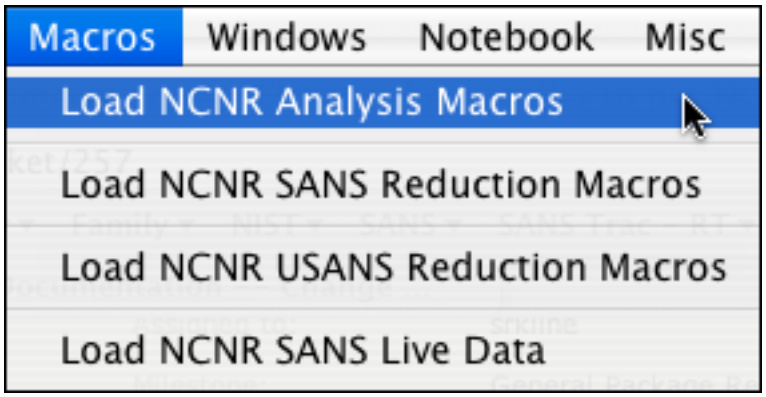
- **SANS Data Analysis Documentation**

6/2008 version 4.00
04/2010 version 4.10 (Package 7.0)
12/2010 version 4.10 (Package 7.04)
03/2012 version 4.10 (Package 7.10)

This revision of the SANS analysis software provides new functionality in an improved interface, making it easier to plot and analyze SANS and USANS data. Once the macros are installed, you can start an analysis experiment by selecting "Load NCNR Analysis Macros" from the Macros menu:



For the highlights of the new features, see the What's New in SANS Analysis section.

If you use this software to analyze ro reduce 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>

This help file is divided into three major parts:

1) Learning how to use these models to predict scattering or analyze data:
SANS Data Analysis Tutorial

2D SANS Analysis

2) Learning more about supplied packages that perform special tasks:

Fit Manager

This is the starting point that allows you to load, plot, and fit models to your data. It allows efficient handling of multiple data sets, models, and coefficient tables all from a single panel.

SANS Model Picker

This panel allows you to load (or remove) model functions into your analysis experiment.

Plot Manager

This allows you to load and plot multiple files, as well as (re)plot and append data sets that you have already loaded.

Global Curve Fitting of SANS Data

This allows you to fit multiple data sets with the same (or different) model, such as a series of contrast variation measurements, or samples that were measured on both the SANS and USANS instruments. For simultaneous fitting of two data sets (especially USANS+SANS), you can use Simple Global Fitting that has a greatly simplified interface.

Calculate Scattering Invariant

This package allows you to calculate the scattering invariant from your data, along with extrapolating your data to large and small Q-values.

Linearized Fits

This package makes it easy to perform a variety of linearized fits, such as Guinier, Kratky, and Zimm plots.

Sum SANS Models

This package allows you to make a new model that is a linear combination of two existing models.

Genetic Optimization

Must be installed as a separate download. This provides an option other than Igor's built-in gradient method for non-linear fitting. Courtesy of Andrew Nelson at ANSTO.

Auto Fit (or Batch Fitting)

This package provides the capability to batch fit a single model to a large number of data sets to speed up analysis of a large set of data. Once the starting information is gathered, the fits run unattended and save reports of the results.

3) Troubleshooting, Resolution Smearing, and a description of the input file format
Frequently Asked Questions About SANS Analysis

Overview

The scattering functions available here are designed to fit models of a given structure to your SANS or USANS data. In this documentation, I have used SANS and USANS interchangeably, since the data can be treated in the same way with the same models.

In this curve fitting approach to modeling scattering data, you propose a structure, and then try to fit that model to your data. If the model does not fit the data well, the proposed structure is not correct. The converse not strictly true - that is a model that fits the data well

does not guarantee that the model is a perfectly accurate description of your physical sample. But given your a priori knowledge of what is in the sample, what structures and sizes are likely to be present, and what you know to be physically reasonable, a good model fit is likely to be the correct answer. Therefore it is in your best interest to have as much information about your sample as you can from other measurement techniques as well as a good understanding about how your sample physically behaves. If possible, simpler, model -independent analysis should be done too (Rg, I(q=0), Invariant, etc.). Simply putting a totally unknown sample in the beam and hoping to fully characterize it from a single SANS measurement is quite unrealistic.

Documentation of all of the model functions and details of their use (with references), is given in a separate help file, SANS Model Function Documentation

The SANS Data Analysis Tutorial guides you through the steps of modeling your averaged (1-D) SANS data using available model functions and IGOR Pro's built in non-linear least squares fitting routines. Detailed statistical information about the goodness-of-fit are provided, including chi-squared error, uncertainty in fitted parameters, confidence intervals, and covariance. This simple analysis only uses a fraction of IGOR's curve fitting capabilities. Refer to IGOR Pro's online Curve Fitting help for the full details.

Requirements

NOTE: You DO NOT need to purchase IGOR Pro to model your data. You can use either the (free) Demo version of IGOR Pro, or the full version. IGOR Pro 6.0x or higher is required. (*The use of certain trade names or commercial products does not imply endorsement of a particular product by NIST, nor does it imply that the named product is necessarily the best product for the stated purpose.)

IGOR Pro is available at: <http://www.WaveMetrics.com> .

Demo users can perform all of the curve fitting and analysis as described in this manual. Publication graphics, of course, cannot be saved or printed. Fitted model curves can be exported as ASCII data for plotting with other software. Fitted parameter tables can be hand copied. Borrow a pencil if necessary.

What's New in SANS Analysis

Package version 7.2 (05/2013)

Auto Fit (or Batch Fitting)

This package provides the capability to batch fit a single model to a large number of data sets to speed up analysis of a large set of data. Once the starting information is gathered, the fits run unattended and save reports of the results.

In version 4.1 (Package 7.14) (02/2013)

• A new option has been added to the Fit Manager, a panel to allow rescaling of the data axes. See Rescaled Axis.

• The quality of data fits can be monitored in several new ways:
(1) The standard deviation of the fitted parameters is displayed directly on the FitWindow table after a fit is complete. If the relative errors are > 50% of the nominal parameter value, then the standard deviations are show BOLD and RED. You'll need to figure out which parameters are ill-determined.
(2) The correlation matrix can be viewed. This is a direct indicator of model parameters that are correlated and leads to non-unique solutions. See the WaveMetrics help for and explanation of the Correlation Matrix.
(3) Chi-squared can be mapped out as any chosen parameter is varied. This provides an empirical view of how sensitive the model fit is to any parameter, and confirmation that the parameter is at a minimum at the solution.

In version 4.1 (Package 7.10) (03/2012)

• A beta version of real-space modeling has been added, allowing Debye's sphere method to be used to calculate the scattering from 3D structures in real-space. FFT version of the calculation provides 2D information, and a binned distance method provides a much faster calculation. See Real-Space Modeling of SANS Data

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In version 4.1 (Package 7.04) (12/2010)

• New options added to curve fitting. Residuals and a TextInfoBox can be appended to the graph.

• The standard deviation of the fitted parameters is now automatically added to the table in the main Fit Panel.

• 2D resolution smearing has been added.

In version 4.1 (Package 7.0) (04/2010)

• A Simple Global Fitting module has been added that is simpler to set up global fitting for the special case of two data sets, typically one USANS set and one SANS set from the same sample.

• Genetic Optimization has been added as an optional search method for non-linear fitting. (Andy Nelson, ANSTO)

• 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.

• Reduced 1D data in canSAS standard XML format can be loaded for analysis.

• Complex constraints of coefficients can be entered as well as simple bounds. See Parameter Constraints

• Experimental data that has been modified (trimmed, rescaled, etc.) can be easily saved to disk.

In version 4 (2/2008):

• The "Fit Manager" now provides a unified interface to load and plot data, plot and append models, adjust coefficients, and setup and perform fits to data. This largely shields a user from needing to know how Igor operates, and lets them just do what they want with their data. Much of the user interaction that was previously needed to select data and options for fitting are now automatically selected.
• Coefficient tables for models are now confined to the Fit Manager window, reducing clutter.
• More feedback about the fit results is presented on the Fit Manager window.
• 2D SANS Analysis is now available. Model functions are courtesy of the DANSE project.
• Model functions are available as a compiled XOP and threaded for multiple processors when practical for a speed boost of 6-7x for the XOP, and an additional 0.9*Nprocessors for threading.
• USANS slit-smearing calculations now use a matrix calculation method that is oodles faster.
• Reports that show the details of the fit and the graph in a convenient one-page notebook can be generated.
• Global fitting has been updated to be more generic, allowing different functions for each data set. It has also been streamlined to be (somewhat) easier to set up.
• A Plot Manager has been added to allow easier loading and plotting of data.
• Smeared models can be plotted multiple times, with each instance attached to a specific data set and its proper resolution function. Especially useful for SANS and USANS data plotted together.
• Direct link to a web page for feedback, bug reports, and feature requests.

- **SANS Data Analysis Tutorial**

Overview of Fitting
Loading SANS Data
Plotting a Model Function
Testing the Model
Setting up the Fit Parameters
Fit Results
Plotting a Resolution Smeared Function
Parameter Constraints
Exporting SANS Models
Freeze SANS Models for Comparison

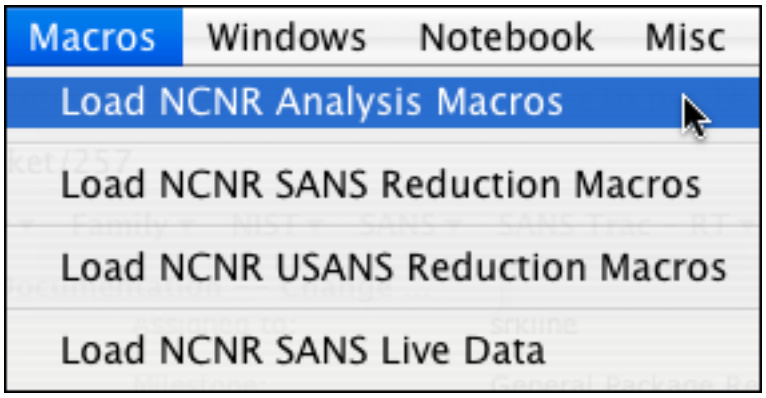
see also: Fit Manager
Loading USANS Data
2D SANS Analysis

Overview of Fitting

The general procedure for fitting a model to your data is:
1) Load in your SANS data
2) Plot a model function
3) Visually adjust the model parameters
4) Set up the curve fitting parameters
5) Do the fit
6) Make publication-quality graph

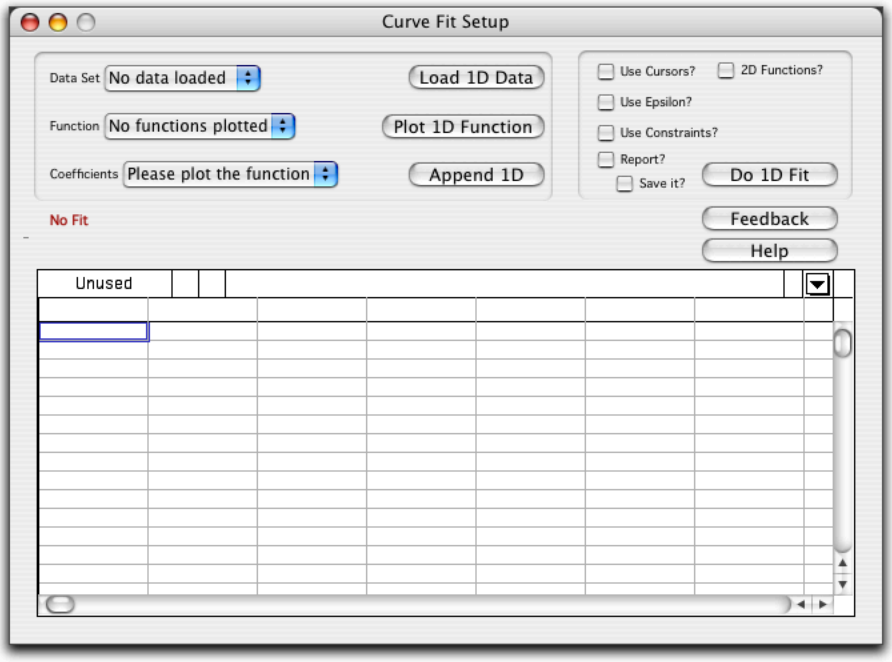
This tutorial will use a real SANS data file "Apoferritin.abs" located in the Sample Data folder that was downloaded as part of the NCNR macros package. This data "Apoferritin.abs" is the output data file from the SANS Data Reduction tutorial.

To get started, choose "Load NCNR Analysis Macros" from the Macros menu:

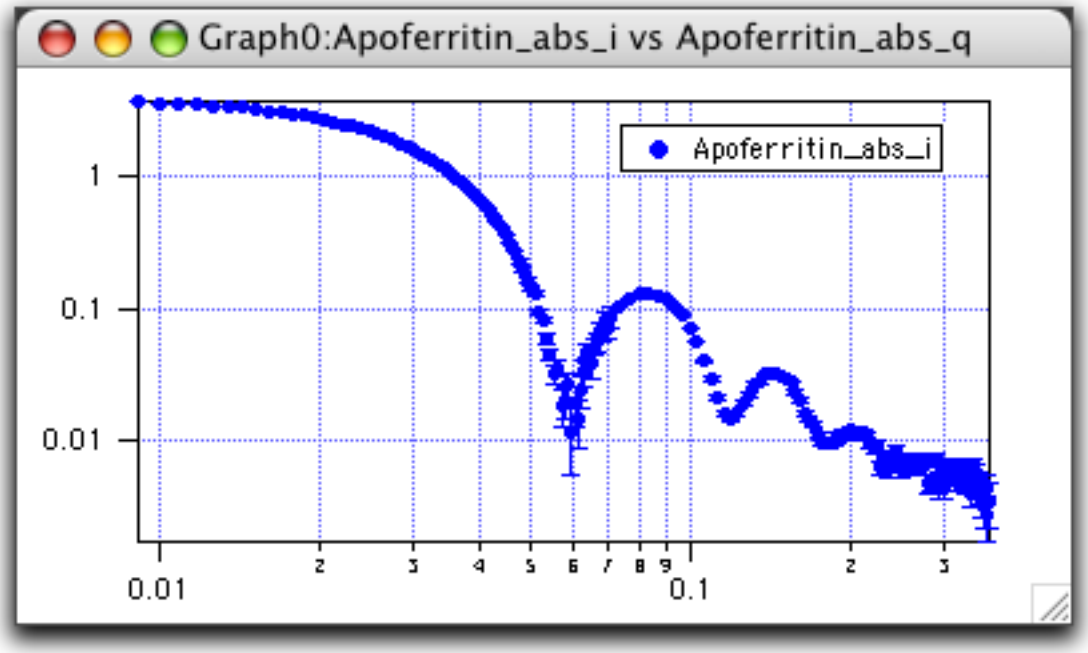


Loading SANS Data

Upon loading the NCNR Analysis Macros, the Fit Manager and the SANS Model Picker will open, and a SANS Models menu will appear. To load a data set, use the "Load 1D Data" button on the Fit Manager:



and you will be prompted to select a data file. Choose the Apoferritin.abs file, and it will automatically be loaded and graphed.



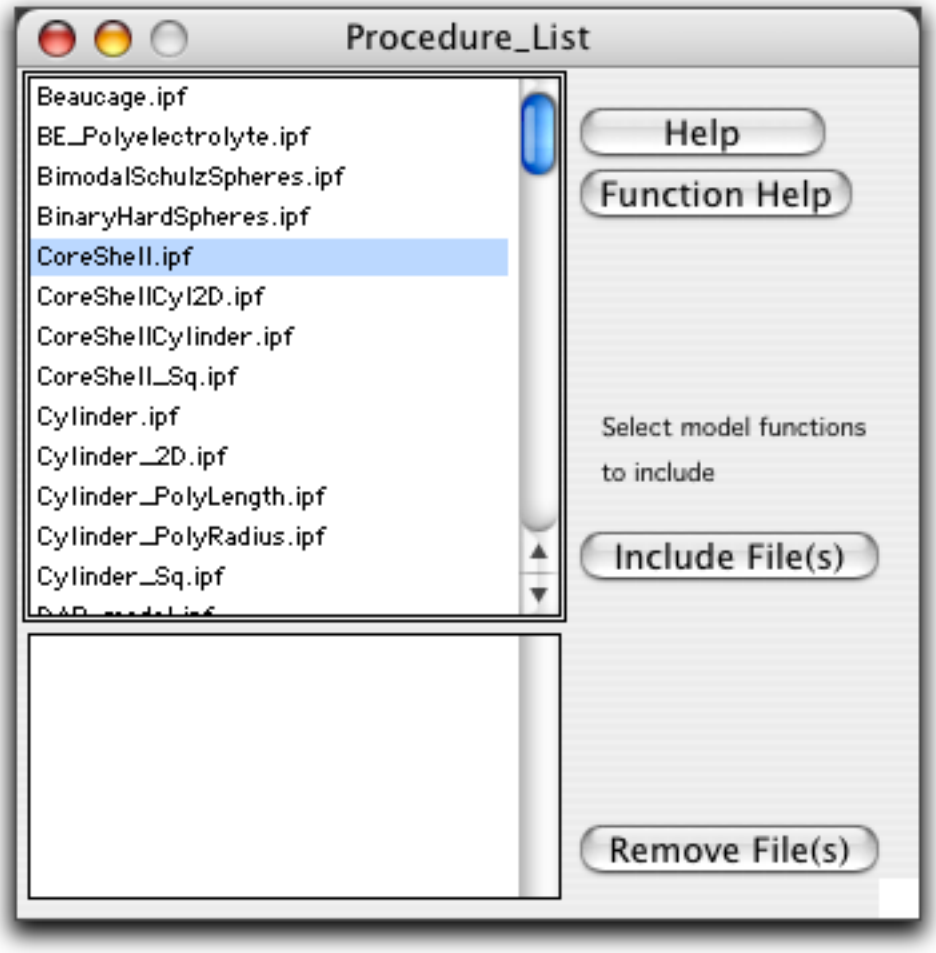
The Apoferritin.abs data file is loaded into a data folder, and the macro automatically names and tags each column of data to uniquely identify them. If you're curious, select the Data Browser from the Data menu, and you will see a data folder "Apoferritin_abs", which contains 4 "waves":

Apoferritin_abs_q "q" = q-values

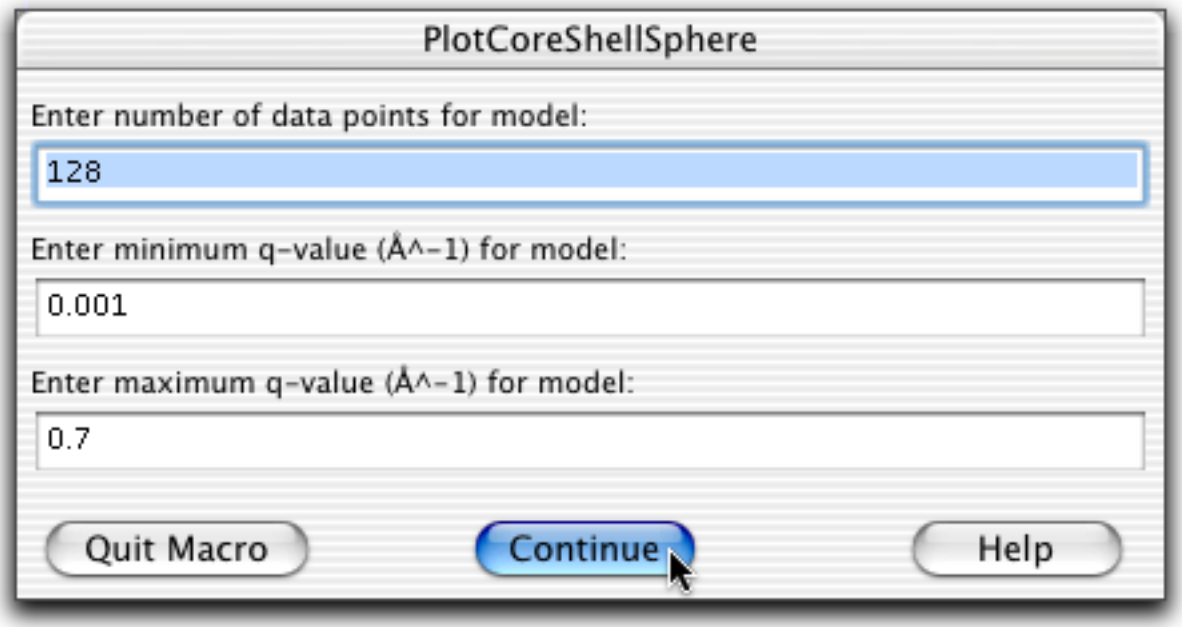
Apoferritin_abs_i	"i" = intensity
Apoferritin_abs_s	"s" = standard deviation of intensity
Apoferritin_abs_res	"res" = the instrument resolution information

Plotting a Model Function

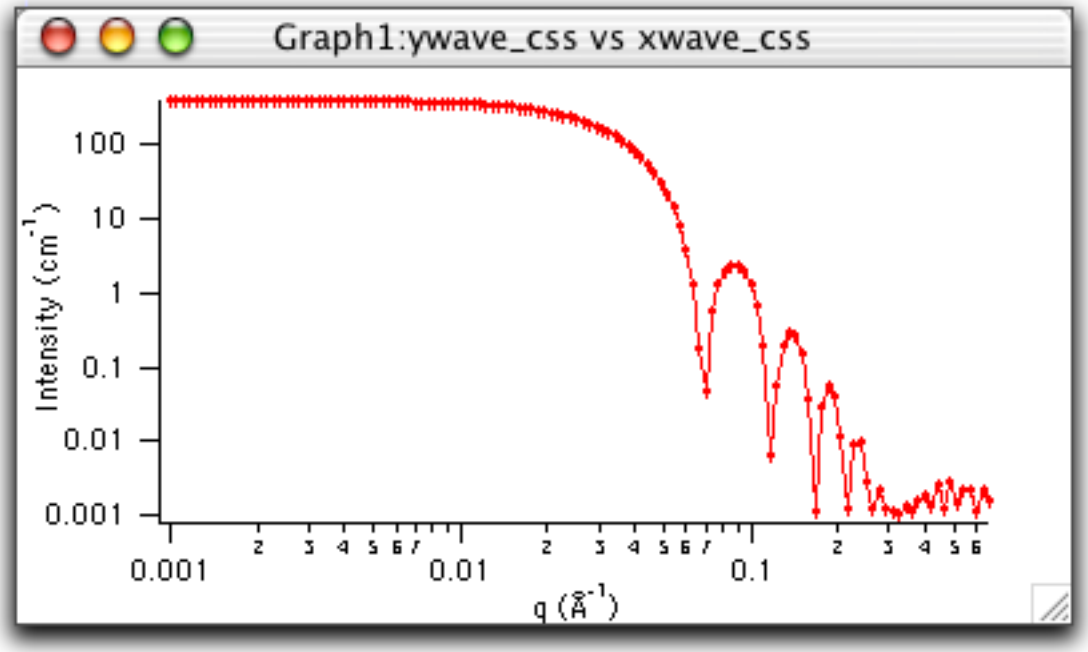
When the analysis macros are initially loaded, there are no model functions available. Each model must be included individually, as needed. For this tutorial, include the CoreShell model by selecting it in the list, and clicking "include". The file will appear in the lower list of files that are currently included, and the CoreShell model will appear under the "Function" popup on the Curve Fit Setup panel (the Fit Manager).

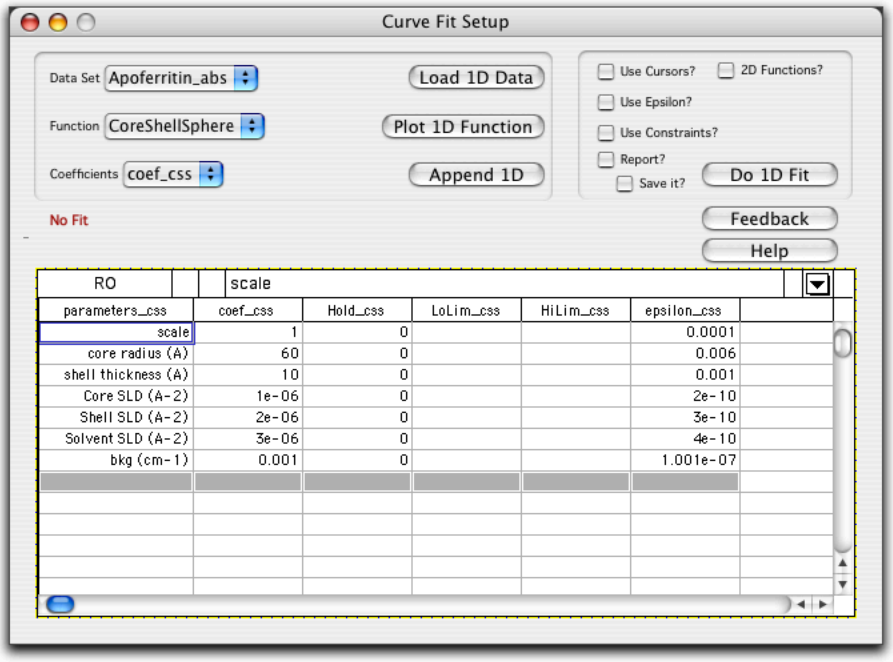


Model functions are plotted by selecting the appropriate function from the popup, either resolution smeared, or unsmeared and then the "Plot 1D Function" button. These "Plot" macros will create the x and y waves of model data, a table of adjustable parameters, and graph the model function. Plot the CoreShellSphere function from the panel, taking the default number of points and q-range:



click "continue" to accept the default ranges, and the following graph is generated, and the coefficients for the model function are inserted in the table.

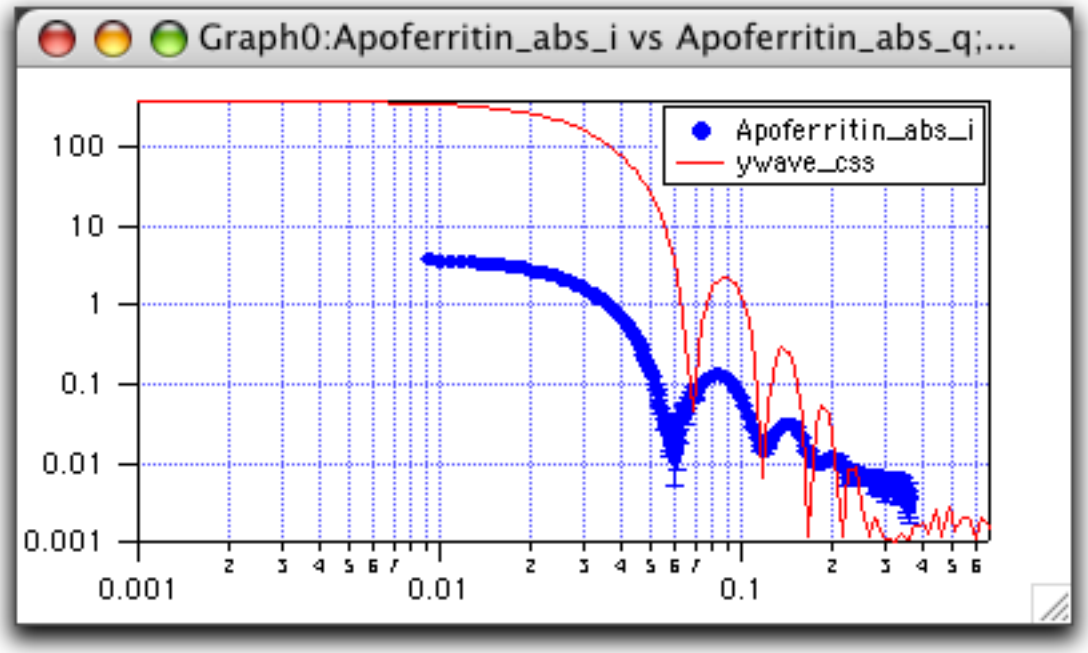




The table of fitting coefficients appears directly below the set of popups. Plotting a model function creates x and y values with appropriate extensions, xwave**_ext** and ywave**_ext.** Coefficient and parameter waves are likewise created for the table. For the Core-shell sphere model, the extension is "**css**". If you're curious about the details of the model calculation, documentation of each model is available and the code is visible under the Windows->Procedure Windows menu.

Testing the Model

What we really want to see is how the model compares to the experimental data. Add the model data to the experimental data by bringing the graph of the experimental data to the front, then choosing the "Append 1D" button on the Fit Manager. Note that you will be appending the "active" function (whatever is currently selected in the popup) onto the "active" window (whatever is on top).

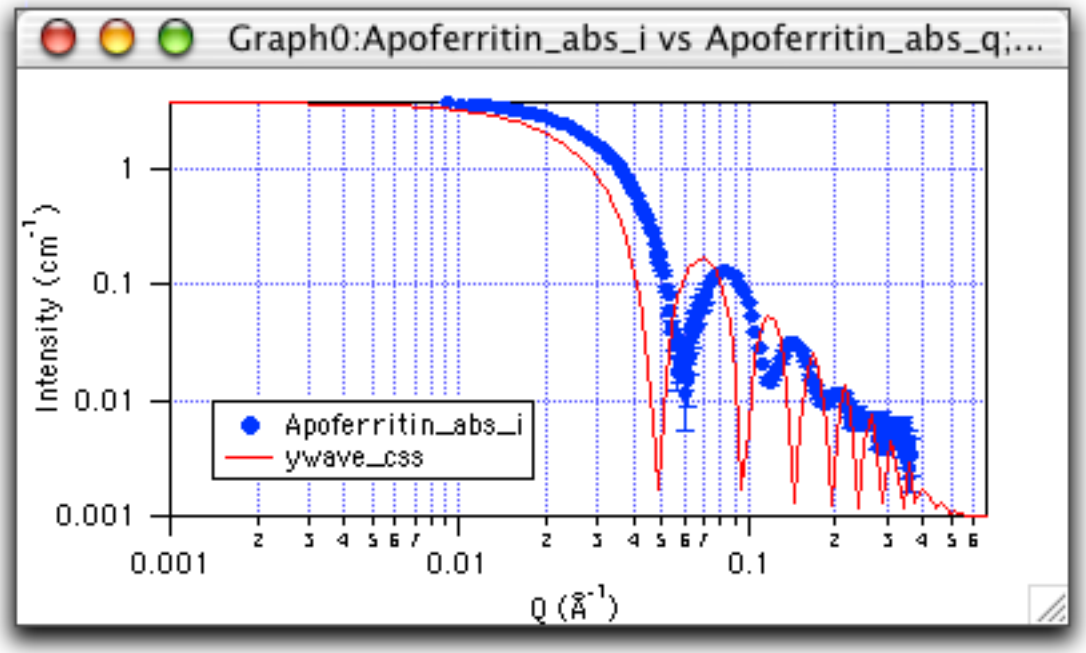


The model data has been appended to the graph, and is in fact a poor representation of our experimental data. Let's see how changing the parameters affects the model. The model intensity "ywave_css" is a "dependent object" - that is, the wave depends on the parameter values in the table - change any of the values, and the data in the graph is automatically updated. For the apoferritin sample, we know that it was prepared in deuterated water at a concentration of 1% by volume. From the crystal structure of the protein, it is also known that the structure resembles a hollow spherical shell of protein. So set the scale equal to the volume fraction, and the scattering length densities of the solvent and the core (which is filled with solvent) to the scattering length density of D_2O. If you don't know this number, a very useful tool for calculating scattering length densities can be found at: <http://www.ncnr.nist.gov/resources/sldcalc.html>, along with a growing list of tools for planning your experiment at NIST.

The coefficients in the table should look like this:

R5			6.35e-06	
parameters_css			coef_css	Hold_css	Lo
scale			0.01	0	
core radius (A)			60	0	
shell thickness (A)			10	0	
Core SLD (A-2)			6.35e-06	0	
Shell SLD (A-2)			2e-06	0	
Solvent SLD (A-2)			6.35e-06	0	
bkg (cm-1)			0.001	0	

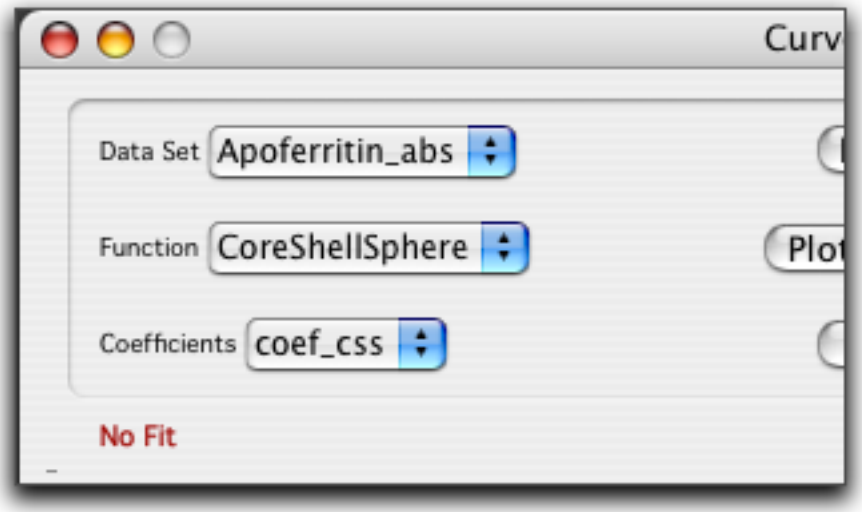
and the graph, now much closer to the data:



You can play with the parameters more, if you like. These values should be close enough to use as initial guesses for the non-linear fitting. Depending on the particulars of the model, the initial guess can be very poor, or may need to be relatively close.

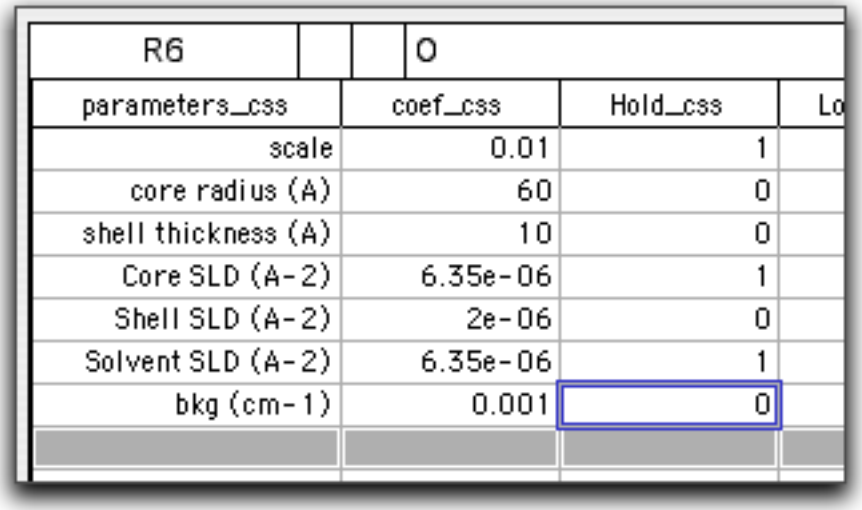
Setting up the Fit Parameters

You're ready to fit the core-shell model to the data now. All of the curve fitting setup can be done from the Fit Manager Panel. First, make sure that the data set and function are properly selected, like this:



This will set the data set to fit (using the appropriate statistical weighting, and resolution if fitting to a smeared model) and the function to use, and your initial guesses for the parameters.

Since we know the values of the scale and two of the scattering length density inside and outside (both D2O), we want to hold these values fixed during the fitting. Enter "1" in these rows of the "Hold_css" column of the table. Values of "1" will be fixed at your guesses, and "0" will be automatically adjusted during fitting. The table will now look like this:



R6 | | | O

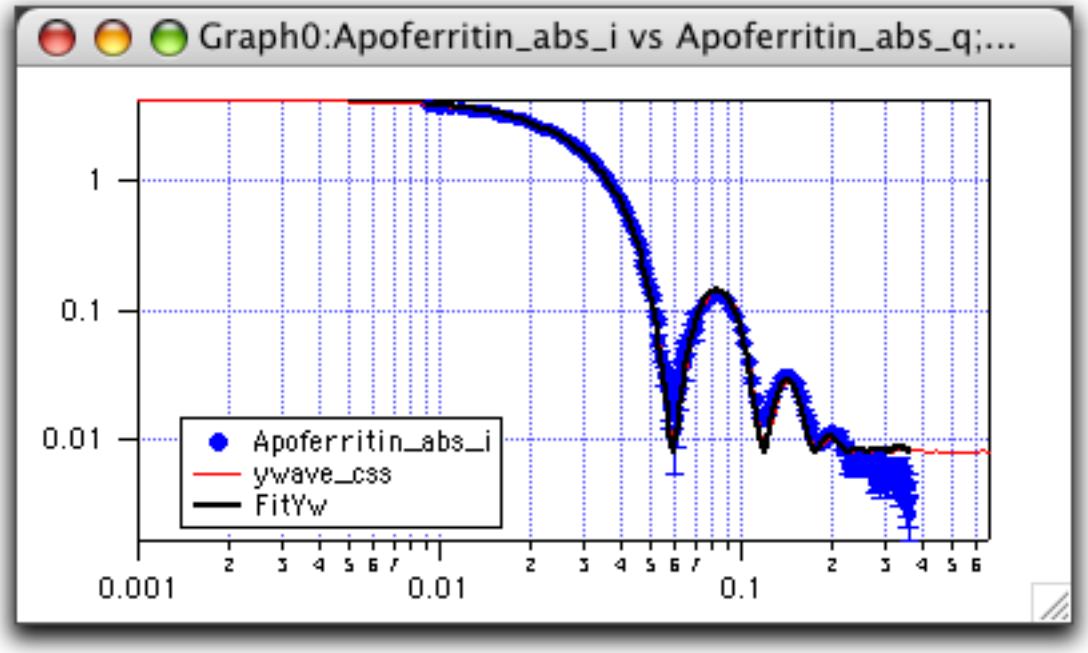
parameters_css	coef_css	Hold_css	Lo
scale	0.01	1	
core radius (A)	60	0	
shell thickness (A)	10	0	
Core SLD (A-2)	6.35e-06	1	
Shell SLD (A-2)	2e-06	0	
Solvent SLD (A-2)	6.35e-06	1	
bkg (cm-1)	0.001	0	

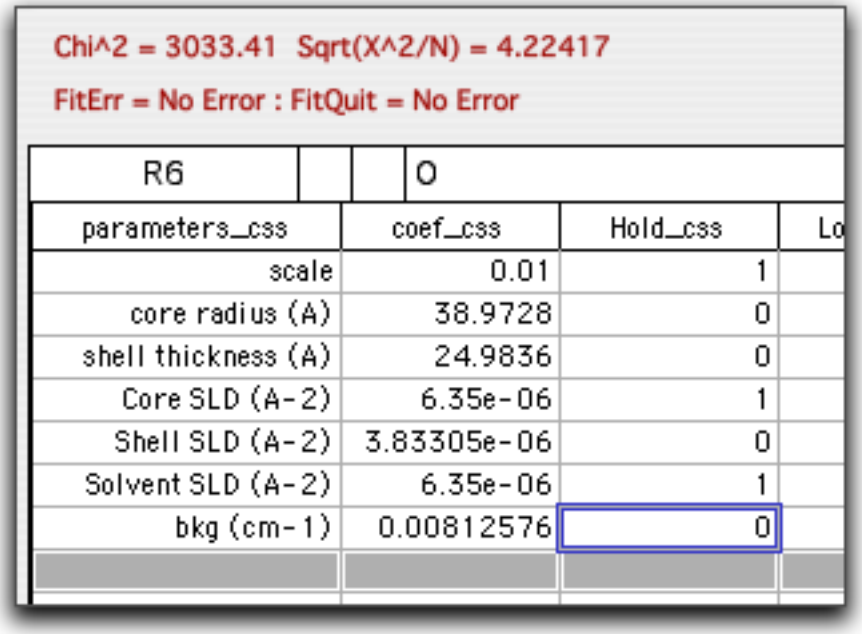
Simple Parameter Constraints can also be entered on this table and is discussed later. For now, leave the LoLim_css and HiLim_css columns empty.

Fit Results

Click "Do 1D Fit, and the fit will be performed, updating the model as it (quickly) converges to

a solution. The best-fit parameters and one standard deviation are reported to the command window at the bottom of the screen, and reflected in the table. The W_sigma column at the far ritght of the table represents one standard deviation of the fitted parameters. ALWAYS think about whether the returned values are physically reasonable based on what you know about your sample. Unphysical results may indicate an error in setting up the fit operation or indicate that the model is a poor representation of the sample. "FitYw" is the fitted result, appended automatically to your graph. The model ywave_css also reflects the best-fit coefficients.





