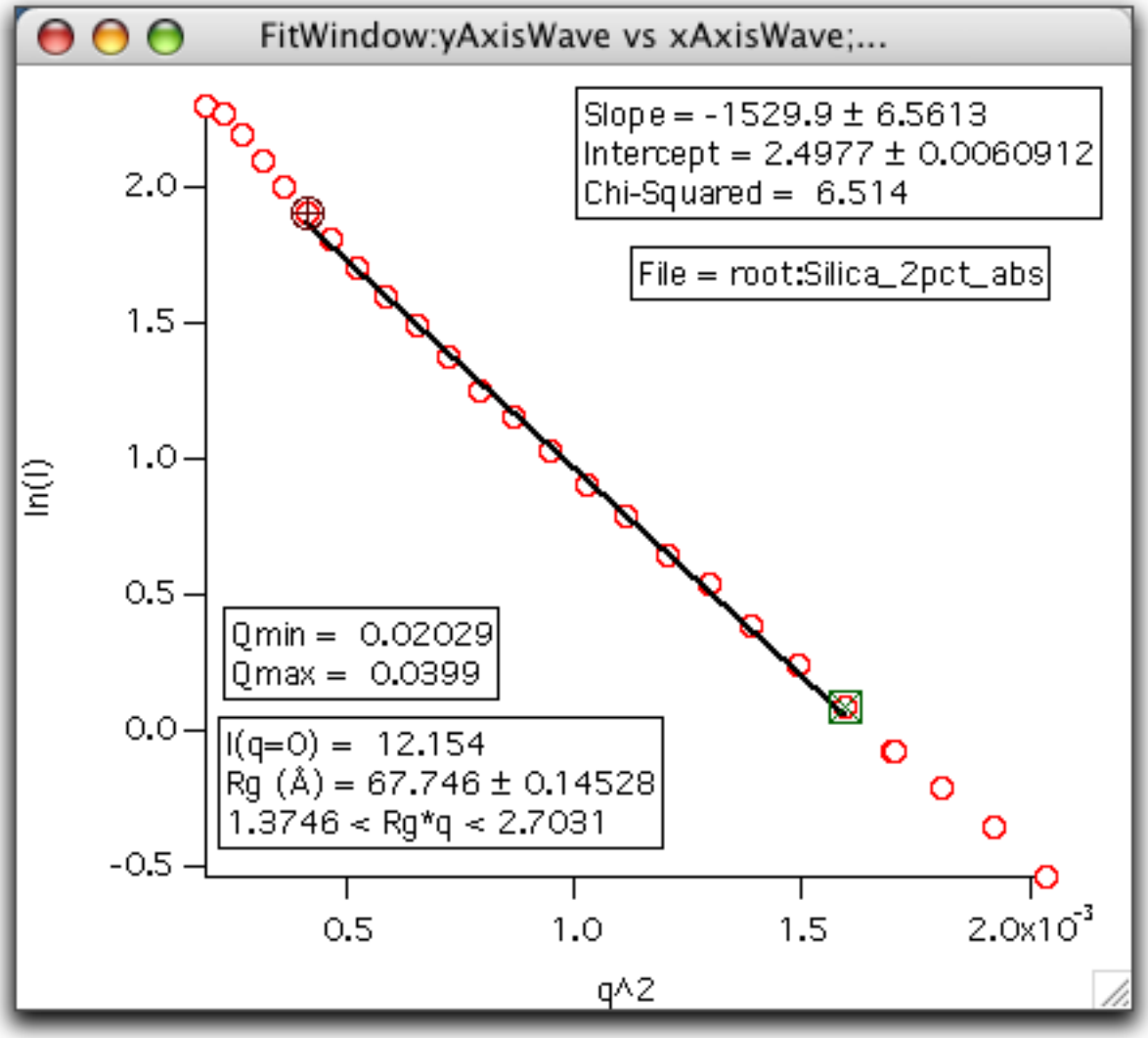
How: The reduced data file Silica_2pct.abs is scattering from some sort of protein, and appears to have a Guinier region at low q. From the 1-D Ops tab on the Main Panel, click "FIT". The following panel will appear.



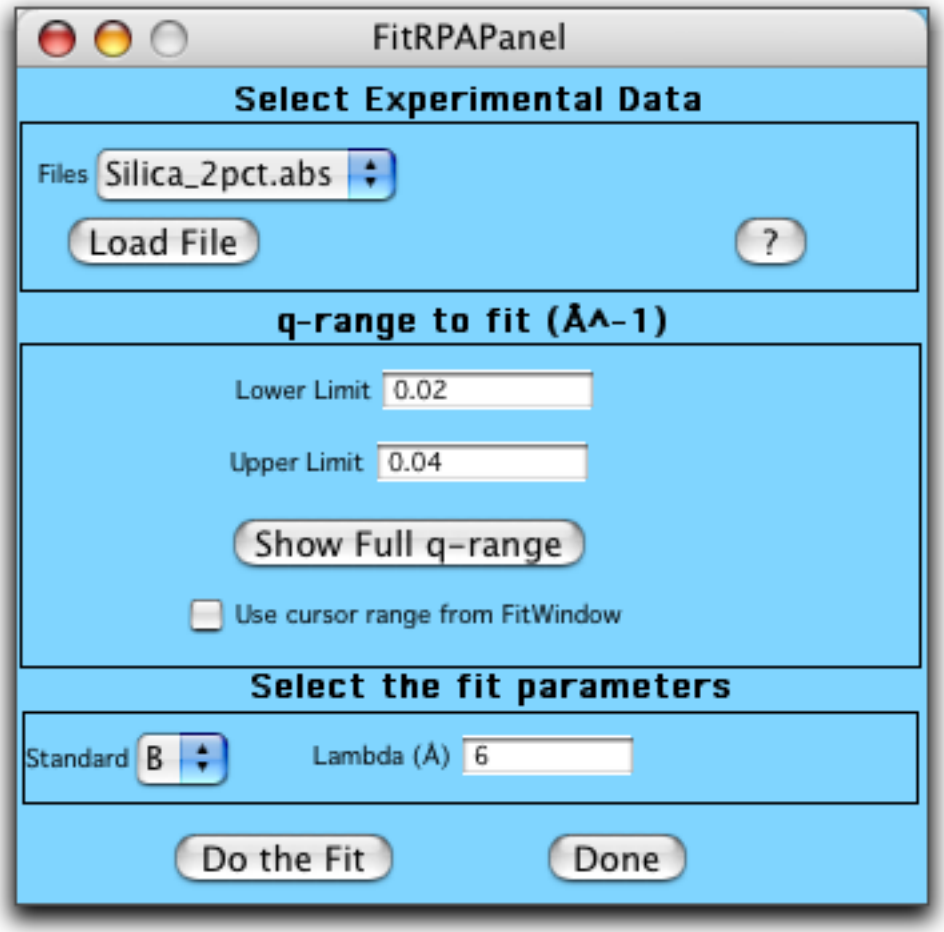
Choose the Silica_2pct.abs data file in the first popup list. We want to determine the radius of gyration of the silica. We do not know whta the correct q-range to fit is (yet) so we'll use the default range of (0.02 to 0.04) (1/A), and adjust the fit from there. To fit the data to a Guinier plot, select a y-axis scaling of "ln (I)" and an x-axis scaling of "q^2". 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*Rg.



The fit is not bad, 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). For this silica data, the range is not perfectly linear (chi-squared is relatively high), and Rg*Q is more than one for the entire fitted range. Ideally for the Guinier approximation, Rg*Q < 1. It is left as an exercise for the reader to adjust the fit range, to see what effect it has on the results.



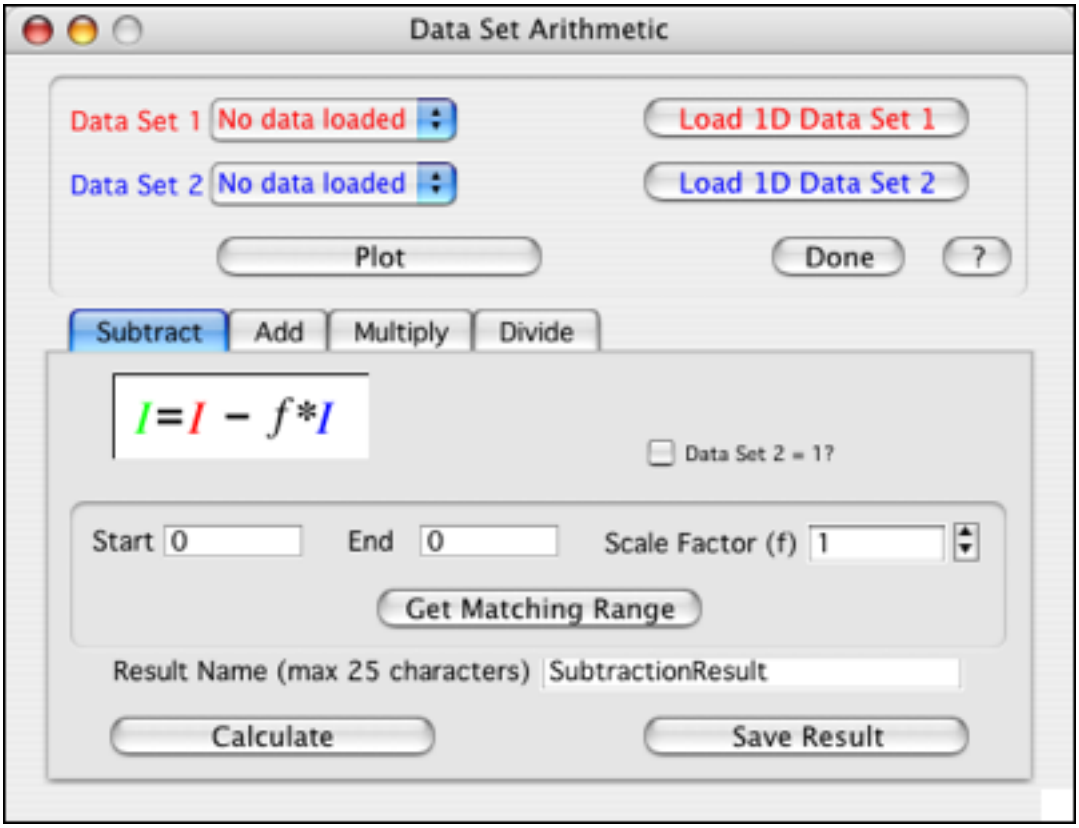
The secondary polymer standards are fitted with an RPA model (Random Phase Approximation) in order to extract the absolute scaling parameters. This panel "Fit/RPA", also from the 1-D Ops tab on the main panel, behaves much like the FIT panel. The model is specific for the polymer standards, so you need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



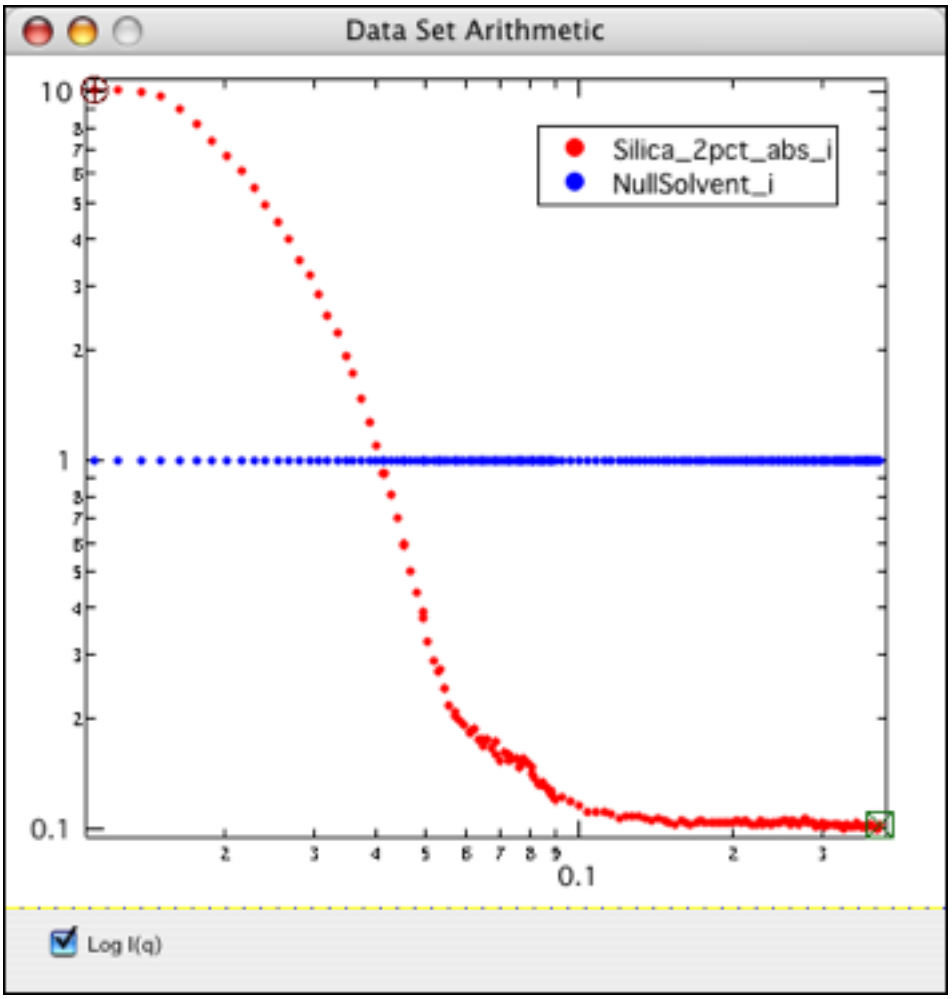
Data Set Arithmetic

What: Subtract, add, multiply, or divide two 1D data files (.ABS or .AVE). Most useful for subtracting a solvent "blank" from the sample + solvent scattering. Often this can be done more accurately after both files have been reduced to 1D data sets. A constant (q-independent) background can also be subtracted from a single data set.