Chi^2 = 3033.41 Sqrt(X^2/N) = 4.22417

FitErr = No Error : FitQuit = No Error

R6 | | | O

parameters_css	coef_css	Hold_css	Lo
scale	0.01	1	
core radius (A)	38.9728	0	
shell thickness (A)	24.9836	0	
Core SLD (A-2)	6.35e-06	1	
Shell SLD (A-2)	3.83305e-06	0	
Solvent SLD (A-2)	6.35e-06	1	
bkg (cm-1)	0.00812576	0	

The fit is not too bad, but could be better. The "V_chisq = 3033.41" that Igor reports is the sum of the chi-squared values for all of the data points fitted (V_npnts = 170).

$$V\_chisq = \chi^2 = \sum \left(\frac{y - y_i}{\sigma_i} \right)^2$$

Chi-squared values are typically reported as a reduced chi-squared, or:

$$Sqrt\{\chi^2/(N - f - 1)\}$$

Where N is the number of data points and *f* is the number of degrees of freedom in the fit (the number of free parameters). From the definitions, it is clear that a reduced chi-squared of one would signify that, *on average*, the model fit is within one standard deviation of each data point. Note that the error estimates on the intensity will give unrealistic chi-squared values if they are not truly representative of the statistical uncertainties.

For this fit, the reduced chi-squared is 4.22 (since there are 4 free parameters). Statistically (and even visually) the fit is certainly not the best representation of the data. The CoreShellForm model did not take the instrumental resolution function into account, and for this example, is likely the cause of the artificially high background value at high q (q > 0.2 $Å^{-1}$).

Plotting a Resolution Smeared Function

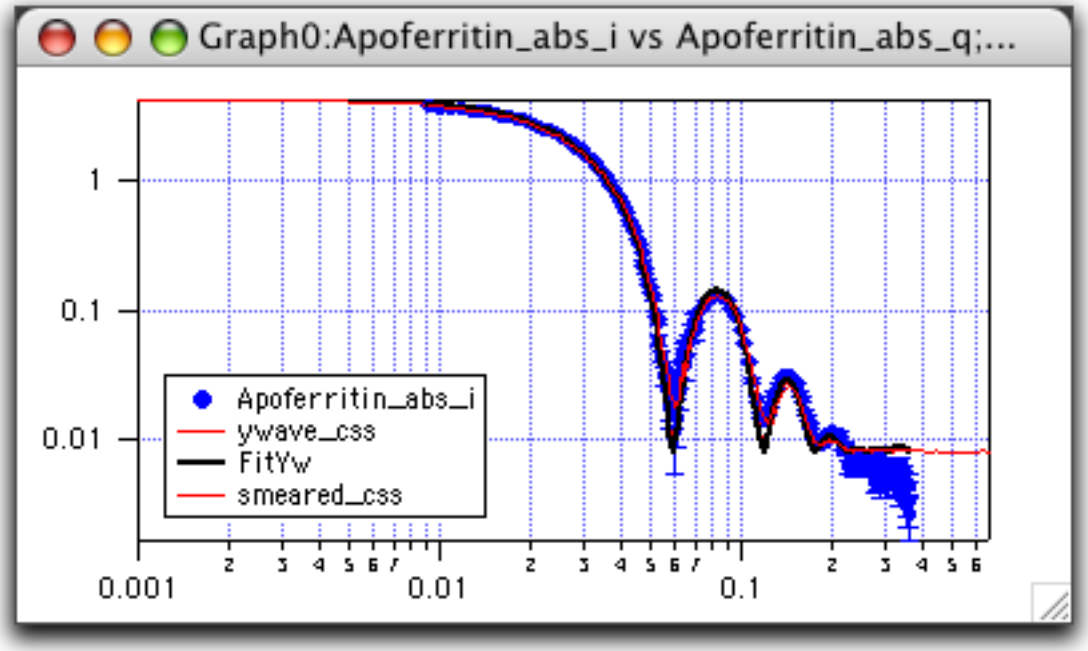
Including instrumental resolution effects into the model calculation is easy, and in some cases can have a significant effect on the best-fit parameters. The resolution information is automatically generated in the apoferritin data file (and in all NIST SANS and USANS data files) and describes the "smearing" effect of the wavelength distribution, apertures, detector resolution, etc... The model function is smeared with the resolution information, and then the

smeared model is fitted to the (smeared) experimental data. More information about Resolution Smearing can be found in the Frequently Asked Questions About SANS Analysis section at the end of this help file.

NOTE: In older versions of the SANS Analysis macros, the resolution information that is used for the smearing calculation was taken from the most recent data file that was read into the experiment. In this version, smeared models are specifically attached to data sets, so that the correct resolution is always used.

Select "SmearedCoreShellSphere" from the function popup, with the Apoferritin_abs data set selected. Note that the coefficients tab now reads "Please plot the function", since the smeared CoreShellSphere has not been plotted for the Apoferritin data set. "Plot 1D Function" will plot the model, and generate a graph that quickly disappears. No dialog to select the number of data points or the q-range is presented, since these values are set by the experimental data.

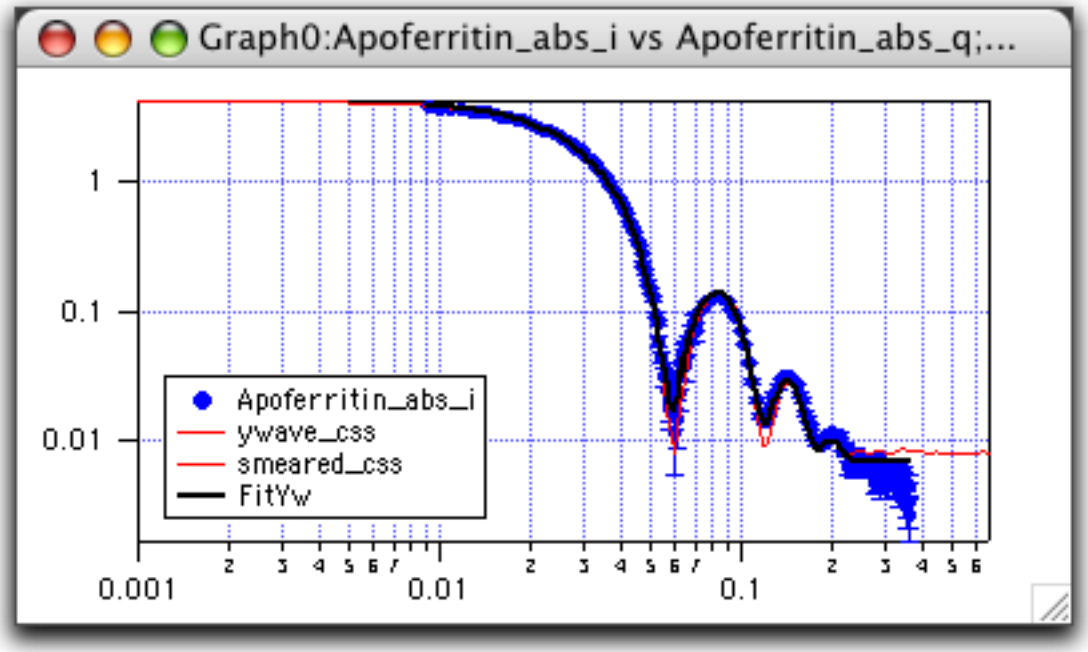
Be sure that your data is the top graph (by clicking on it). "Append 1D" will append the smeared_css model to the graph. Change the smeared coefficients to the best-fit values from the unsmeared model, and you should have a plot something like this, where the oscillations of the model have been smeared out by the resolution function. There is not a large difference here, but it is clear that the sharp minima are reduced somewhat in the smeared model. Setting the background to zero in each of the smeared and unsmeared models provides a more clear view of the effect of instrument resolution.



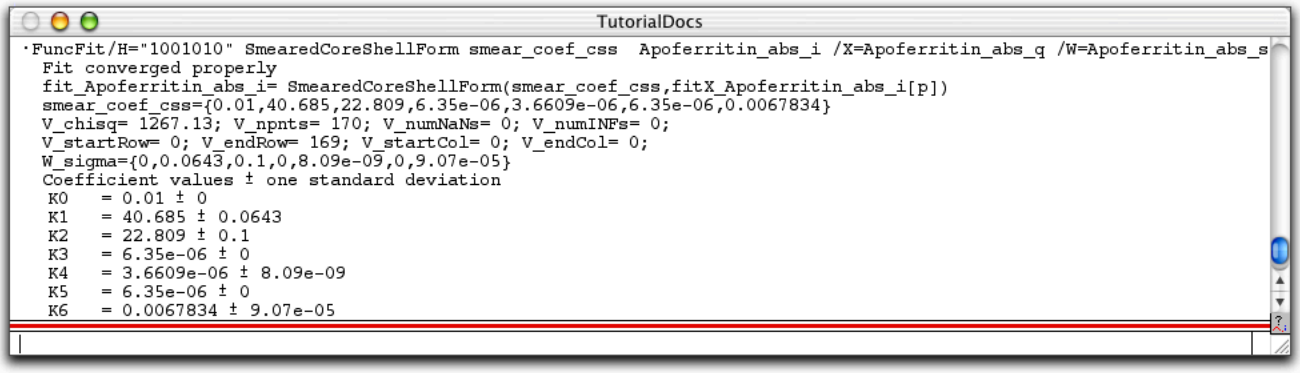
Fitting the smeared model to the data follows the same sequence as for the unsmeared model. Set the "smear_coef_css" values to the results of the unsmeared fit, and set the Hold_css values to "1" for the same parameters, like this:

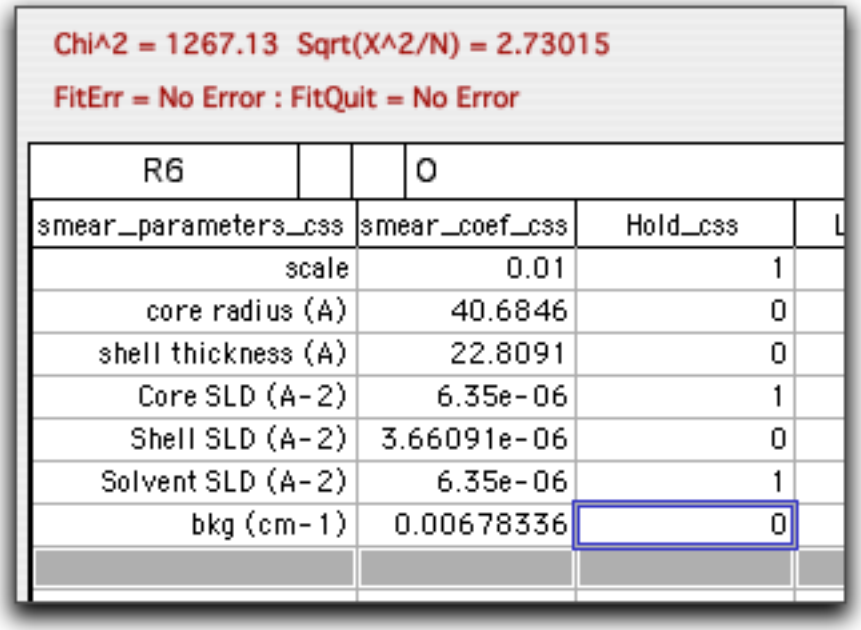
R6			O	
smear_parameters_css		smear_coef_css	Hold_css	L
scale		0.01	1	
core radius (A)		38.9728	0	
shell thickness (A)		24.9836	0	
Core SLD (A-2)		6.35e-06	1	
Shell SLD (A-2)		3.83305e-06	0	
Solvent SLD (A-2)		6.35e-06	1	
bkg (cm-1)		0.00812576	0	

If the column names are not "smear...", be sure that you have the "SmearedCoreShellSphere" function selected from the popup, which automatically updates the "smear_coef_css" coefficients. Once all is set, click "Do 1D Fit", and the fit is done. The fit should be rather quick this time, since the initial guesses are very good. The final fit is visually "better" when resolution is included, and is also numerically better since the resolution smeared model is a better representation of the measured intensity.



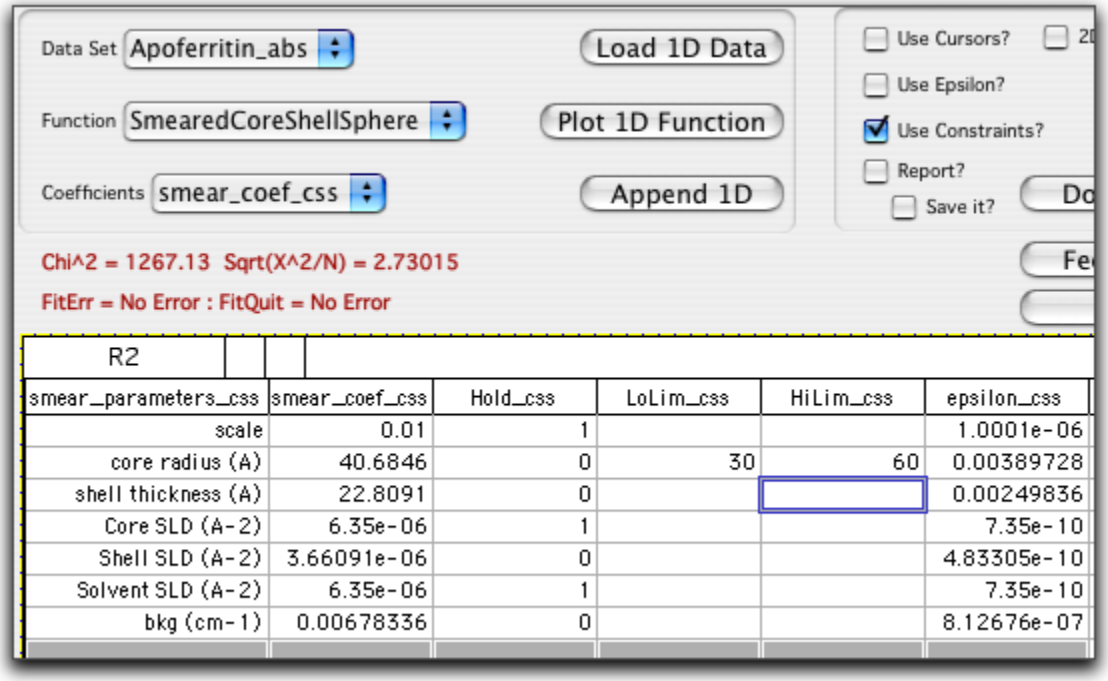
The best-fit coefficients from this fit are also reported in the command window, and can be compared to the results of the unsmeared fit. Chi-squared has improved significantly, and the parameter values have changed slightly.





Parameter Constraints

Although not necessary in this simple example, constraints can be placed on coefficient values during the fitting. Bounded coefficients are often critical for highly nonlinear functions, or helpful in cases where a range of allowable values can be set. Constraints are set in the fit Manager in the table of coefficients. You can, for example, set simple bounds on the core radius to values which you know are physically reasonable. First, check the box "Use Constraints?", then enter the values for the lower limit in the "LoLim_css" and the upper limit in the "HiLim_css" columns. Fitting will be constrained to these bounds. Setting these simple bounds can be helpful in keeping a very non-linear fit to within physically reason for your sample.



smear_parameters_css	smear_coef_css	Hold_css	LoLim_css	HiLim_css	epsilon_css
scale	0.01	1			1.0001e-06
core radius (A)	40.6846	0	30	60	0.00389728
shell thickness (A)	22.8091	0			0.00249836
Core SLD (A-2)	6.35e-06	1			7.35e-10
Shell SLD (A-2)	3.66091e-06	0			4.83305e-10
Solvent SLD (A-2)	6.35e-06	1			7.35e-10
bkg (cm-1)	0.00678336	0			8.12676e-07

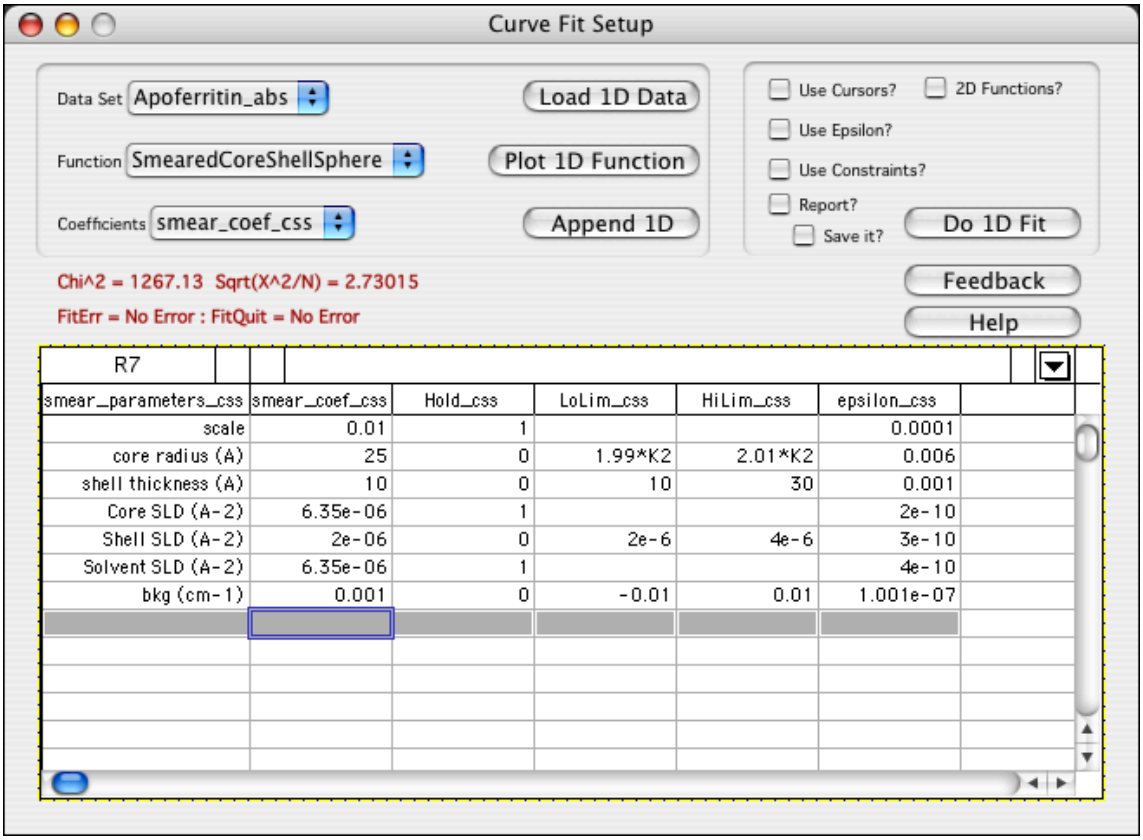
Simple bounds can be set here, or more complex relations between the variables can be created very similar to the techniques used in linear programming. That means inequalities, and nothing that is non-linear. See the IGOR Pro help file Fitting With Constraints for all the details. A simple example is shown below:

- For this type of constraints, the coefficients are referred to by Igor's internal variable notation K(0-n). Here there are 7 coefficients, K0 through K6.

Lower limits are interpreted as:
Kn > value K1 > 30 in the panel above
Upper limits are interpreted as:
Kn < value K1 < 60 in the panel above

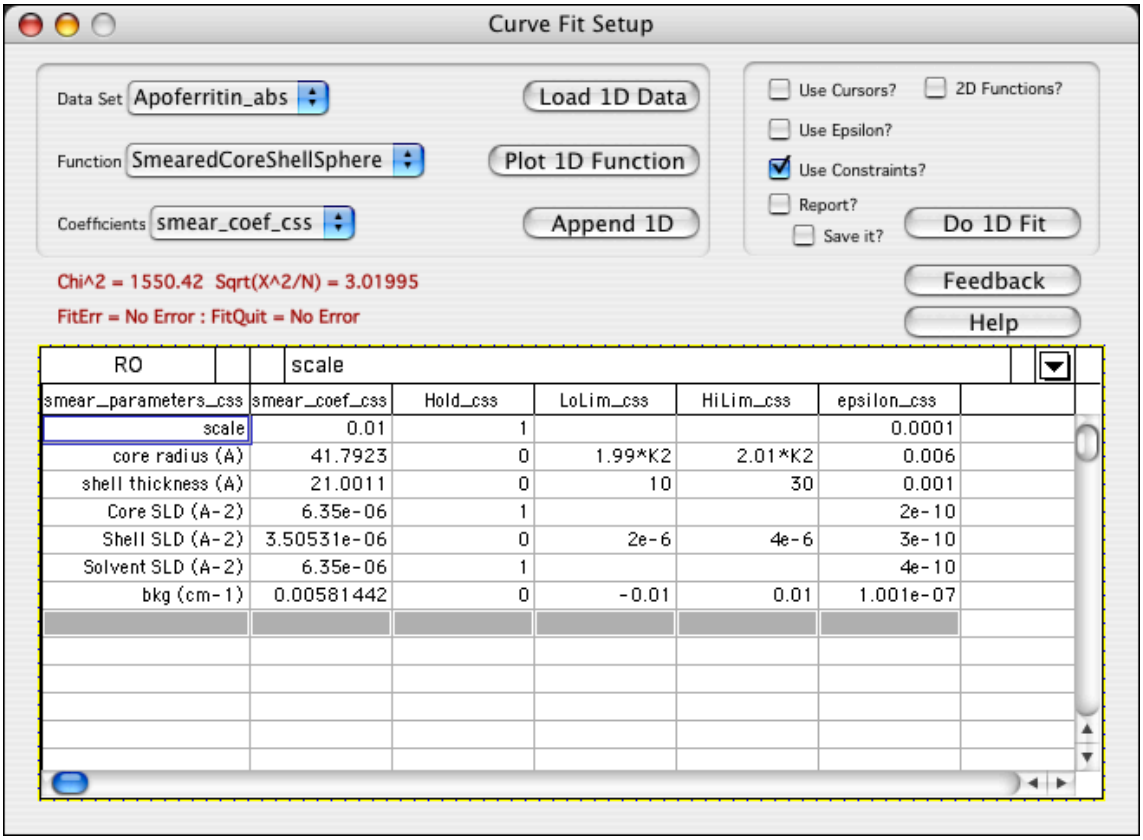
So simple bounds constrain K1 (the core radius) to be between 30 and 60 (Angstroms). If you want equality, the preferred way is to hold it fixed. Otherwise you can set very tight inequality relations to "pinch" the value to what you want.

For more complex constraints, like a completely fictional requirement that the core radius be equal to 2x the shell thickness, you can set it up like this: (remembering that equalities are not allowed, and don't put in initial guesses that grossly violate the constraints):



This lets the shell float to its optimal value, given the constraints that:
K1 > 1.99*K2 and
K1 < 2.01*K2 (effectively making the core radius = 2* shell thickness)

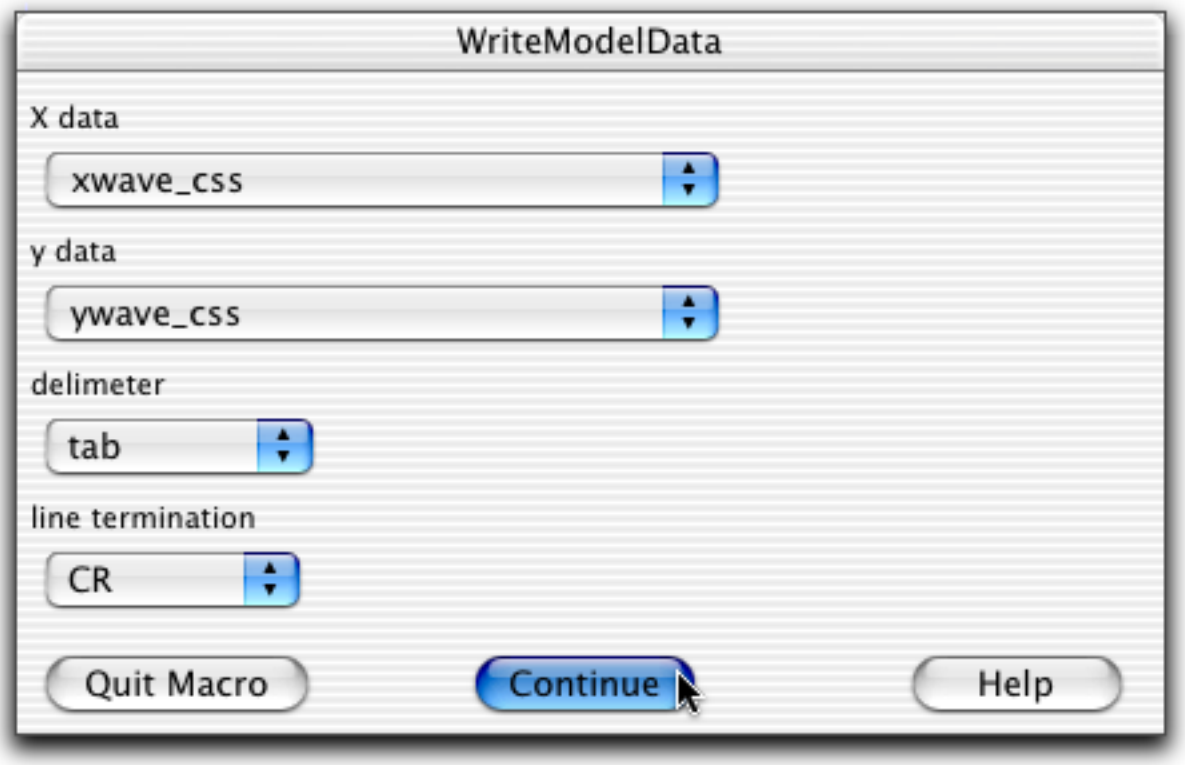
And the result of the fit is:



You can see that the fitted core radius is at the lower limit of the constraints (21*1.99 = 41.8) and is not much different from the upper limit (21*2.01 = 42.2). You could pinch the bounds in tighter if you like. Compared to the fit where the core and shell are independent, this constrained fit has a slightly poorer chi-squared, but is still quite good.

Exporting SANS Models

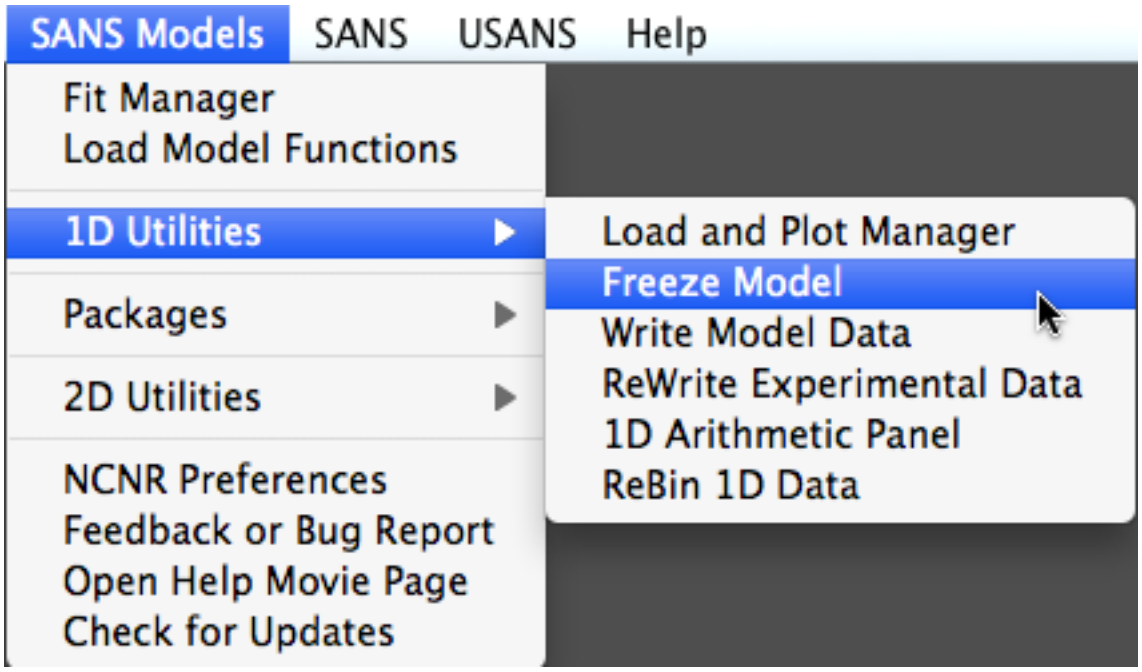
You can export the model calculations as x-y data, in a two-column ASCII format. Choose "WriteModelData" from the Macros menu, and the following dialog appears:



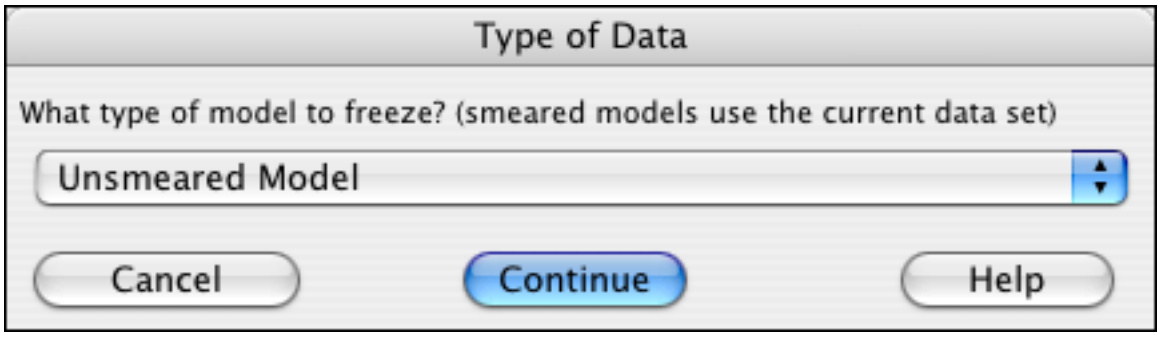
Choose the desired waves from the popup menus, select the delimiter (either a tab or 3 spaces) and the line terminator. Macintosh uses a carriage return (CR), Unix uses linefeed (LF) and Windows uses both (CRLF). Continue, and you will be prompted for a filename for the exported data. If you have a full version of IGOR Pro, you have a variety of other save options available using "Save Waves..." under the data menu.

Freeze SANS Models for Comparison

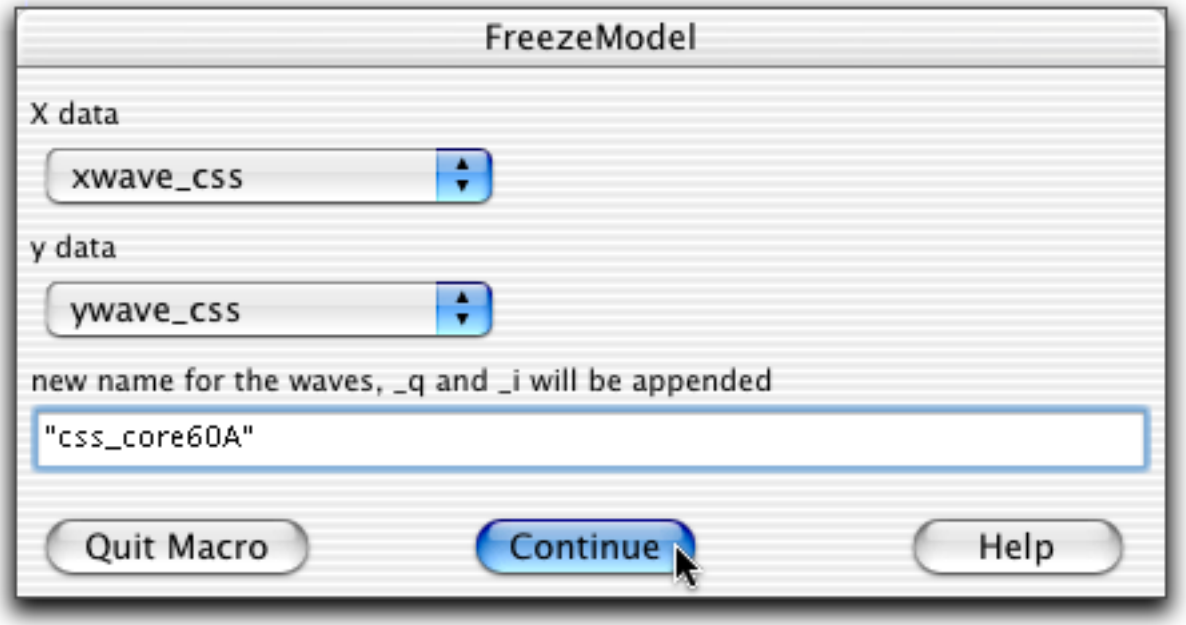
When planning an experiment it is helpful to simulate the scattering for various conditions to optimize the expected signal, or to optimize the desired q-range for the instrument. When you have a model function plotted, from the SANS Models Menu, choose "1D Utilities -> Freeze Model":



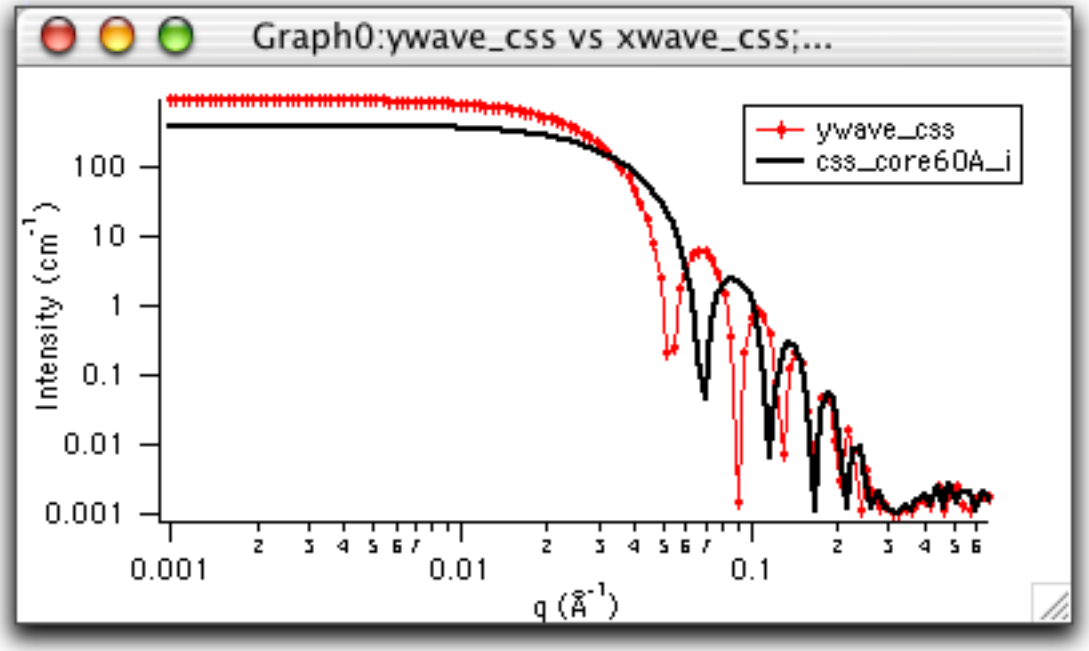
This will present you with a dialog for you to select the model intensity that you would like to keep a copy of, "frozen" with whatever parameters are in the table. You'll be presented with a dialog to choose either an unsmeared or smeared model:



In this example, it is an unsmeared core shell sphere model with its default parameters of a core radius of 60 A. So for the saved name, choose something appropriate. These two waves are created with "_q" and "_i" tagged at the end to keep the notation consistent. Note that the waves are NOT saved to disk - they are in memory, and will be saved with your experiment. If you want to save the waves to disk, use "WriteModelData" to do this.



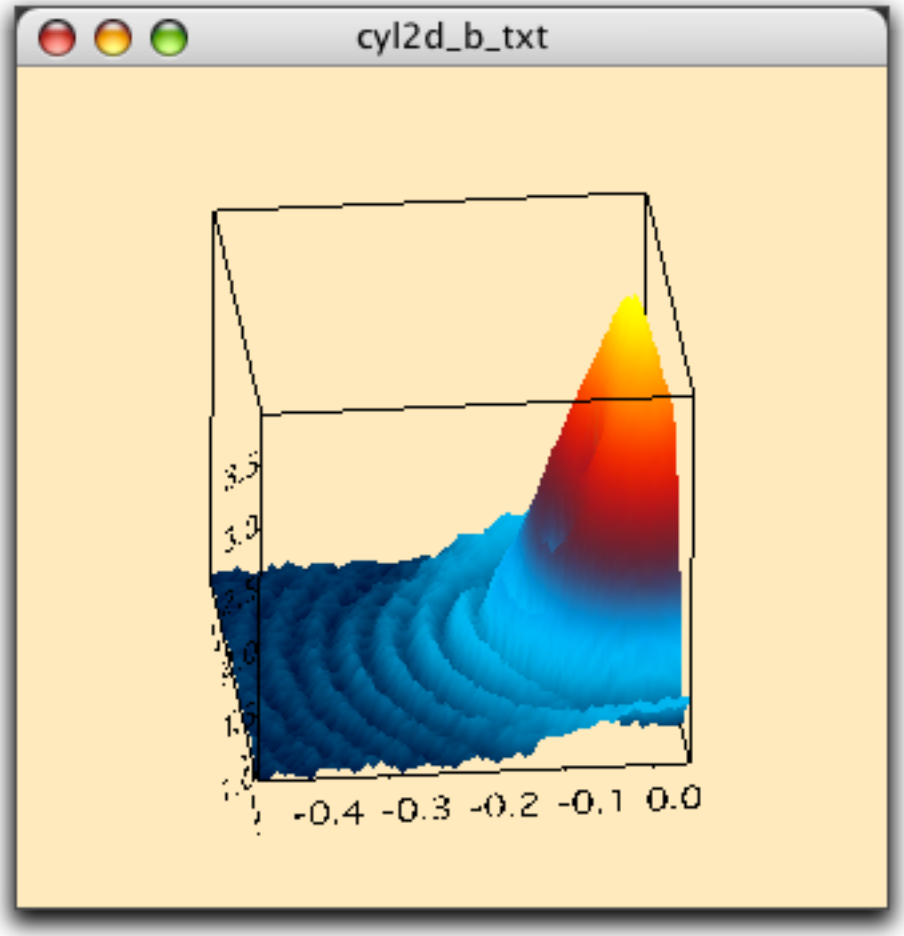
The "frozen" I(q) that you have just made will be appended to the top graph, typically the original model calculation. You won't see it initially, since it's exactly the same as the current model. But changing the core radius to 80 A in the CoreShell model changes ywave_css, and it is clear that this increase in radius shifts the form factor minima to lower q-values, since the radius is larger versus the 60 A radius in the frozen model.



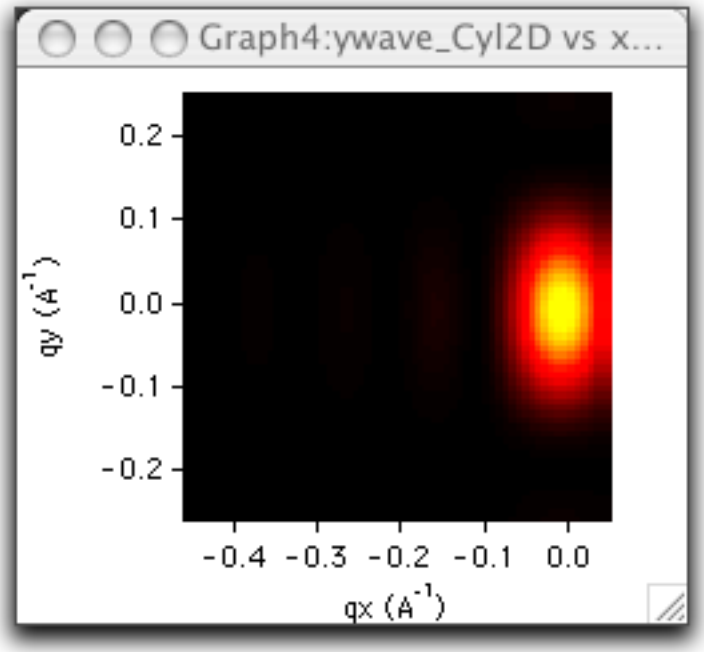
2D SANS Analysis

Anisotropic SANS data can be modeled in a full 2D format from the Fit Manager when the "2D Functions" checkbox is selected, enabling the 2D functionality. The input format for the 2D data files is the "QxQy ASCII" output from the NCNR SANS Reduction package. If you want to simulate data, you can create a "fake" QxQy data set using Macros->Fake QxQy and choosing an appropriate Qx Qx range.