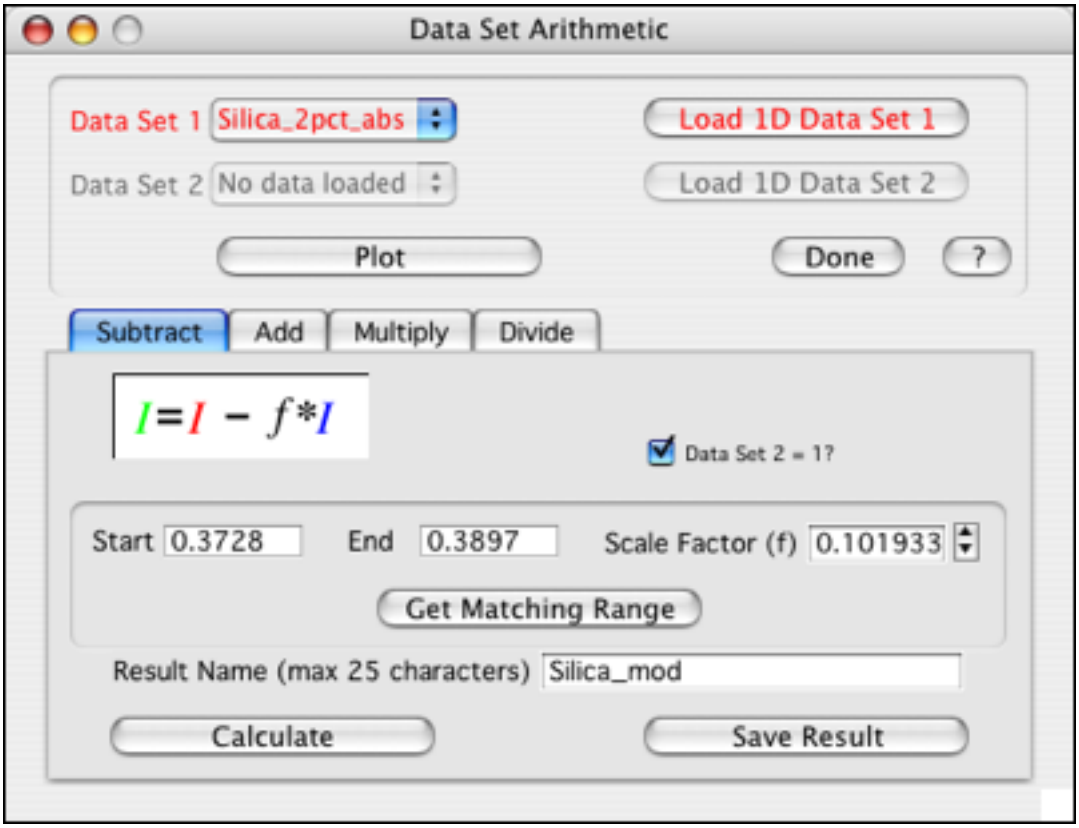
How: Reduce your data to 1D ASCII files, sort and combine to get data sets that are free from data points obscured by the beamstop and excessively noisy data at the detector edges. From the 1-D Ops tab on the Main Panel, click "1D Arithmetic". The following panel will appear. If you have previously loaded some 1D data, you can simply select the data sets from the Set 1 and Set 2 popups. Here, no data has been loaded, so click on "Load 1D Data Set 1" to load in the silica data, then "Plot".



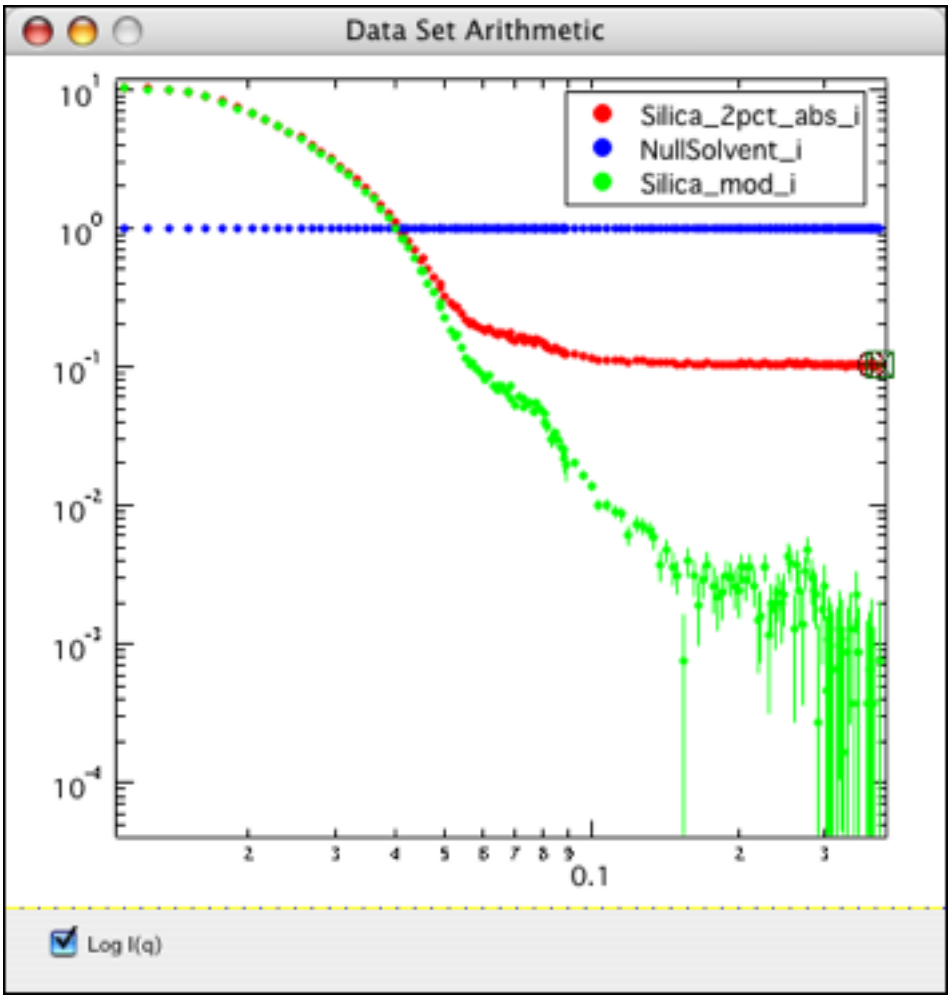
For this example, the reduction protocols subtracted only the empty quartz cell and blocked beam scattering from the sample scattering. So the Silica_2pct.abs data is the scattering from the silica in D2O. The scattering contribution from D2O is a flat incoherent background. One could either measure the (flat) scattering from a sample of D2O, and subtract that scattering from the silica+D2O, or simply subtract the incoherent scattering level from the data measured at high (enough) Q. I'll use the second method, done by checking "Data Set 2 = 1", to subtract flat background. A data set "NullSolvent" is added to the plot



The cursors on the graph are both on the sample data set. Adjust the cursors to move them to the high q end of the scattering data set. The data range defined between the cursors will be the "Matching Range" where the subtraction will be scaled (by the factor "F" in the panel) such that the result has an average value of zero in that range. Click on the "Matching Range" button and the starting and ending q-values will appear in the panel. Note that you can zoom in on the graph by clicking and dragging a rectangular region on the graph (say around the cursors) and then click inside the marquee to get a contextual menu, and select "Expand". To see the whole axis range again, type CMD-A (Mac) or ctrl-A (Win).



Once you've set the cursors to an appropriate range, and clicked to set the "Matching Range", enter a name for the result in the box. A data folder will be created with the result, but not yet saved to disk. Click "Calculate" on the panel. The result (in green) should appear something like this, and should look something like this:



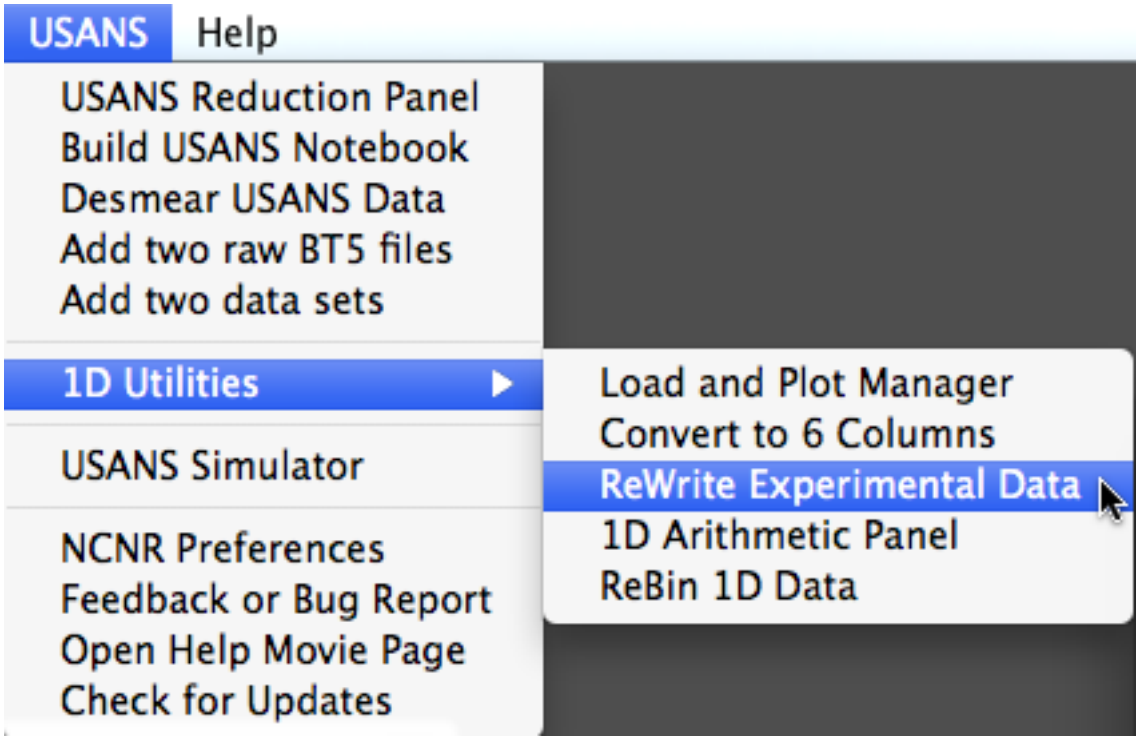
The matching range can be further adjusted, or the fraction of solvent subtraction can be set manually to fine-tune the subtraction. Clicking "Calculate" will update the result (asking if you want to overwrite - usually you'll want to say yes). Once you're satisfied, the resulting subtraction can be saved, using "Save Result". You do not need to use the same name for the saved data set as you used in the panel.

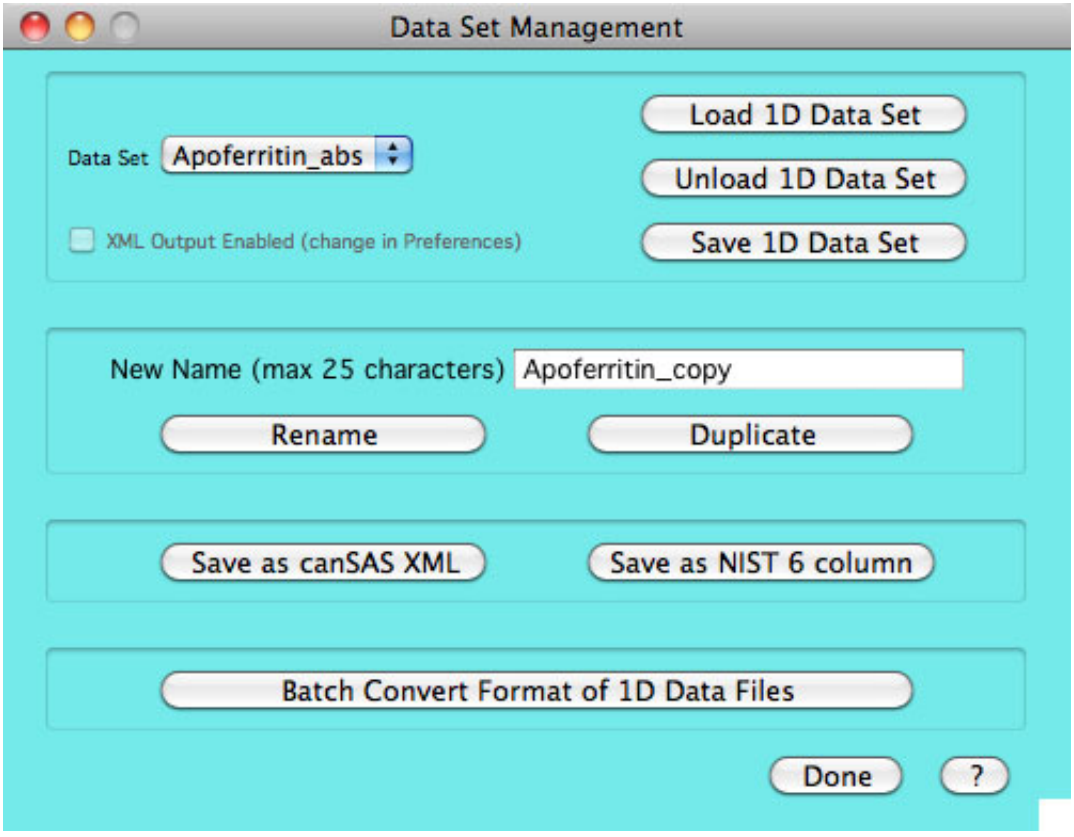
Data sets can be added, multiplied, or divided in a similar way. The output data is in the same format as the original data. Since the result is stored in a data folder internally, it can be immediately used in the Plot Manager or in data analysis without the need for re-loading the data.

Data Set Management

What: This panel allows you to do some common manipulations of 1D data files, such as re-saving data that has been modified or batch conversion of the format of the reduced data files.

How: From the 1-D Utilities Menu, Select "ReWrite Experimental Data". (The screenshot is from the USANS menu, but the data manegement panel is avaialble from all of the analysis and reduction menus.