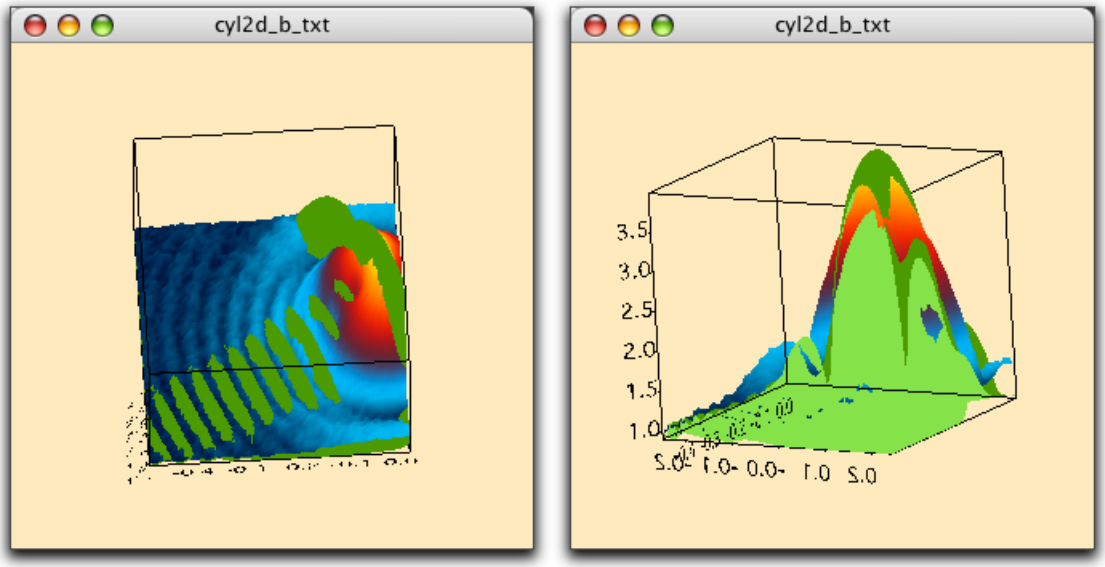
Load the 2D Sample data set cyl2d_b.txt using the "Load 2D Data" button. The data is displayed as a surface plot that can be rotated to view at any angle. The graph below has been toggled to a logarithmic intensity scale:



Next, load in a 2D model function, Cylinder_2D.ipf using the Model Picker. Then select the data set "cyl2d_b_txt", the function "Cylinder2D", and plot the 2D function. An image plot of the model is drawn, and the coefficient table is updated.



Finally, "Append 2D" will overlay the model surface on the surface plot of the data. The model function is shown as a solid green, darker on the top of the surface, and lighter on the underside (so you know which way is up).

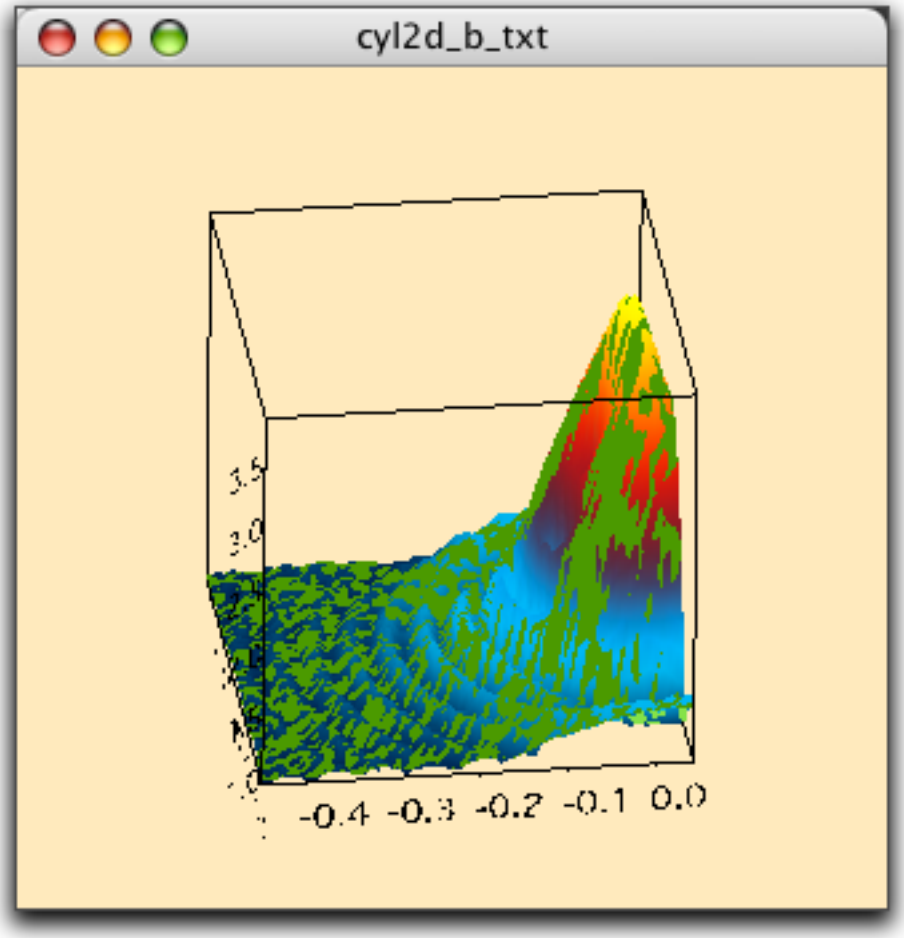


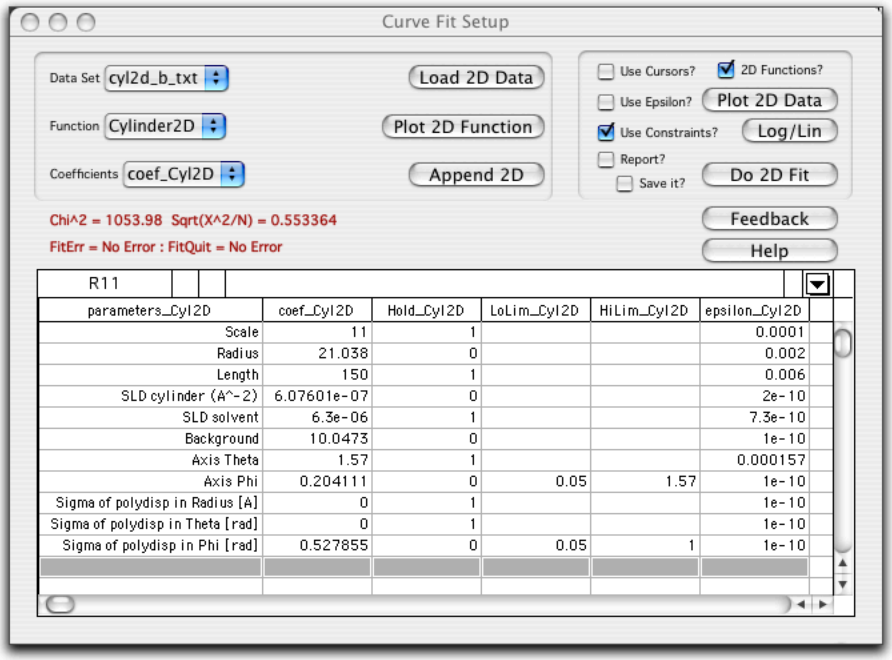
There is clearly a lot more complexity in a 2D model, so it is much more important (and difficult) to get a good starting point for the fit. Since this is a contrived example we can adjust the coefficients for a good "guess". Set the parameters to the following values, along with the Hold_Cyl2D and the LoLim and HiLim of the angle Phi. Be sure that the "Use Constraints" checkbox is selected too.

R11

parameters_Cyl2D	coef_Cyl2D	Hold_Cyl2D	LoLim_Cyl2D	HiLim_Cyl2D
Scale	11	1		
Radius	23	0		
Length	150	1		
SLD cylinder (A^-2)	2e-06	0		
SLD solvent	6.3e-06	1		
Background	12	0		
Axis Theta	1.57	1		
Axis Phi	0.5	0	0.05	1.57
Sigma of polydisp in Radius [A]	0	1		
Sigma of polydisp in Theta [rad]	0	1		
Sigma of polydisp in Phi [rad]	0.7	0	0.05	1

With these initial guesses, "Do 2D Fit" should converge quite rapidly. Instead of a fitted that passes through 1d data, the result is a fitted surface that intersects the data surface. Ideally, a good fit will visually have a "speckled" appearance as the smooth model calculation intersects the scatter in the experimental data, and have a numerically good chi-squared.

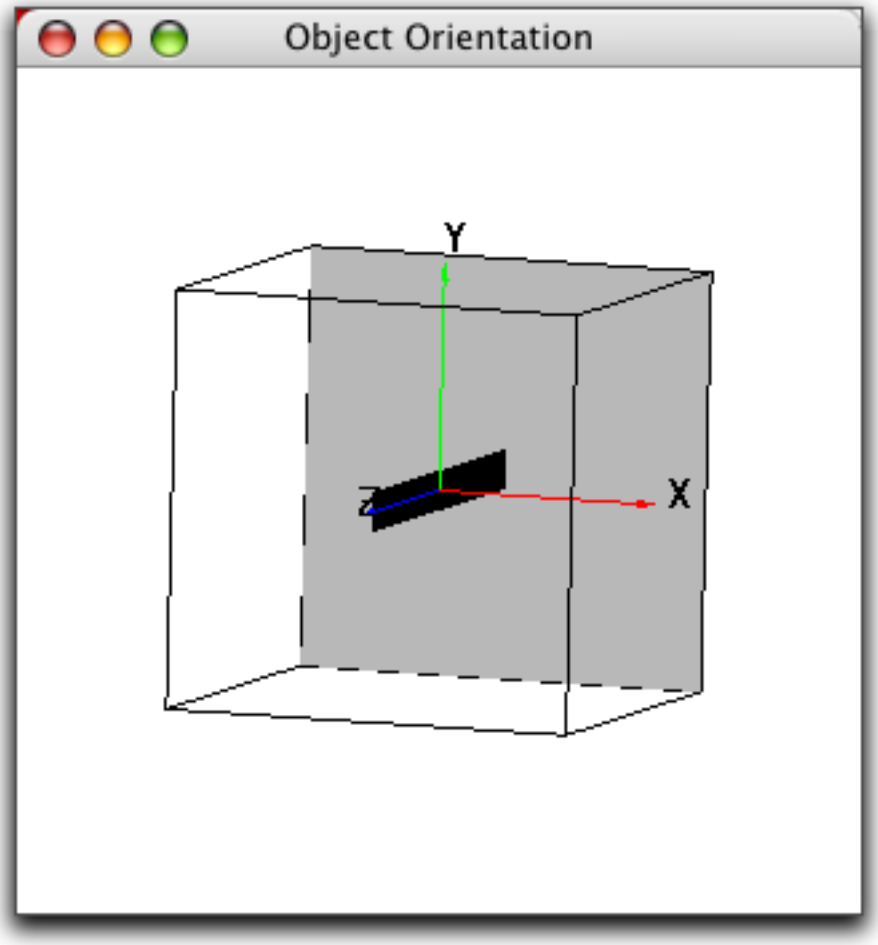




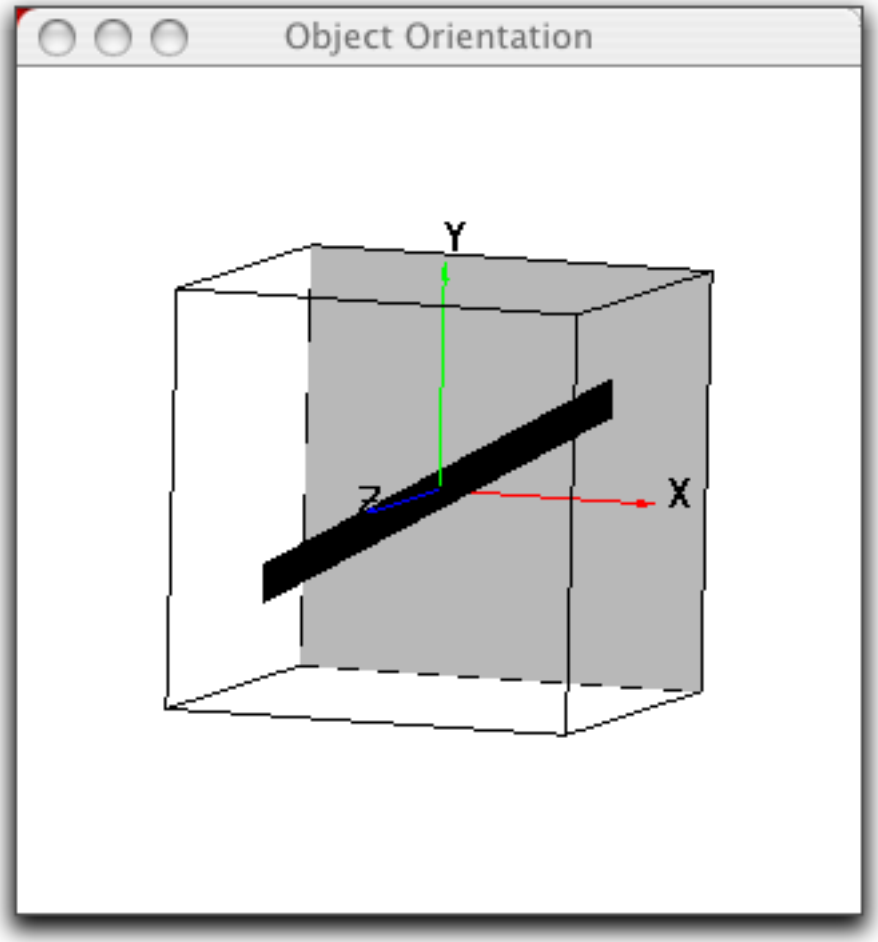
parameters_Cyl2D	coef_Cyl2D	Hold_Cyl2D	LoLim_Cyl2D	HiLim_Cyl2D	epsilon_Cyl2D
Scale	11	1			0.0001
Radius	21.038	0			0.002
Length	150	1			0.006
SLD cylinder (A^-2)	6.07601e-07	0			2e-10
SLD solvent	6.3e-06	1			7.3e-10
Background	10.0473	0			1e-10
Axis Theta	1.57	1			0.000157
Axis Phi	0.204111	0	0.05	1.57	1e-10
Sigma of polydisp in Radius [A]	0	1			1e-10
Sigma of polydisp in Theta [rad]	0	1			1e-10
Sigma of polydisp in Phi [rad]	0.527855	0	0.05	1	1e-10

What do the angles Theta and Phi mean? Check out the function help (on the Model Picker Panel) for the documentation. For a physical picture, choose "Show Cylinder Orientation" from the Macros menu (this may find a new home...). The default displayed orientation is

Theta=Phi=0 (degrees, sorry). XY is the detector plane, and the Z-axis is pointing from the detector towards the sample (that is, opposite to the flight of the neutrons). Theta is the angle between the cylinder axis and the Z-axis. Phi is the angle between the cylinder axis and the X-axis:

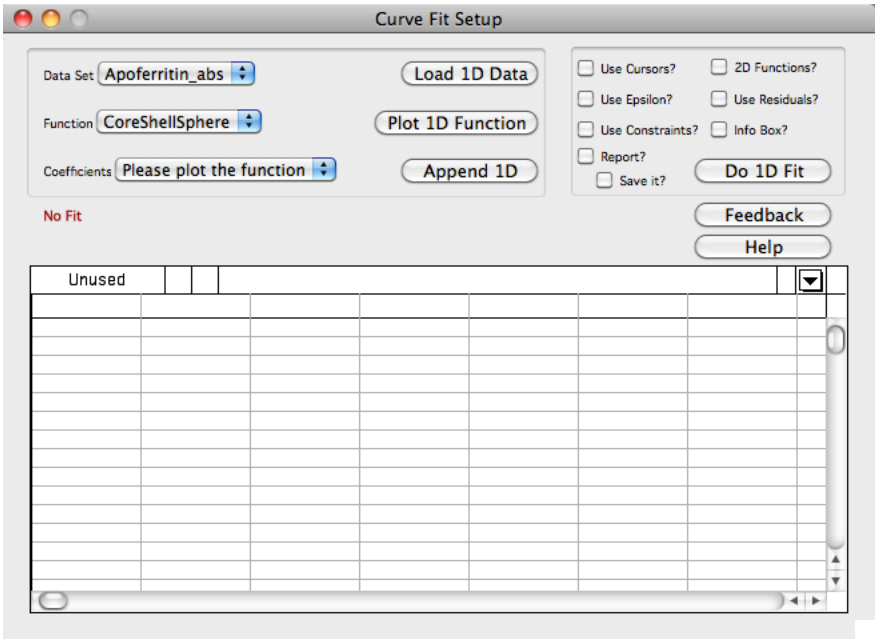


So the fitted result for the example above corresponds to Theta = 90 and Phi = 30 (degrees, noting that the model is in radians). Rotate the display to get a good view of what the cylinder orientation really is.



Fit Manager

The Fit Manager (Curve Fit Setup) window is the main panel for data analysis.



What is on the panel:

• In the upper left, three popup menus and three buttons:

- Data Set Popup: is a list of the currently loaded data sets. Whatever data set you have selected here, is the data set that is "active", that is the data set that will be fitted, and impacts the action of the function and coefficient popups

- Function Popup: a list of the available functions that have been included using the SANS Model Picker. The function selected here can be plotted using the "Plot 1D Function".

- Coefficient Popup: is the coefficient set for the selected function. You do not need to set this popup, it is automatically selected based on the function. This is also the coefficient list that is displayed in the table at the bottom of the panel. If the popup reads "Please plot the function", then the particular function selected has not yet been plotted (and the coefficients do not yet exist)

- Load 1D Button: loads a single 1D data set, either SANS or USANS

- Plot 1D Function Button: plots the function that is selected in the function popup. If it is an unsmeared model function, it is not attached to any specific data set, so you will be prompted for a number of points and a q-range for the model. If it is a resolution smeared model, you must have the proper data set selected and then the smeared function will be plotted using the resolution of the selected data set, and is permanently attached to that data set. That is, if you plot a smeared sphere model for data set A, and then load data set B, you will need to plot the smeared sphere for data set B.

- Append 1D Button: appends the function selected to the top graph (your data set is a good choice). Plotting any function will not automatically append it to anything. You get to do it here.

• In the upper right, there are a lot of checkboxes for curve fitting options, and a button to do the fit:

- Use Cursors?: adds cursors to the top graph, that you can move to delimit the range of data you would like to fit. If this is not selected, the entire data set will be fitted

- Use Epsilon?: manually set the derivative step during optimization. Uses the epsilon column in the table. For nearly all cases, this is unchecked, and not necessary.

- Use Constraints?: uses the constraints (upper and lower bounds) as specified by you in the

LoLim and HiLim columns of the table.

- Report?: Generates a report of the fit, including statistical information of the fit, and a graph of the results. If "Save It?" is checked, the report will be automatically saved to disk. This a good way to archive the results of a good fit.
- 2D Functions?: enables 2D operations if checked.
- Use Residuals?: plots the residuals at the top of the graph, after the fit, if checked.
- Info Box?: adds a textbox with fit information to the graph, if checked. Often it is rather large and unwieldy. Double-click on the box to change its formatting, or to delete it. Often the Report is a much better format.
- Rescale Axis?: Opens a panel to allow rescaling of the Y axis and X axis of experimental or model data, and exporting of the rescaled data.

- Feedback button: opens a web browser (if you have an active internet connection) where you can send comments, bug reports, feature requests, suggestions, or anything else you might like the software to be able to do.
- Help button: takes you to this help file.

• In the middle, there is a dark red text display of the results of the curve fitting. Chi-squared and a reduced chi-squared are reported, along with the status of the fit. If all was successful, FitErr and FitQuit should be "No Error". If there was a problem, it will be reported. Whatever the error, it is usually remedied by starting with a better set of initial guesses, holding additional parameters fixed (or constrained), and re-running the fit. See the section Frequently Asked Questions About SANS Analysis for additional help.

• At the bottom is a table of coefficients for the model function, and additional columns for setting up the curve fitting. The columns in the table are (for a model "abc"):

- parameters_abc: these are the names of the coefficients, and their units.
- coef_abc: these are the coefficients for the model, and are dynamically linked to the model function. Any change in these coefficient values initiates a recalculation of the model function, and a redisplay of the new result in the graph (if it has been appended somewhere)
- Hold_abc: initially filled with zeros. When fitting, there almost always will be some parameters that are known values and can be held fixed during fitting. Enter a one for any parameter you want to hold fixed, leave a zero for parameters you want to be automatically optimized during curve fitting.
- LoLim_abc: initially blank. Enter a numerical lower limit (lower bound) for the corresponding parameter. The "Use Constraints?" checkbox must be checked for these limits to be used during fitting. Constraints do not apply to held parameters, and they are ignored.
- HiLim_abc: initially blank. Enter a numerical high limit (upper bound) for the corresponding parameter. The "Use Constraints?" checkbox must be checked for these limits to be used during fitting. Constraints do not apply to held parameters, and they are ignored.
- epsilon_abc: These values set the step size for numerical derivatives during curve fitting. They are typically not necessary to set manually, but if a fit seems to be making slow progress towards a solution, the "epsilon" values can be set. Initially set to 1E-4 * (default parameter value). The "Use Epsilon?" checkbox must be checked for these step sizes to be used during fitting.

The width of the columns can be resized by dragging the separator at the column heading. Be sure to "enter" values in the table for them to be recognized, either with <enter> or <return>, or moving off of the cell with an arrow key.

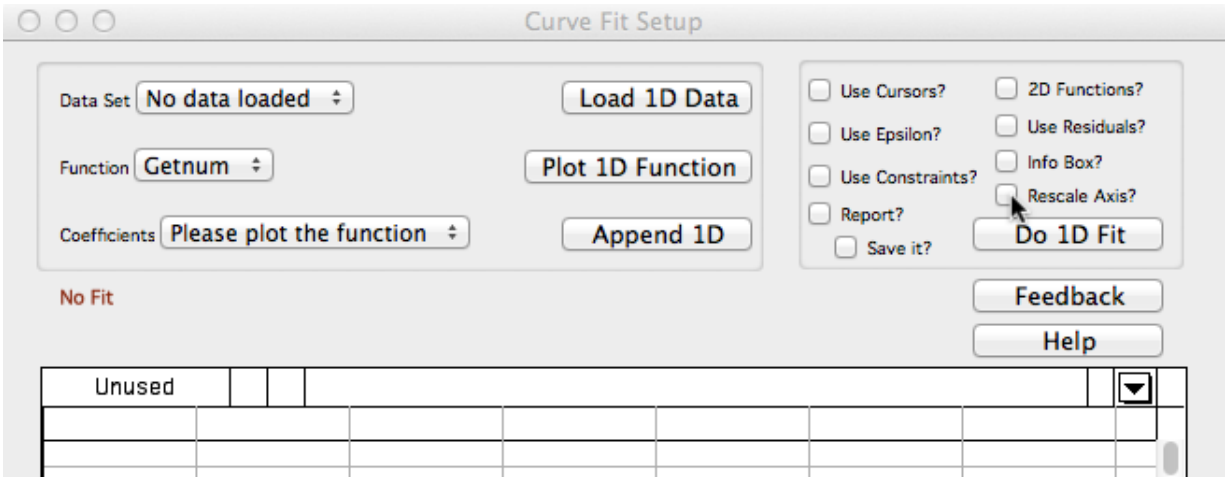
When in "2D" mode, the Load/Plot/Append/Fit buttons are for "2D" data, and two additional buttons appear - one to "Plot 2D Data" (the selected data set) and one to toggle the intensity scaling of the active display from "Log/Lin".

Rescaled Axis

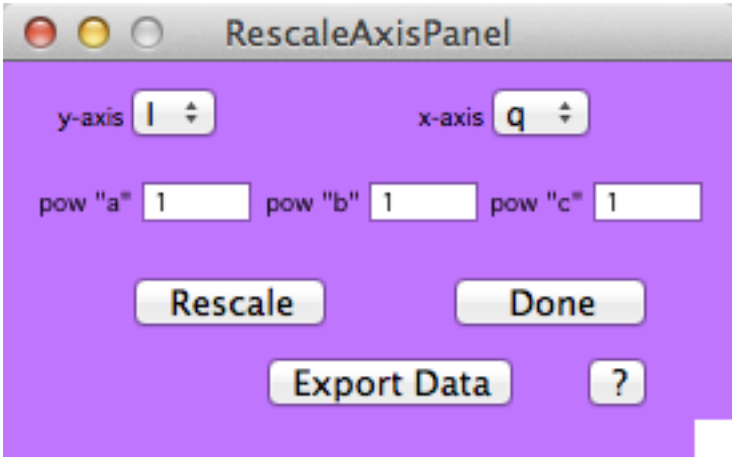
For different analyses it is sometimes useful to visualize the data plotted differently from the standard I(q) vs q. Using the Rescaled Axis Panel it is possible to convert either the x-axis or the y-axis or both to an alternate scaling.

Instructions for use:

1) Tick the tickbox labeled "Rescale Axis?" found on the fit manager.

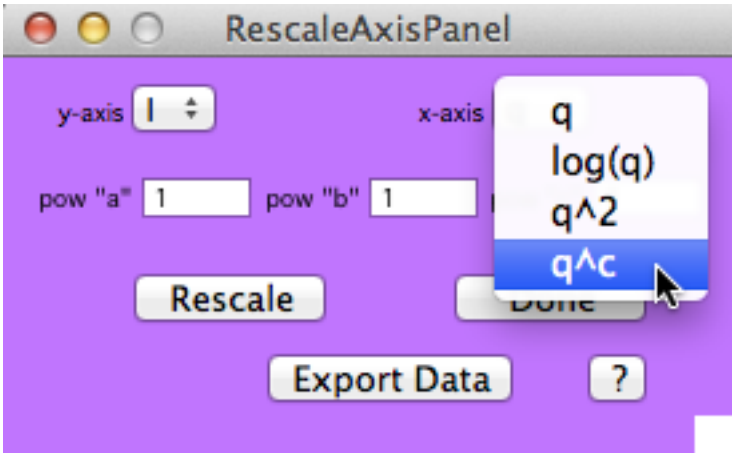


The Rescaled Axis Panel will then appear.



2) The drop down boxes labeled y-axis and x-axis let you choose the scaling for the axis required. Some rescaling options require user input values, called "a", "b", and "c". Value "a"

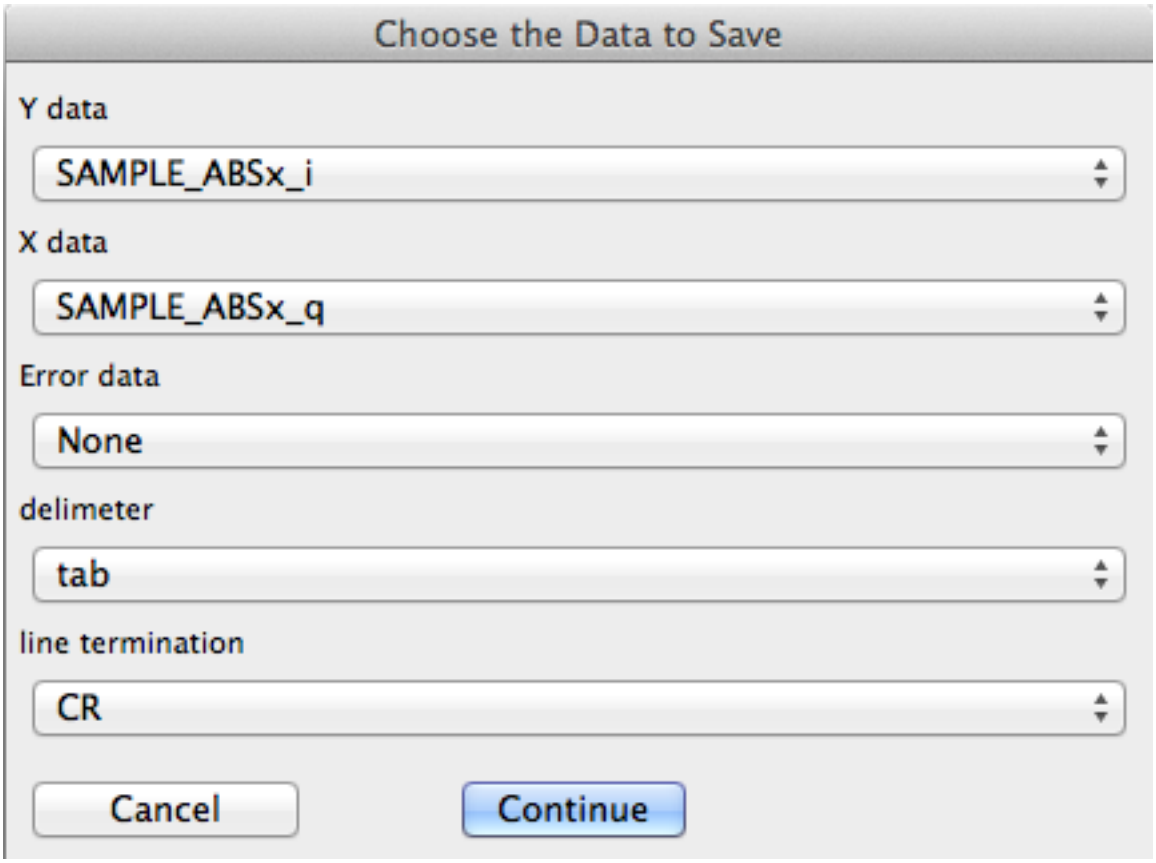
must be between -2 and 10, values "b" and "c" must be between 0 and 10.



3) The "Rescale" button will take all data sets from the top graph and rescale them according to the choices made for y-axis and x-axis. If a model calculation is on the top graph it will be rescaled but it will no longer change when the model parameters are changed. This functionality can be recovered by replotting the graph as I vs q.

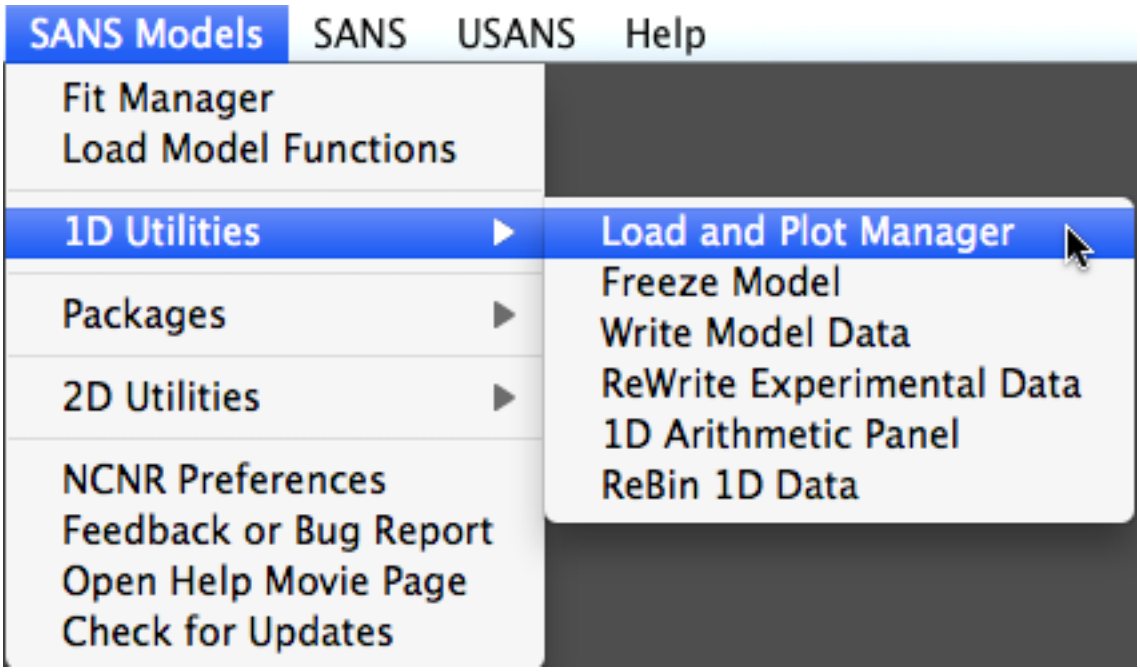
4) The "Done" button closes the Rescale Axis Panel but does not change the scaling.

5) The "Export Data" button opens a diaglog allowing the user to export data sets as a three column text file from the top graph. Y data and X data are are chosen in the dropdown boxes. Error data can be chosen, however if there is none then the choice of 'None" will stop an error column from being written.

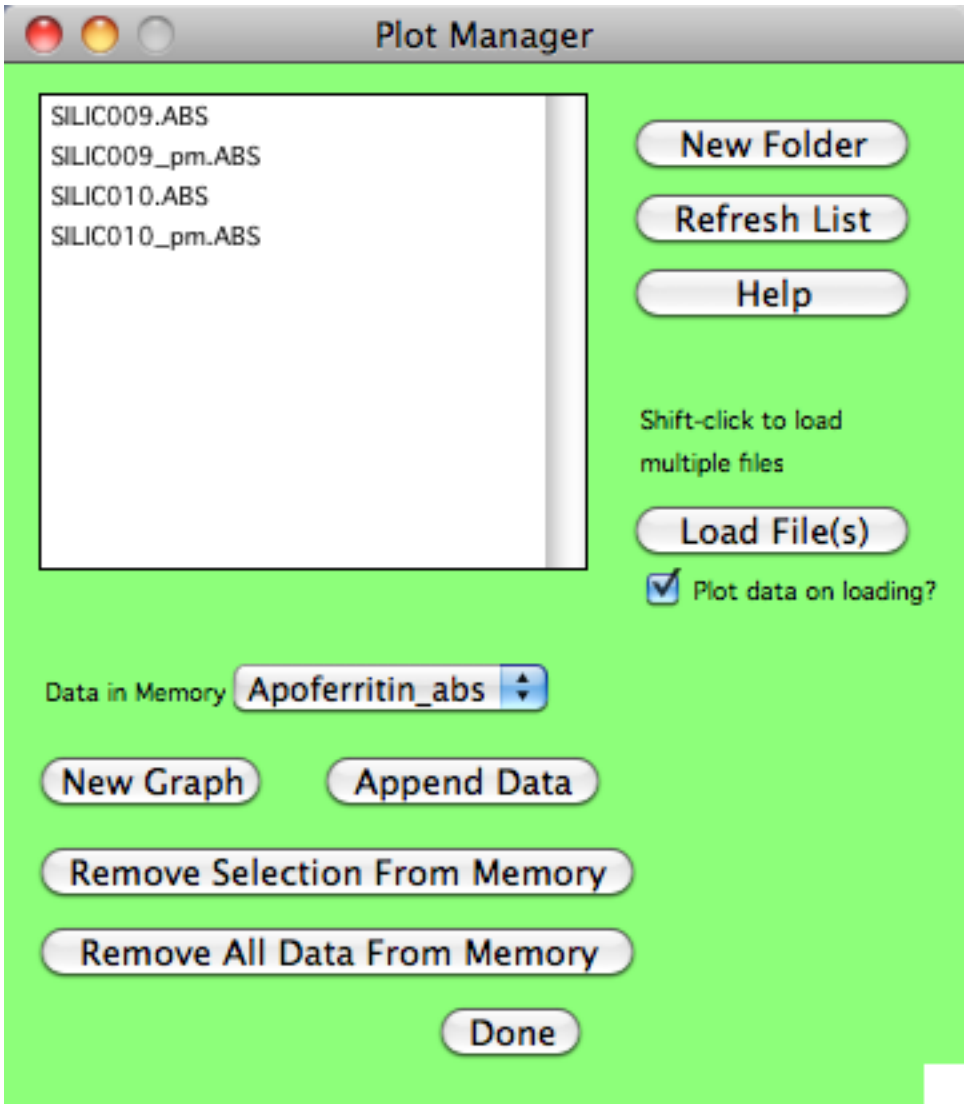


Plot Manager

The Plot Manager allows an easy way to load data, graph it, and append multiple data sets to a single graph. The Plot Manager is opened from the SANS Models menu:



And the panel looks like this:



If you have not set the OS path to the folder where your data is stored, you will be asked to do so, by using the "New Folder" button, and selecting the data folder from the dialog. What is on the panel:

The upper part of the panel has:
- A list of what files are on the disk, in the selected folder.
- You can change the folder at any time with the "New Folder" button.
- "Help" brings you here. But you're here already.
- "Load File(s)" will load the selected file(s). If you have multiple files selected, they will be loaded sequentially (prompting for a slope if they are USANS), and you will be asked if you want to append the set to the top graph. This makes a quick way to load and plot a series of data. If the "Plot data on loading?" box is unchecked, the data will only be loaded, not plotted.
- If data has already been loaded, you will be notified, and asked if you want to re-load the data, overwriting what was already loaded. If you haven't modified your data, there is no harm in re-loading the data.

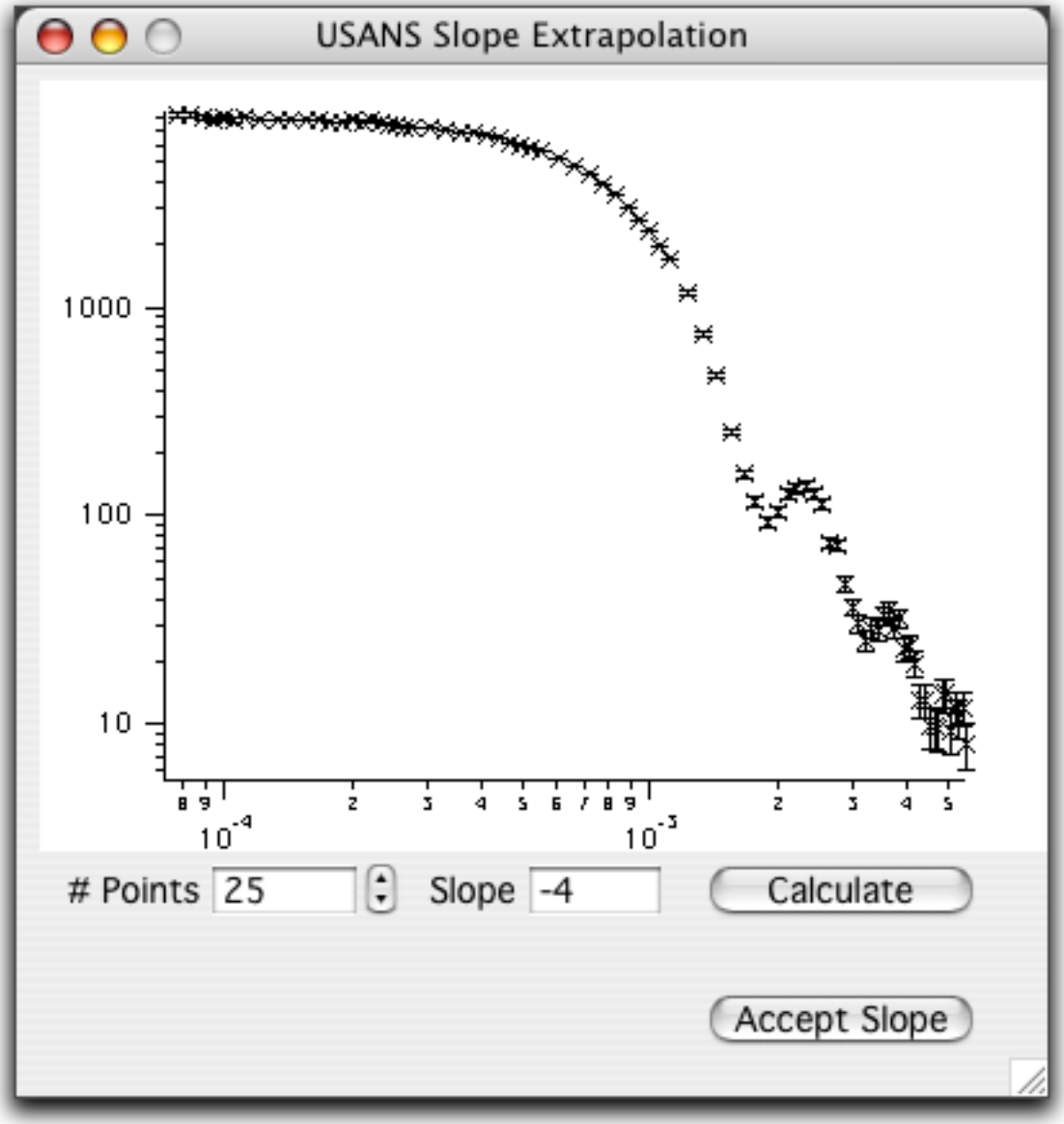
In the lower part of the panel, you can manage data that has already been loaded:
- The popup has a list of the data sets that have already been loaded. Selecting a set from the popup allows you to:

- Make a "New Graph" with just this data set (default is log-log, with error bars)
- "Append Data" to append this data set to the top graph
- "Remove Selection From Memory" will do just that, if you are finished with the data. Note that this does NOT delete your data on disk - it simply erases it from Igor's memory. Note also that you can't remove data that's currently being used in a graph.
- "Remove All Data From Memory" will remove any data that is not currently in use.
- "Done" closes the window. Recreate it from the SANS Models menu.