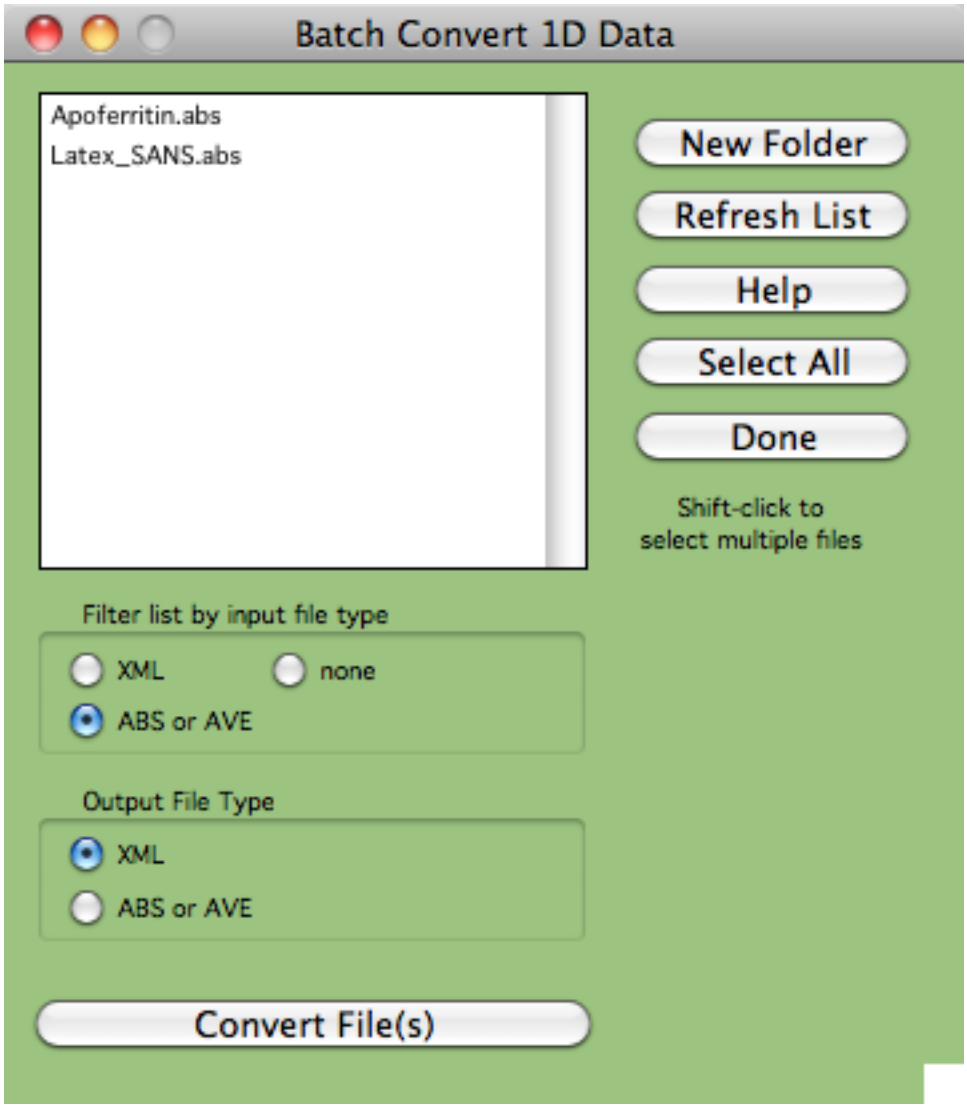




From the input panel, you can (from top to bottom):

- Load, unload, or save any data set. "Save 1D Data Set" will save in the selected format as noted in the check box to the left of the button.

- Rename a data set that is currently loaded
- Duplicate a data set that is currently loaded
- Save 1D data in either canSAS XML format or the NIST 6-column format. Either format is fully compatible with the NCNR data analysis routines. The 6-column format is often more convenient for exporting the data to other analysis packages that may not be XML-friendly.
- Batch convert data between XML and 6-column formats. This eliminates the need to re-reduce data if the preference was incorrectly set during reduction. Batch conversion opens its own panel:

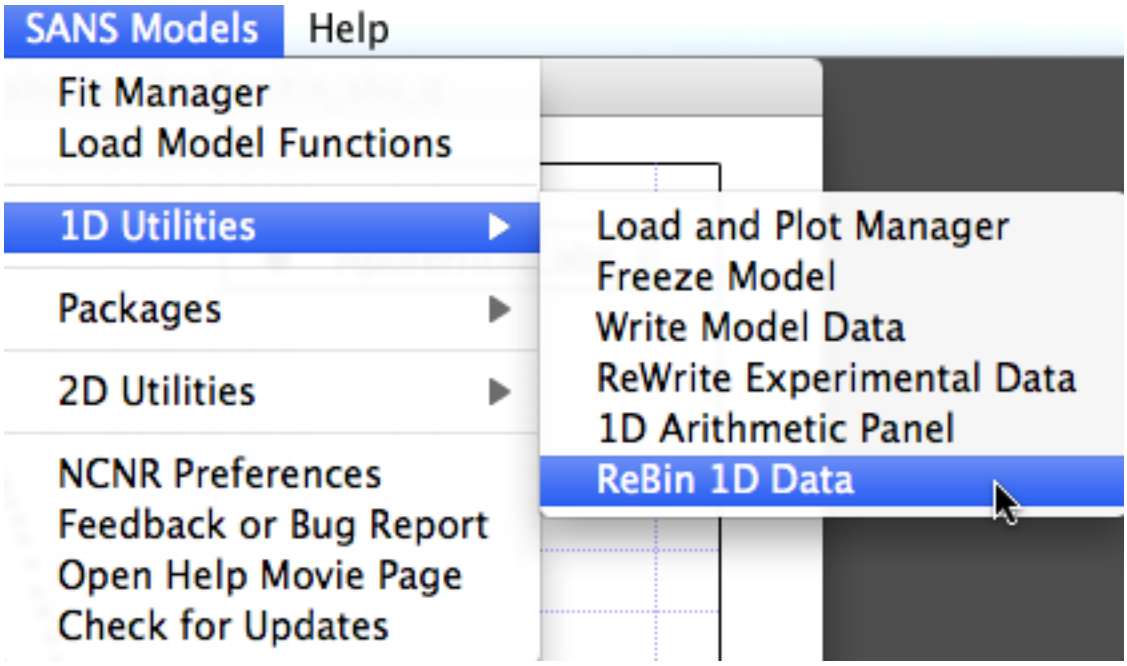


From this panel, the selected files in the list will be converted from XML to NIST 6-column (or the reverse). Files are automatically named during the conversion so no intervention is necessary.

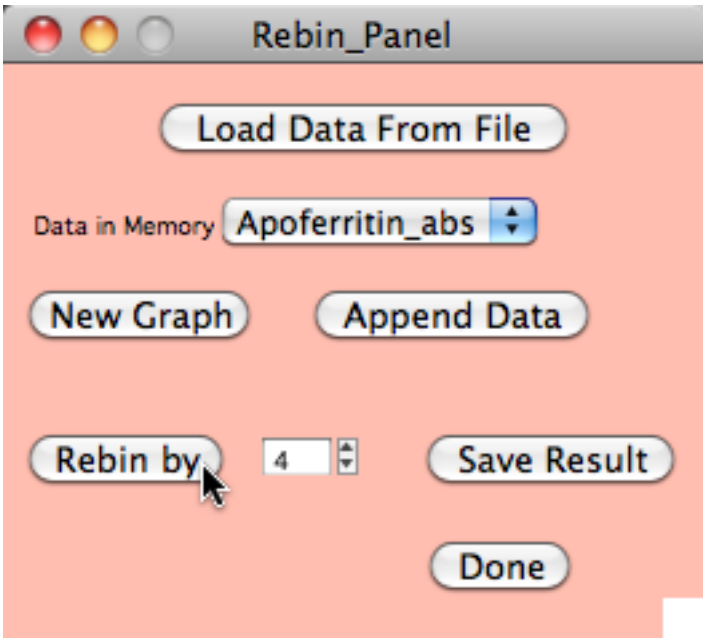
Re-Bin Data

What: This operation allows you to re-bin 1D data in order to improve counting statistics at the expense of q-resolution. Rebinning of data can also be accomplished by increasing the Averaging Bin Width during the data reduction. See the SANS tab of the SANS Preferences Panel for details.

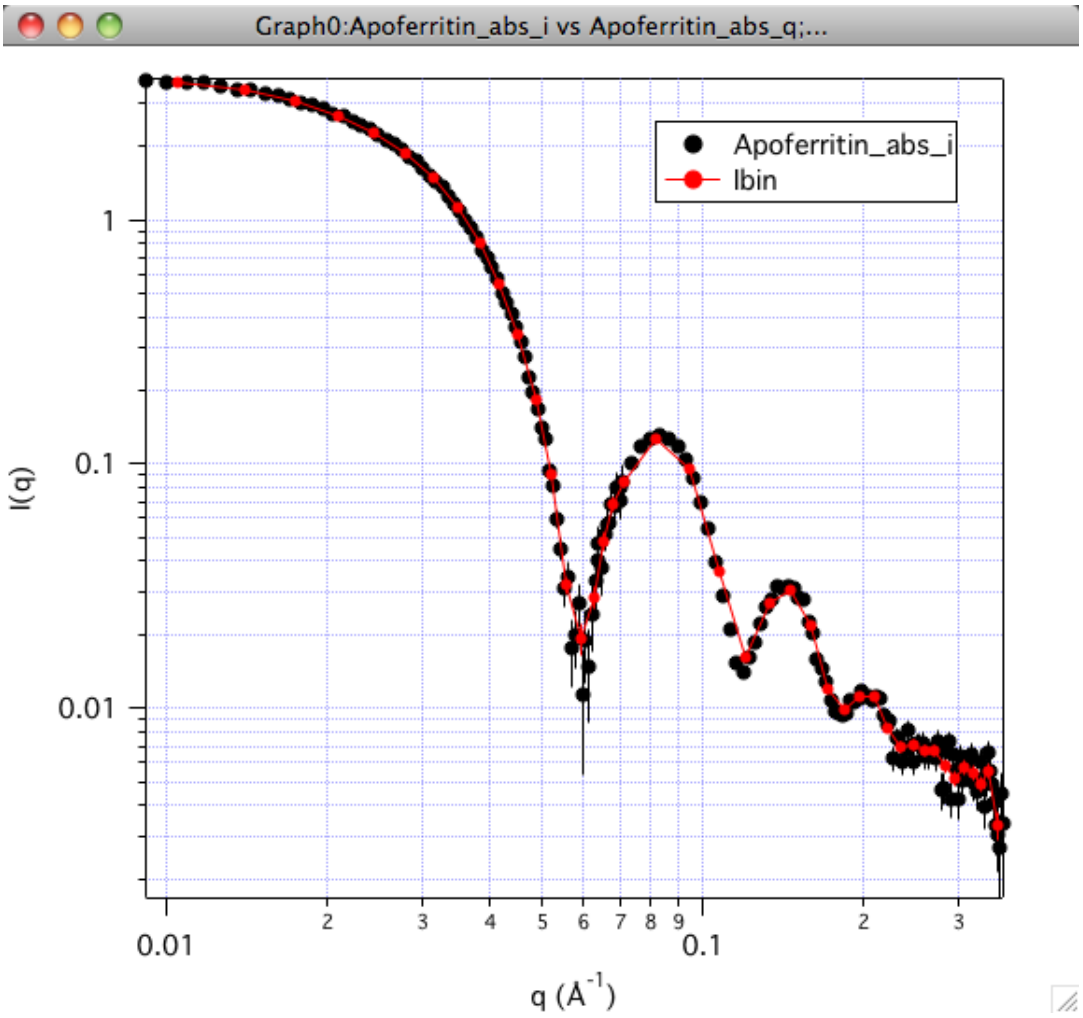
How: From the 1-D Utilities Menu, Select "ReBin 1D Data"



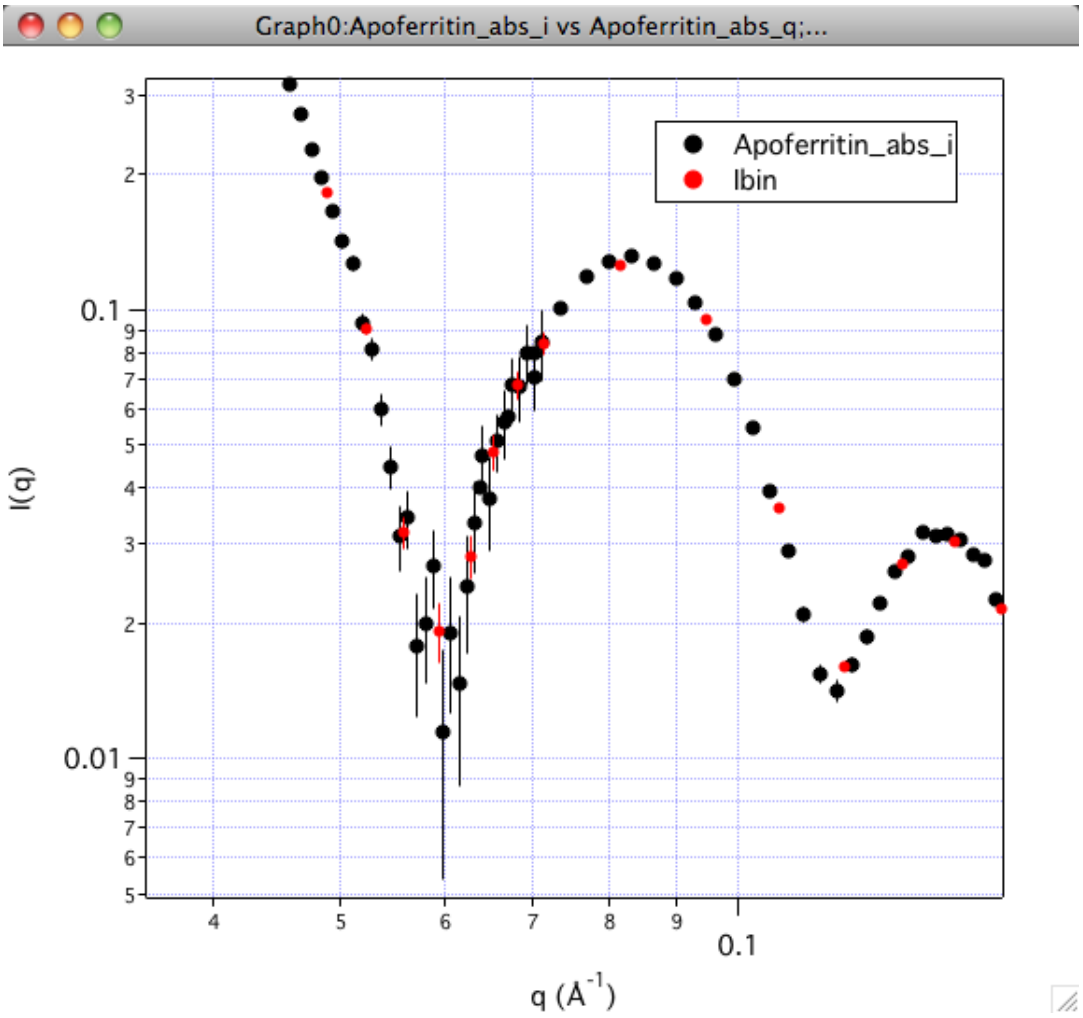
Then from the input panel, you can:



- Load a new data file -or- Select an existing data file. Existing files can be plotted fresh or may be on the topmost graph. With the data selected and the graph on top, The "Rebin by" button will combine the set number of points into a single point. The averages of the q, data, errors, and resolution information are appropriately calculated, and the result is plotted on the top graph as "iBin":



In this example, the number of points is reduced by a factor of four, and the error bars on the intensity are significantly reduced.