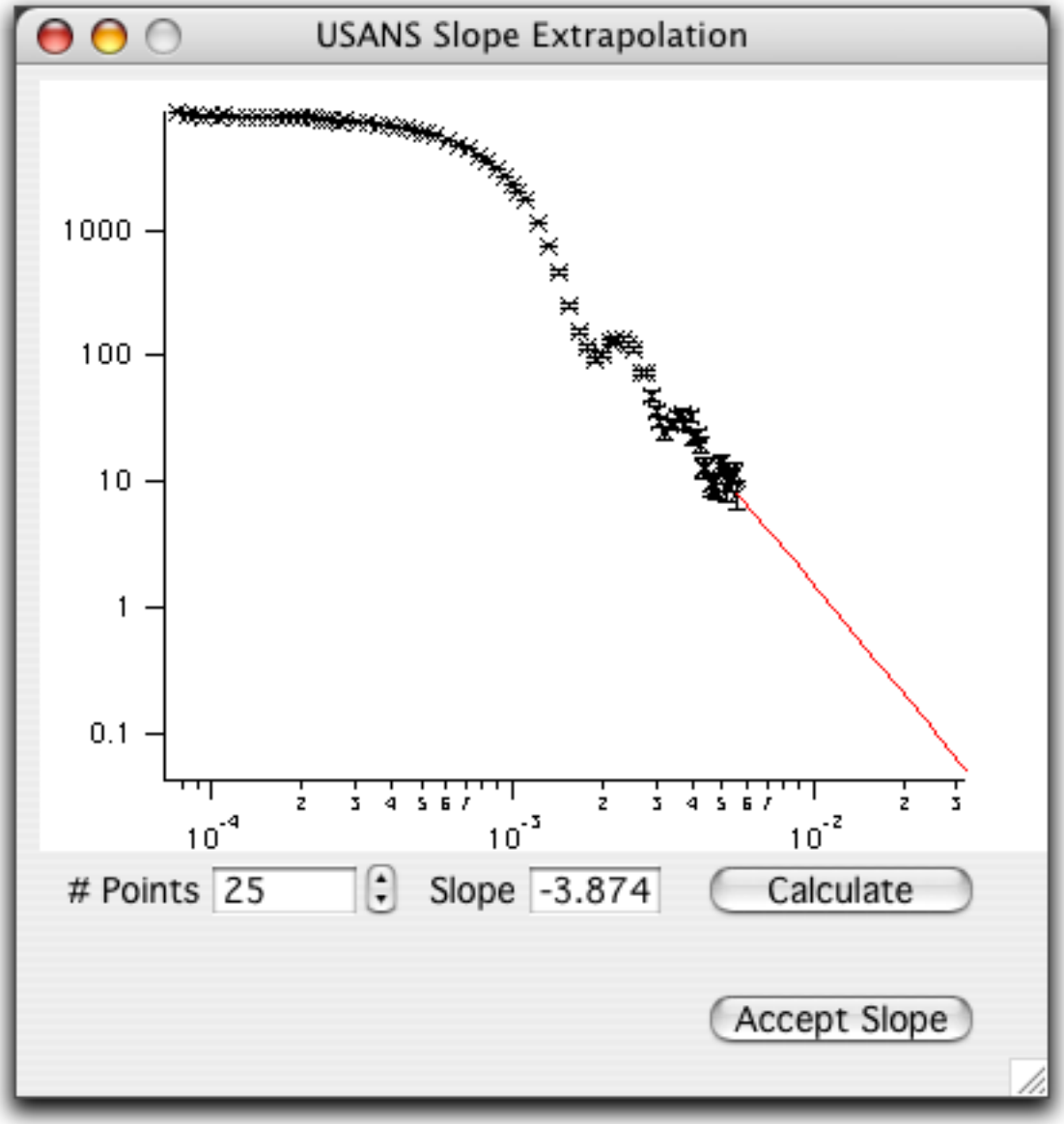
Loading USANS Data

Loading slit-smeared USANS data now requires an extra interactive step to determine an appropriate high Q slope for extrapolation. This power law slope is used to calculate a resolution matrix that dramatically speeds up the calculation of resolution smeared models for USANS. It does take a few seconds to calculate the matrix, but this is a one-time operation (unless you use the cursors to fit a sub-range of your USANS data, then the matrix must be recalculated). Loading USANS Data proceeds as follows:

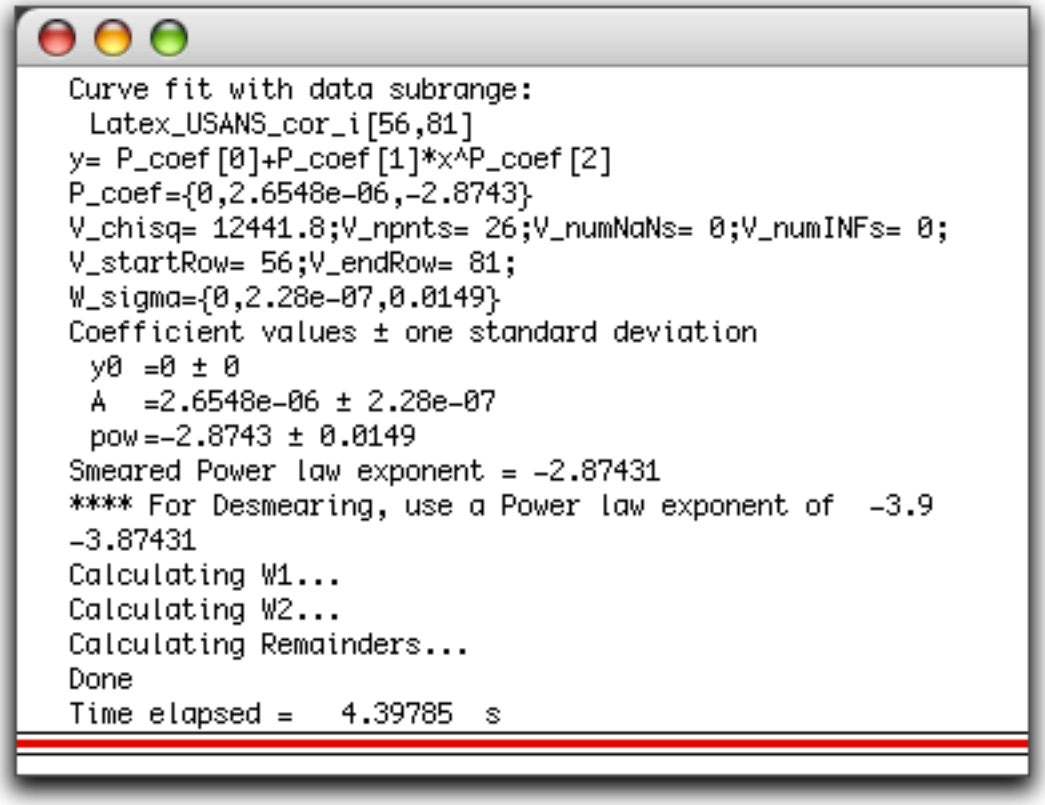
Starting with the "Load 1D Data" button on the Fit Manager, select a slit-smeared USANS data file (typically ends in .cor). You will be presented with a panel like this:



Clicking "Calculate" will use the last 24 points of the data set to fit to a power law, and then show the result:



If the slope looks wrong, change the number of points to fit (try 15 or so) and calculate again. This looks good, so "Accept Slope" will close this window and start the calculation of the resolution matrix. The progress is shown in the command window, and the USANS data will be plotted when the calculation is complete. At this point, you can model the USANS data with and appropriate resolution smeared models.

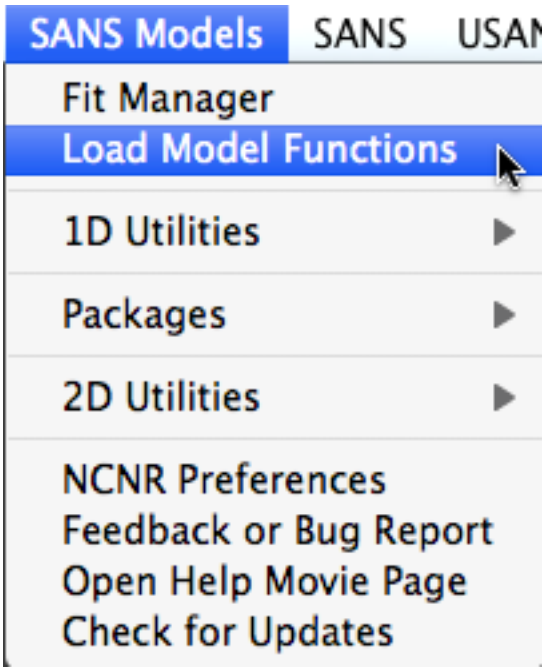


SANS Model Picker

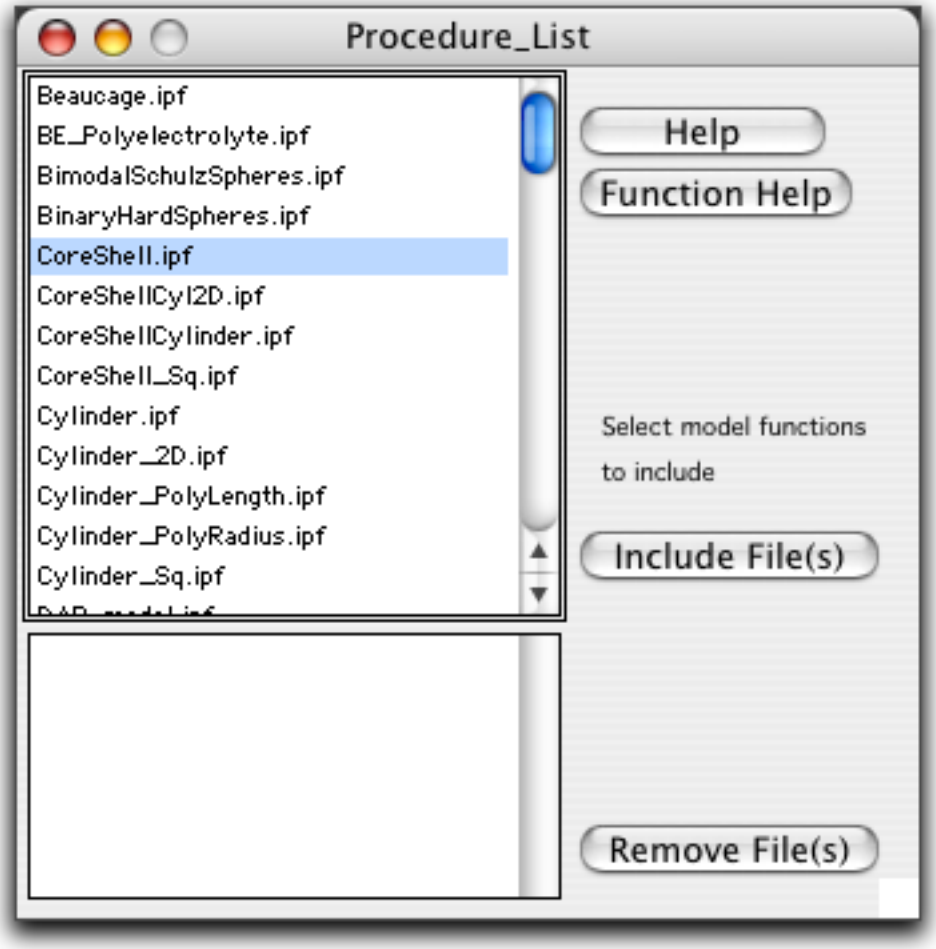
The SANS Model Picker allows you to load into a single experiment the select models that you want to use for curve fitting. This is useful to avoid clutter of models that aren't appropriate for your data.

Instructions

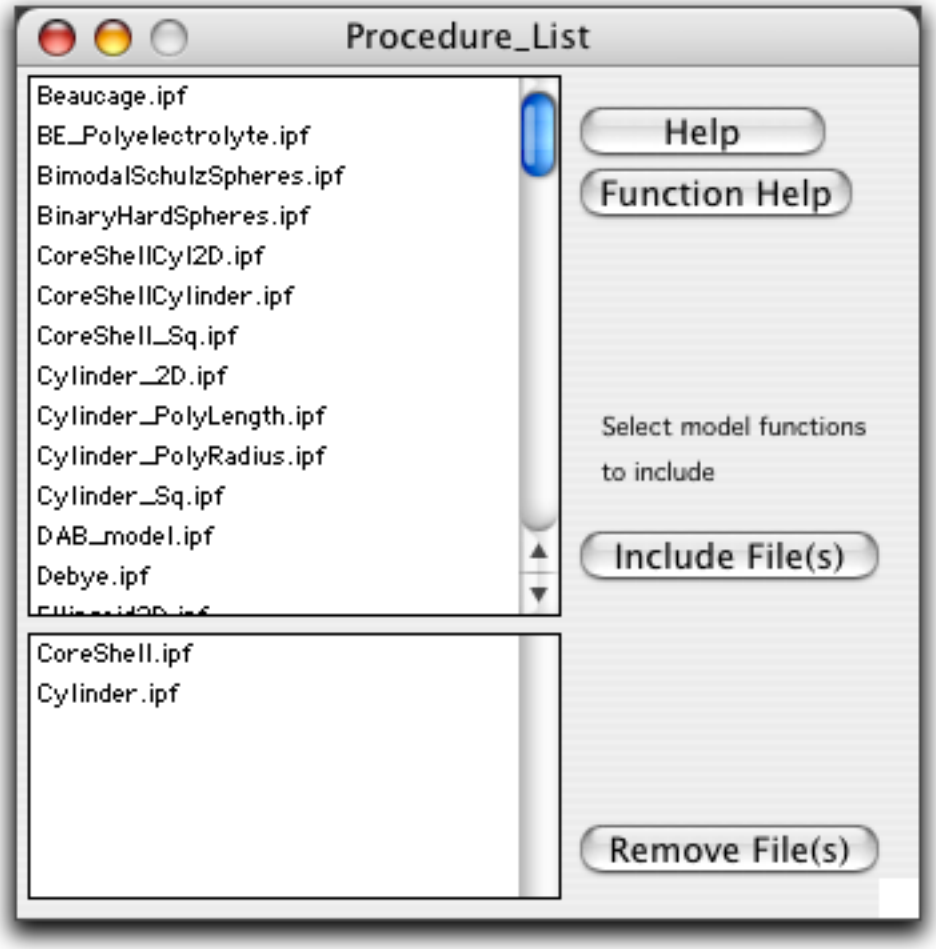
1) If the Procedure List Panel opens is not open, or is not visible. From the SANS Models menu choose Load Model Functions:



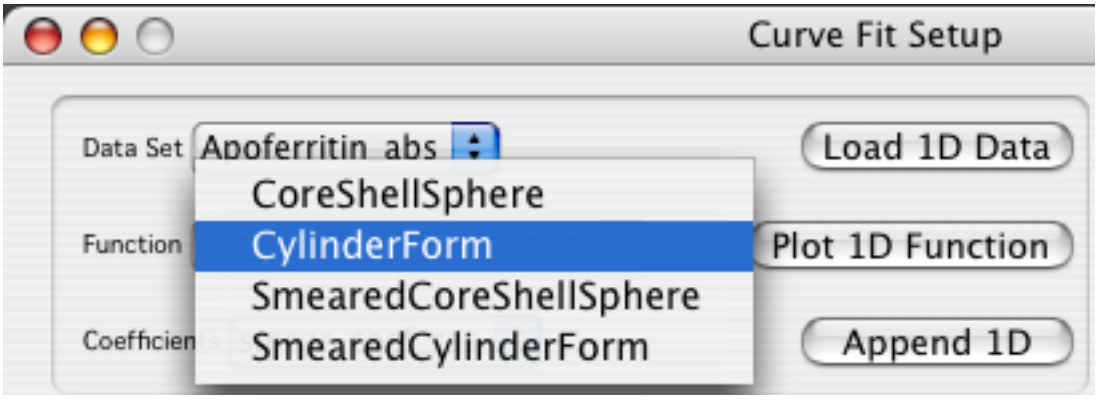
The list in the upper box is the list of models that you can add, and the lower box is the models that have been added (initially there are none). Clicking "Help" will bring you back to this help document. If you select a model function file (.ipf) and click "Function Help", you will be taken to the documentation for that particular model - which will tell you the actual name of the function, its use, scope, reference, and a sample graph.



2) Select the file(s) from the list to include them in the experiment. They are automatically compiled when you click the "Include" button. You can shift-click to select multiple files.



3) Your selected models will now appear under the function popup on the Fit Manager Panel.



4) To remove model functions that you don't want to use anymore, select the file from the lower panel, and click the "Remove" button. The model will no longer appear in the menu.

Note that some models can't be removed. For example, if you are using a model of polydisperse spheres, the sphere form factor model will appear in the menu, even though

you didn't include it yourself. That is because the polydisperse model is based on the monodisperse model, and is automatically included.

Error messages, and what they mean

• Why do I get an error dialog that says "File "xxxx.ipf" not found"?

- Igor is looking for the model function (actually the procedure file) with that name, in the User Procedures Folder. Be sure that the downloaded model functions have been copied or moved to the User Procedures Folder as described in the instructions that came with the model functions.

- Another, less common reason, is that you have an alias (or shortcut) in the User Procedures Folder that points to the model functions. In this case, you need to turn off file checking. See below in the Tips for the Adventurous for how to do this.

• Why can't I find the model function that I want in the SANS Model Menu?

- Because it's not there. Functions are in the popup on the Fit Manager.

General Curve Fitting Tips

Non-linear optimization is full of mathematical pitfalls, no matter how smart the software claims to be. Some suggestions are:

- Make sure that you have all the correct waves selected (Data Set + Function popups)
- Make sure you're using a model that is an appropriate physical description of your data
- Use a better initial guess - find it by manually adjusting the coefficients
- Make sure your starting guesses are non-zero
- Hold more (nearly all) of the parameters fixed, then release them one at a time
- Check the function documentation to make sure that the parameters are reasonable
- Constrain the parameters to physically reasonable values

Also see the built-in documentation that describes how Igor does the non-linear fitting. To see this help file:

1) From the Windows menu, choose Windows->Help Browser
2) Select the "Help Topics" tab

3) Choose "Curve Fitting" or one of the other sub-topics
4) Click on "Show Selected Topic"

Tips for the Adventurous:

• If you have your own procedure(s) that you want to add to the list, you can do this by running the command:

```
AddProcedureToList("ProcedureFileString")
```

where ProcedureFileString is the full name of your procedure file, including any extension (in quotes). Your procedure file will now appear at the bottom of the list.

• Now that you've added your extra procedures, you don't want to have to add them every time you open the Picker template. You can save this list of procedures by making a custom "template". Open the original Picker template, add your procedure(s), then save the experiment with a ".pxt" extension, designating it as a template (this is also called a "Stationery" file on the Mac).

• If you have an alias (or shortcut) in the User Procedures Folder that points to the model functions, you will receive an error dialog stating that the file cannot be found, and is not included. This safety net is to try to prevent non-existent files from being included, which then can't be compiled, which then can't be removed (actually very easy to remove, see below). Turn off this file checking by selecting the following line, control-click (or command-click) and choose "Execute Selection" from the contextual menu.

```
root:FileList:checkForFiles=0
```

• If you've accidentally included a file that doesn't exist, the compiler says it can't find the "#include" file, and now the buttons on the panel won't work because you need to compile the procedures. How do you fix this?

- You need to manually remove the offending line that is trying to include the "bad" file. Control-M (or Command-M) will open the built-in procedure window. There will be a list of #include statements. Look for the line with the "bad" file on it, and simply delete that line. Click on the (tiny) "compile" button on the bottom bar of the window, and the procedures should compile successfully. Close the procedure window and proceed as usual.

Global Curve Fitting of SANS Data

Frequently, analysis of experimental data requires fitting the same function to several data sets. In many cases, experimental conditions dictate that some physical parameter or dimension is common to all data sets, while others are local and different for each set. In these cases, it is desirable to fit all the data sets simultaneously in

order to gain the benefits of a larger number of points and several measurements. This is often referred to as global analysis.

This experiment demonstrates a procedure file, "Global Fit", that automates the tasks associated with global analysis. The procedures in this package will allow you to fit any number of data sets (limited by your memory and patience) to virtually any combination of fitting functions. The parameters to the function may be "LINKED" or local. Linked parameters will be fit with the same value for all linked data sets, while each data set gets its own best-fit value for local parameters.

There is a great deal of flexibility built into the Global Fitting Panel. This panel is based on the WaveMetrics-supplied version of <Global Fit> based on Igor 6, and as a result, large portions of this documentation look quite similar to the WaveMetrics documentation. As a result of the flexibility, the panel is rather complex. Suggestions for improvements are welcome.

---Tips from a user ---

What you need to do before using the global analysis program:

- Carry out the model fitting on the separate scattering curves to find the best model (or two) to use.
- Keep an ordered record of the best-fit parameters for all the scattering curves. These are needed to enter beginning values to enter in the extensive table for the global fit.
- Have a list of the parameter names for the model. This is easily done by printing at least one report. Then, label these parameters as K0...Kn so you can keep track of them. Note the number of parameters is one more than the highest label number.
- Using the cursors to limit the ranges of the fit in the global format is somewhat more clumsy than for the individual fits. It can be helpful if data out of the useful range--such as the points inside the beam stop--is simply omitted from the files by editing before attempting a global fit.

What can you do with the global analysis program:

The global analysis program allows you to tie the parameters of one model for all the runs together or to let them vary for each curve individually. For example, if you have a set of solvents with different contrast, such as having different H/D ratios, you can lock the structural parameters to a single fitting value while letting the solvent SLDs be different. Both the locked sets and the individual curve variables can be set to vary or held to fixed values for the fit.

Three checkbox options are available: Setting the statistical weighting, setting the cursors to limit the regions for the fitting, and setting limits on the values of the parameters so they will not be allowed to converge to some absurd values. The weighting protocol is straightforward.

Setting the cursors is unfortunately named masking, which should not be confused with the data mask used in the data reduction. Each curve must have cursors set individually--there is no global cursor choice. After checking in the masking box, a popup requires you to do the following for each curve: choose the line of the data in the box, click "show the cursors," then set the cursors on the graph, and then click on ”mask from cursors.”

Checking the constraints box provides a popup that is sensible, but it helps to recognize that not all the parameters are shown for all the curves. All the parameters are listed for the first curve, but below that only the uncoupled parameters are listed

for the remainder of the curves.

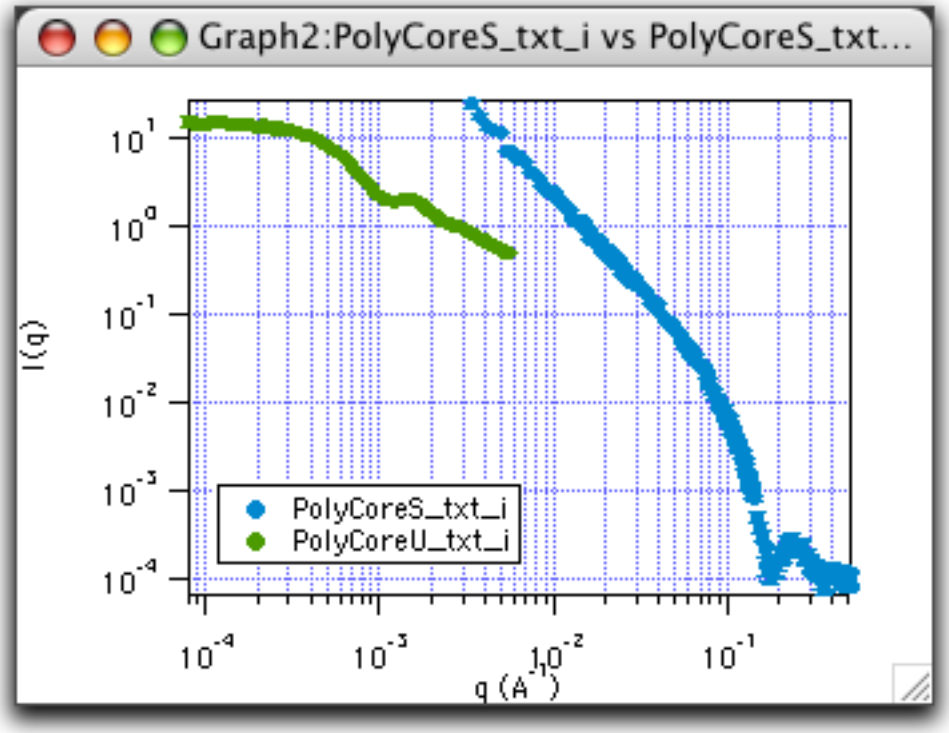
Finally, for saving the extensive table of values in the "coefficient control" tab, there are buttons at the top of the window for saving and retrieving the values. The setup at the bottom of the window saves not only the parameters, but all the values in both tabs of the window.

Basic Operation

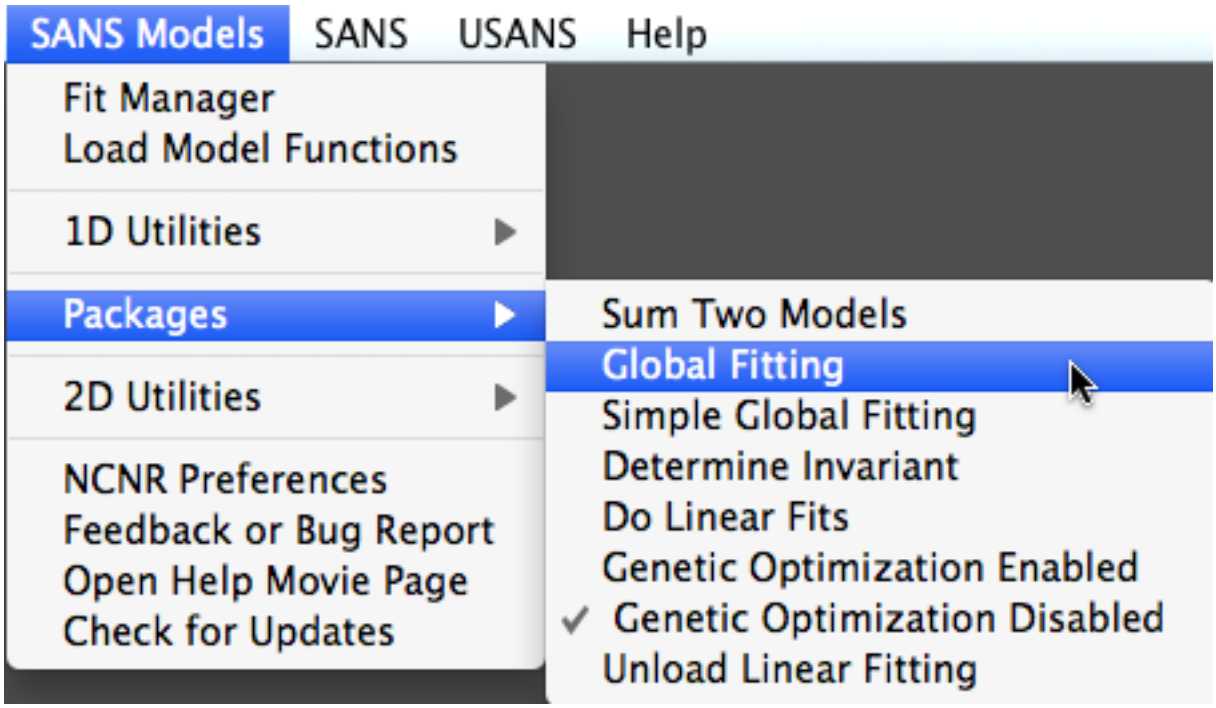
It is recommended that you are familiar with fitting individual data sets before attempting to perform a global fit. It is also very helpful to fit each data set individually so that these fit results can be used as (very good) initial guesses to the global fit. If the model doesn't fit the individual data sets, it'll never be able do the global fit.

From this point, it is assumed that you have done these individual fits and have plotted the model that you want to use for the global fit, and the desired model has already been included through the SANS Model Picker.

1) Load all of the data sets that you would like to fit, appending them all to the same graph. For this example, load the sets PolyCoreS.txt and PolyCoreU.txt which are simulated data for polydisperse core-shell particles. The two data sets are for (S) SANS and (U) USANS, respectively. Note that there are significant scaling and slope differences between the slit-smeared USANS data and the pinhole-smeared SANS data. The USANS data will be several orders of magnitude lower in intensity than desmeared data, and the slope will in general be more shallow than the desmeared data. Don't expect the data sets to overlap - due to the different instrumental resolution, SANS and USANS data should never overlap! See Resolution Smearing for more of the details why this is so.



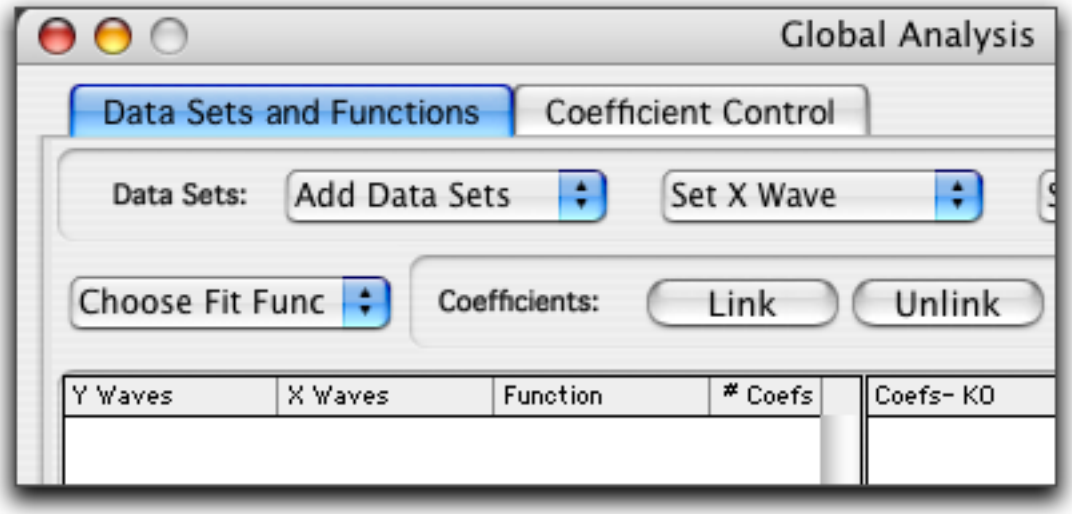
2) Load the Global Fit package by selecting Packages->Global Fitting from the SANS Models menu.



When the package loads, it displays the Global Fit control panel. At any time, you can bring the control panel to the top by selecting Global Fit from the Macros menu.

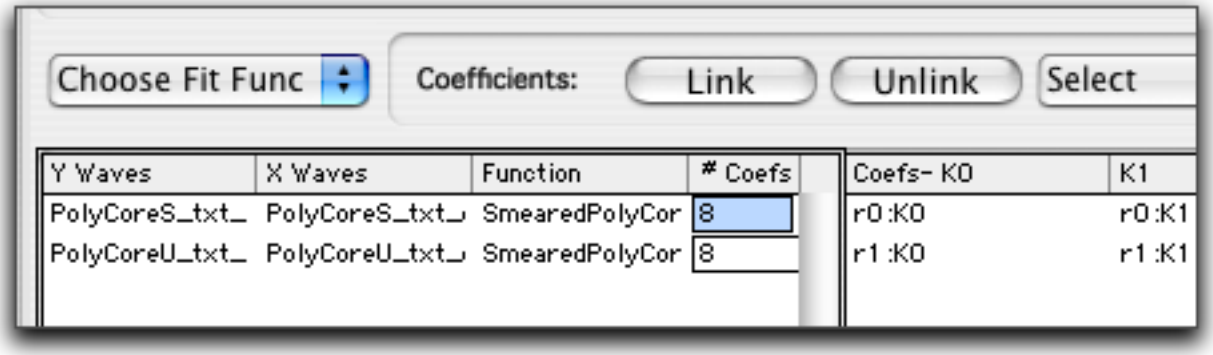
3) Select the data sets using the "Add Data Sets" popup. "All from top graph" will add both of

the data sets to the file list.

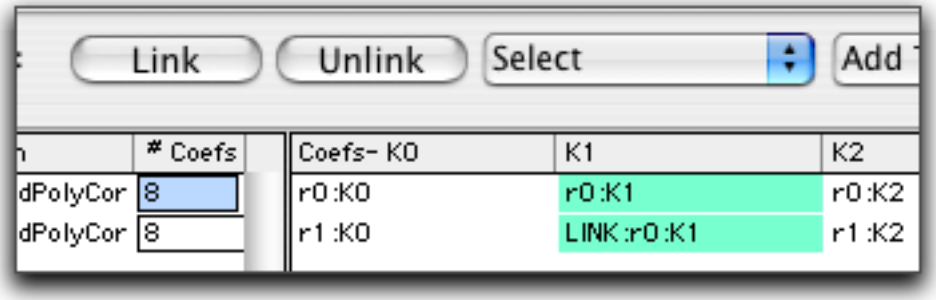


4) Choose the fit function for each of the data sets. They could be different, but in this example, we want them to be the same, the SmearedPolyCoreForm model. Click on the empty "function" box next to the first data set, and choose the function from the popup. The name will fill in the box. Do the same for the second data set.

The fitting function has 8 parameters (count them in the coefficient table). Set "# coefs" to 8 for the first data set. The second set is automatically filled in, since it's the same model. The table should look like this at this point.

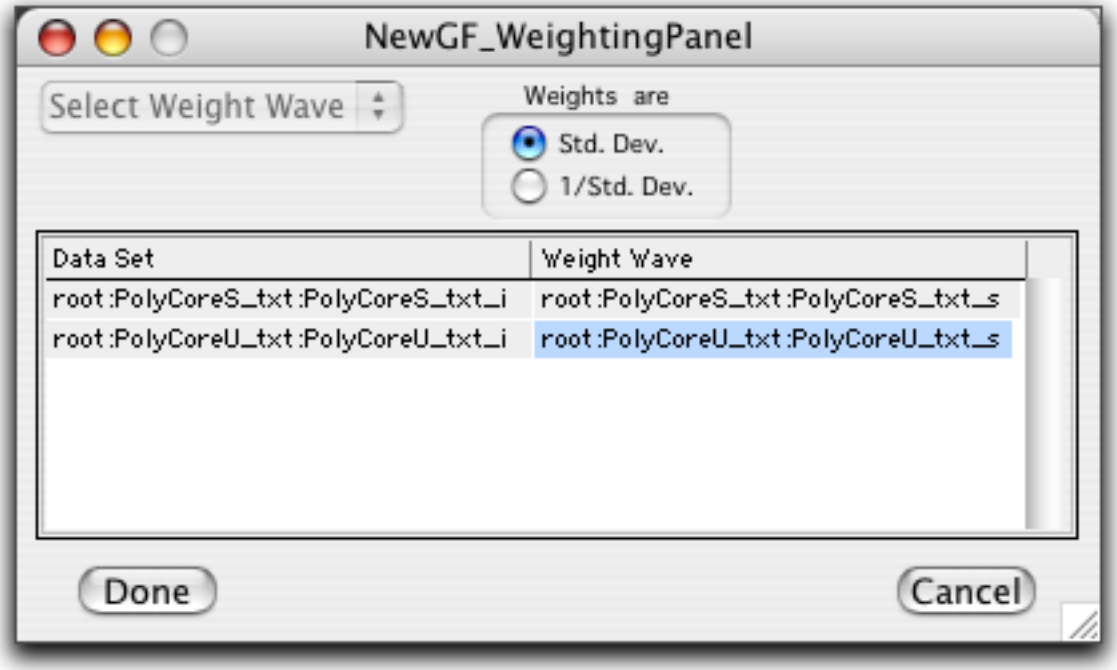


5) The right half of the table is where the "linked" coefficients are set up. For this example of SANS and USANS data from a single sample, the physical dimensions of the particles and their SLD's don't change, so they are global. The scale factor and the background (coefficients 0 and 7) can be left local, since there may be differences in absolute scaling and background on each instrument. In the table, the coefficients don't have nice names, but rather are indexed K0-K7. We now want to link coefficients K1 through K6 between the two data sets. From the "Select" popup, choose "SmearedPolycoreForm:K1", and then click "Link". You should see:



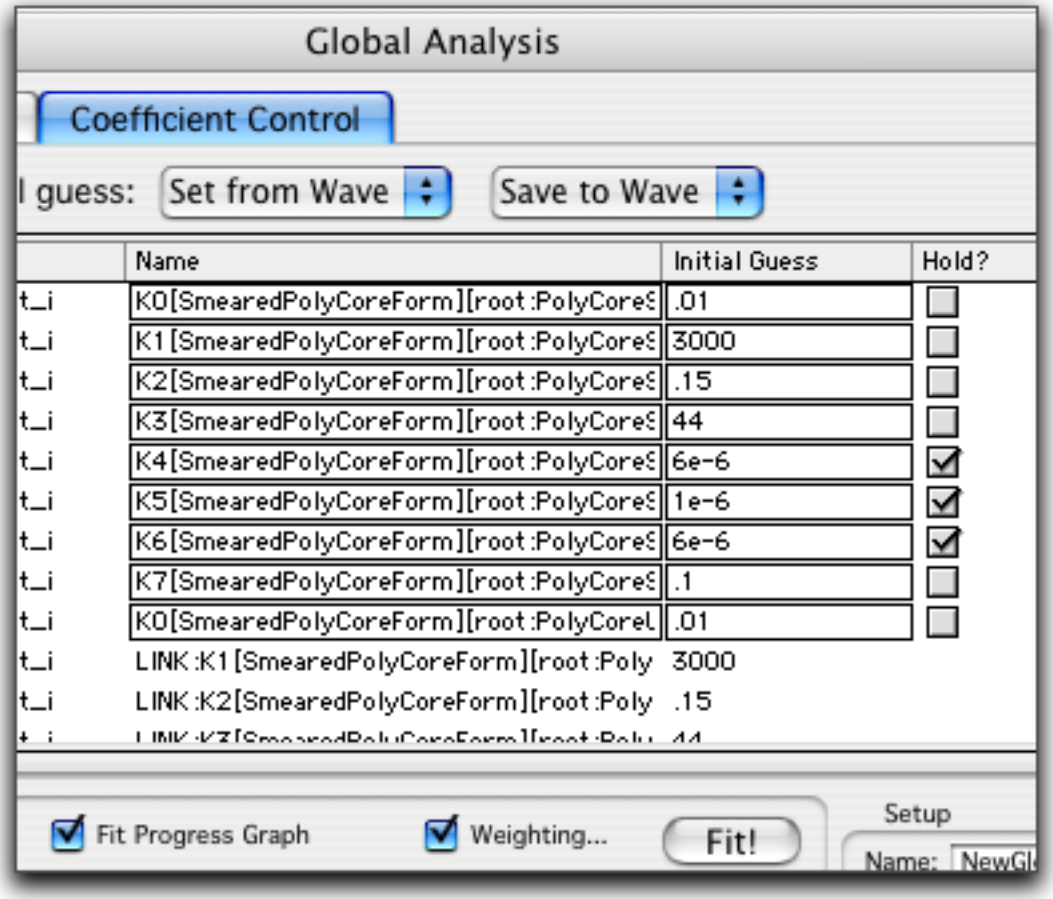
Do the same for parameters K2 through K6.

6) Next, set the weighting waves to use, which is the error in the intensity. Click the "Weighting..." checkbox below the table of linked coefficients. A new panel appears. Simply click in the empty "Weight Wave" box next to each data set. The proper data is automatically identified. Then click done to close the panel.



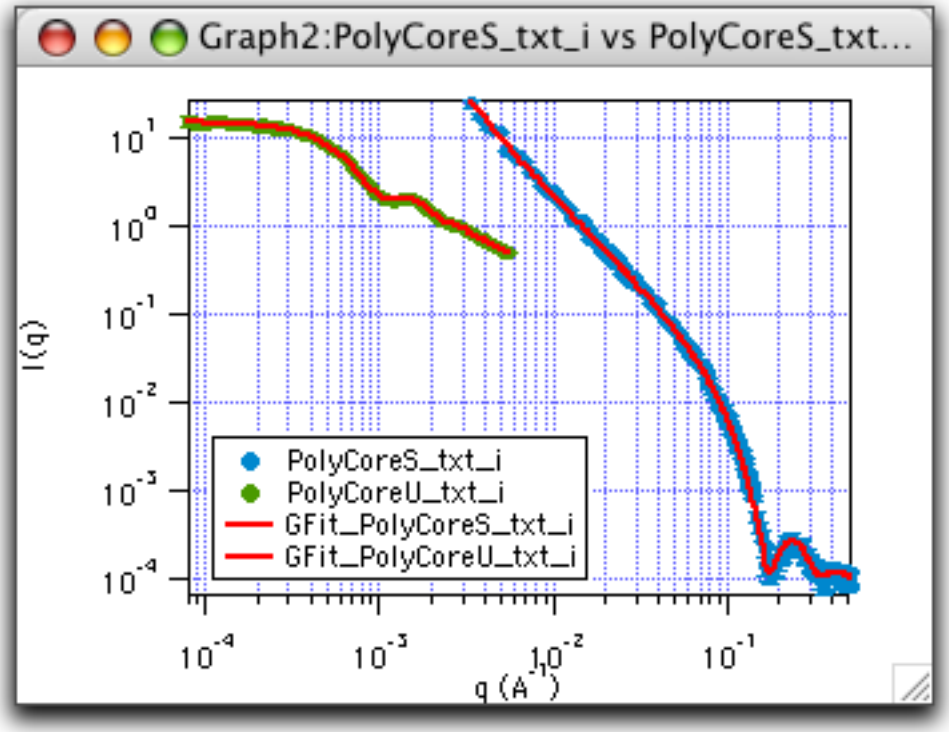
7) Click on the Coefficient Control Tab at the top of the Global Fit Panel, where we can enter the initial guess for the coefficients, and set which are to be held fixed. The coefficients again are indexed K0-K7 for each data set. Enter the initial guesses as shown below. This is where you should make use of the results from the best (or close) fits to each of the individual data sets that you have already done. Be sure to scroll down and enter a guess for the background (K7) of the second data set (0.1 is OK)

In this fabricated data, the SLD's of the solvent, core, and shell are known values. They are global to all data sets and should be held fixed during the fitting. Be sure to check these boxes to hold these three parameters.



8) Fit!

9) A report is automatically generated and saved, showing the results of the fit. Coefficients that are HELD or LINKED are marked as such. The results are also added to your original graph as "GF_" data. This example, of course, worked wonderfully.



10) There is no step 10. One may be added in the future.

11) If you want to exclude some of the data points from the fit, apply constraints to the parameters, calculate the covariance (highly recommended), or calculate residuals see the specific instructions below.

12) Click the Fit! button and watch the results.

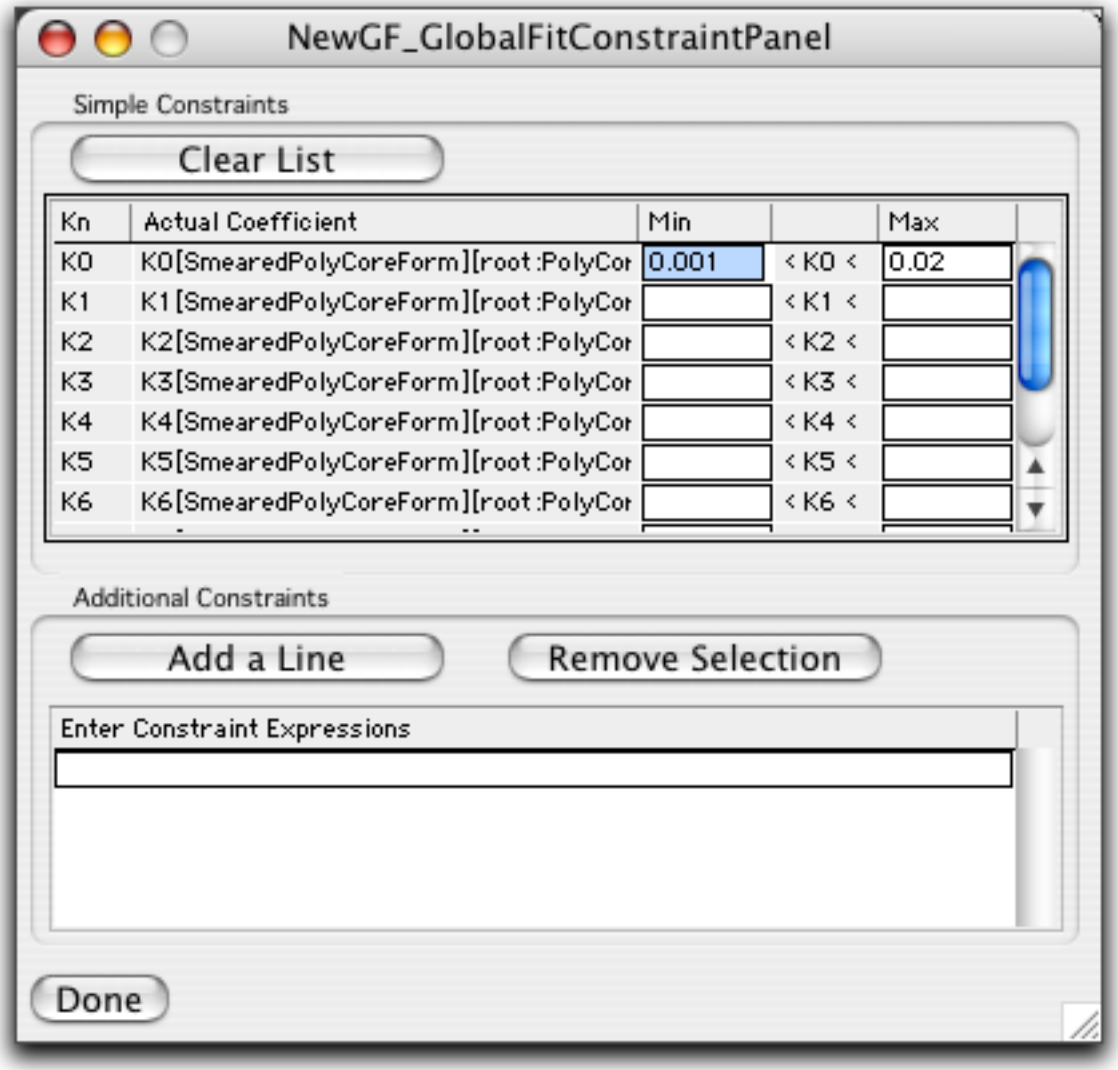
Saving Parameter Guesses

If the parameter list is long, it can be tedious to re-type a set of initial guesses. A set of guesses can be saved to a wave that you create by selecting "Save Setup" from the bottom right corner of the panel.

Constraints

You can apply constraints to the coefficients to make sure they remain within prescribed limits. Click the Constraints... checkbox in the bottom part of the control panel. When you turn on this checkbox, a control panel is created that allows you to enter constraints. The upper part of the panel allows you to enter simple limits on the coefficient values. The lower part allows you to enter arbitrary expressions involving combinations of the coefficients.

Note that the constraint expressions use "Kn" to refer to the n'th fit coefficient. When doing a global fit, n refers to the entire collection of fit coefficients, not to the coefficients in your fitting function.



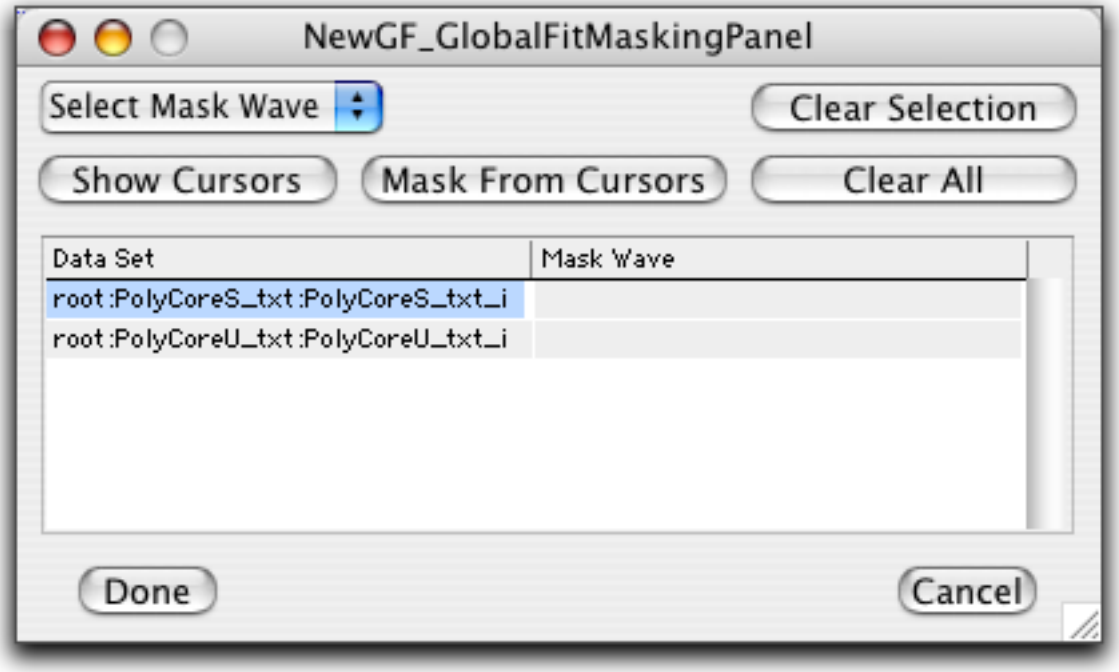
For more information on fitting with constraints, see Fitting with Constraints in the Curve Fitting help file.

Data Masking

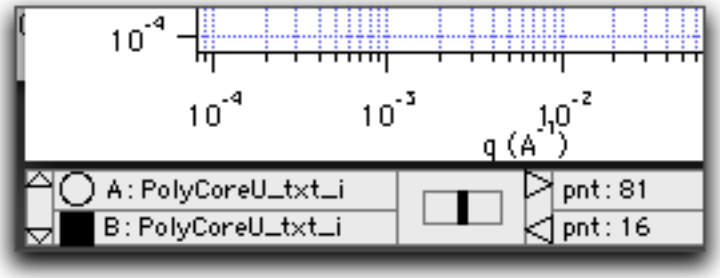
It may be that you don't want to fit all the points of all your data sets. If that is the case, you can prepare a mask wave for the data sets for which you want to exclude some points. You do not have to select a mask wave for each data set. If you leave the

mask wave blank in any row, the fit will use all of that data set. If you wish to use masking waves, check the Masking... checkbox in the bottom part of the Global Fit control panel to display a control panel where you can create mask waves.

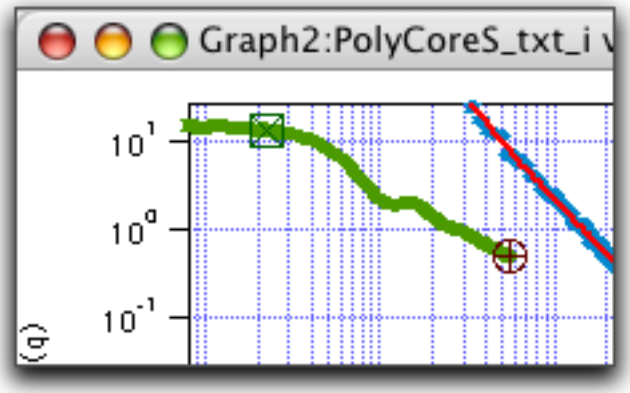
To create a mask wave for a data set, click a data set in the list to select it. Then choose Show Cursors above the list. This will add cursors to the first data point of the selected data set.



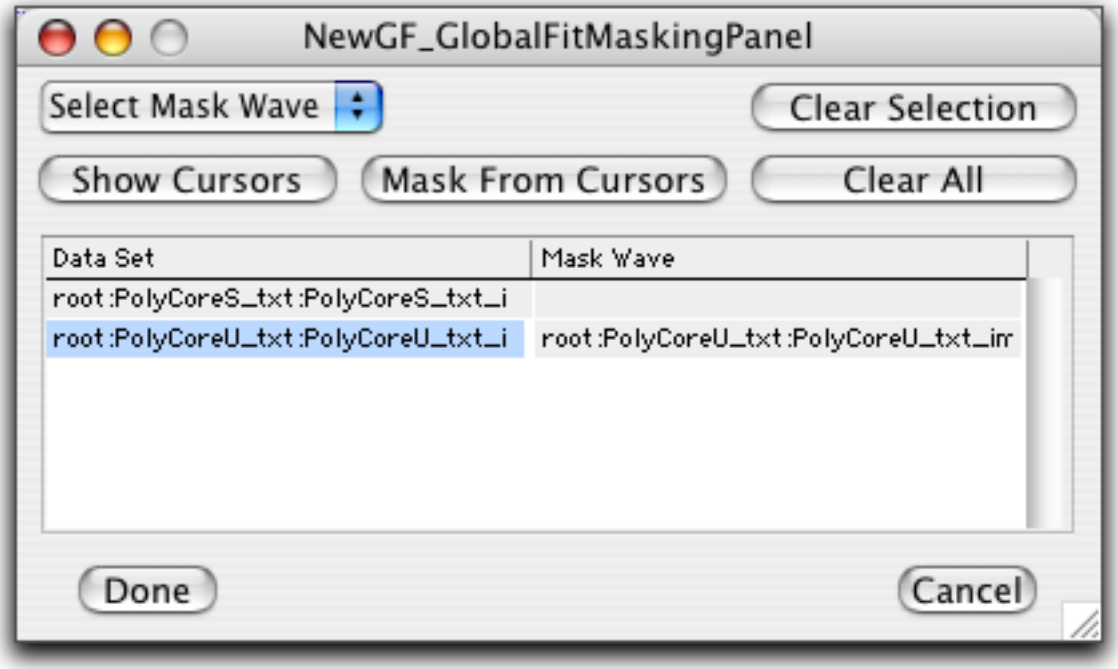
Initially both cursors are "active", and solid black in the lower left of the graph. Clicking the circle or square will toggle that cursor. When solid black, the cursor will move along the data set using the right/left arrow keys. Only data between the cursors will be included in the data fitting.



Move the "A" cursor using the arrow keys to exclude some of the low Q data.



When satisfied, select "Mask from Cursors" on the panel. A masking wave is created, and added to the list box. When finished creating data masks, "done" will save your selections, and dismiss the panel. If you fit the data again, it will use the entire SANS data set, but use only your selected region of the USANS data set.



Simple Global Fitting

There is a great deal of flexibility built into the Global Fitting Panel that is based on the WaveMetrics-supplied version of <Global Fit>, and as a result, the panel is rather complex. One of the most common uses of global fitting is simultaneous fitting of a SANS and USANS data set with a single model. Then a simplified interface is much more appropriate.

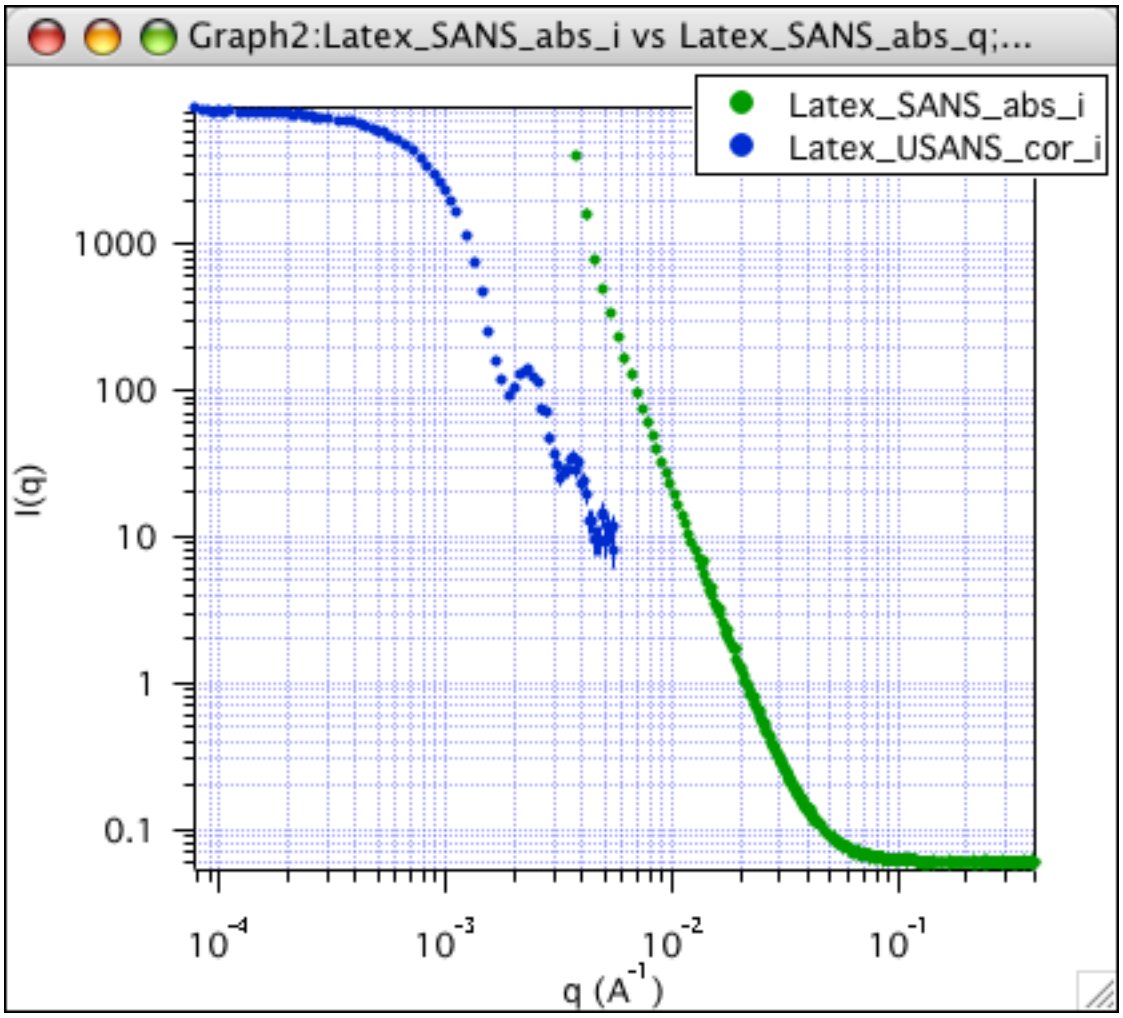
Basic Operation

It is recommended that you are familiar with fitting individual data sets before attempting to perform a global fit. It is also very helpful to fit each data set individually so that these fit results can be used as (very good) initial guesses to the global fit. If the model doesn't fit the individual data sets, it'll never be able do the global fit.

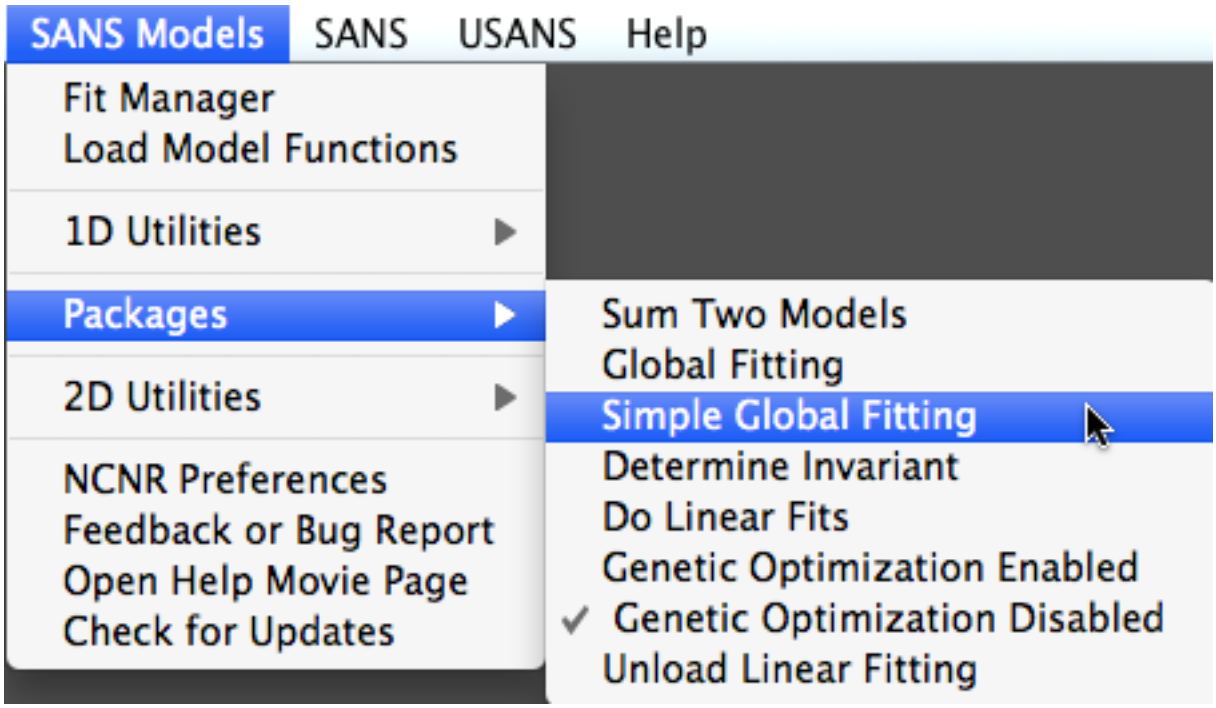
From this point, it is assumed that you have done these individual fits or at least have plotted the model for each data set and gotten the coefficients close by hand.

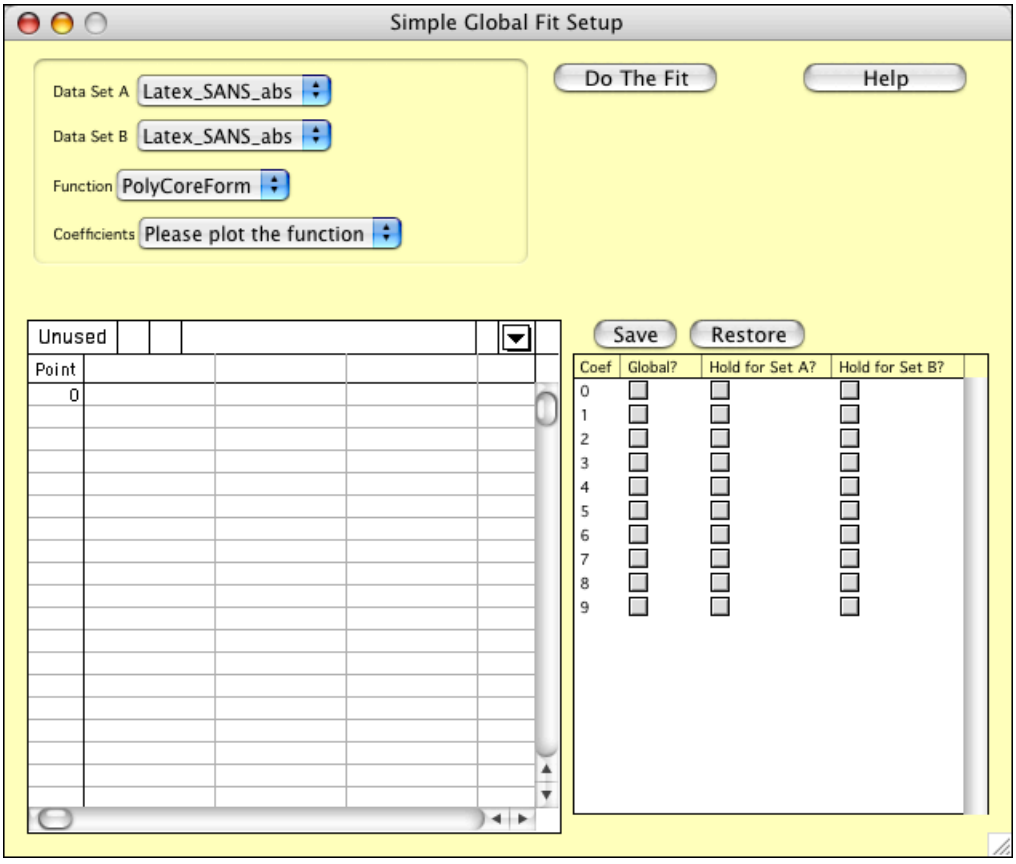
1) Load the two data sets that you would like to fit, appending them to the same graph. For this example, load the sets Latex_SANS.abs and Latex_USANS.cor that are experimental data for nearly monodisperse latex particles in D2O. Note that there are significant scaling and slope differences between the slit-smeared USANS data and the pinhole-smeared SANS data. The USANS data will be several orders of magnitude lower in intensity than desmeared data, and the slope will in general be shallower than the desmeared data. Don't expect the data sets to overlap - due to the different instrumental resolution, SANS and USANS data should never overlap! See Resolution Smearing for more of the details why this is so.

For this example, the data is fitted with SmearedSchulzSpheres, so this model has already been loaded and plotted for each data set. If the models are not plotted, you won't be able to continue with the global fitting.



2) Load the Simple Global Fit package by selecting Packages->Simple Global Fitting from the SANS Models menu.



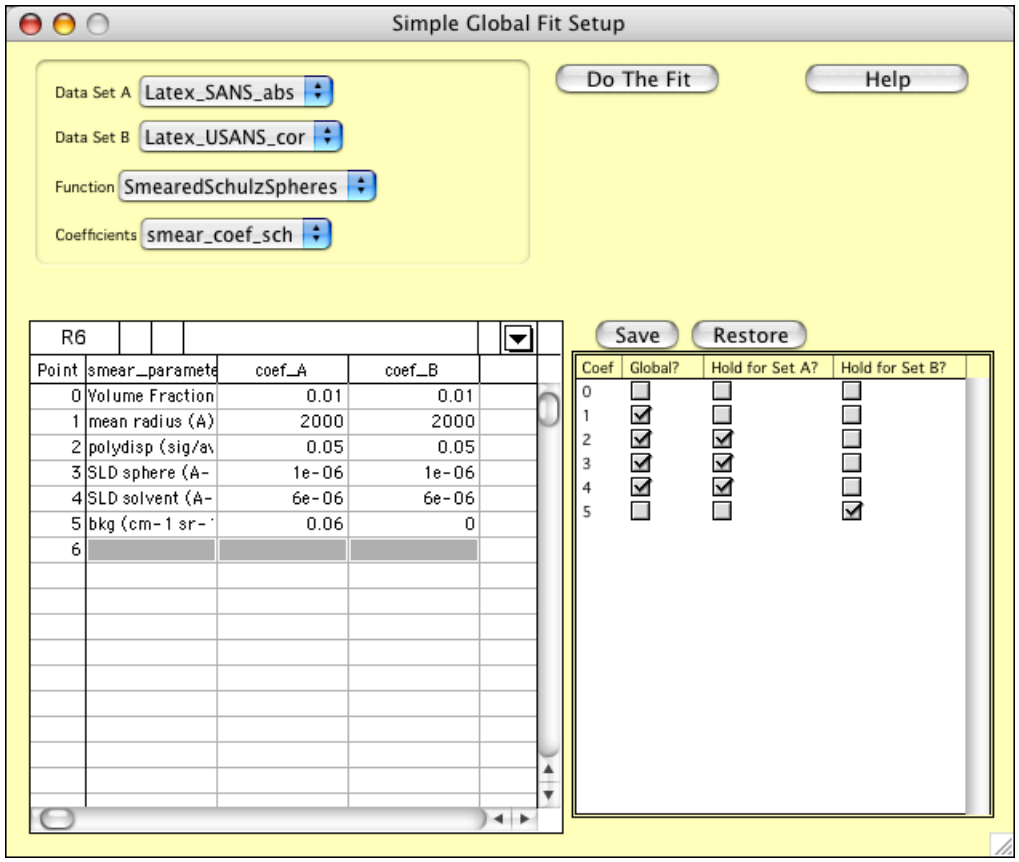


When the package loads, it displays the Simple Global Fit control panel. At any time, you can bring the control panel to the top by selecting Simple Global Fit from the SANS Models menu.

3) Select the data sets (A and B) using the popups. The data sets can be in either order, with the only note that the initial guess for the coefficients will be copied from the coefficients that are associated with set A. They will be editable later, however.

4) Choose the fit function for each of the data sets. In this simplified interface, a single model is fitted to both data sets, in this case, SmearedSchulzSpheres. Click on the "function" popup, and choose the function from the list. Then choose the correct coefficients from the popup. There should be only one item in this popup if all is working correctly. Once the coefficients are selected, the coefficient values are filled into the table, and the checkboxes are adjusted to reflect the correct number of coefficients for the model.

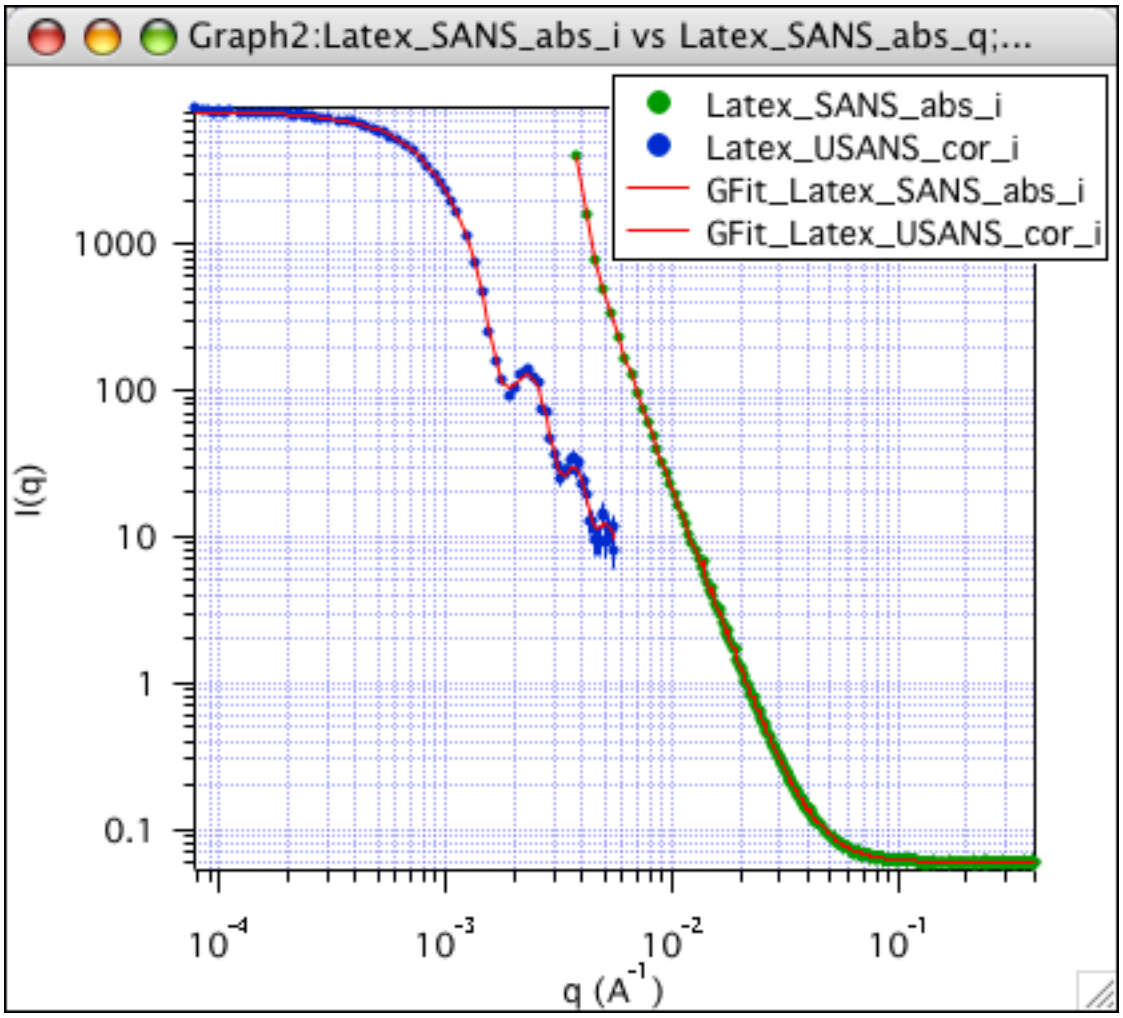
5) The right half of the table is where the "linked" coefficients are set up. For this example of SANS and USANS data from a single sample, the physical dimensions (radius and polydispersity) of the particles and their SLD's don't change, so they are global. So check these as global. In addition, the SLD's and polydispersity are known values, so they need to be held fixed too. Check the hold box for either set A or B (or both). Holding a global value for at least one set is equivalent to holding it for all data sets. The scale factor may be different for each data set since the absolute scaling may be slightly different (a few percent). Ideally, they both should be identical and equal to the volume fraction of latex particles. So, leave that coefficient as not global, and not held for either set. Keep in mind that after the optimization, the results must be physically reasonable... Finally, the background value is fitted for the SANS data set, and is held fixed at zero for the USANS data set. Enter the coefficients in the table, and hold the value for the USANS data set. Now the starting coefficients (reasonably close values) and the table setup looks like:



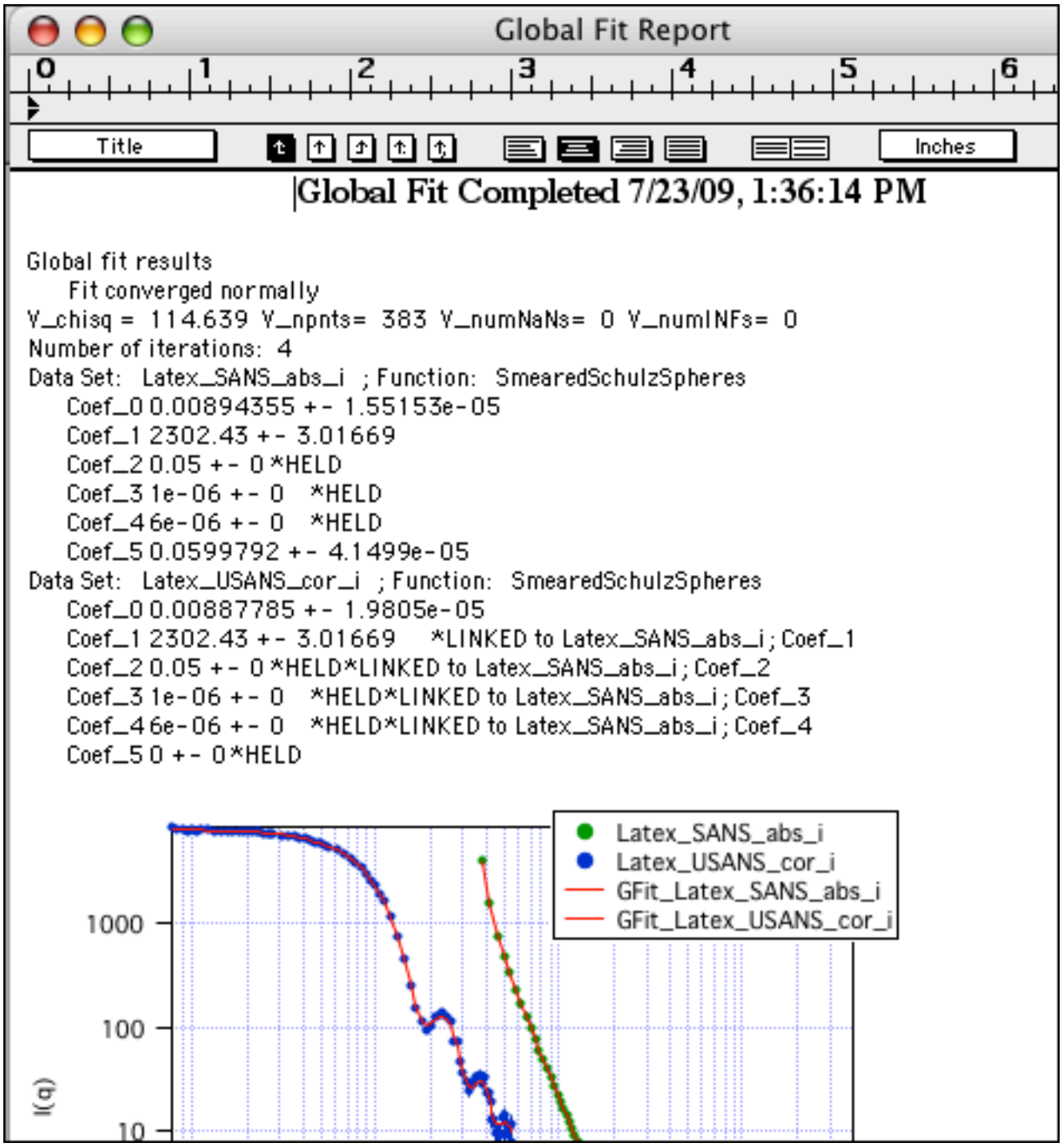
6) The state of the checkboxes is saved with "Save" and restored with "Restore" if you are trying out different combinations of global parameters in the fit. Coefficient values are not saved, as they can be easily copied (cut and paste) from the coefficients for each model from the Curve Fit Setup panel. All that is left is to do the fit. The weighting waves, the error in the intensity, are automatically selected for each set as the fit is performed.

7) So click Do The Fit already!

8) A separate window is generated showing the progress of the fit, and disappears when it's done. The fit results are automatically appended to the graph. In addition, a report is generated and saved to disk, showing the results of the fit. Coefficients that are HELD or LINKED are marked as such. The results are also added to your original graph as "GFit_" data. This example, of course, worked wonderfully.



And the report looks like:



9) If you want to exclude some of the data points from the fit, apply constraints to the parameters, calculate the covariance (highly recommended), or calculate residuals, you'll need to use the full Global Fitting package (see Global Curve Fitting of SANS Data).

Calculate Scattering Invariant

The scattering invariant is a model-independent quantity that can be easily calculated from the scattering data. The invariant is defined as the integral:

$$Q \equiv \int_0^\infty q^2 \frac{d\Sigma}{d\Omega}(q)\, dq$$

For two-phase systems where there are two distinct phases with volime fractions $\phi 1$ and $\phi 2$ such that $\phi_1 + \phi_2 = 1$, and with scattering length densities ρ_1 and ρ_2:

The invariant is related to the volume fraction, ϕ, using the relation:

$$Q = 2\pi^2 \Delta\rho^2 \phi(1-\phi)$$

where $\Delta\rho$ is the contrast, $\rho 1 - \rho 2$, the difference in scattering length densities between the two phases.

In an ideal two-phase system with sharp interfaces between the phases, the intensity should decay as q^{-4}; hence the Porod constant is defined as the large q limit of the intensity:

$$\lim_{q\to\infty} q^4 \cdot \frac{d\Sigma}{d\Omega}(q) \equiv C_p = 2\pi S_v (\Delta\rho)^2$$

and can be found as the scaling factor in a Porod plot.

The quantity Sv is the surface area per unit volume of sample (also called the specific surface area) can be determined in cases where the volume fraction is independently known. The scattering length densities of each phase are not required. With this normalization, the scattered intensity does not even need to be in absolute units.

$$S_V = \frac{\pi\phi(1-\phi)C_p}{Q}$$

The zero angle scattered intensity (on absolute scale) is related to a "correlation volume":

$$\frac{d\Sigma}{d\Omega}(0) = \phi(1-\phi)(\Delta\rho)^2 v_c$$

and normalizing by the invariant:

$$v_c = \frac{d\Sigma}{d\Omega}(0)\frac{2\pi^2}{Q}$$

In some cases the correlation volume can be related to the size of the domains in the two phase material, but be careful with this - see the discussion in G&K, Chapter 2 (written by Porod) for the warnings.

For the special case of particulate systems, the invariant still is true even if there are interparticle interactions present. The Porod constant is also correct, since at high enough q values, the effect of interparticle interactions vanishes. For particles, the surface to volume ratio can be related to the average particle dimensions. For a sphere, Sv = 3/R, and then the radius of each sphere (if your sample really is composed of spherical particles) is:

$$R = \frac{3Q}{\pi C_p}$$

For an infinitely long cylinder of radius R, Sv = 2/R.

But your sample must be dilute enough that there are no interparticle interactions to measure the correct zero-angle intensity or radius of gyration. If the particles are dilute enough, then the zero-angle intensity is related to the particle volume:

$$\frac{d\Sigma}{d\Omega}(0) = \phi(\Delta\rho)^2 V_p$$

and can be determined easily even if the volume fraction and contrast are not known:

$$V_p = \frac{d\Sigma}{d\Omega}(0)\frac{2\pi^2}{Q}$$

Slit-Smeared Data:

Slit-smeared data from the USANS instrument is collected with a different instrument resolution from pinhole SANS data, and in the infinite slit approximation (valid for our USANS instrument) the "smeared" invariant is defined slightly differently,

$$Q = \Delta q_v \int_0^\infty q\,\frac{d\Sigma_s}{d\Omega}(q)\,dq$$

including the value of the vertical resolution for the slit height, Δq_v. The limiting slope for the smeared intensity of a two-phase system is $I_s(q) \sim q^{-3}$, rather than q^{-4}, so the smeared Porod constant is defined as below, and simply related to the true Porod constant.

$$\lim_{q\to\infty} q^3 \cdot \frac{d\Sigma_s}{d\Omega}(q) \equiv C_{P,S} = \pi C_P / (4\ \Delta q_v)$$

When slit-smeared data is loaded into the Invariant calculator, it must be marked as slit-smeared data, entering the slit height if it cannot be found in the data file. Then the proper integration can be done for the invariant and the values reported are *already corrected* for the slit-smearing effect.