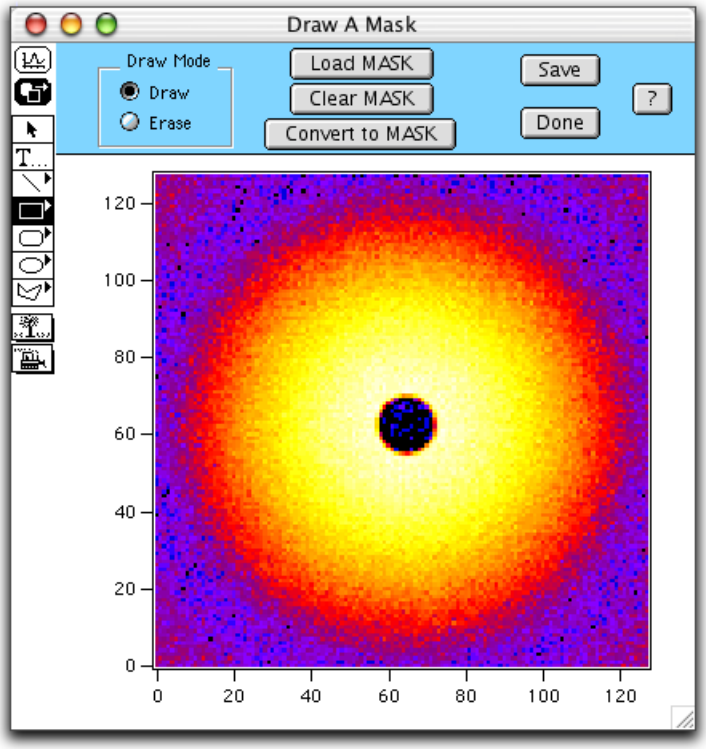


When you are satisfied with the rebinning, you can save the result. The rebinned data will be saved in the format specified (either XML or 6-column) in the SANS Preferences.

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.

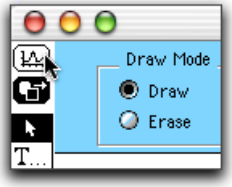
Clear Mask: clears ALL of the mask that is currently being drawn, giving you a clean slate to work from.

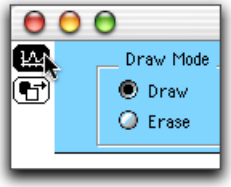
Convert to Mask: takes the current draw objects and converts them to the current mask (cumulatively), drawing or erasing pixels depending on the mode setting **when the objects were drawn**.

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.

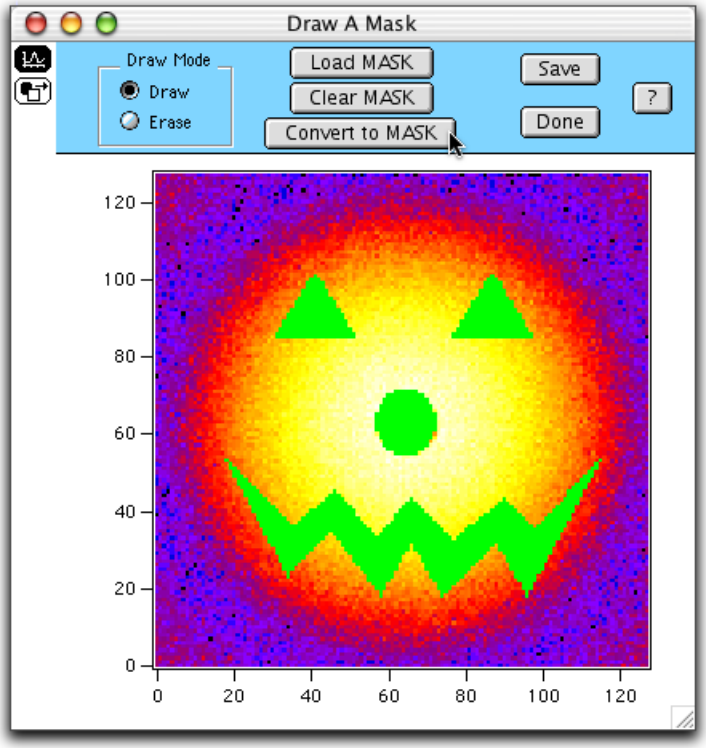
Tools/Graph Toggle: switches between modes where the Tool Bar is visible (below, left) or hidden (below, right). When the Tool Bar is visible, the buttons in the top control bar are inactive. When the Tool Bar is hidden, the control buttons are activated.





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

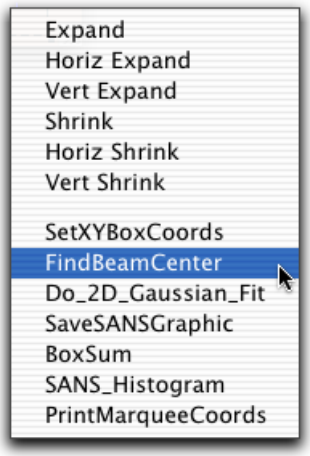
text drawn will not be added to the mask. Draw the desired objects, and hide the tools. Click "Convert To MASK", and the (white) draw objects will be replaced with a green mask image. Mistakes can be "Erased", or "Clear MASK" will start fresh again. Be sure to save your mask before leaving. Once saved, 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:

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 and displayed in a graph of counts versus run number.

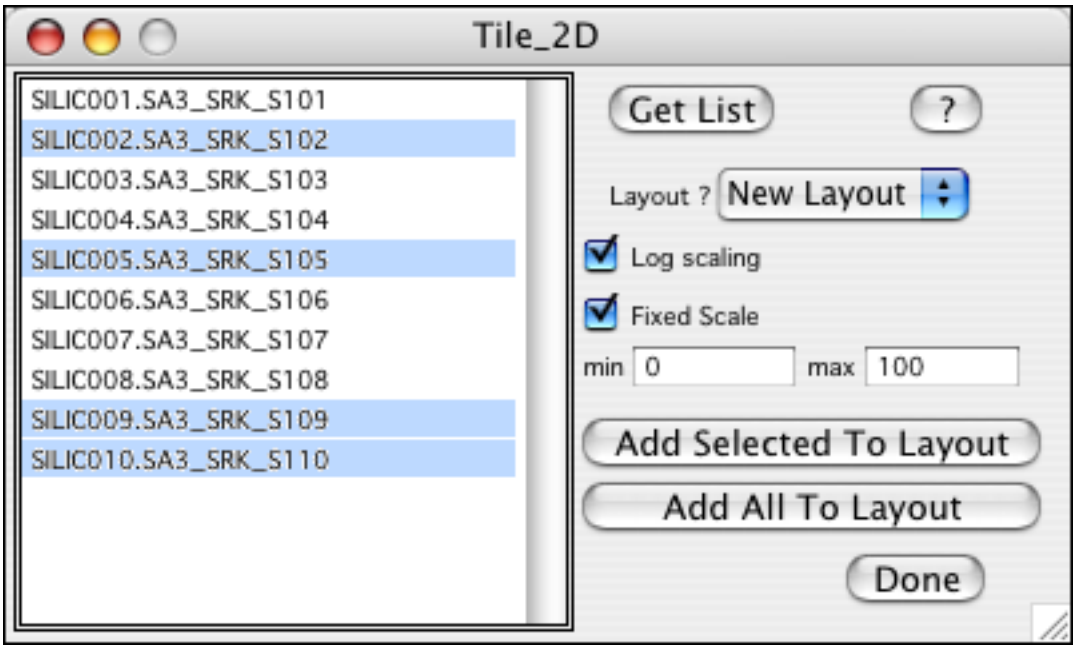
SANS_Histogram: generates a histogram of counts vs. pixel location in the selected region. Positive values are displayed in red, negative values in blue. Very useful to check the balance of counts around the beamstop for alignment.

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

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:

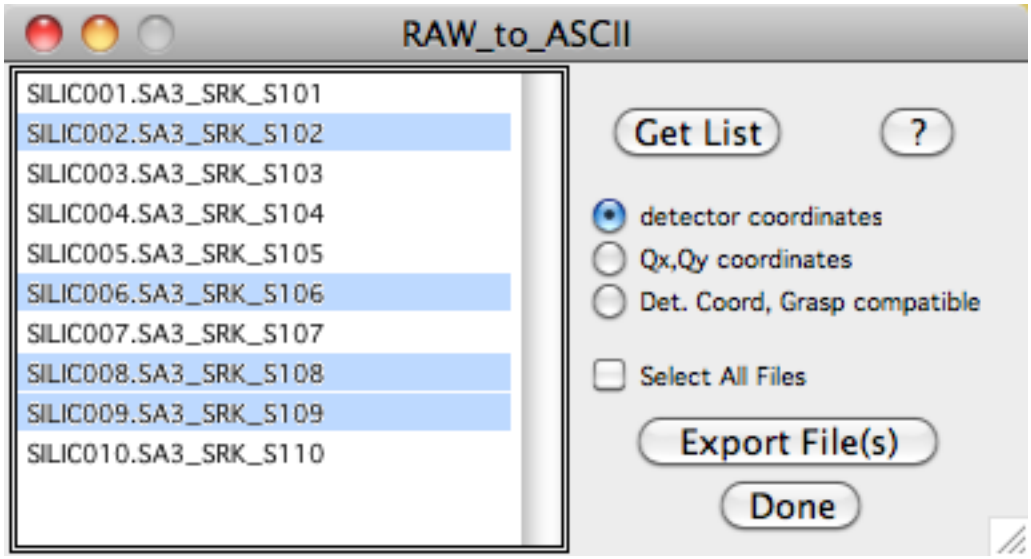


Click "Get List" to see a list of available raw SANS data files. Shift-click to select the desired files. You can choose log or linear scaling of the colors. To better compare a series of data, you can also fix the minimum and maximum values of the color mapping to be the same for all of the selected 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. "Add All to Layout" will put all of the files into a layout, up to 40 images per layout. More layouts will be generated as needed. 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 "SILIC002.ASC".

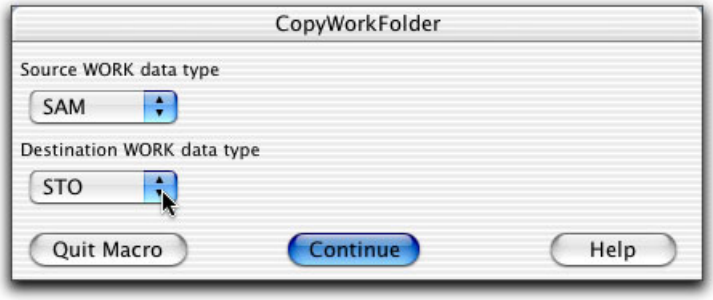


- Data exported in detector coordinates is written with a header followed by a single column of data, containing 128*128=16384 elements.
- Data exported as Qx, Qy coordinates are written as eight columns: Qx, Qy, I(Qx,Qy) plus 2D resolutionk information
- Data exported as "Grasp Compatible" is a specific format for import into GRASP software (C. Dewhurst, ILL)

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.



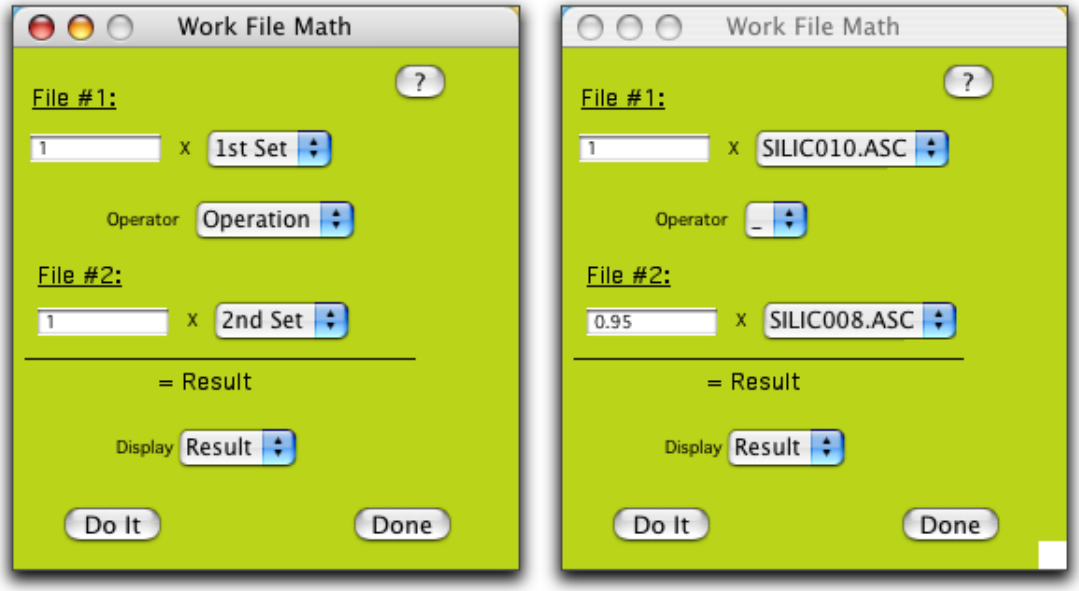
2-D Work File Arithmetic

What: Allows simple arithmetic operations on previously saved 2D ASCII data files, and is particularly useful for fine-tuning background corrections or finding differences in 2-D datasets. Results of the operation are viewed directly, and can be averaged or saved.