However, the zero-angle intensity and Porod slope are slit-smeared values since they are found by directly fitting the smeared data set. Slit smearing does not affect the Guinier slope, so no correction is needed for the radius of gyration. For proper calculations, the other values must be corrected as follows to get the true, unsmeared values:

$$\frac{d\Sigma}{d\Omega}(0) \approx \frac{2R_G\,\Delta q_v}{\sqrt{3\pi}} \frac{d\Sigma_S}{d\Omega}(0)$$

.

$$C_P = C_{P,S} \frac{4\ \Delta q_v}{\pi}$$

Important Notes:

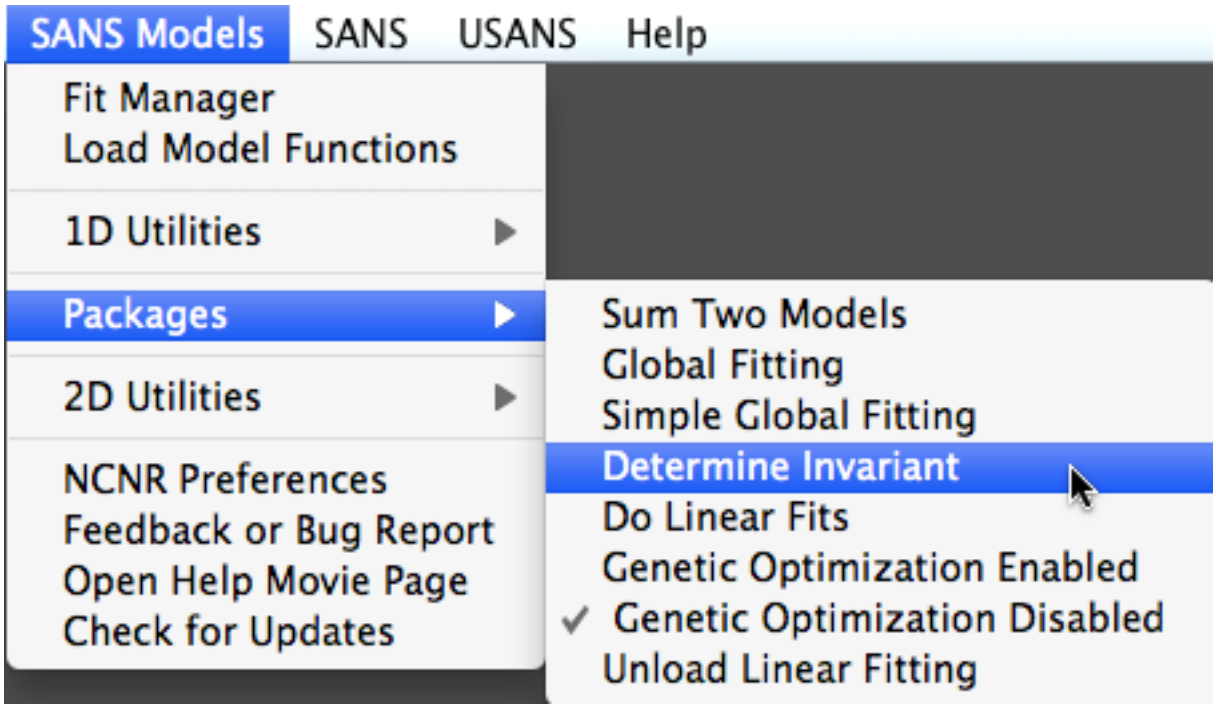
- Either pinhole SANS data or slit-smeared USANS data can be used. No corrections are made for smearing effects in pinhole smeared SANS data. USANS data is properly corrected using the slit height so that the invariant reported is the true, unsmeared value.
- You must subtract any incoherent background before calculating the invariant - See Data Set Arithmetic in the SANS Reduction Package.
- This calculation expects that the data are on an absolute scale. If your data is not on absolute scale, the calculations where the invariant is used for normalization are still valid.
- Clearly it is important to measure the scattering over as wide of a q-range as possible to get an accurate integration.
- The current routines calculate the invariant for the measured q-range, and for extrapolations to high and low q.
- The invariant calculation from each region is reported separately to show the relative contributions.
- More complex expressions for three-phase systems can be found in the literature.

- Polydispersity of the particles adds additional corrections to the lengths, since the integral quantities use different moments of the size distribution.

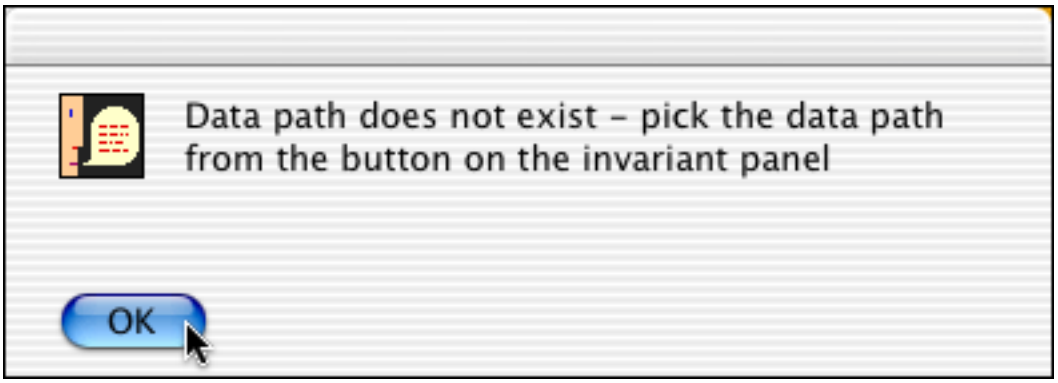
- Reference: Porod's chapter (2) from O. Glatter and O. Kratky, "Small Angle X-Ray Scattering", Academic Press, New York, 1982. A classic. The notation is geared towards x-ray scattering, but it still applies. It has been out-of-print for many years and is somewhat hard (darn near impossible) to find a copy, but a PDF version can be downloaded directly from Otto's web page: <http://physchem.kfunigraz.ac.at/sm/>

Instructions for use:

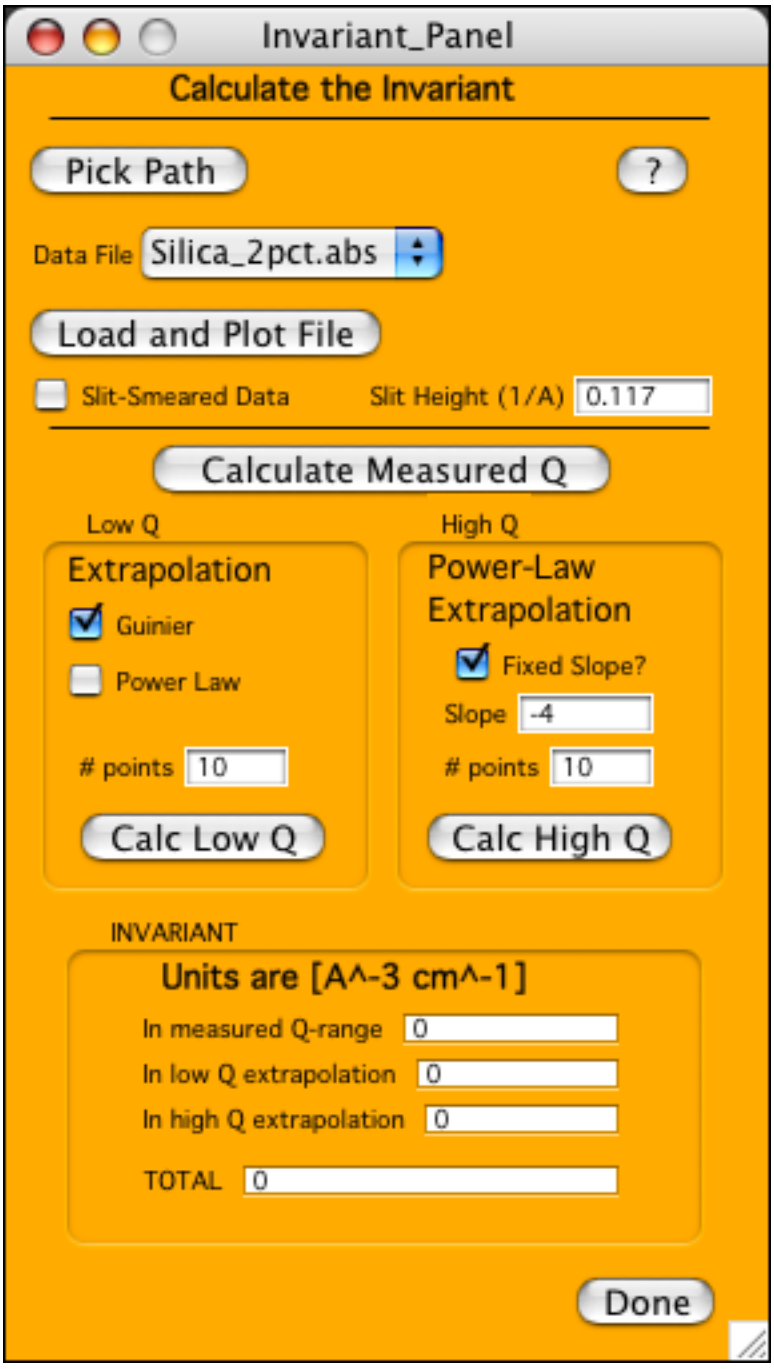
1) Open the Invariant Panel from the Macros menu, choosing Packages-> Determine Invariant



The Invariant_Panel will be drawn, and if you haven't already chosen the data path, an alert will be presented.



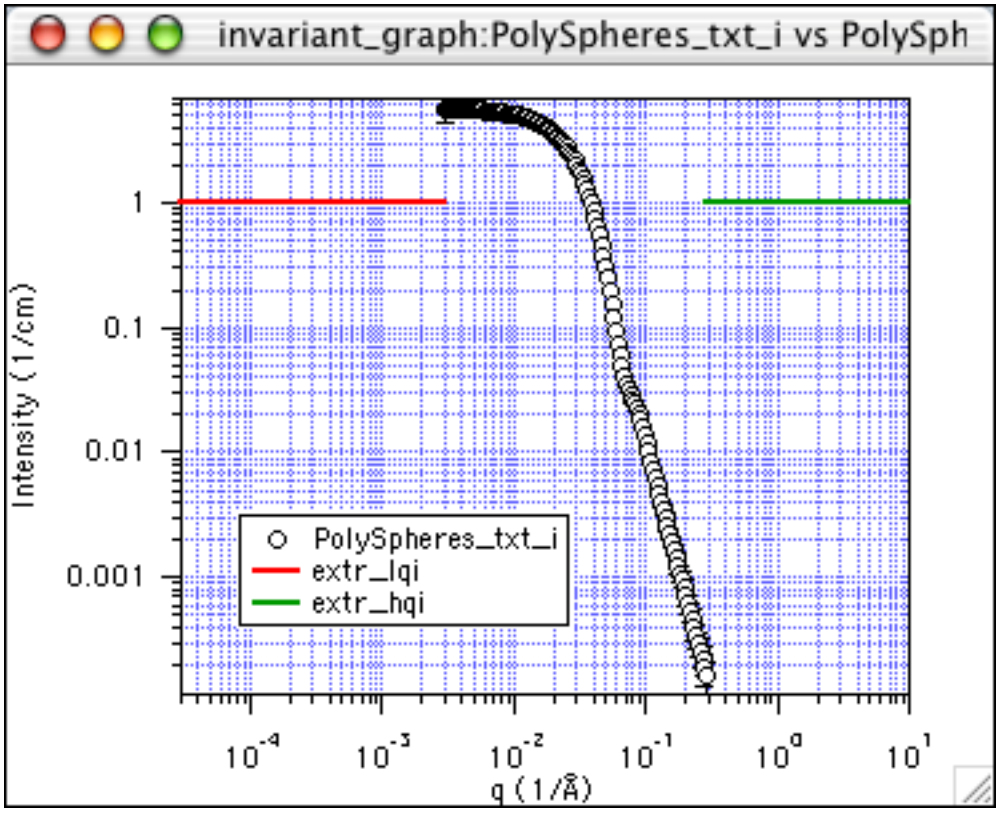
Follow the instructions and pick the path to the data you would like to analyze. Once you have set the path, you will be present with the following panel and the "Data File" popup menu will have a list of available files.



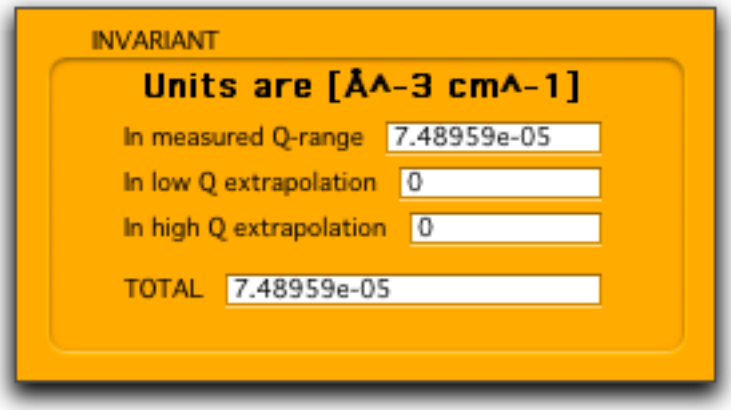
2) The example data file "PolySpheres.txt" is model data of polydisperse spheres. PolySpheres.txt data is not slit-smeared data, so leave the "Slit Smeared" box unchecked. If the input data is slit smeared, check the box and load the data set (either order). The file loader will try to determine the slit height from the data file. If it cannot, you will be

instructed to enter the proper value, or warned that the input data is not really slit-smeared data.

Load and Plot the file. A graph is drawn. The loaded data is represented as points. On each side of the data, there are dummy waves (set to 1) that will be used later for extrapolation to low and high q.

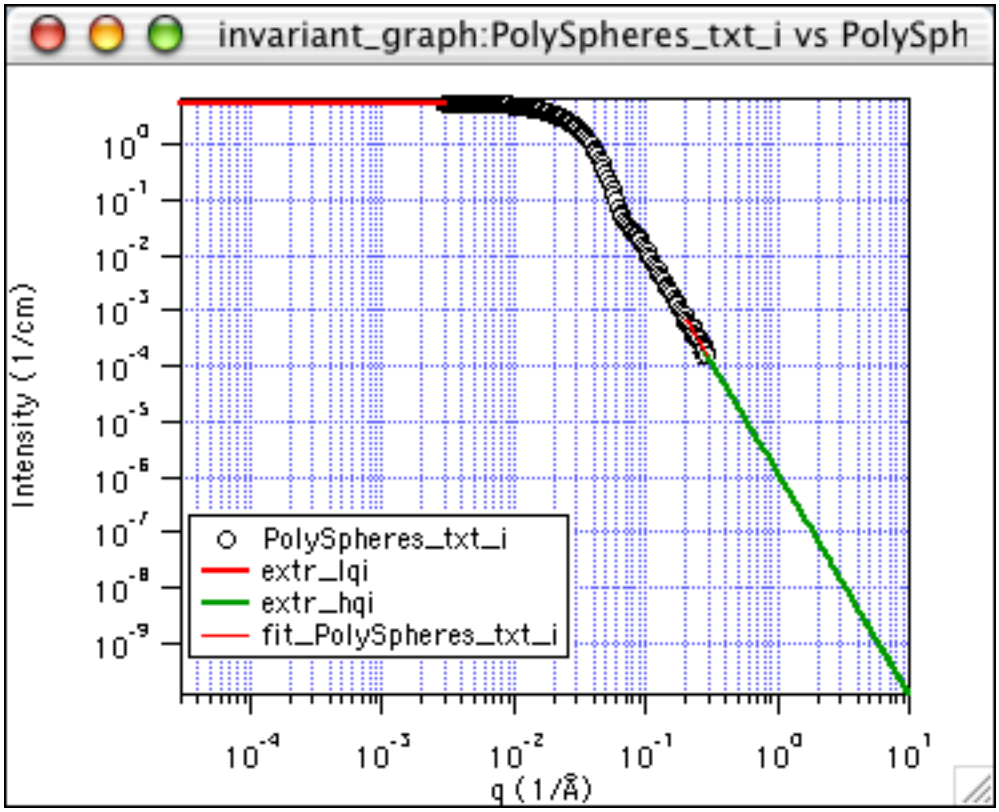


3) Calculate the measured Q range by clicking the button on the panel. The value of the invariant is reported in the panel and in the command window at the bottom of the screen. The command window also shows the details of the q-range evaluated. Note that the units of the invariant are 1/(A^3 cm^-1), which are the "natural" units of the data with q [=] (1/A) and I(q) [=] (1/cm)

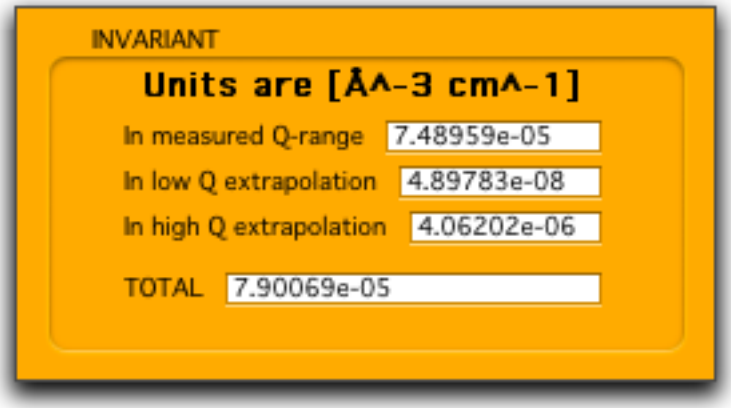


4) Since you can't measure an infinite q-range (at least not with the instruments at NIST), you may want to calculate the contribution of extrapolating the data to low Q. A Guinier extrapolation is usually best if the data has begun to level off at low Q. Adjust the number of points as appropriate. The low q contribution and grand total of the invariant is reported to the panel, and the details of the extrapolation are reported in the command window. You can re-calculate the extrapolation as many times as you like. The latest value is the only one retained.

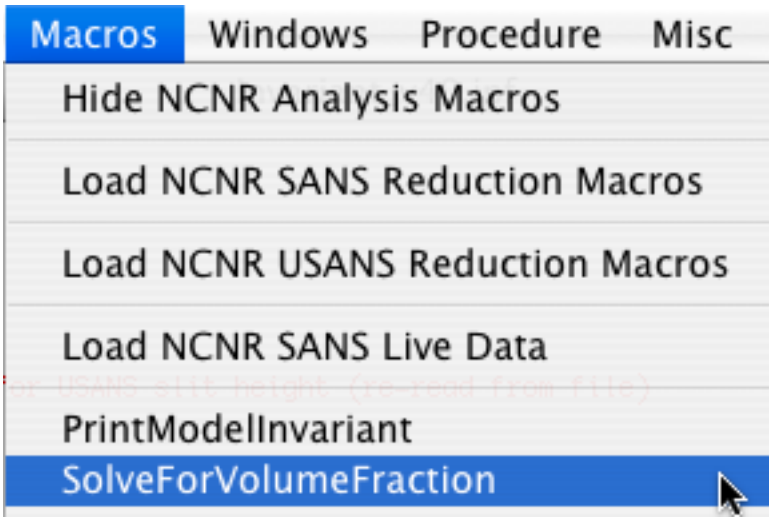
5) Now do the high Q extrapolation, using 20 points. A power-law extrapolation is most appropriate here, hopefully in the Porod region for your sample. Adjust the fit as needed, making sure the extrapolation is reasonable. The "Pre-exponential" reported in the command window is the Porod constant (if you held the slope to -4). This extrapolation is more likely to go haywire than the Guinier extrapolation - so look critically at the results.



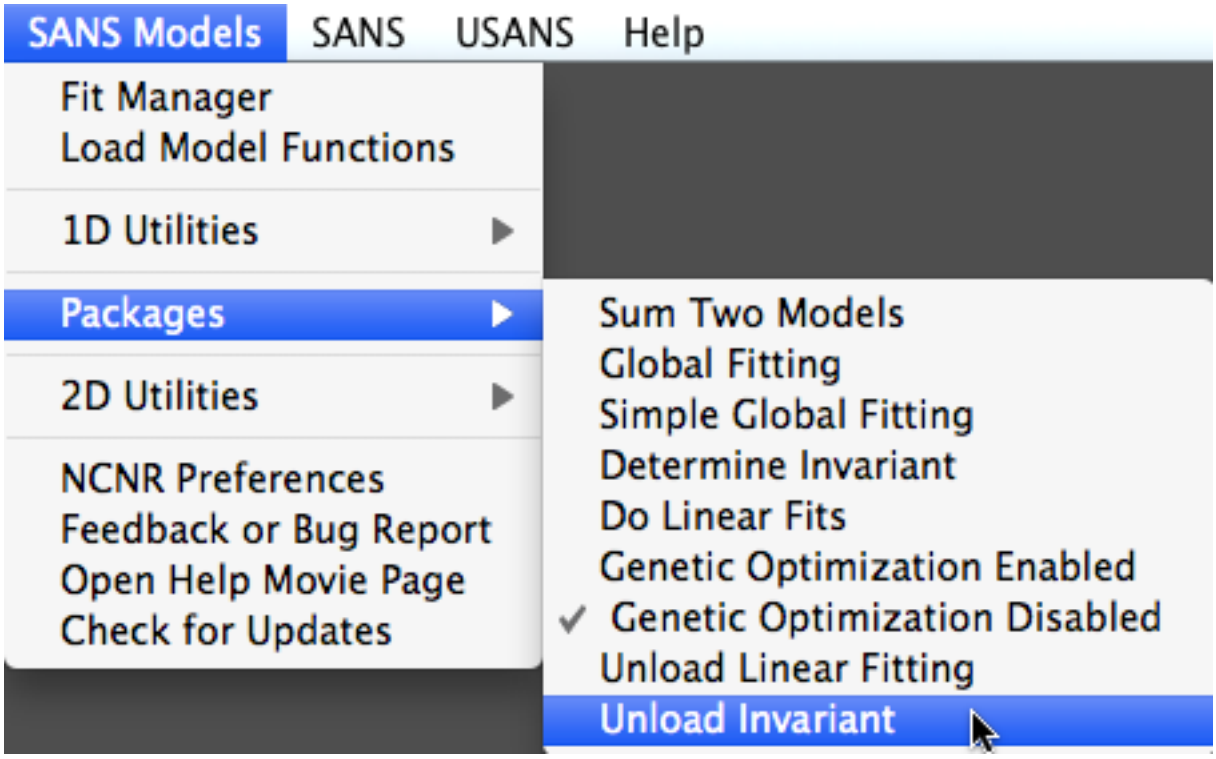
In this example, the data is model data (with random noise added) of polydisperse spheres. The volume fraction = 0.01, and the contrast = 2E-6 (1/A^2). The "perfect" calculated invariant is 7.817E-5 (A^-3 cm^-1) is quite close to the calculated value, as expected. Note the relative contributions of the low and high Q extrapolations to the measured Q range. The high Q is much more significant - since the integral is weighted by Q^2.



6) If you want, you can use a calculator from the Macros menu to calculate the volume fraction, given the calculated invariant and the contrast. Other calculations must be done by hand at this point.



7) If you are done with the Invariant package, you can unload it from the experiment using the SANS Models menu selection

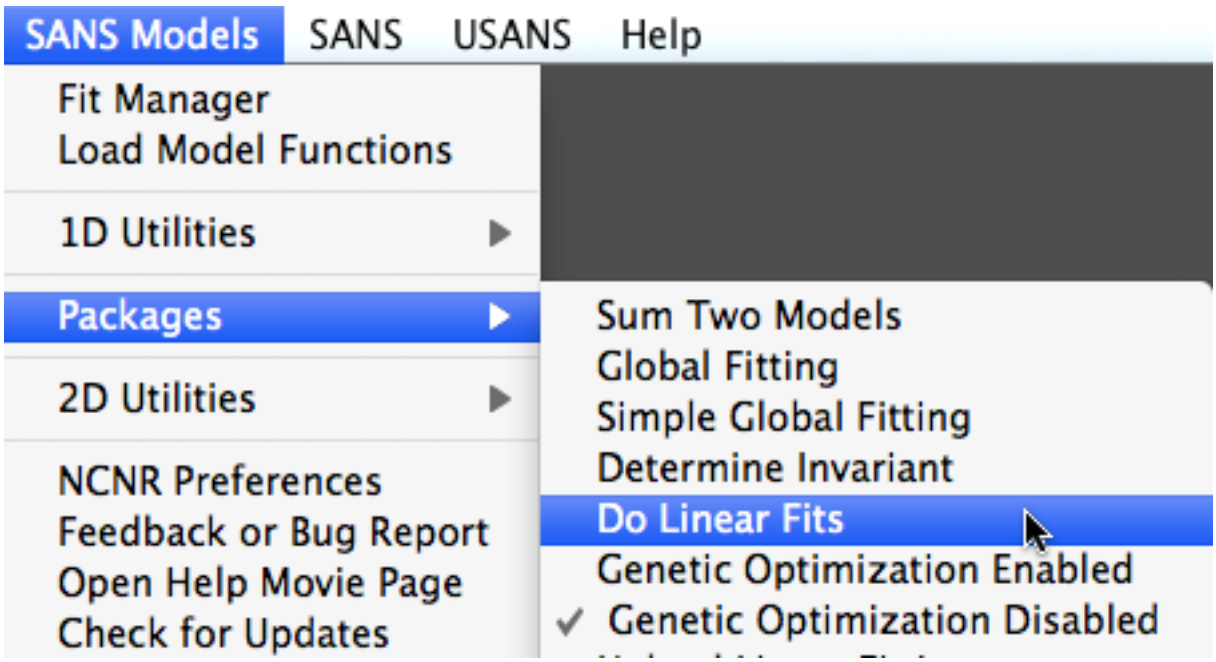


Linearized Fits

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. These linearized fits are also available as part of the SANS Reduction procedures to provide quick analysis tools as your data is being collected.

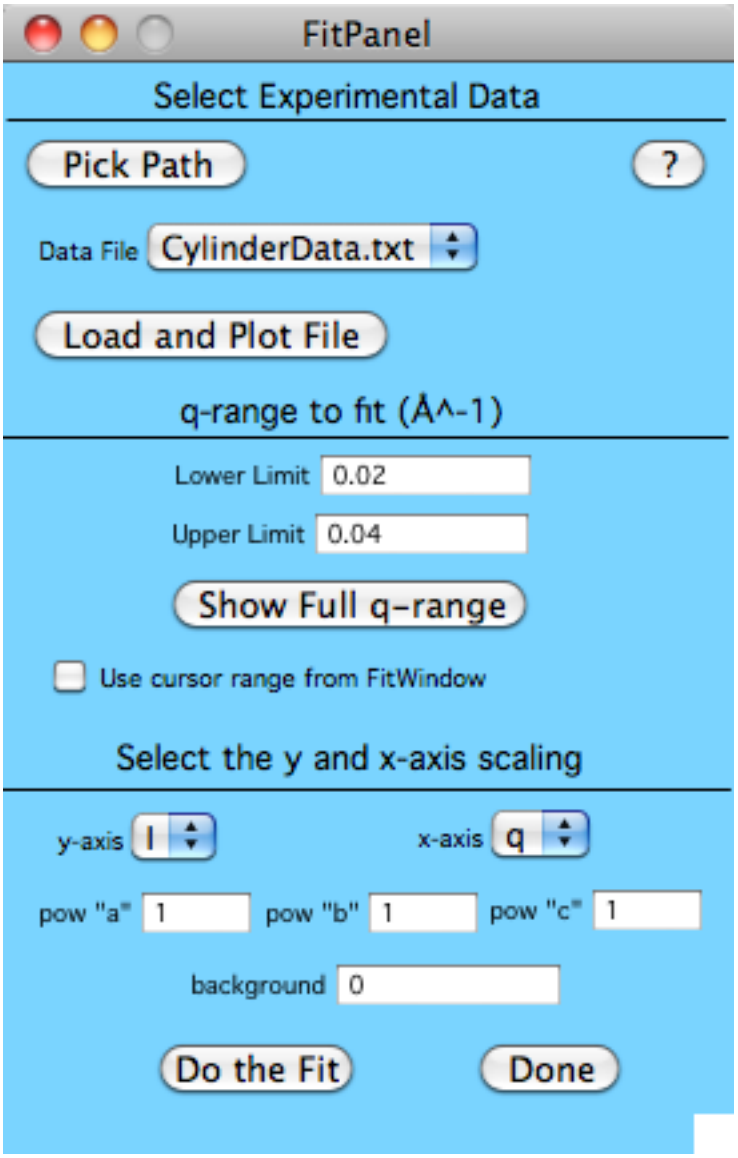
Instructions for use:

1) Open the Fit Panel from the SANS Models menu, choosing Packages->Do Linear Fits

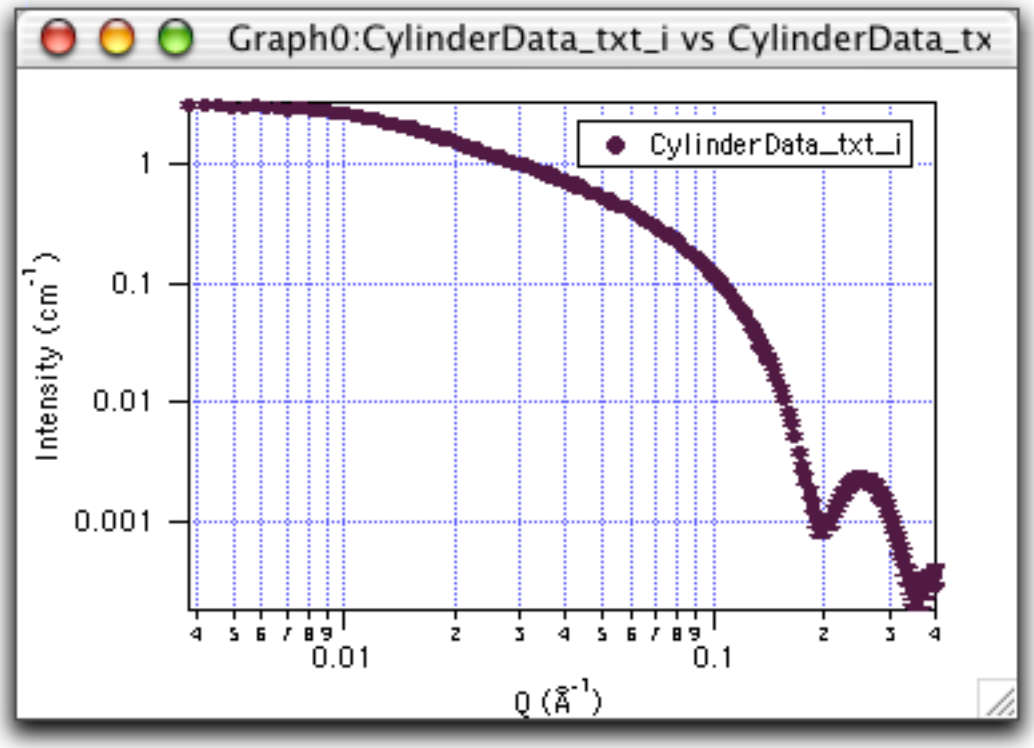


The FitPanel will be drawn, and a dialog may appear:

If you see this, follow the instructions - and Pick Path, choosing the folder that contains the data you wish to fit. Once you have picked a path to the data, the "data file" popup menu will have a list of available files.

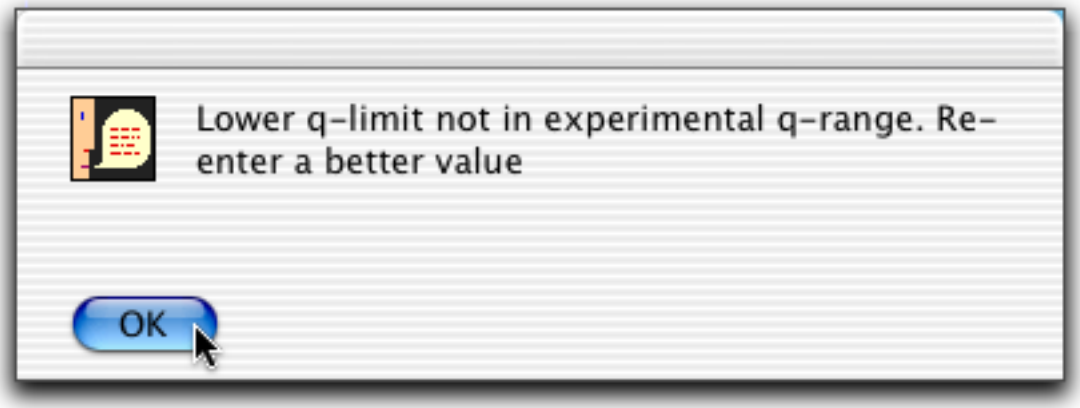


2) The file CylinderData.txt is model data for a cylindrical particle. Before plotting it from the "Load and Plot" button on the fit panel, load the data as usual from the SANS Models menu. This will allow you to more easily inspect the data and visually make a first guess at where the Guinier region(s) are for the cylinder data.



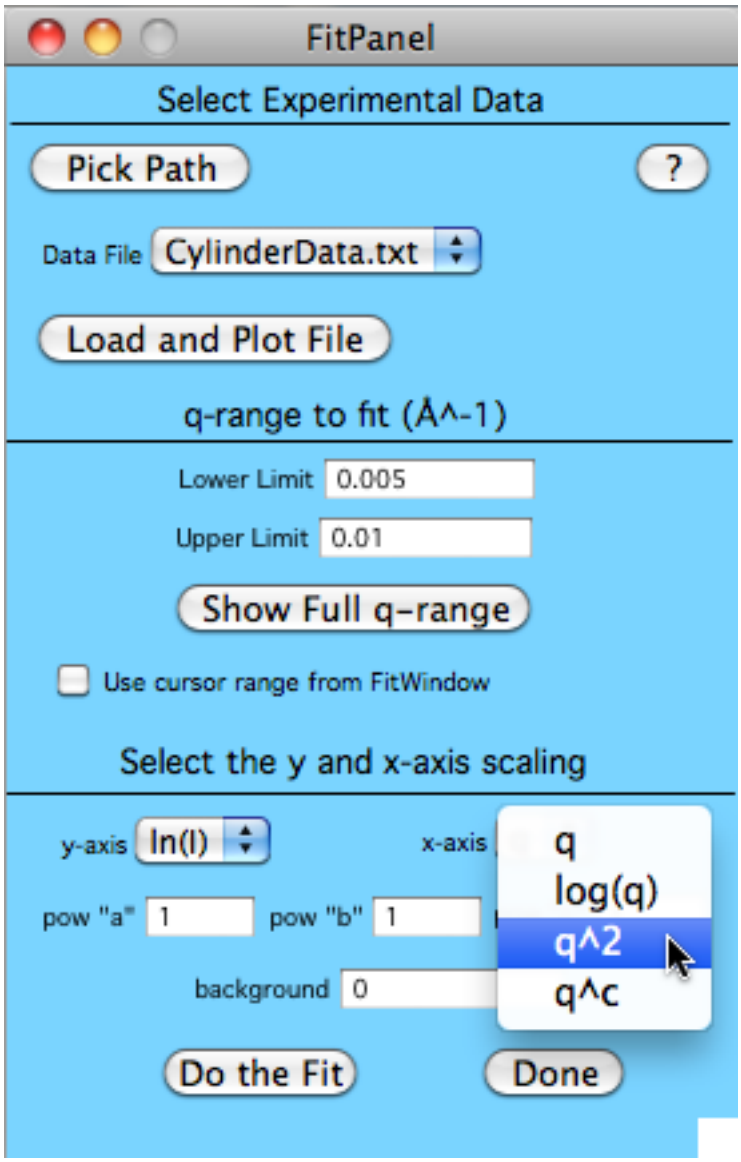
There are two Guinier regions for a cylindrical particle. To get an estimate of total size of the cylinder, fit the low Q region of the data to ln[I(Q)] vs Q^2. The Guinier region looks to be from approximately (0.005 to 0.015) [1/A].

Select the file in the popup menu on the FIT panel, and click "Load and Plot File". It will try to plot your data with the default Q-range of (0.02 to 0.04) [1/A]. This is in the q-range of the data loaded. If not - the following "warning" appears. If this happens for your data, simply click OK, and enter a more appropriate range for the plotted data.

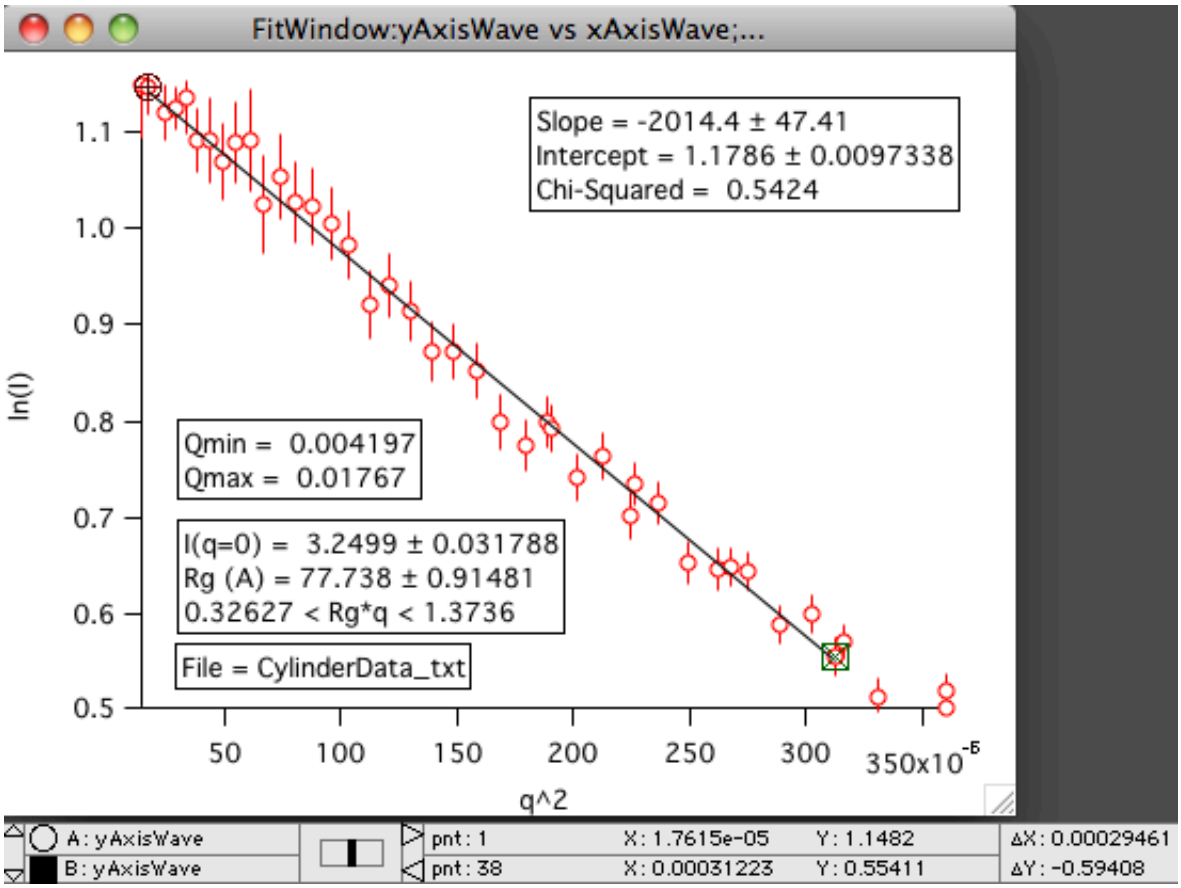


3) To fit the data to a Guinier plot, select a y-axis scaling of "ln (I)" and an x-axis scaling of

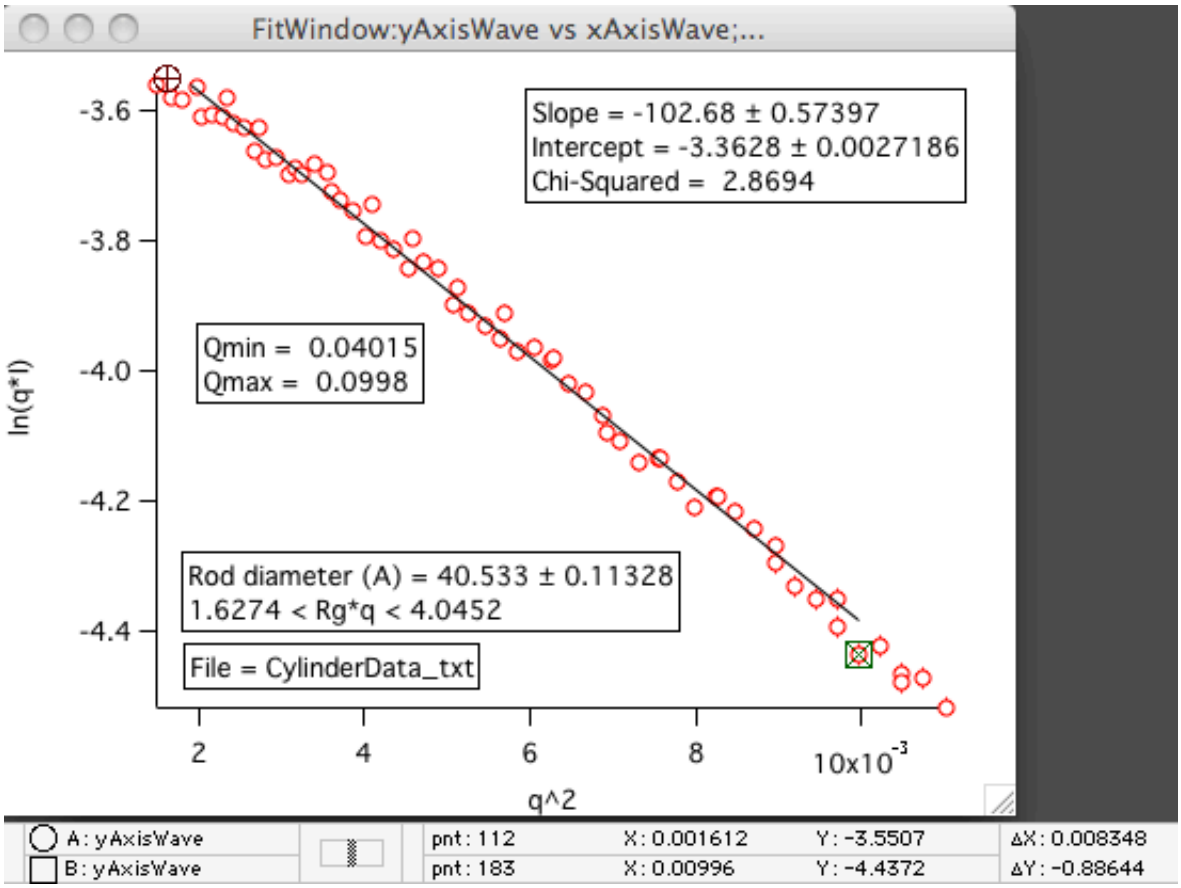
"q^2". The powers a, b, and c apply to different axis scalings, and we do not need to subtract any background before doing the fit. Enter the lower and upper limits for fitting of q = 0.005 (1/A) and q = 0.01 (1/A) in the boxes. You can (and should) adjust the values and re-fit the data if you don't like what you see.



4) Once you've entered the fitting range (or selected it with the cursors) and chosen the axis scaling, then click "Do the Fit", and the data is scaled and fitted, with all the results displayed on the graph. One standard deviation is reported along with the radius of gyration and range of q*Rg. Guessing a fitting range of q = 0.005 (1/A) to q = 0.01 (1/A) did not use many points, so in the plot below, The cursors were used to select a larger q-range (which is still nicely linear) for the fit.



5) For a cylinder, there is a second Guinier region at higher Q. This represents the radius of gyration of the "cross-section" of the cylinder, rather than the radius of gyration of the cylinder as a whole. This region is recognized on the plot as the "break" between the Q^-1 slope and the first steep minimum of the cross-section scattering. This is a q-range of approximately q = 0.04 (1/A) to q = 0.1 (1/A). Enter these values in the Range boxes (be sure to un-check "use cursors"). For the fit type, choose a "Cross-section" Guinier plot, ln[Q*I(Q)] vs Q^2. Then do the fit, with the following result - note that the actual cross section diameter is reported, since this form of ln[Q*I(Q)] vs Q^2 assumes that the particle is cylindrical.



6) If you are finished using the linear fitting package, you can unload the procedures from the experiment using the Macros menu selection.

Sum SANS Models

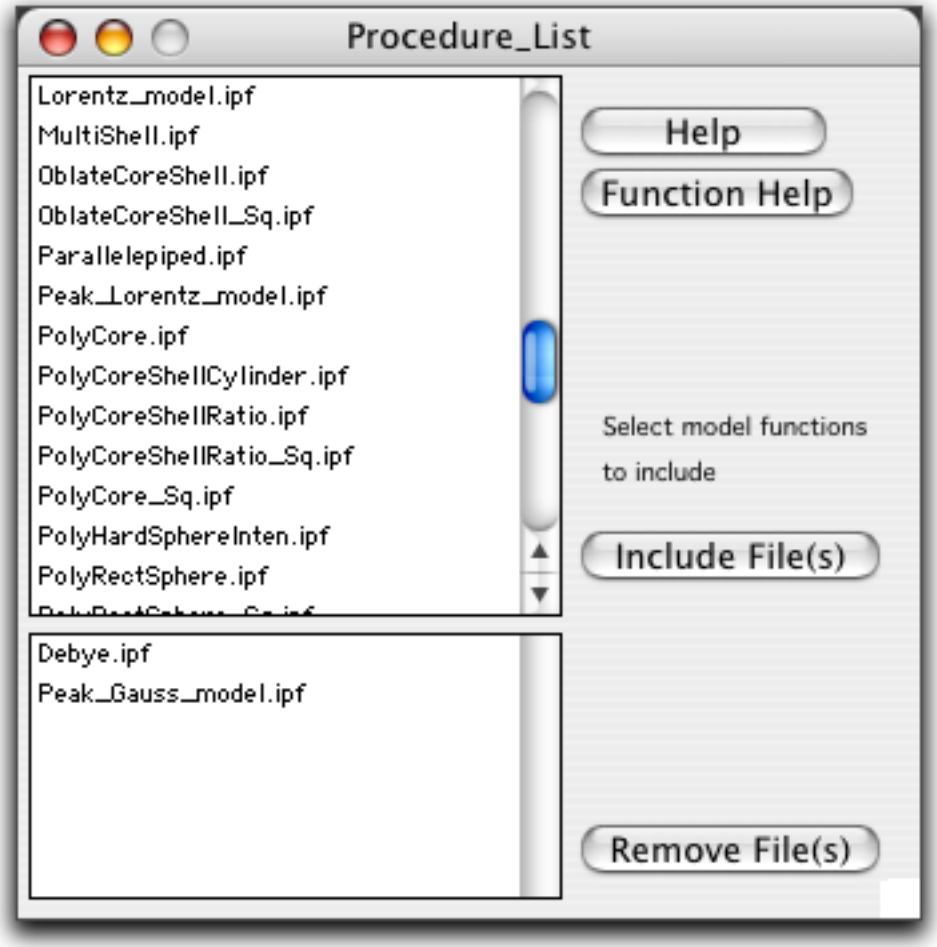
Sometimes scattering data arises from systems where there are two or more different microstructures present. In an ad hoc way, scattering from these systems can often be approximated by a simple linear combination of two model functions.

Keep in mind that this linear combination is an approximation. YOU must justify that the approximation is valid. The presence of these procedures do not justify their applicability in all situations. They simply allow easy addition of models that may or may not provide more insight into the true nature of the scattering.

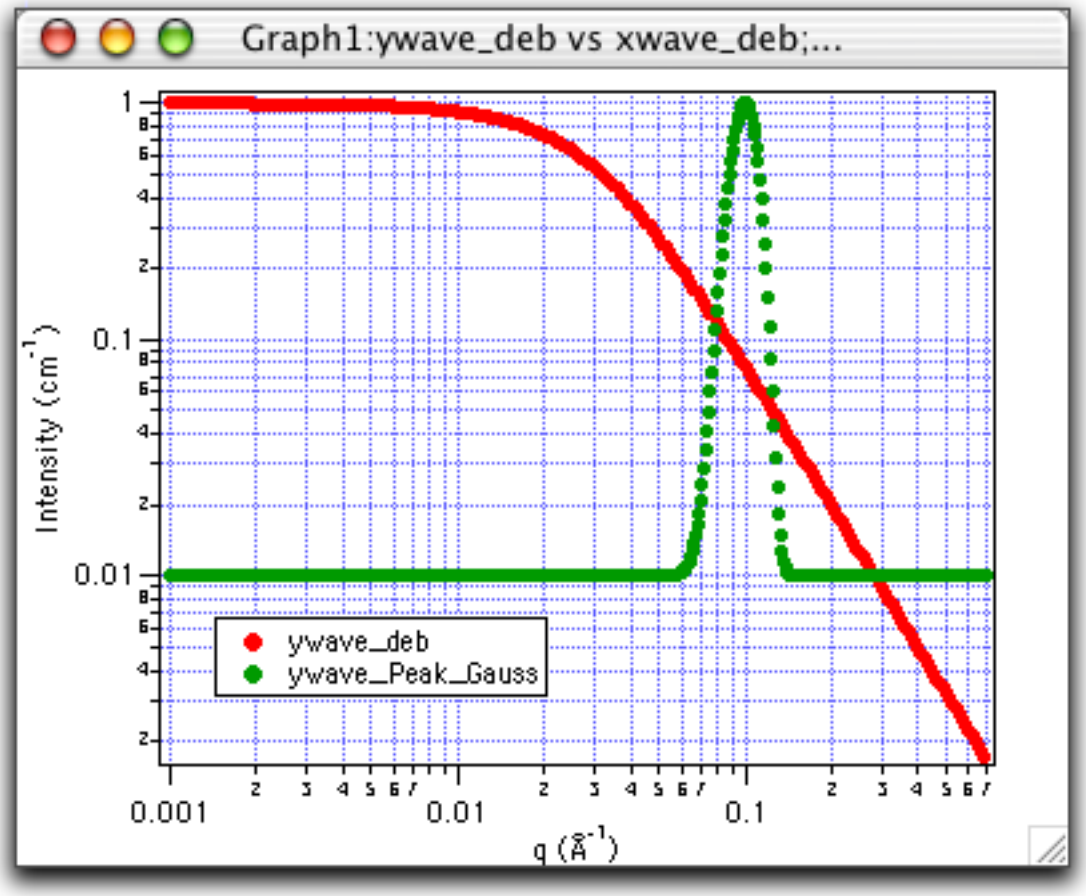
The summed model is a simple linear combination of the two models. It is done under the assumption that the two structures are dilute enough that they do not interact at all with each other. In a dilute binary mixture of particles, the partial structure factors Sii(q) = 1, and the cross structure factor Sij(q) = 0, hence no cross term (cross-correlation) is included. In the case of non-particulate scattering, the assumption is the same - that the two structures that produce the scattering are uncorrelated.

Example of Operation

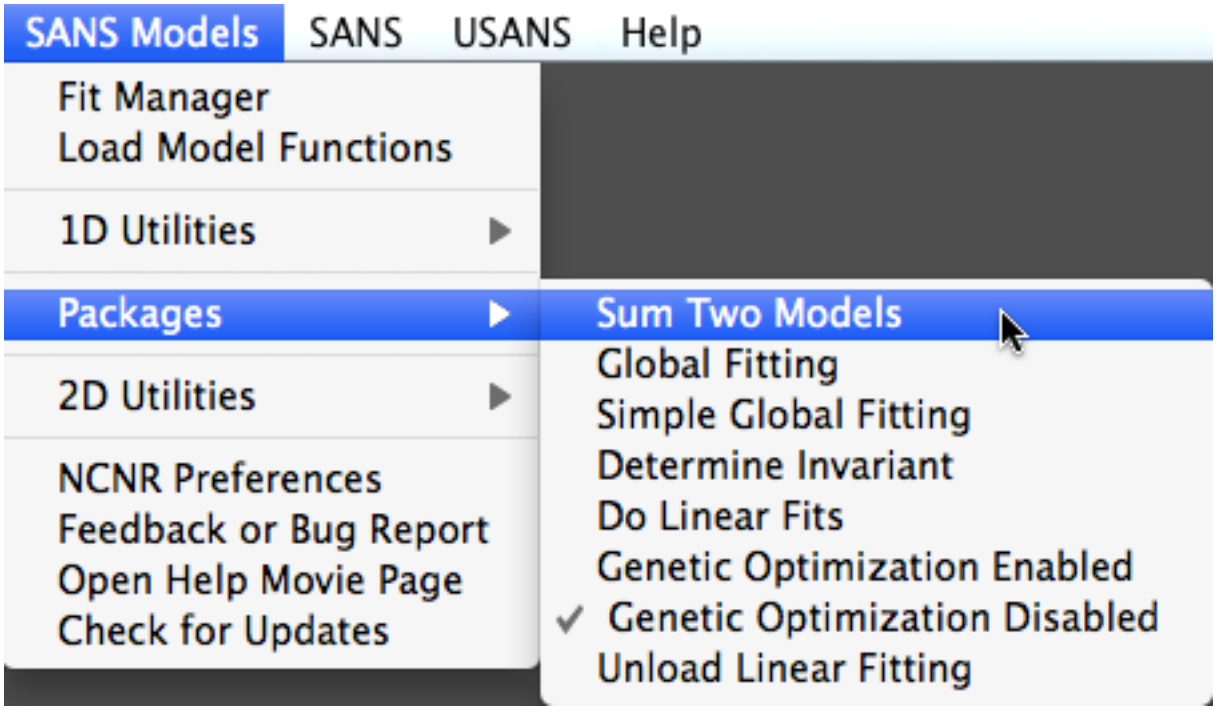
1) Include two models using the Model Picker. For this example, include the Debye function and a Gaussian peak. This has no physical significance for any real system that I know of, but it makes a nice example.



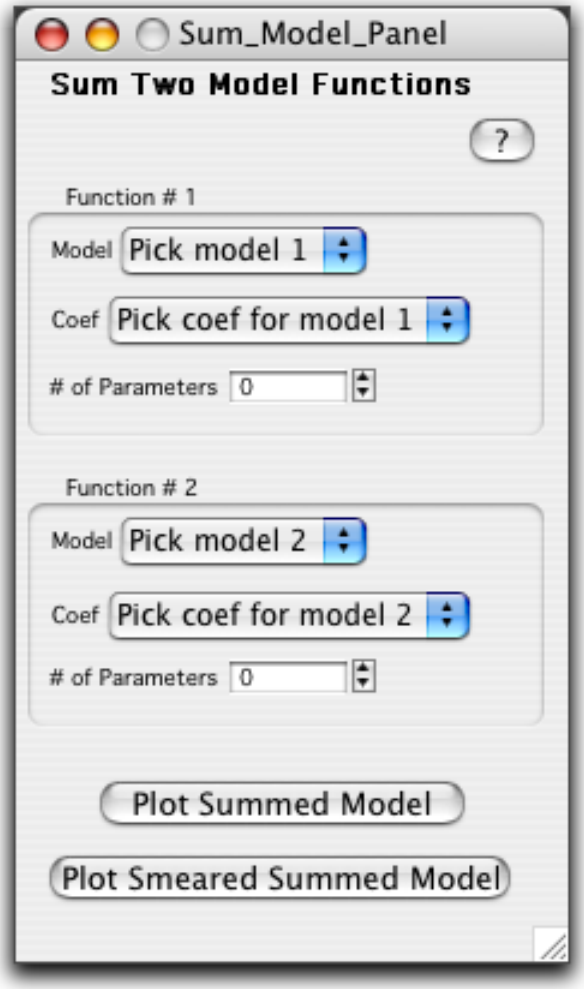
2) Plot both of these models on the same graph to see how they combine. You will need to do this to see how many parameters there are in each model, and what each parameter physically means. Remember to plot the NON-smeared models from the function popup on the Fit Manager.

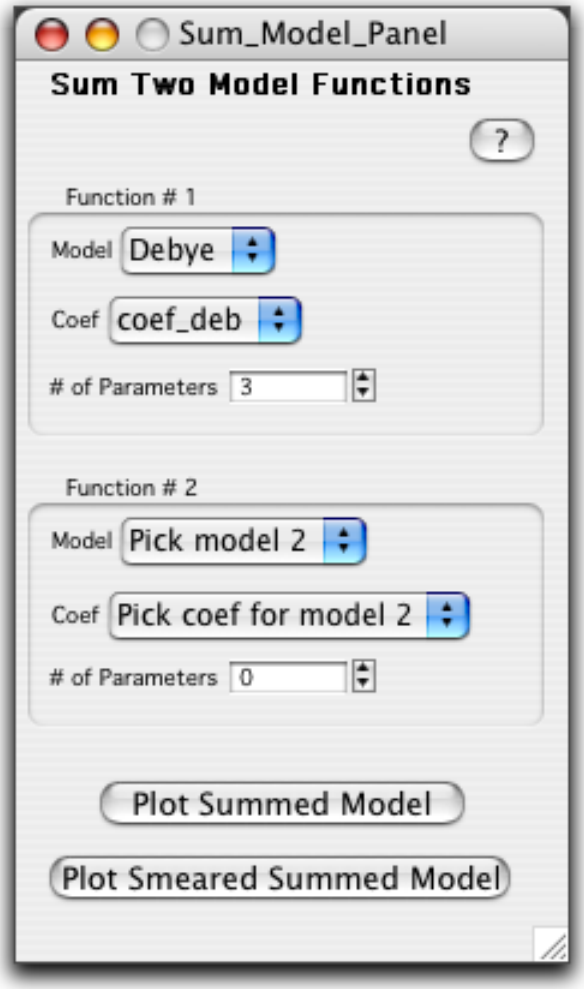


3) Open the Sum Two Models Package from the SANS Models menu:

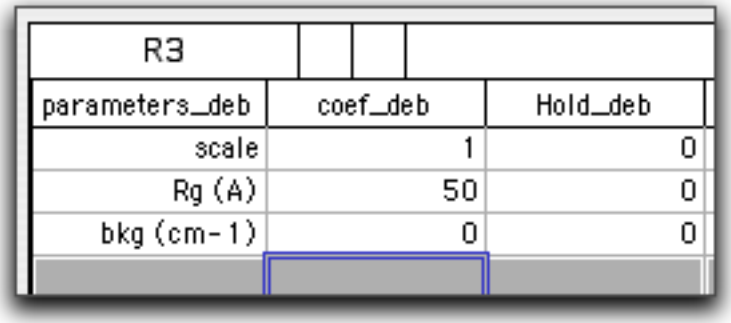


4) Set the first function to sum by choosing the model "Debye" from the popup:


Sum_Model_Panel
Sum Two Model Functions
?
Function # 1
Model
Pick model 1
Coef
Pick coef for model 1
# of Parameters
0
Function # 2
Model
Pick model 2
Coef
Pick coef for model 2
# of Parameters
0
Plot Summed Model
Plot Smeared Summed Model



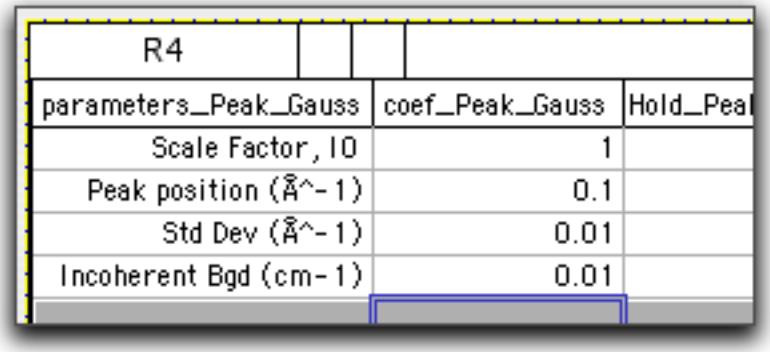
There are three parameters for the Debye model. Set the coefficient wave in the popup and the number of parameters to three. The panel should look as the upper right panel.



R3

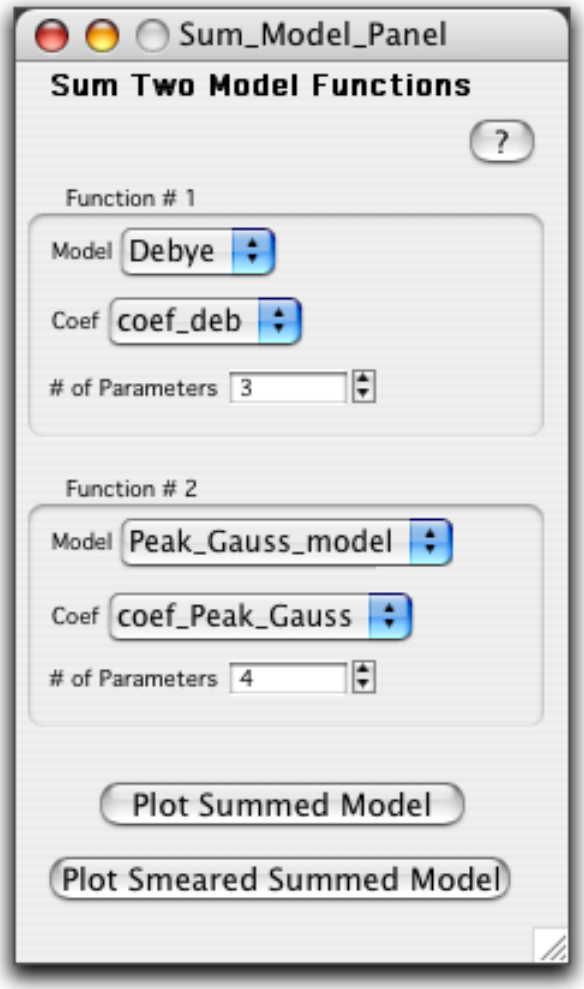
parameters_deb	coef_deb	Hold_deb
scale	1	0
Rg (A)	50	0
bkg (cm-1)	0	0

5) Set the second function to sum in the same way as the first. The Gaussian peak model has four parameters.



R4			
parameters_Peak_Gauss	coef_Peak_Gauss	Hold_Peal	
Scale Factor, I0	1		
Peak position (Å^-1)	0.1		
Std Dev (Å^-1)	0.01		
Incoherent Bgd (cm-1)	0.01		

The panel should now look like this:



6) Plot the summed model. You can plot a smeared version if you have previously loaded experimental data. Several waves are created:

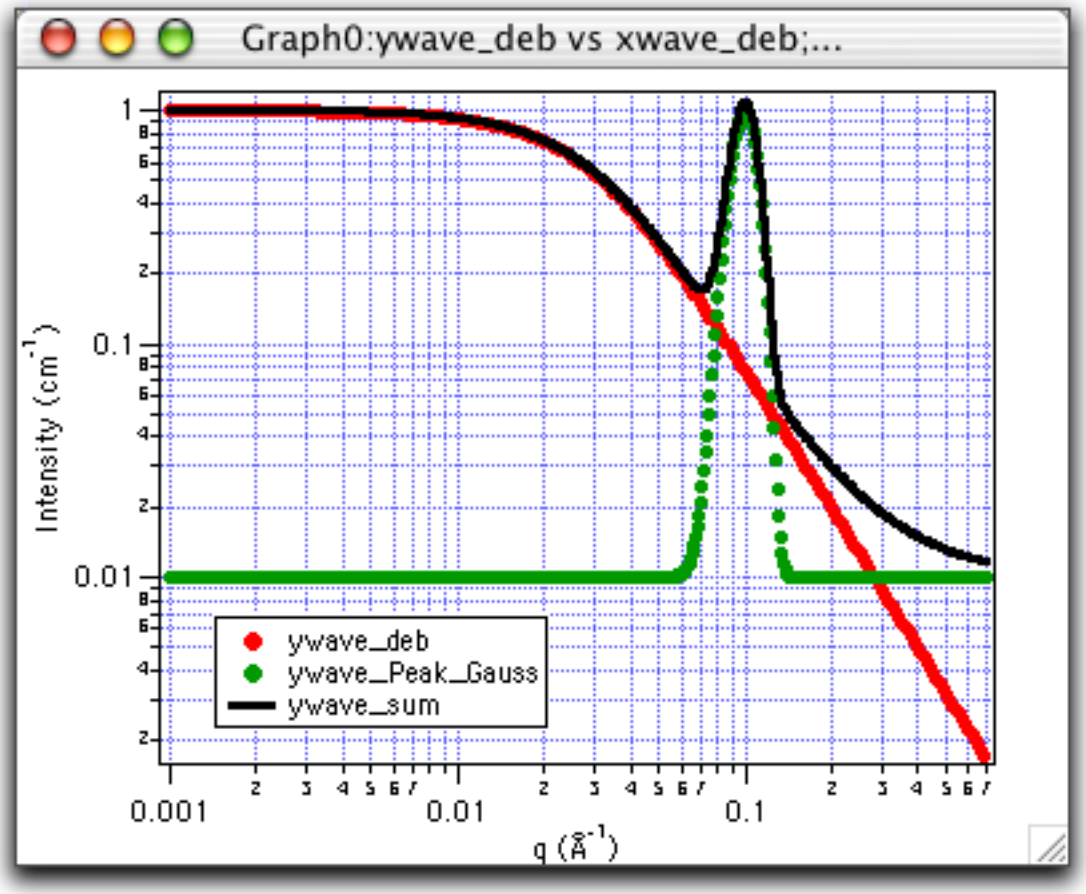
- coefficients: coef_sum

- parameters: parameters_sum

- Model function: Sum_Model(w,x) or Smeared_Sum_Model(w,x)

- XY data: ywave_sum vs xwave_sum

A graph of the model function and a table of the combined parameters is created. You can kill the graph if you like, and append the summed model to the graph with the two individual models. Sum_Model and Smeared_Sum_Model now show up in the Function Popup just like any other model functions.



7) The coefficients for the summed model are simply a concatenation of the coefficients for the individual models.

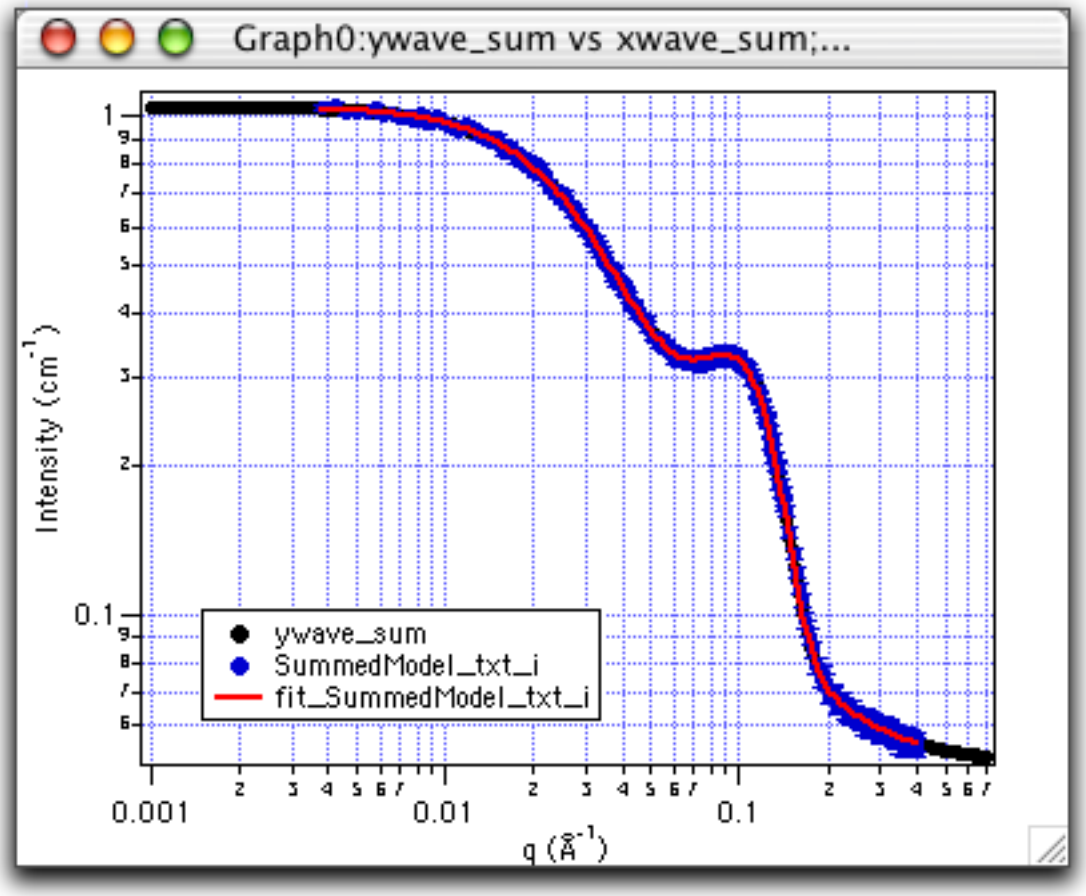
RO			scale
parameters_sum		coef_sum	Hold_sum
scale		1	0
Rg (A)		50	0
bkg (cm-1)		0	0
Scale Factor, IO		1	0
Peak position (Å^-1)		0.1	0
Std Dev (Å^-1)		0.01	0
Incoherent Bgd (cm-1)		0.01	0

For these two models, there are two independent scale factors that determine the scaling of each individual model. In a real sample, the scale factors are often linked by the material balance - that describes how material is distributed in the sample.

NOTE that there can be duplicated parameters depending on the models selected. Scale factors and background are commonly duplicated. It is your responsibility to make sure that duplicated parameters are held fixed at appropriate values during fitting. Two or more perfectly correlated parameters during curve fitting is a very bad thing.

There are two incoherent background parameters. One of these (either one) should be set to zero, and held fixed for any curve fitting done.

8) This summed model can be used for curve fitting as is, or can be used with the Global Fitting panel. Load in the fake data file "SummedModel.txt", and append the summed model that you just made. You can then fit the test data as usual, being sure to hold one of the incoherent background values fixed (it doesn't matter which). You should get a nice fit like this...



9) If you are finished with the Sum Model package, you can unload it from the experiment. Be aware that unloading the Sum Model package will kill the panel AND your model function.

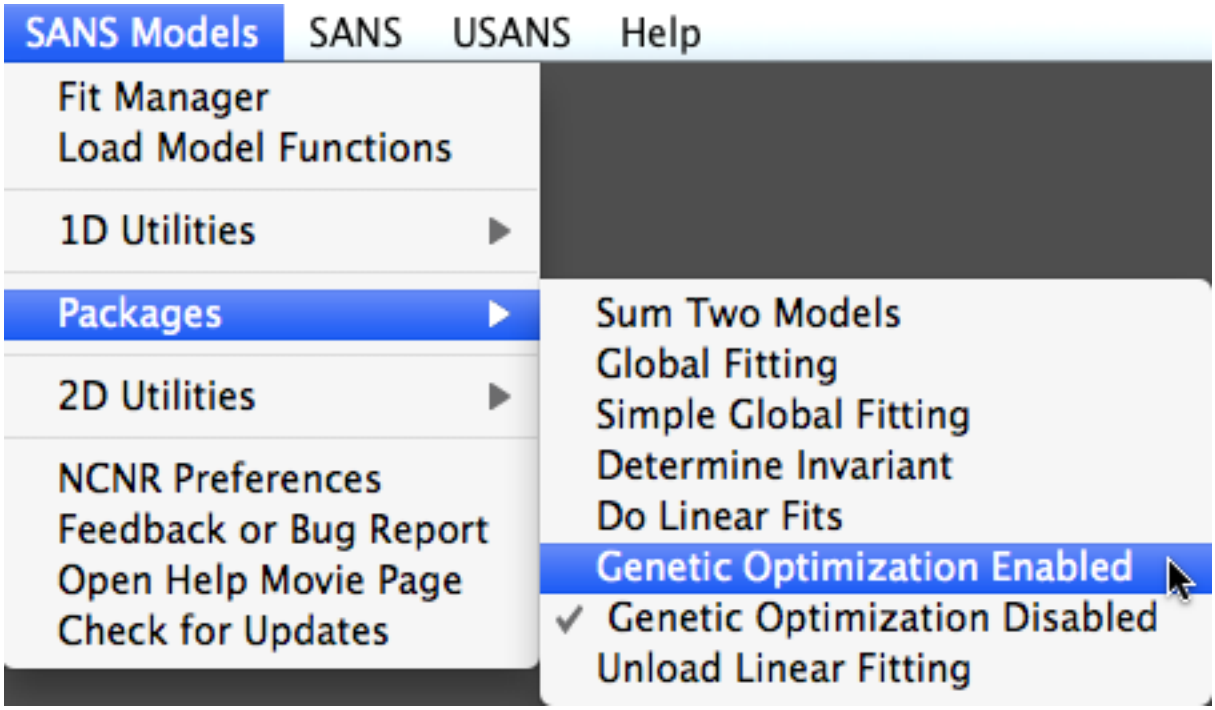
Genetic Optimization

(Courtesy of Andrew Nelson, ANSTO)

The model fitting uses Igor's built-in curve fitting package. See Overview of Curve Fitting for all of the details. In some cases where the solution surface is pitted with many local minima, gradient-based optimization methods may fail to reach a global minimum. In such cases, another search strategy such as Genetic Optimization may work.

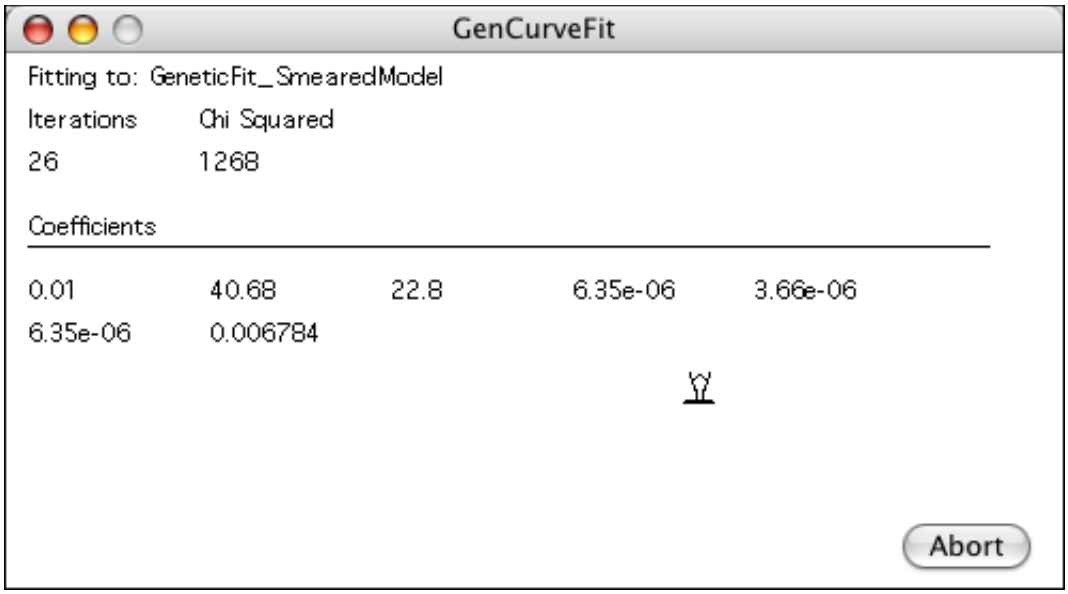
To enable Genetic optimization, you must first download and install the package which is found at:
<http://www.igorexchange.com/project/gencurvefit>

Once installed (you'll need to quit and restart Igor), you can enable Genetic Optimization from the SANS Models menu.



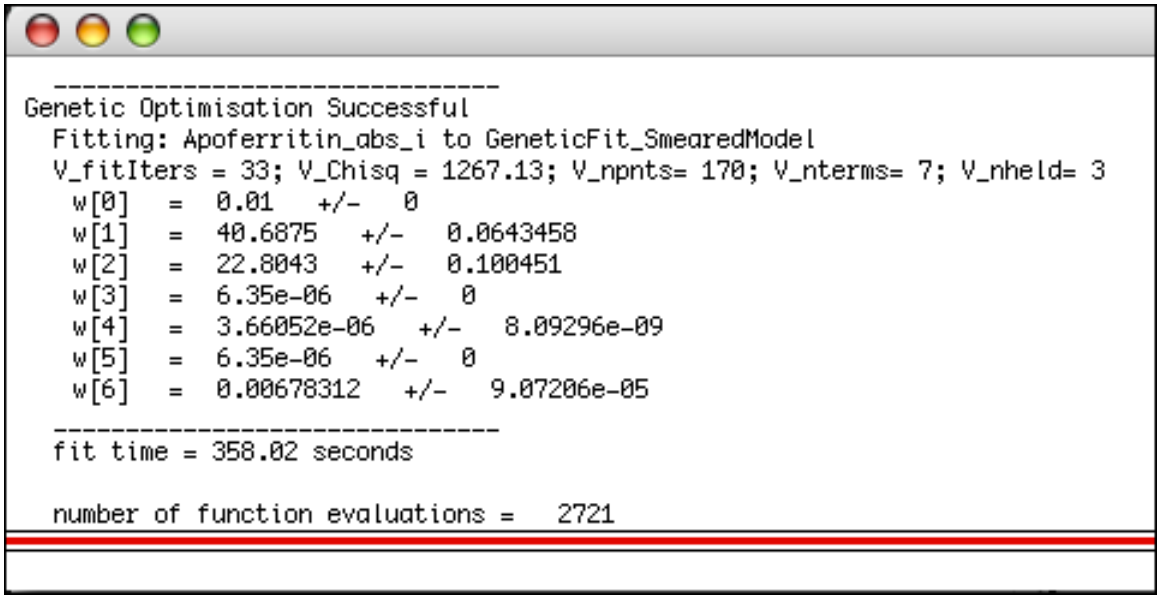
Set up your fit in the usual way using the Curve Fit Setup panel. **Be sure to set low and high limits for each of the coefficients that are not fixed **. These bounds define the search space for the algorithm. If they are missing, you will be asked to fill them in before the fit will proceed.

Now when you initiate a non-linear fit from the Curve Fit Setup panel, a different fit progress window will be displayed:



Currently, the results of the Genetic Optimization appear in the command window at the bottom of the screen (not the Curve Fit Setup). For the example data of apoferritin, both methods converge to the same solution. Although robust, the genetic optimization method is

much slower to converge than traditional gradient methods.



If you want to return to Igor's built-in optimization, select "Genetic Optimization Disabled" from the menu.

See also GenCurveFit help (this may or may not be installed as part of the GenCurveFit package)

- **Auto Fit (or Batch fitting)**

vers 1.0 DEC 2003
Updated JUL 2011
Release MAY 2013

This package provides the capability to batch fit a single model to a large number of data sets to speed up analysis of a large set of data. Once the starting information is gathered, the fits run unattended and save reports of the results. Not all curve fitting features are accessible, but the basics are there. The results can be compiled into tables where the results can be compared and plotted.

- Any smeared or unsmeared model can be used
- Initial parameter guesses are individual to each data set
- Held parameters, constraints, and fitted range are also individual to each set

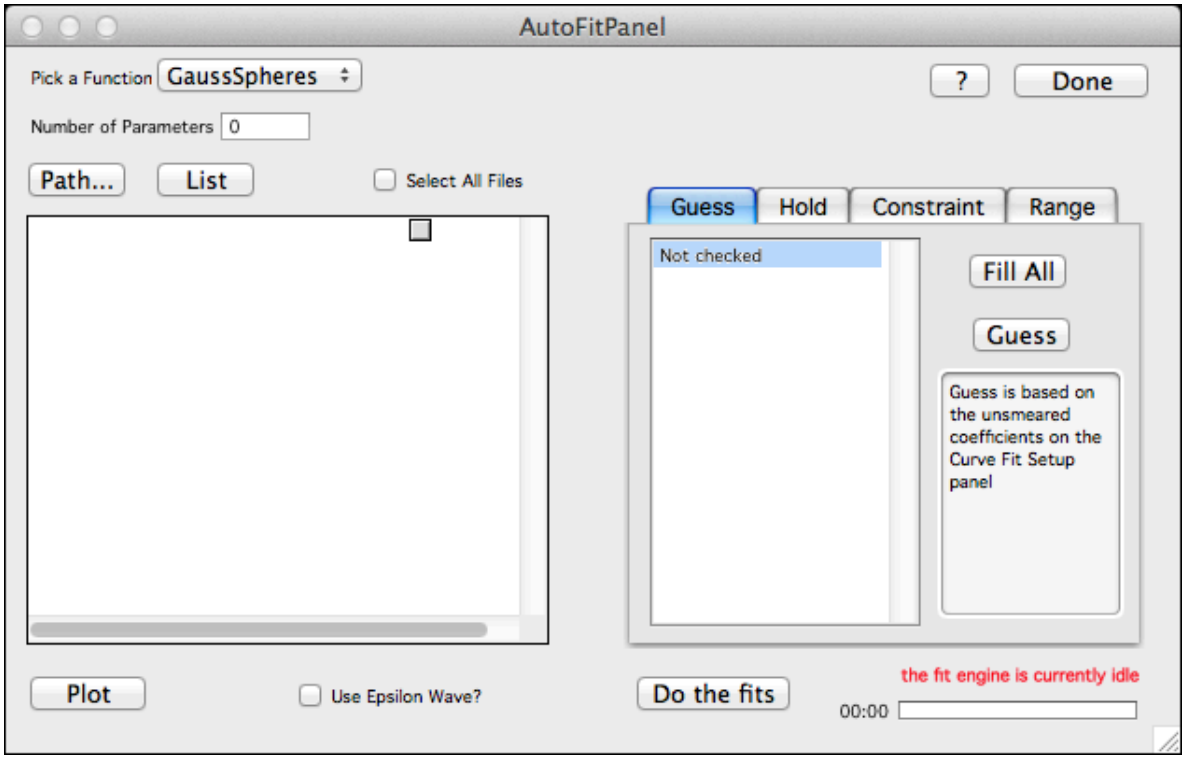
Note that this is not a global fit. Each of the data sets are fit independently.

To Batch Fit a Series of Data:

1) Load the Analysis package, and include a model function. Plot the unsmeared model. This will be used later to generate decent initial guesses for input to the fitting. For the example data, load and plot the GaussSpheres model.