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 data set to display which is typically the result. Select the appropriate files from the popup menus for the two data files. These files must be 2D ASCII files saved from a reduction protocol, from the Average Panel (see Average Options), or from Raw 2-D ASCII Export. An option for the second operand to be a unit matrix is also available.

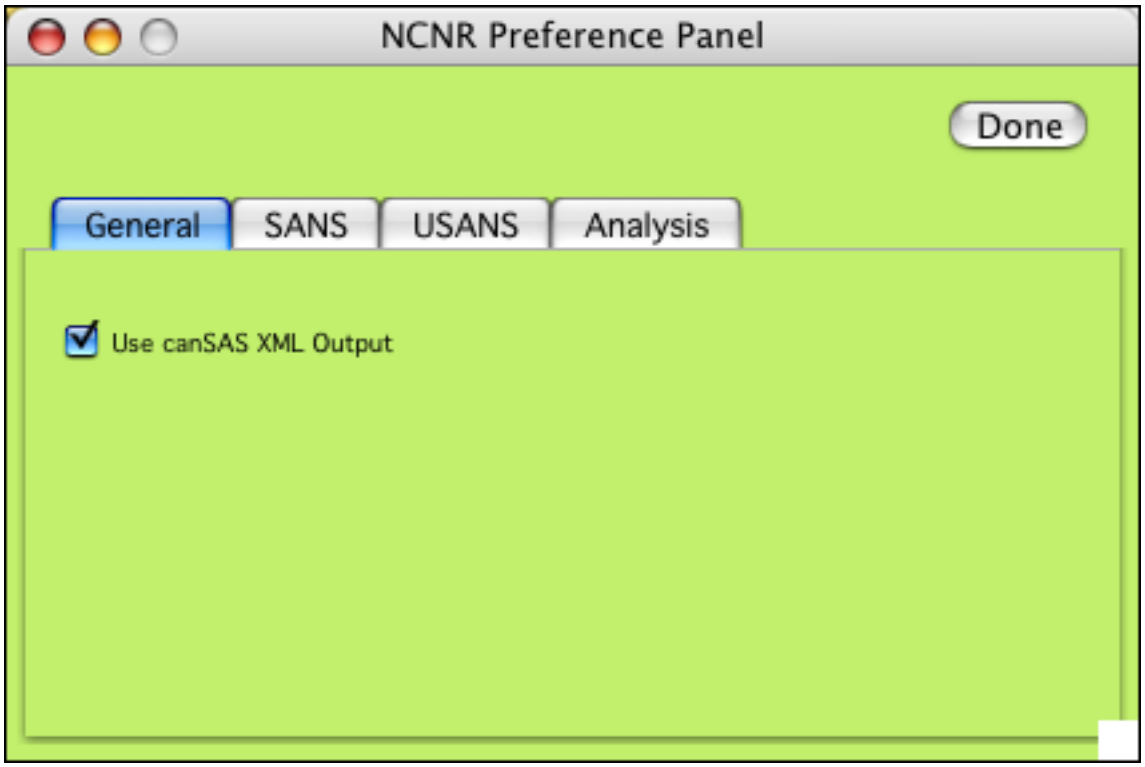
In the example on the right (below), 0.95*SILIC008.ASC will be subtracted from SILIC010.ASC. The result of the calculation is deposited in a "Result" data set, which will be displayed. The calculation performed will also be echoed to the command window at the bottom of the screen. The result is not automatically saved, but can be averaged or saved as 2D ASCII using the controls on the SANS data display window.

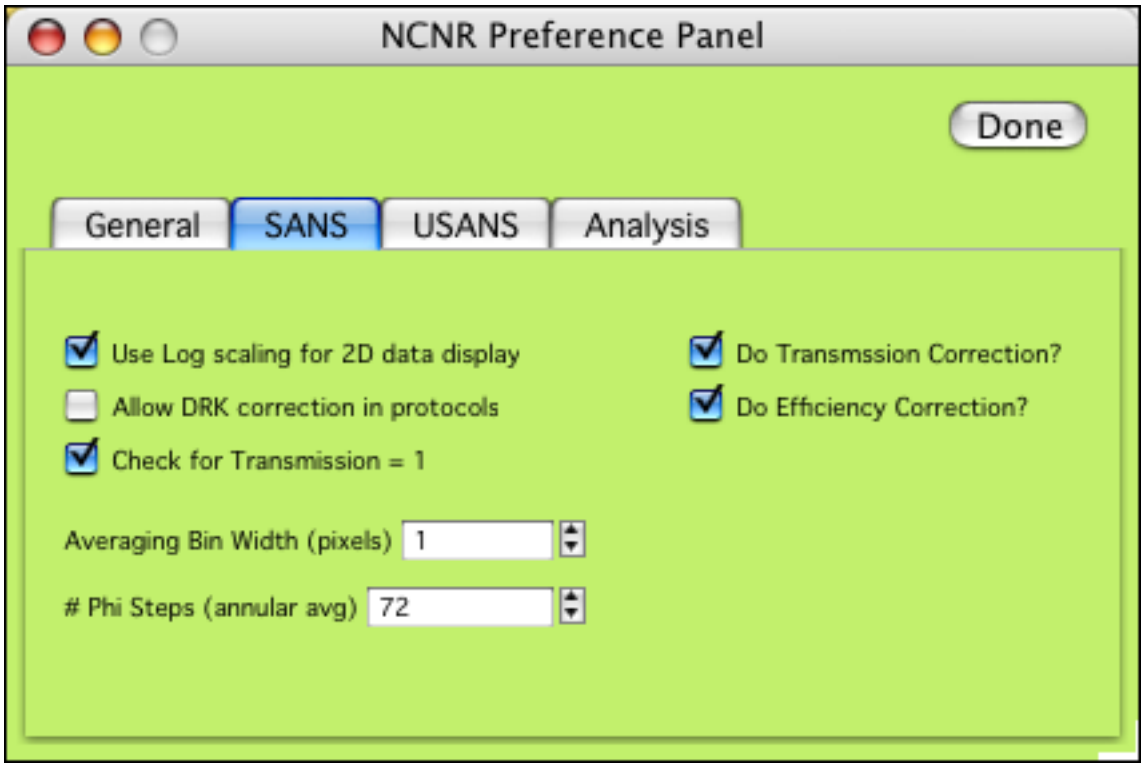


SANS Preferences

What: Set a few display and averaging preferences.

How: From the Misc Ops Tab on the Main Panel, click on "Preferences", or the preferences can also be found in other packages under their menus by selecting the item "NCNR Preferences" The values shown in the panel are the default values. The default values can be reset by selecting "Initialize" from the SANS Menu.





From this panel, you can set preferences for:

General:
- XML output. This will write out 1D data in a standardized XML format, supported by many other analysis packages. Unchecking this will revert to the NCNR ASCII output.

SANS:

- the default display for the 2D SANS data, either log or linear scaling of the counts
(note that this will also set the scaling for saves of PNG graphics as saved from the Protocol Panel)
- allow DRK correction step in data reduction protocols (default is no)
- enable checking for Trans = 1 during data reduction (default is YES do the checking)
- the bin width for 1-D averaging (default is one pixel)
- the number of bins used for an annular average (default is 72)
- turn off the angle-dependent transmission correction.
- turn off the angle-dependent detector efficiency correction.
** both of these corrections MUST be left ON for data collected at the NCNR. **
USANS:

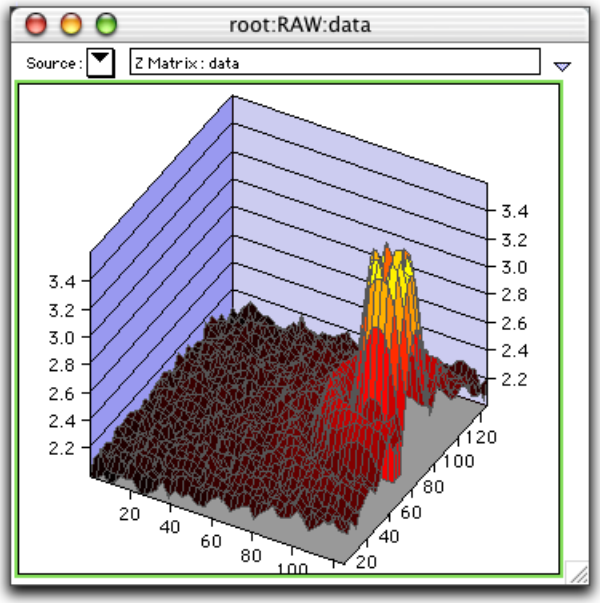
-nothing specific to USANS
Analysis:

- nothing specific to Analysis

Note that the preference are set for the current experiment. Re-opening an experiment will not change the modified values, but starting a completely new experiment WILL start with the default values.

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.

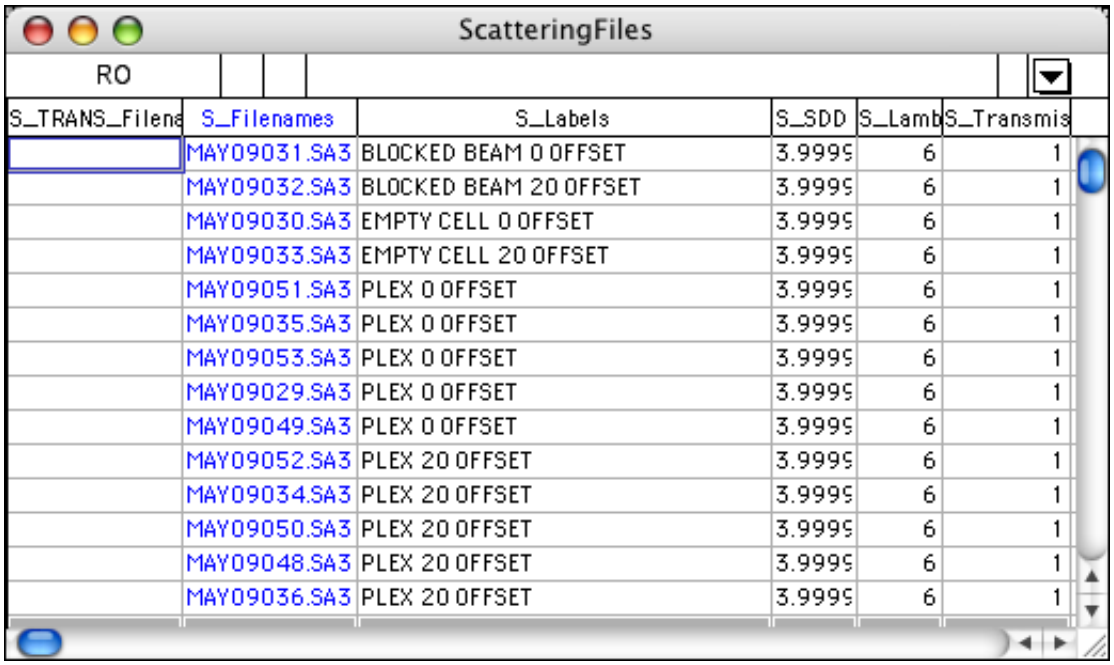


Detector Sensitivity File

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.

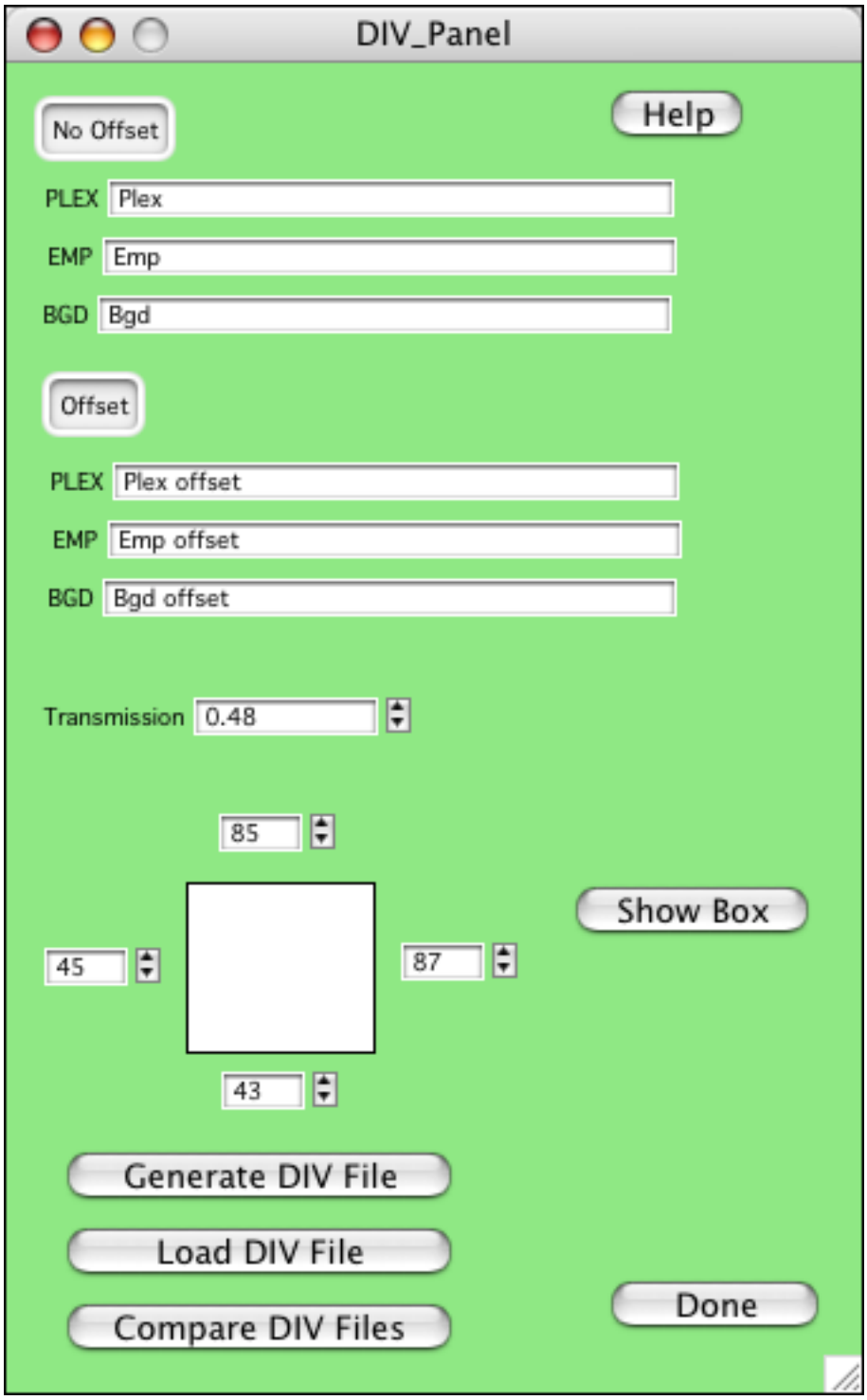
How: Get a file listing of the raw data files. Sorting them by label from the transmission

panel is most helpful for grouping the data by label. Be sure that all of the data files have the correct beam center, and that the plex data has the correct transmission:

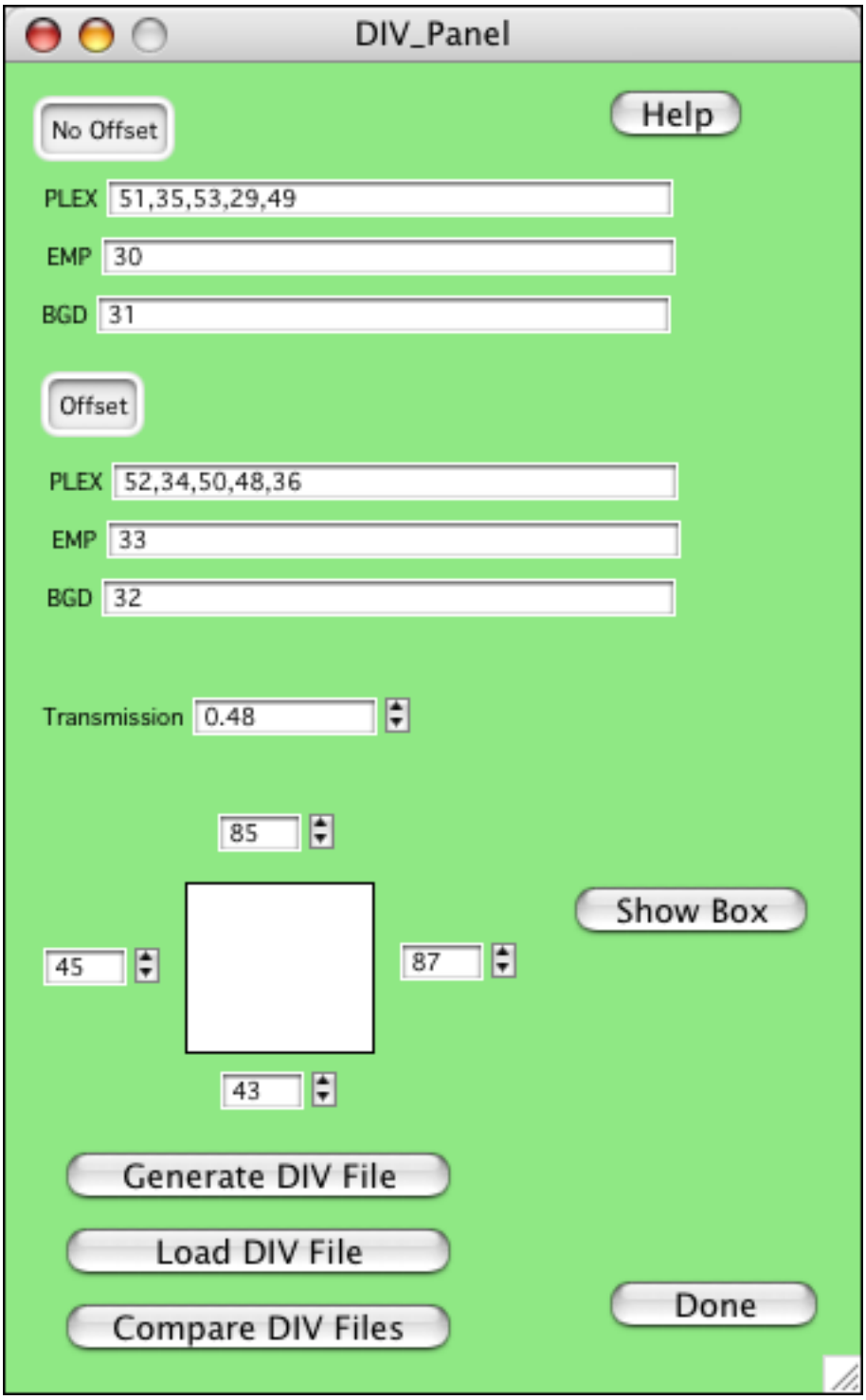


S_TRANS_Filens	S_Filenames	S_Labels	S_SDD	S_Lamb	S_Transmis
	MAY09031.SA3	BLOCKED BEAM 0 OFFSET	3.9995	6	1
	MAY09032.SA3	BLOCKED BEAM 20 OFFSET	3.9995	6	1
	MAY09030.SA3	EMPTY CELL 0 OFFSET	3.9995	6	1
	MAY09033.SA3	EMPTY CELL 20 OFFSET	3.9995	6	1
	MAY09051.SA3	PLEX 0 OFFSET	3.9995	6	1
	MAY09035.SA3	PLEX 0 OFFSET	3.9995	6	1
	MAY09053.SA3	PLEX 0 OFFSET	3.9995	6	1
	MAY09029.SA3	PLEX 0 OFFSET	3.9995	6	1
	MAY09049.SA3	PLEX 0 OFFSET	3.9995	6	1
	MAY09052.SA3	PLEX 20 OFFSET	3.9995	6	1
	MAY09034.SA3	PLEX 20 OFFSET	3.9995	6	1
	MAY09050.SA3	PLEX 20 OFFSET	3.9995	6	1
	MAY09048.SA3	PLEX 20 OFFSET	3.9995	6	1
	MAY09036.SA3	PLEX 20 OFFSET	3.9995	6	1

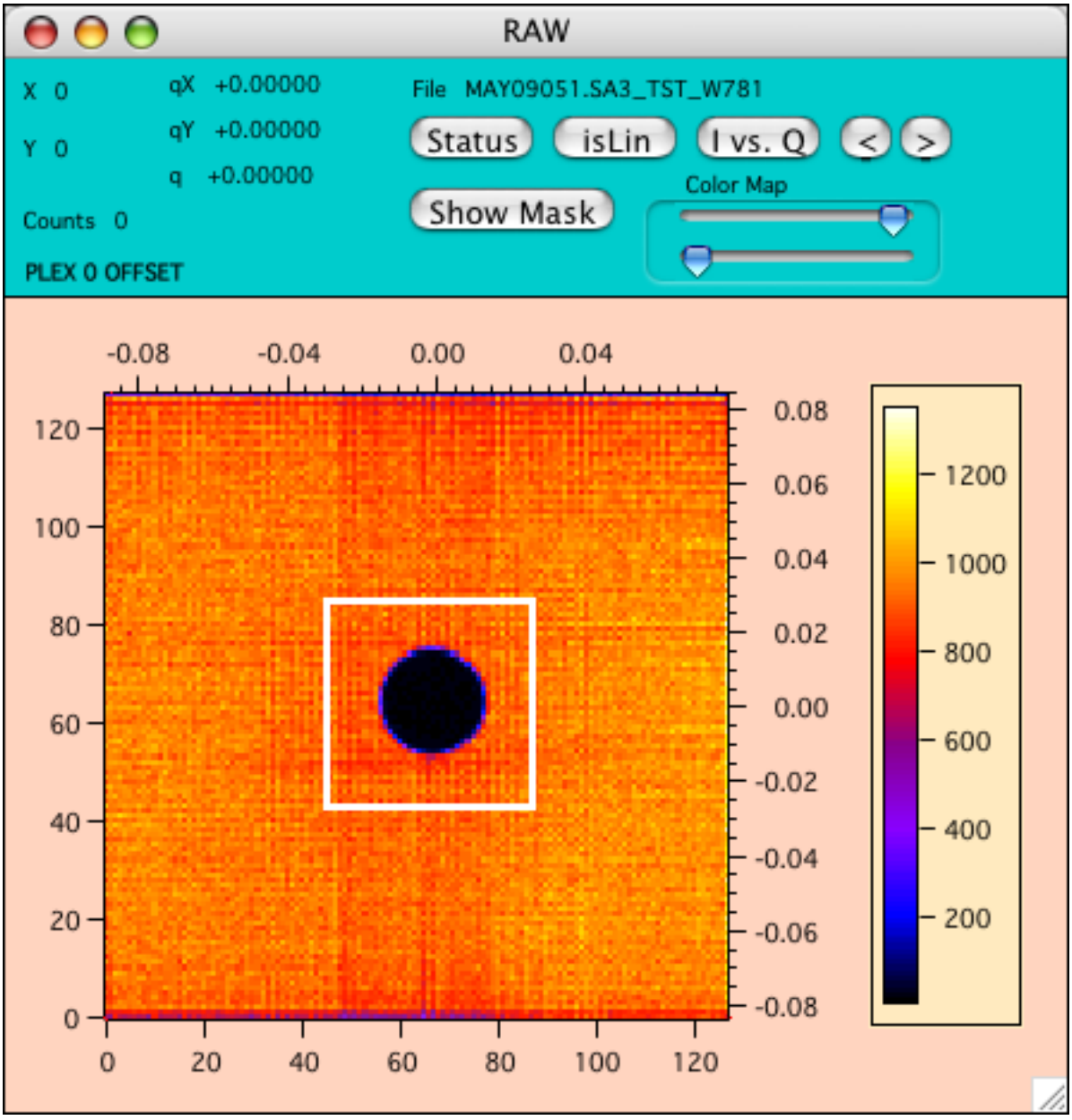
Then from the Misc Ops Tab, select "Make DIV File", and a panel will be presented where you can enter all of the information necessary:



Enter the run numbers for the plex, emp, and bgd data for the "no offset" data (comma-delimited as usual), and then do the same for the data with the detector offset. You of course, must have the data path set properly from the main panel for it to find any of these data files.

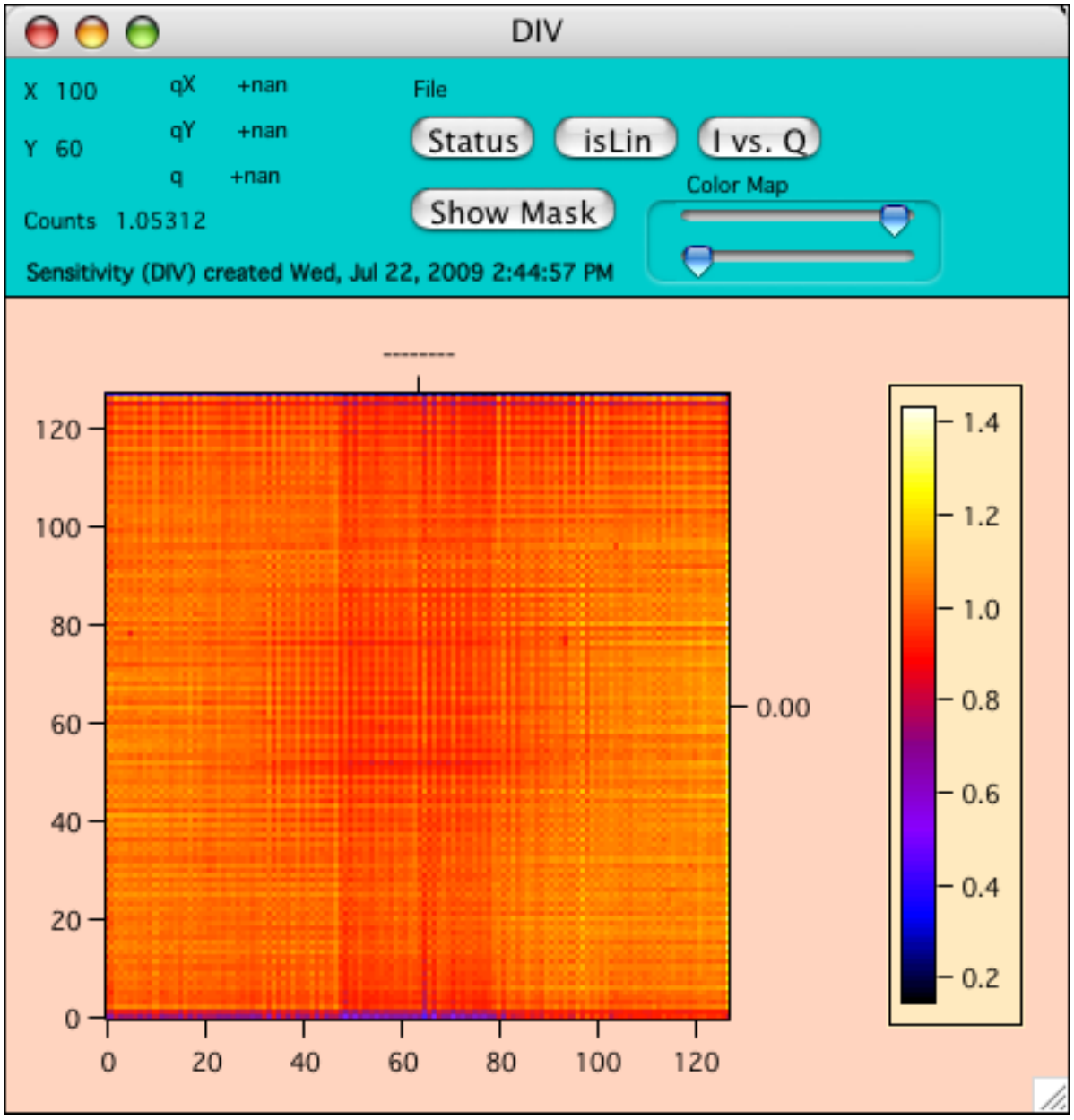


Next, click on "Show Box". This will show the box that will be replaced in the zero offset data with a block of data from the offset data. One of the plex->zero offset data sets will be loaded. For the typical case of the 4" beam stop, the default values are good.

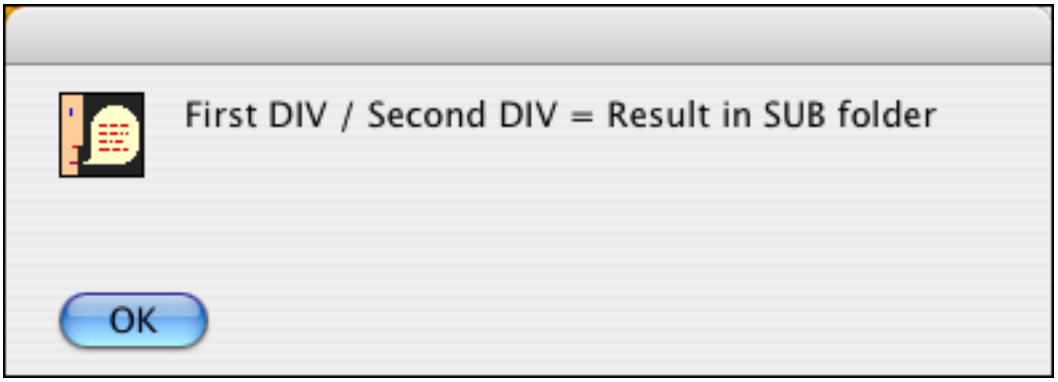


Then, "Generate DIV File" will do all the steps - loading, correcting, replacing the patch of data, and normalizing. The empty cell (aperture) transmission is one, so you can accept that value if the dialog appears. you will then be prompted for the name of the DIV file to save.

You can reload the DIV file, or any other DIV file, using "Load DIV File". This also prints the wave stats to the command line.

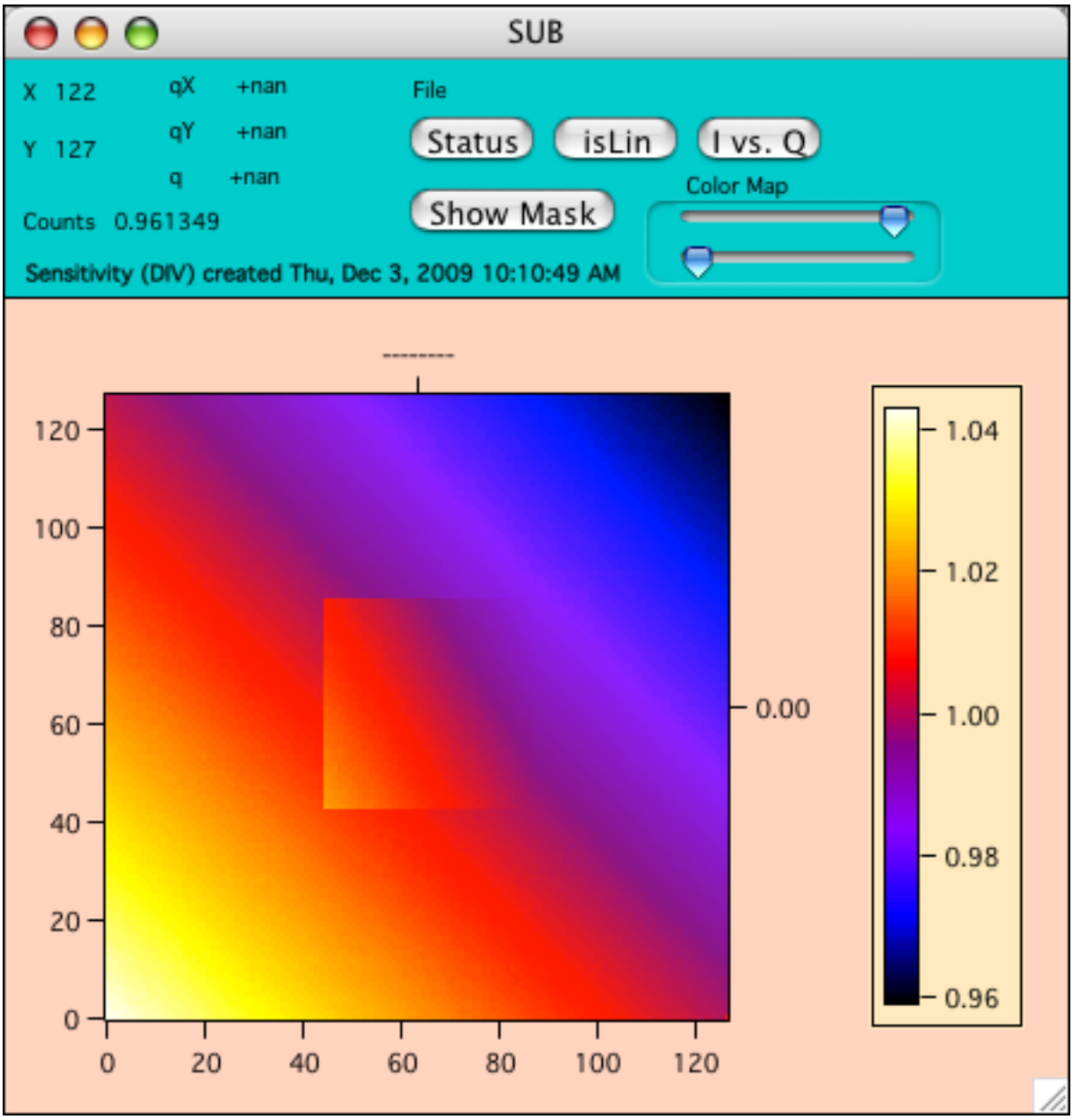


To compare two DIV files as a ratio, click "Compare DIV files":

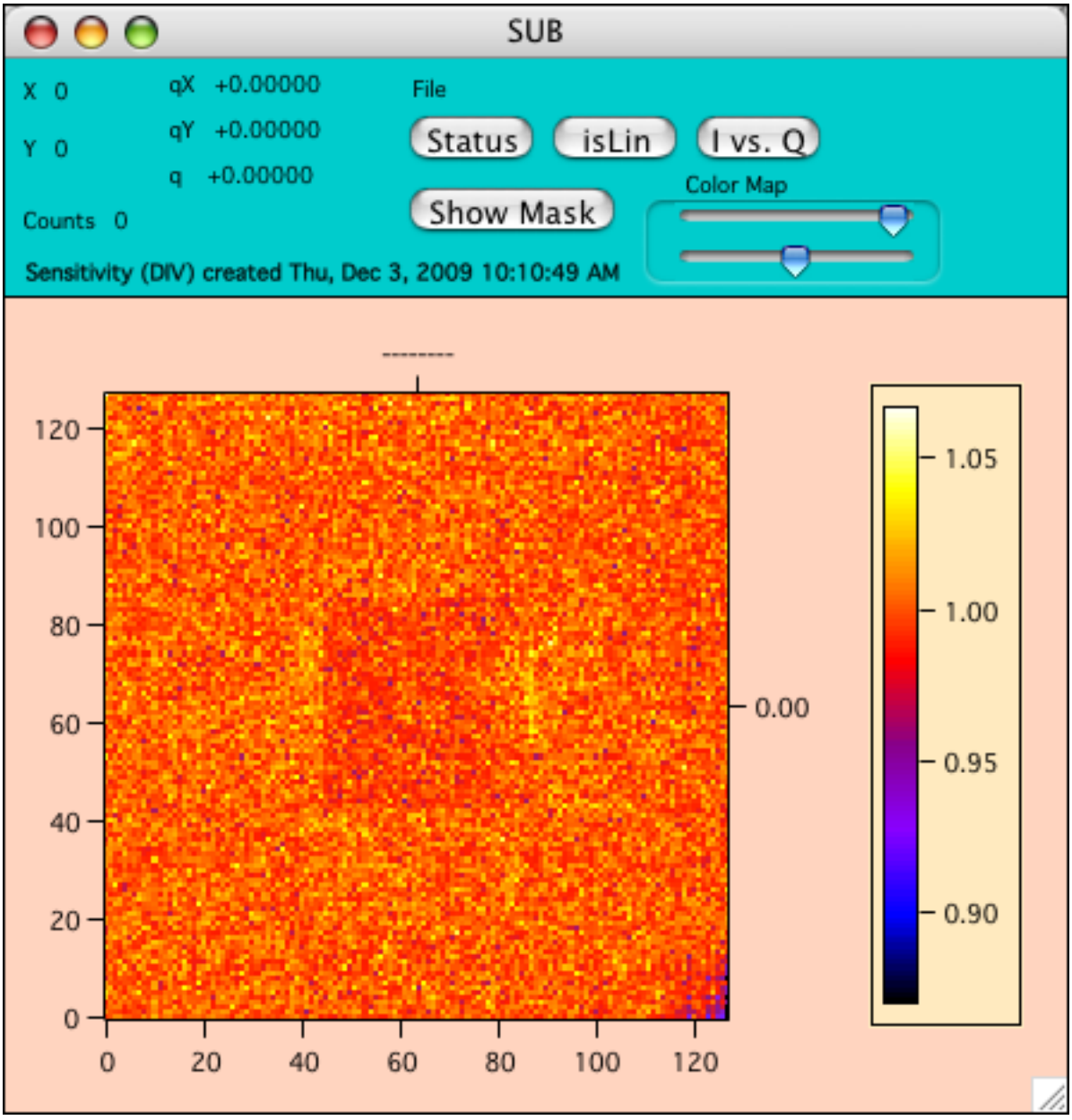


After the two files are selected, the ratio is plotted. In this example, one of the DIV files was reduced

with correct beam centers, while the other set was reduced with (0,0) as the center. The result is a skewed difference.



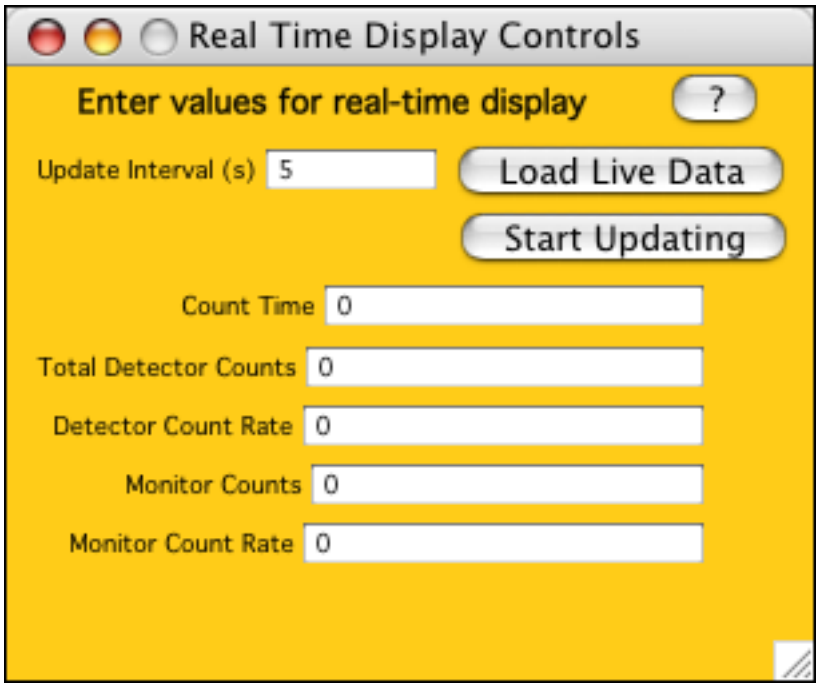
A proper difference looks like below. In this case the difference is statistical fluctuations and a different patched block.



Real Time Data Display

What: Show the live detector image during data collection. Currently this is used when ICE is being used for data acquisition.

How: From the Raw Data Tab on the main panel, click on "RealTime Display" to bring up the following panel:



Click on "Load Live Data" to load the "live" data set. Check with your local contact for the location and name of this file as it may change. Click "Start Updating", to initiate a refresh of the data displayed. In this case, display will be refreshed every 5 seconds (the detector only sends new data on an interval of a few seconds).

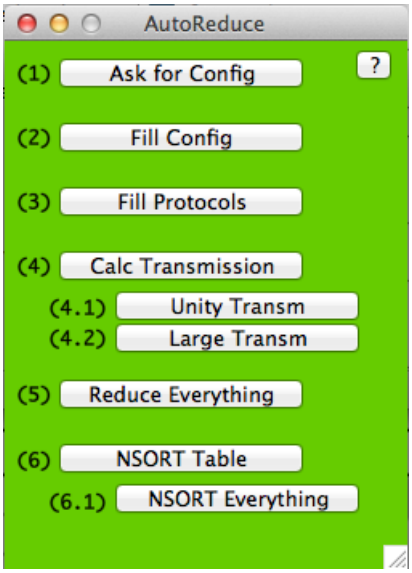
- **Automated SANS Data Reduction**

A bunch of (beta) functions in an attempt to automate data reduction
SRK OCT 2014

The basic idea here is to be able to reduce an entire set of SANS data with a minimum of intervention from the user. The more consistently all of the files are labeled, the more likely the operations will be successful. Also, I expect that only "standard" experiments will work with automation. Special cases will require special handling.

The most obvious danger in automation is that the user is "insulated" from actually looking at their data. Issues apparent in the raw data that are a result of instrumental issues or sample issues are going to be missed. Other issues during the processing steps that are obviously wrong in the real world are perfectly fine for a computer. So with that said, these are testing procedures, so please use good (human) judgment on what each step produces. And when things happen that are unexpected or just plain wrong, let me know. Feedback is infintely useful.

So -- as a first attempt to make automation happen, a simple panel has been created to walk a user through the steps in a very simple fashion. Much of this is simple scripting of the reductions steps that are already present in the SANS package. However, many procedures were written to automatically identify files, beam centers, etc. so that the necessary information could be fed into the scripts with a minimum of user intervention.



0) First, complete the basics of setting up a SANS reduction experiment.

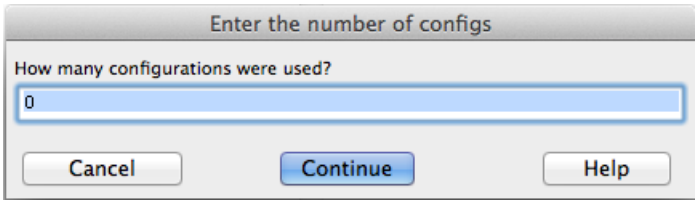
From the Main (Yellow) panel:

- Pick Path -- to set where the data is located
- File Catalog -- to get a listing, you will want to verify files
- Save the experiment -- somewhere for the results to go

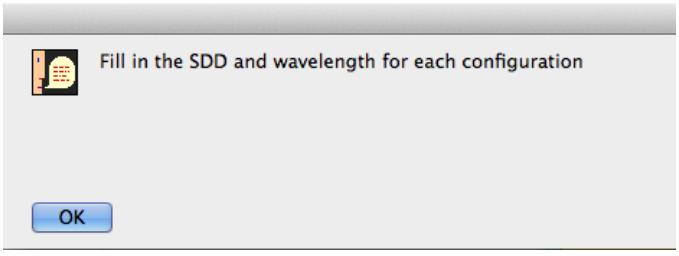
1) For the automation, start with gathering some basic information.

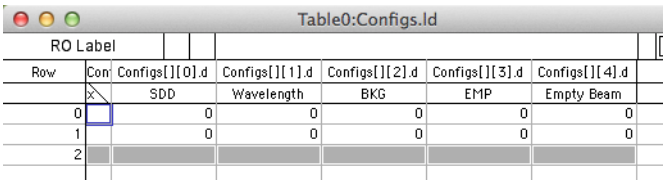
Button (1) Ask For Config

You'll be asked for the number of configurations that you used:

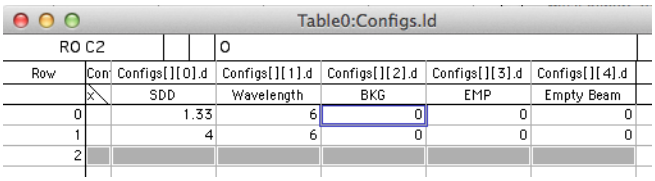


and then be asked to fill in only the SDD and wavelength for each configuration. The order doesn't matter in the table.





The SDD and wavelength are in the Data File Catalog (that's why it's there)

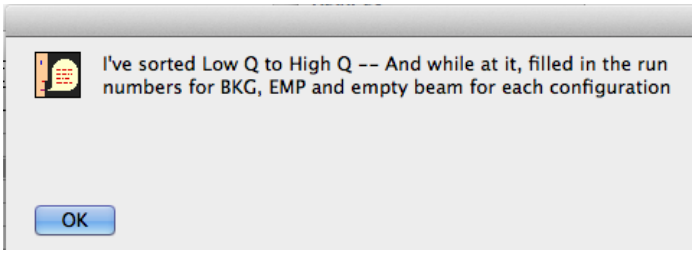


2) Next, Fill in the run numbers for each configuration.

Click the button, and Igor will attempt to fill in the blocked beam, empty cell, and empty beam files from the (hopefully) well-labeled samples. It will also sort the configurations in the table from low Q to high Q.

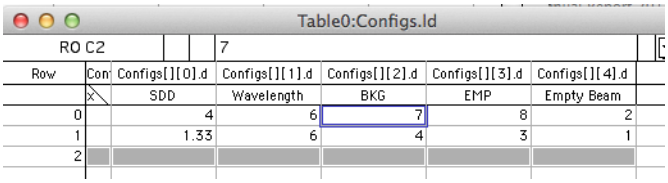
Button (2) Fill Config

You'll see this dialog when done:



**

Inspect the results to make sure that the run numbers are all correct before proceeding.

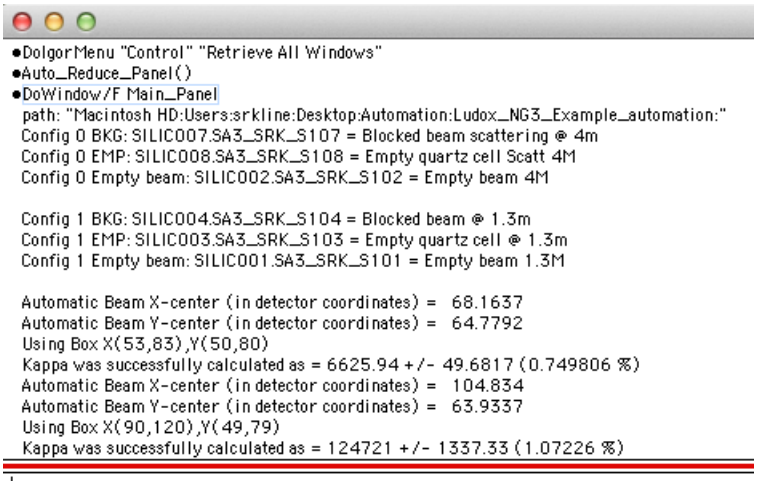


3) Next, fill in the Reduction Protocols.

With all of the run numbers properly identified in the table, there is enough information to set up a reduction protocol for each of the configurations.

Button (3) Fill Protocols

The Protocol Panel will automatically open, and raw data files will open up as the ABS scaling is calculated. Configurations are saved and named "Config_N", where N is the row number in the table with all of the configuration information. If the sorting worked, the q-range for the configurations increases with N. Check the command window at the bottom of the screen to see the results. It will show which files were used, and the calculation of beam centers and kappa values. Check to make sure all makes sense.



Behind the scenes:

- Files are located by run number
- DIV and MASK are filled in if possible.
- ABS will use the empty beam method. The beam center of the empty beam file(s) will be automatically determined and written to the raw data file. The beam center for the empty beam files are often not set correctly during instrument setup (since there is no need to do so). The box to sum is set around the beam center, and all other information to calculate kappa is present.

Some potential issues:

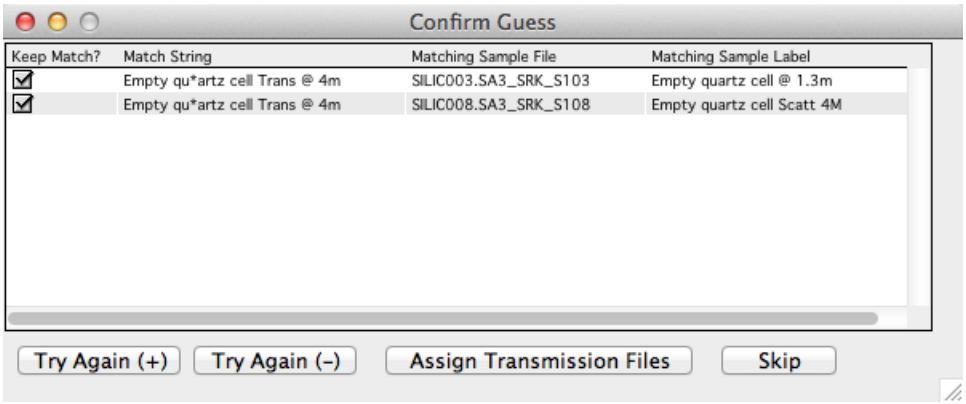
- Igor is looking for a sensitivity file ending in ".DIV". It must be in the same folder as the data, and there must be only one DIV file.
- Igor is looking for a mask file ending in ".MASK" (as in DEFAULT.MASK). If that's not present with the data files, you'll have problems. Also, if you have more than one mask file that you want to use, don't bother with the automation - you've got a special case.

4) Then, it's time to calculate all of the transmissions.

This step still requires some human intervention, but is hopefully a bit easier to work with than doing everything manually.

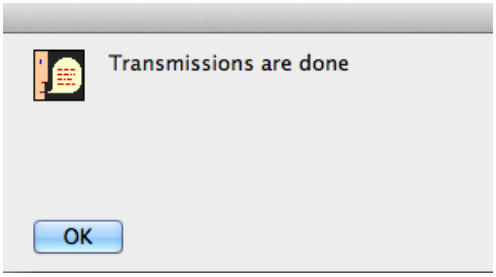
Button (4) Calc Transmission

Igor will open the Transmission Panel, and list the files. All of the empty beam files have been identified, and the correct ones will be matched up as needed based on the wavelength and SDD. Igor will start to loop through all of the transmission files, stopping at each match of scattering files. You'll be presented with a dialog for each set of possible matches, and you'll need to make some judgment of whether it's a correct transmission match or not.



In this dialog, you have a few new choices. The "keep match?" checkbox is just that. If a few stray files are "found" that are not really matches, uncheck them, and the transmission assignment will only be made for the checked rows. The "*" in the match string is at the string length that is attempting to match (with the matching sample label). If you get no matches (or too many) with the default number of characters, Try Again (+) will use one more character, and (-) will use one less. When correct, Assign Transmission Files will do that, and immediately calculate the transmission(s). You will then be presented with the same dialog for the next transmission file, and repeat the process to step through all of the files. "Skip" will skip that particular transmission file, and proceed to the next without making any assignments or calculations. You'll need to assign and calculate the transmission manually for any skipped files before proceeding with the reduction.

When it's done looping through all of the transmission files, you'll get this dialog:



Before finishing with the transmissions, check that all is reasonable (by inspecting the tables) and some automated checks:

Button (4.1) Unity Transm

and

Button (4.2) Large Transm

These two buttons will search for either T=1, or T>1. The results will be printed to the command window. Here, all that is "wrong" is the blocked beam file where the transmission is meaningless. Correct any problems manually before proceeding.

Behind the scenes:

- The empty beam files are identified with the configurations. This process loops through all of the empty beam files, looking for anywhere they may have been used as an empty beam reference for a transmission measurement. Files are filtered out by SDD and wavelength.
- With the help of the user "OK", then all of the assignments and calculations can proceed.
- The groups of sample files that are "OK-d" for transmission assignments are saved, as these are typically the groupings of runs that are a single sample that you'll want to later merge into a single data file. So save that information now, rather than have to as for it (again) later.

Potential issues:

- If the files are poorly labeled, identification of "matches" between transmission files and scattering file will be quite difficult for a computer to accomplish.

5) Reduce all of the data at each configuration

Button (5) Reduce Everything

Click the button and away it goes. The MRED panel opens, files are matched to each protocol,

and reduced. Files will be automatically saved and named as usual.

Behind the scenes:
- Nothing more than MRED, with the exception that it does now filter SDD + wavelength to identify files. This can be important if you have lens data.

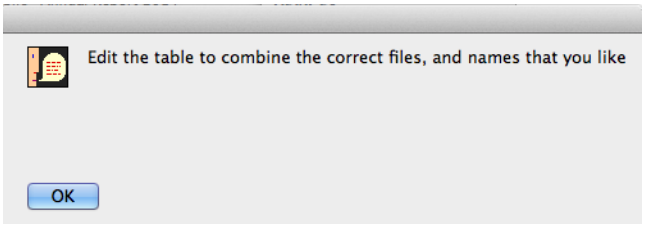
Potential issues:
- Occasionally, you may get a panel flagging "Transmission = 1". If so, make a note for yourself of which file(s) have this problem. It may or may not be a problem. Sometimes it is a "dummy" run for temperature equilibration, or a file where you really want to use T=1.

6) And now, combine + sort the 1D data sets

This will start with a table of the best guesses of which files to combine together. User intervention is needed here to be sure that the correct files are combined. Start with:

Button (6) NSORT Table

You'll get the dialog:

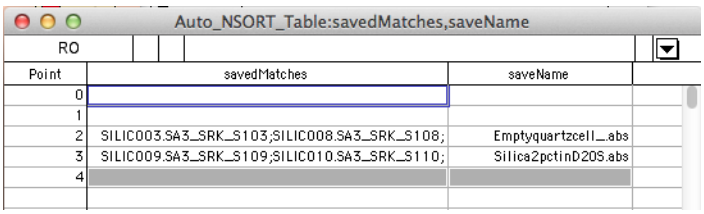


And the Auto_NSORT_Table:

Resize the column widths as needed to see all of the contents. Blank rows will be ignored when processing, so don't worry about them.

One condition where user intervention seems unavoidable is when lens data is present. Then, transmissions are assigned separately (different wavelength) and there is no way to reliably determine which files are from the same sample. So in that case, you'll need to copy/paste that file name into the correct "savedMatches" entry so that all of the data files for a given sample are all together. Be sure to keep a semicolon ";" after each file name. You can delete the stray row of lens data (or any other row you don't want to combine) by clicking on the point number of that row, and from the popup menu (triangle in upper right of the table), select "Delete Points..." and then "OK" from the dialog. You will typically want to delete the row with the empty cell data, since this data is usually excluded from the data reduction, hence these reduced data files won't exist.

Before you're done with the table, be sure that all of the "saveName" are correct for your data files. It is populated with a compressed string from the sample label for each group, so it may or may not be terribly useful as a final combined file name. Note that it may not be unique, either, especially if you used long sample labels that were different only towards the end of the label. Simply edit the file names in the table.



Once you're satisfied with all of the grouped files and the names that will be used:

Button (6.1) NSORT Everything

All of the groups of matched files will be trimmed, concatenated, sorted and saved. Results will be reported to the command window. If any of the reduced 1D files to combine are missing, they will be skipped (like the empty cell files in this example) - but you won't be warned that anything was skipped.

Behind the scenes:

-- A default number of points are trimmed from the high Q end of each file (10 Points)
-- The low Q end is trimmed removing points where the beamstop shadow fs < 0.98
-- NO autoscaling is done whatsoever.

Potential issues:

-- There may be a need to allow for some user feedback here in selecting the exact points to keep/discard. This is still a step where human judgment is rather useful.
-- No autoscaling.
-- Clumsy to edit the table of matched files. Potential here for errors since you can't really see what files are being matched up, except as file names.

7) Finally, plot the data

This step isn't on the automation panel, since the automation is done. Go to the Main Panel (yellow) and on the 1-D Ops tab, "Plot". This will allow you to plot all of the freshly combined and saved files. Big sanity check time here, to be sure that the data makes sense -- trends, scaling, background levels, all samples there, etc.