2) Initialize the AutoFit Panel (Macros menu)

Most of the instructions below refer to the AutoFit Panel, some steps refer to adjusting model coefficients - and these are on the Curve Fit Setup panel)



3) On the AutoFit Panel, pick the function. Even if it's shown on the menu already, pick it again, and the number of parameters should automatically fill in. You're allowed to pick a smeared function even it it's not plotted, as long as the unsmeared model is plotted. (Warning: There is no "save" of the information you'll be entering on the tabs for guesses. If you ever switch the model function, you lose any parameter guesses that you've entered in the table - because using the coefficients from different models doesn't make any sense)

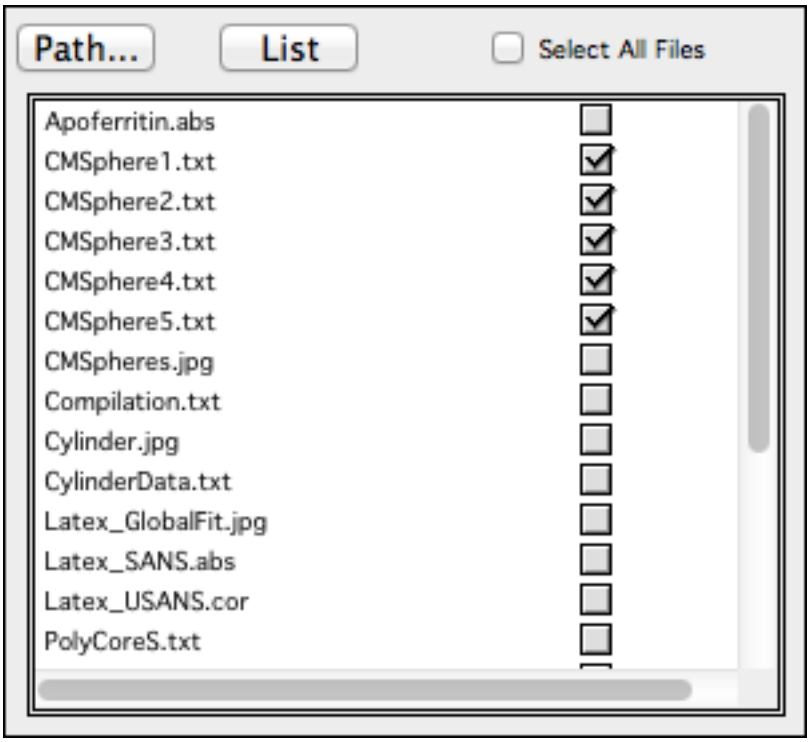
4) Be sure the number of parameters is correct.

5) Pick the data path using the "Path..." button. The example below follows along with the example 1D data that is provided with the downloaded package and can be found in: NCNR_SANS_Package_7.nn/NCNR_SANS_Utilities/Sample_Data/SANS/Analysis/1D_Data Then save the entire experiment now if you haven't done so. Results are automatically saved to the "home" path.

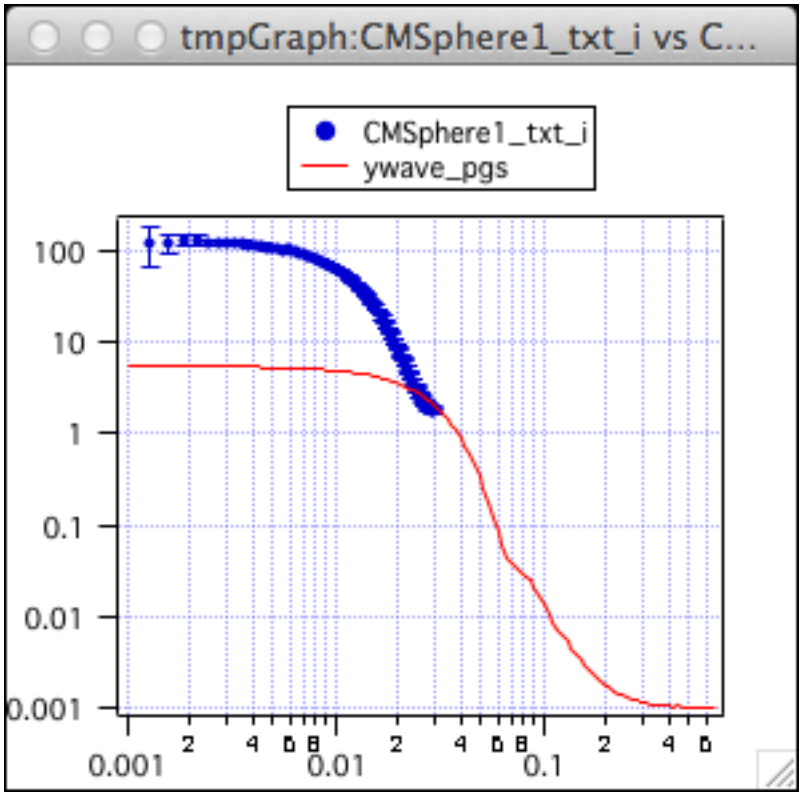
6) Click "List" to get a listing of the files in the folder (this is everything in the folder, so you may want to group data in sub-folders on disk, or at least separate the reduced data from raw data). You will be asked to "initialize" the matrix and all of the guesses. You'll

typically only do this once, since you're listing all of the files, and you can pick and choose which files you want to work with. Everything is there. Select which data sets you want to fit by checking them. You don't need to pre-load them. The files will be loaded as needed.

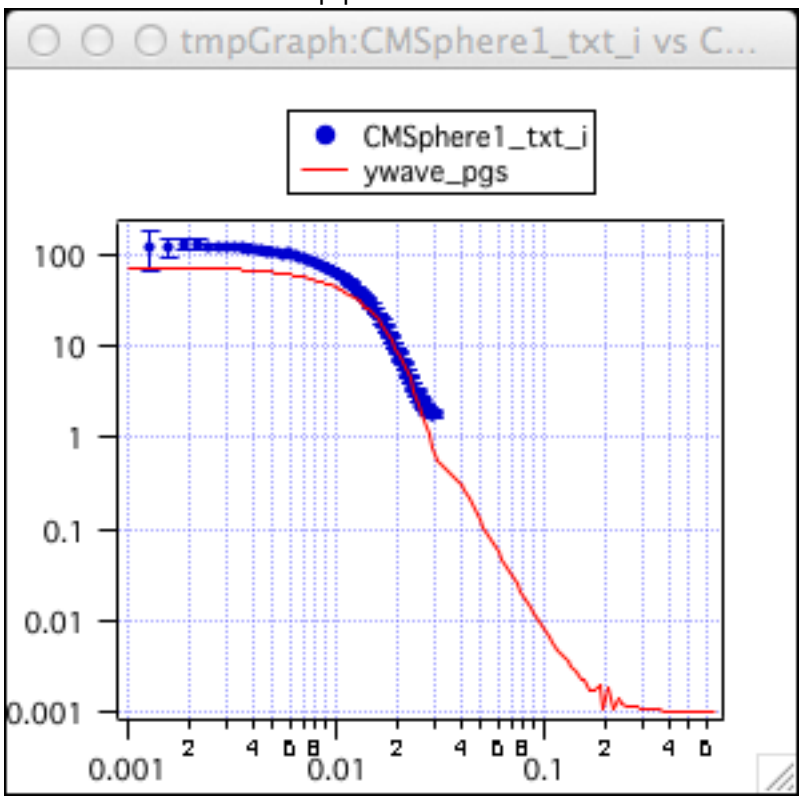
- Check all of the "CMSphere(n).txt files:



7) Select one of the data files by clicking directly on the file name in the list. Plot the selected file using the "Plot" button at the bottom of the list - the ywave of the model will be appended (ywave_ext). You'll see the unsmeared model. If you're fitting with the smeared model, you'll still fit with the smeared model. Plotting the unsmeared model here is a lot faster than requiring the smeared model be plotted for all of the selected files. It's good enough for the initial guess.

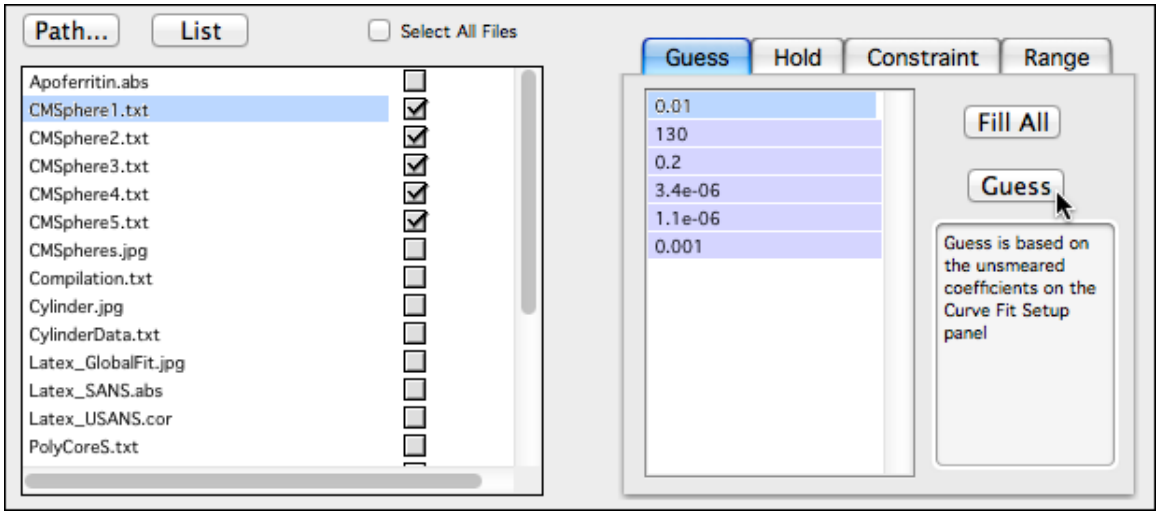


8) Adjust the coefficients as needed to get a good guess. Do this for the unsmeared model coefficients from the Curve Fit Setup panel.

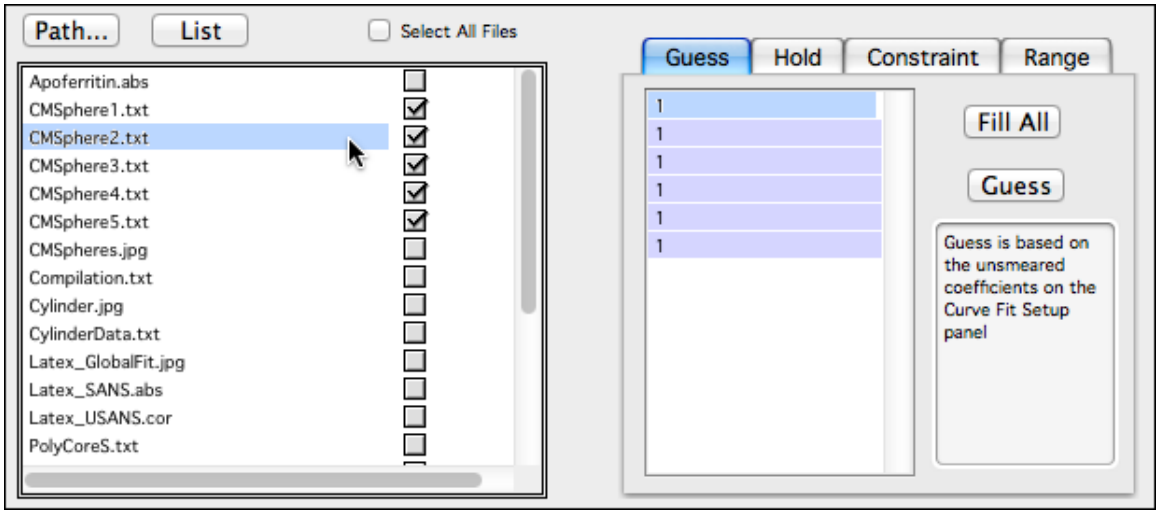


9) On the "Guess" tab, clicking the "Guess" button will set the guess for this file (only) based on coef_pgs in the example, the coefficients of the unsmeared model. If this guess

is good enough for all of the checked files, click "Fill All"



10) If you want to adjust the initial guess for another file, go back to step 7 - Plot will kill/ create a new "temp" graph for the next file. Note also when you select a new data file from the list, the "Guess" values will all be set to 1:

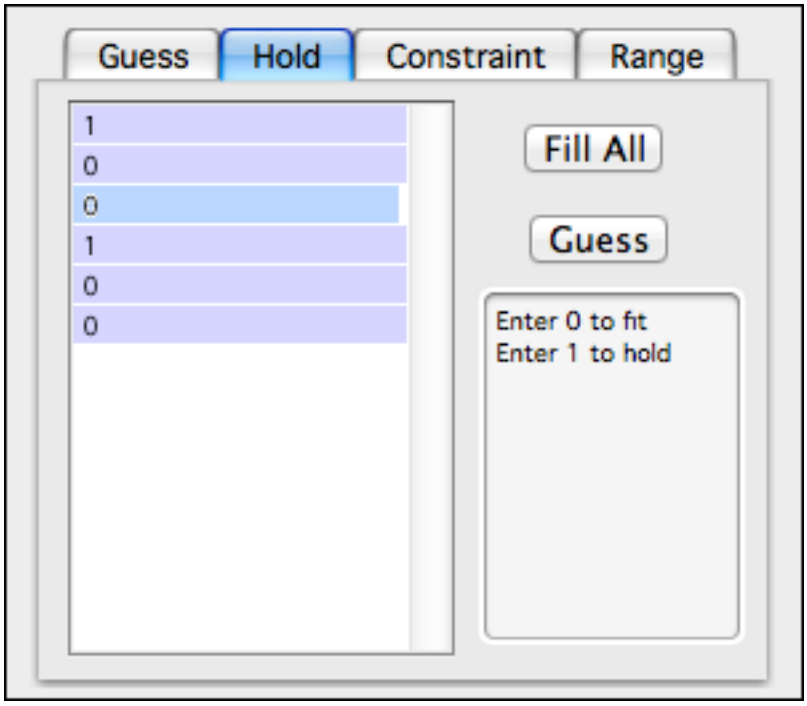


We could have accomplished the same thing by setting the coefficients for the first data set, clicking "Fill All", and then adjusting the solvent SLD and background for each of the data sets.

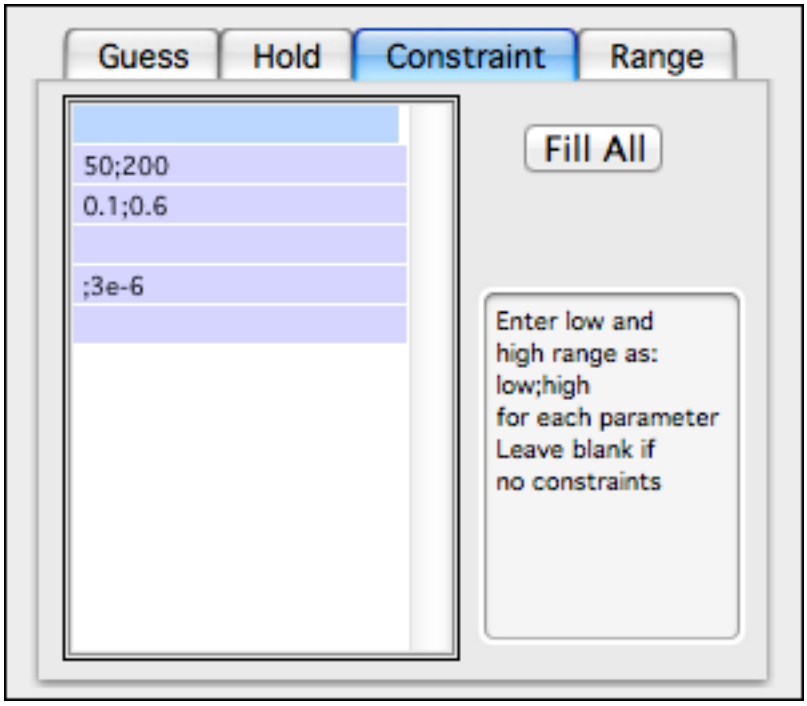
11) Using the tabbed table at the bottom, enter any other guesses, hold values, and constraints. Remember that you are entering values for the highlighted data set only. Sometimes you need to hit return after the last entry. Occasionally if you use the arrow keys, then the edit event can be missed and the value won't get entered.

12) Select the "Hold" Tab. Entering "Hold" == 1 in a given row will hold that parameter fixed. Entering 0 (default) will fit that parameter. For the example here, we want to hold the volume fraction and sphere SLD fixed (parameters 0 and 4), so the hold tab should look like below. If you have set the hold parameters for the unsmeared model, "Guess" will

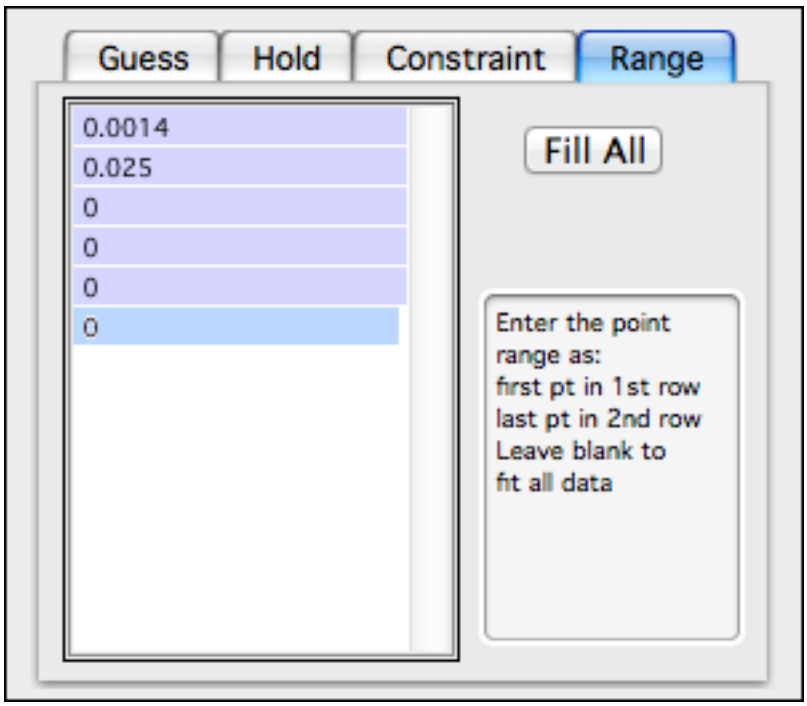
use the values from the Curve Fit Panel. Also, we want to click "Fill All" to use the same free parameters for all of the data sets.



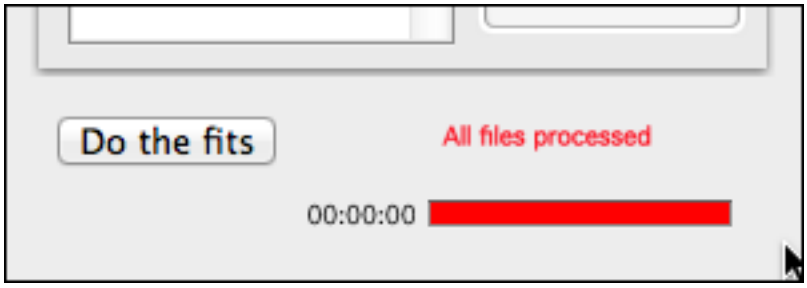
13) Constraints for each parameter are entered row-wise as loLim;hiLim in the desired parameter row. Either value can be omitted. Leaving a row blank means no constraints. In the example, we don't really need constraints, but it won't hurt. Entering the following would constrain the radius as 50 < R < 200, the polydispersity as 0.1 < pd < 0.6, and constrain only the upper limit of the solvent SLD as SLD < 3e-6. Remember that these constraints are for only the selected set. If you want these constraints for all of the data sets, click "Fill All".



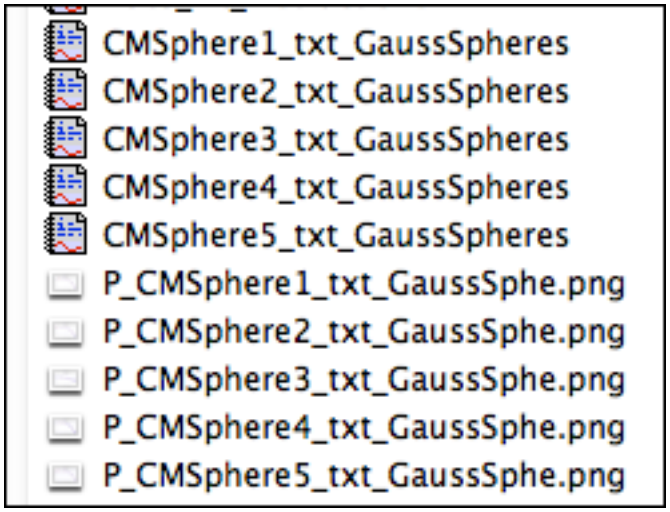
14) Select the fitted range for each set- either all, or a selected (inclusive) or a q-range. Enter the range as the first point number (or low q value) in the first row, and the last data point number (or high q value) in the second row. Leave the other elements blank (zero). If nothing is entered for the range or either entry is missing or invalid, then the full data set is used.



14) Once all of the guesses are set, Do the fits. The progress is noted in the text field and status bar to the right of the button. For each data set, the fit is repeated 3x to be sure that it converges.



15) For each fit, a graph is saved of the final fit, and a report notebook is saved.



Now what?

16) All of your results are in the reports and the graphs, so go find those on disk. Select all of the reports and open them. There you can inspect all of the fits and see if any need to be re-done. If all is well, then with all of the reports open, select Macros->Compile_Reports. You'll be asked to (confirm) the total number of parameters in the model, and a "tag" to identify this set of parameters. The reports will be parsed and the information presented in a table and in a separate notebook.

17) The table: each parameter and its error are listed as par_n. You can rename these as you like. Chi-squared is also reported. As you did with the data reports, check these tables for anything odd or indications of bad fits. Data in the table can be plotted against (something). You'll have to take care of this.

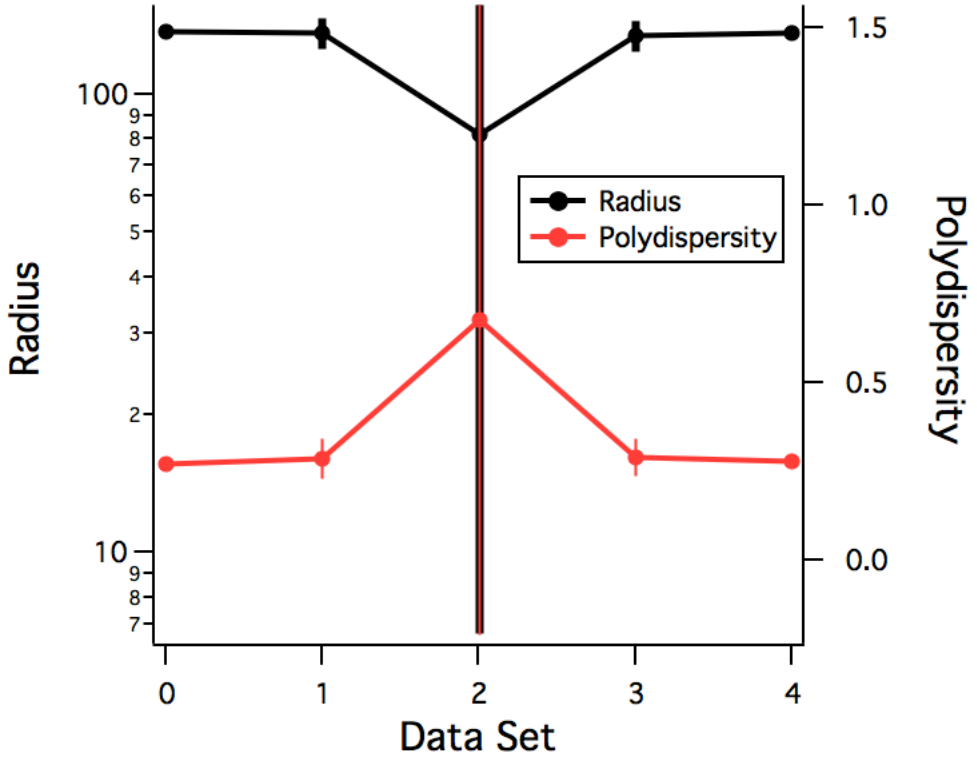
AutoFitResults:fittedFiles_v1,chiSQ_v1,...

R5

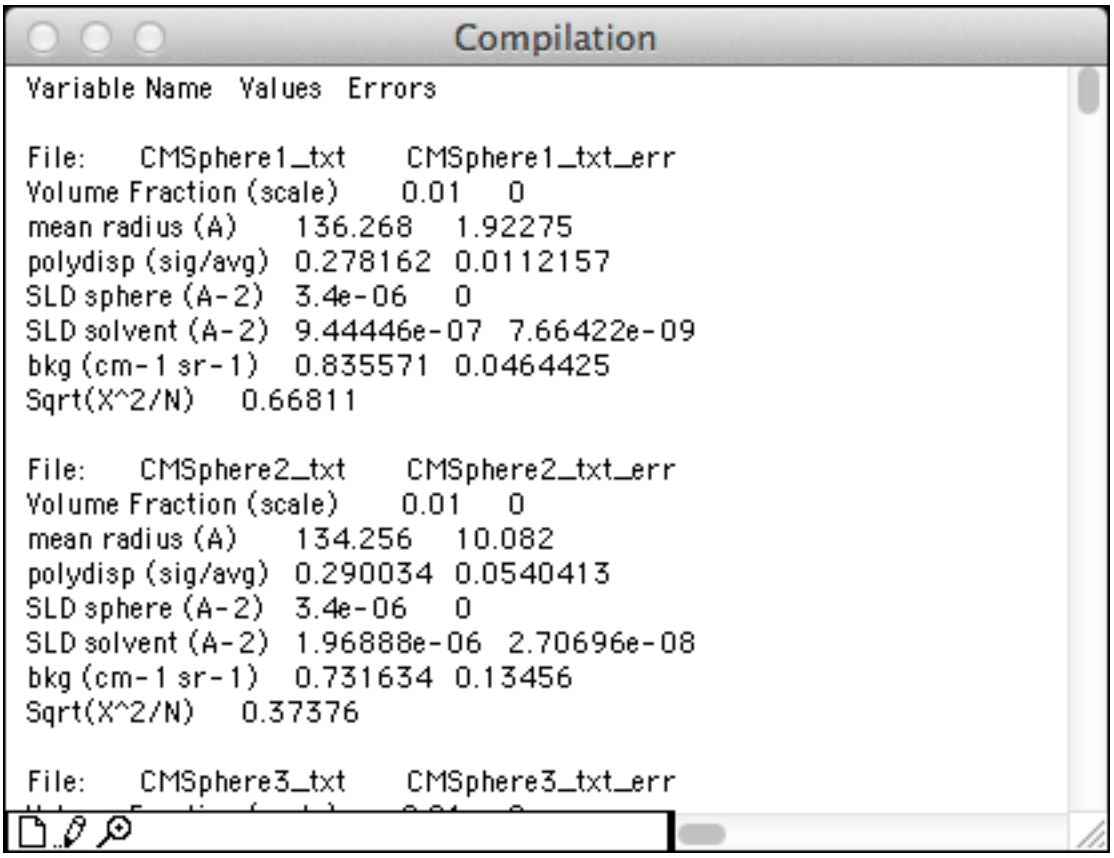
Point	fittedFiles_v1	chiSQ_v1	par0_v1	par0_err_v1	par1_v1	par1_err_v1	par2_v1	par2_err_v1
0	CMSphere5_txt	0.421502	0.01	0	137.178	2.57714	0.271883	0.0151305
1	CMSphere4_txt	0.229407	0.01	0	135.662	10.5895	0.284633	0.0578052
2	CMSphere3_txt	1.26375	0.01	0	81.6081	74.9468	0.678879	0.885166
3	CMSphere2_txt	0.373756	0.01	0	134.256	10.082	0.290034	0.0540413
4	CMSphere1_txt	0.668113	0.01	0	136.268	1.92275	0.278162	0.0112157
5								

Here, it's clear that although the chi-squared for data set [2] is reasonable, there is something wrong with the fit. The error bars on the parameters are way out of line with

the other data sets. The errors are sometimes larger than the parameter value itself. Very bad...



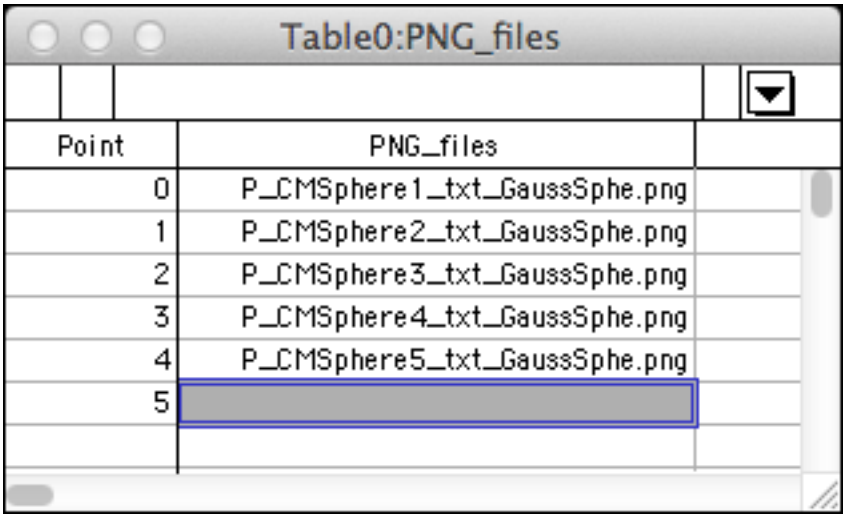
18) The notebook of results is the same information as the table, just presented in a different way. Save it if you like.



19) You can print all of the notebooks from the macros menu (this may be a lot of pages!), or simply close them if you've compiled the results into tables.

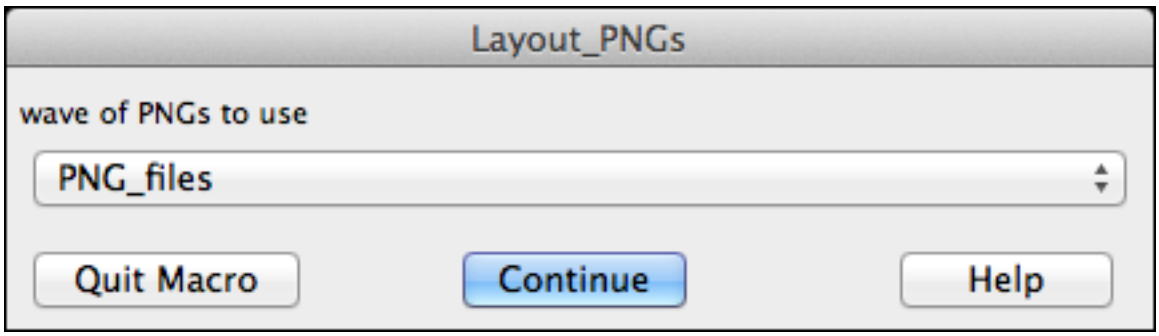
-- the graphs --

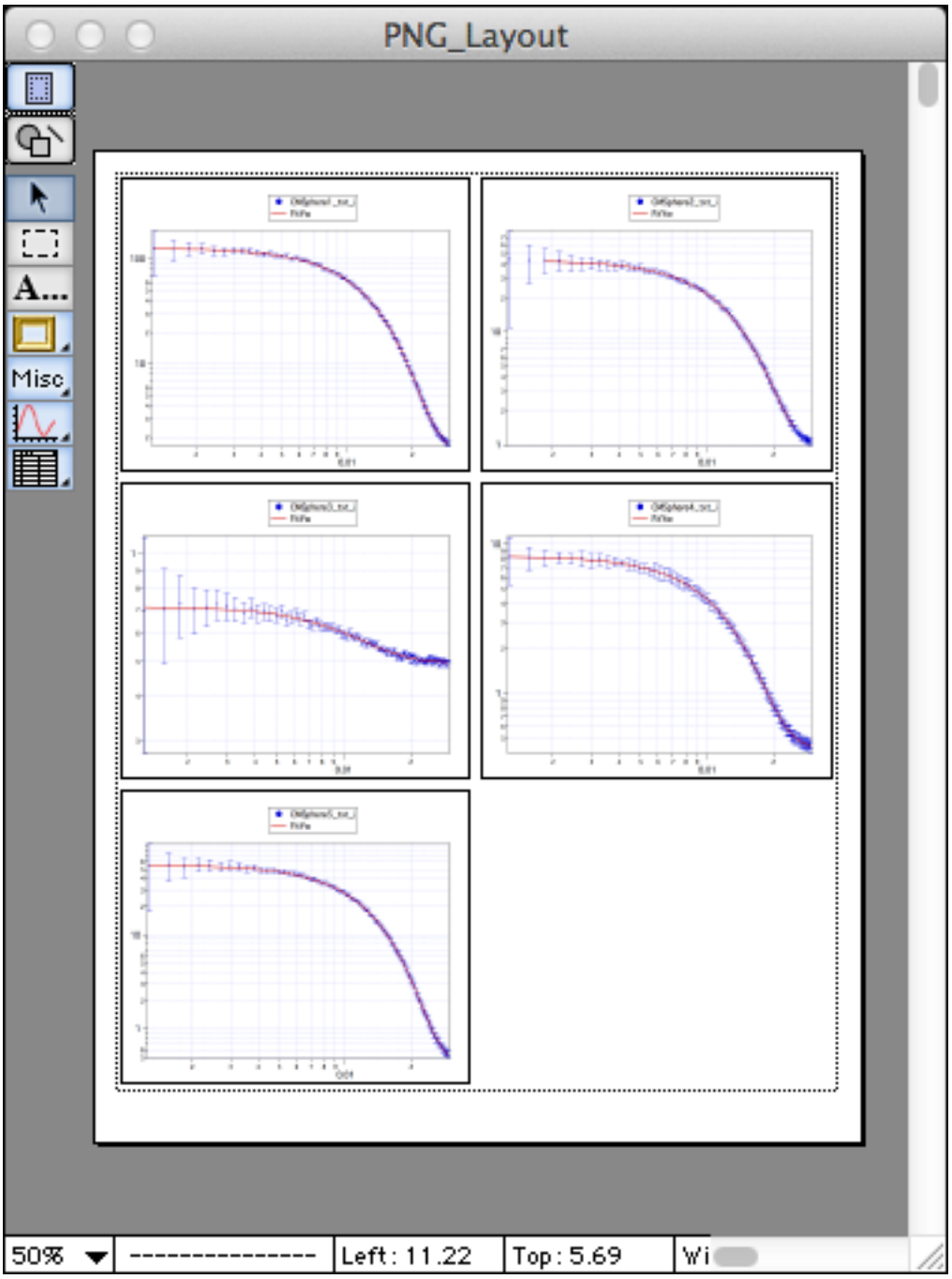
20) The graphs: Sometimes it's easier to see all of the fits together. The graphs are saved to disk as PNG files @2x screen resolution. Select Macros->Generate_PNG_List to create a wave of PNG files that were saved in the "home" folder where the experiment is saved.



Delete points from the wave if you don't want them in the layout, or create a new text wave STARTING WITH "PNG" (must be capital).

21) Then choosing Macros->Layout_PICTS dumps everything in the PNG_files wave into a layout and tiles the images. This is very useful for viewing a series of fits, all at once - for comparison, or to see which ones went bad.





- **Frequently Asked Questions About SANS Analysis**

The FAQ's listed here answer some of the more frequently encountered problems with working with the SANS Analysis macros.

1) I can't find the model function I want in the Curve Fitting dialog.

Did you include it using the SANS Model Picker ?.

2) I've downloaded the models, but nothing appears under the Macros menu.

Model functions appear in the "Functions" popup on the Fit Manager only after they have been included (by you). The SANS Models menu will open panels for specific operations, or un-bury panels that have gotten covered. The Macros menu may contain some items that have not found a permanent (more logical) home yet, so don't count on them always being there.

3) My fit is lousy, doesn't converge, or gives an error.

Non-linear optimization is full of mathematical pitfalls, no matter how smart the software claims to be. Some suggestions are:

- Make sure that you have all the correct items selected (Data Set + Function)
- Make sure that you have the desired options checked (or unchecked)
- Make sure you're using a model that is an appropriate physical description of your data
- Use a better initial guess - find it by manually adjusting the coefficients
- Make sure your starting guesses are non-zero
- Hold more (nearly all) of the parameters fixed, then release them one at a time
- Apply constraints to variables that wander to unphysical values
- Check the function documentation to make sure that the parameters are reasonable
- Try Genetic Optimization as a different method that may better converge on an answer.

4)
Resolution Smearing

- What does resolution smearing do to my data, and why is it different for SANS and USANS?
- What happens when I plot a smeared model function using one of the "Smeared..." macros?

- All experimentally measured scattered intensity is smeared to some extent by the resolution of the instrument, since no instrument has perfect resolution. The SANS instruments at NIST are pinhole collimated (the pinholes are of a finite diameter), use a narrow wavelength band (but not monochromatic), and uses a detector with a finite pixel size. All of these factors plus other collimation effects produce pinhole-smeared SANS data. The effect of pinhole-smearing is often slight, especially if there are no sharp features such as peaks or steep slopes in the sample scattering. The pinhole-smeared intensity is calculated as:

$$I_s(q_o) = \int_0^\infty R(q,q_o)\frac{d\Sigma(q)}{d\Omega}dq$$

and the resolution function is represented as a Gaussian as:

$$R(q,q_o) \equiv \frac{f_s}{\sqrt{2\pi V_q}} \exp\left(\frac{-(q-\bar{q})^2}{2V_q}\right)$$

with:

q = q-value
I(q) = intensity
σI = standard deviation of the intensity
σq = standard deviation of the Gaussian approximation to the q-resolution
q(mean) = mean q-value
fs = beamstop shadowing factor (= 0 behind beamstop, =1 away from beamstop)

For details of the calculation of the resolution function from the instrument geometry, see Barker & Pedersen, *J. Appl. Cryst.*, (1995) **28**, 105-114.

- The USANS instrument at NIST is a Bonse-Hart type using triple-bounce silicon crystals for the monochromator and analyzer. As a result, the source collimation for USANS is effectively a very long, narrow slit, rather than a pinhole. So the measured intensity at USANS is slit-smeared according to:

$$I_s(q) = \int_{-\Delta q_v}^{\Delta q_v} P_L(q_v)\, I\left(\sqrt{q_v^2 + q^2}\right) dq_v$$

where $P_L(q_v)$ is the slit height weighting function. qv is the vertical component of the momentum transfer, and q is the horizontal component of momentum transfer selected by the analyzer. the function $P_L(q_v)$ is an even function around zero which can be approximated well by $P_L(q_v) = 1/\Delta q_v$, where Δqv is the maximum extent of the vertical resolution. For the NCNR USANS instrument, Δqv = 0.117 (1/A).

- When you "PlotSmeared..." you are calculating the model function at each q-value, and performing the appropriate smearing integral (numerically) to the model function, based on the resolution function of the data set that you have selected in the popup. When you use a "Smeared..." model for curve fitting, it is the resolution-smeared model that is fitted to your (resolution-smeared) experimental data.

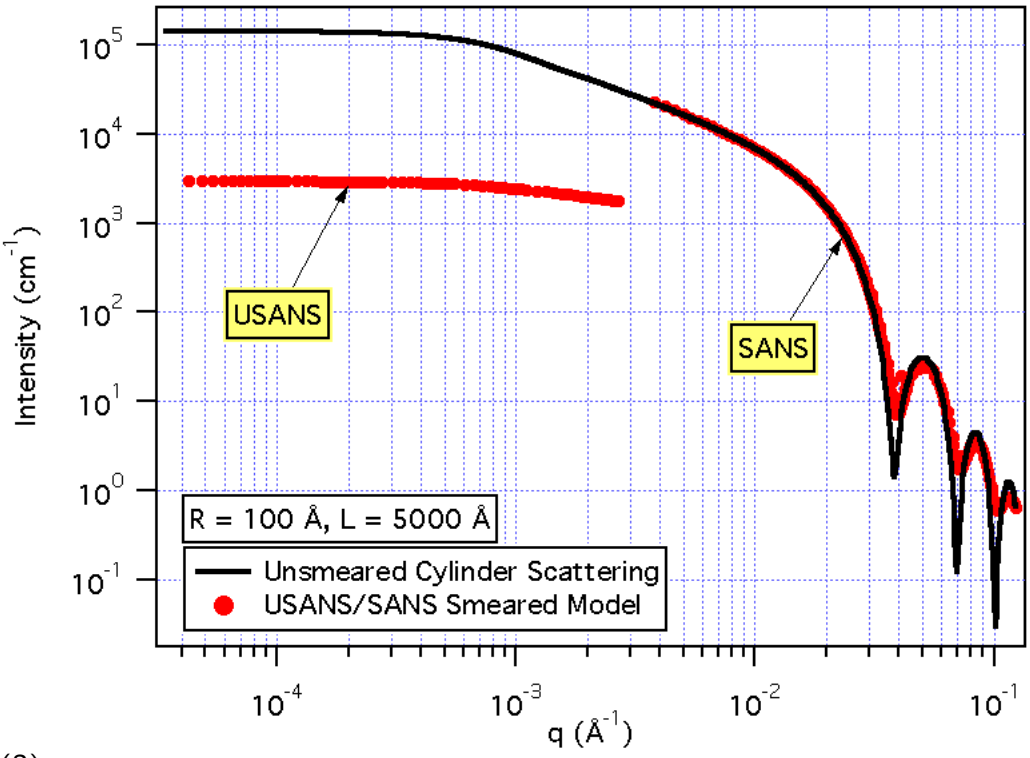
Two examples of the effects of smearing on model data:

(1) is long cylinders with sharp features in the SANS range, and a relatively flat slope in the USANS range. The slope of the USANS data is largely unchanged, but is almost two orders of magnitude lower in scale than the unsmeared model calculation. The pinhole smearing blurs the form factor oscillations, but is very close in scale to the unsmeared model in q-regions where the slope is not very steep.

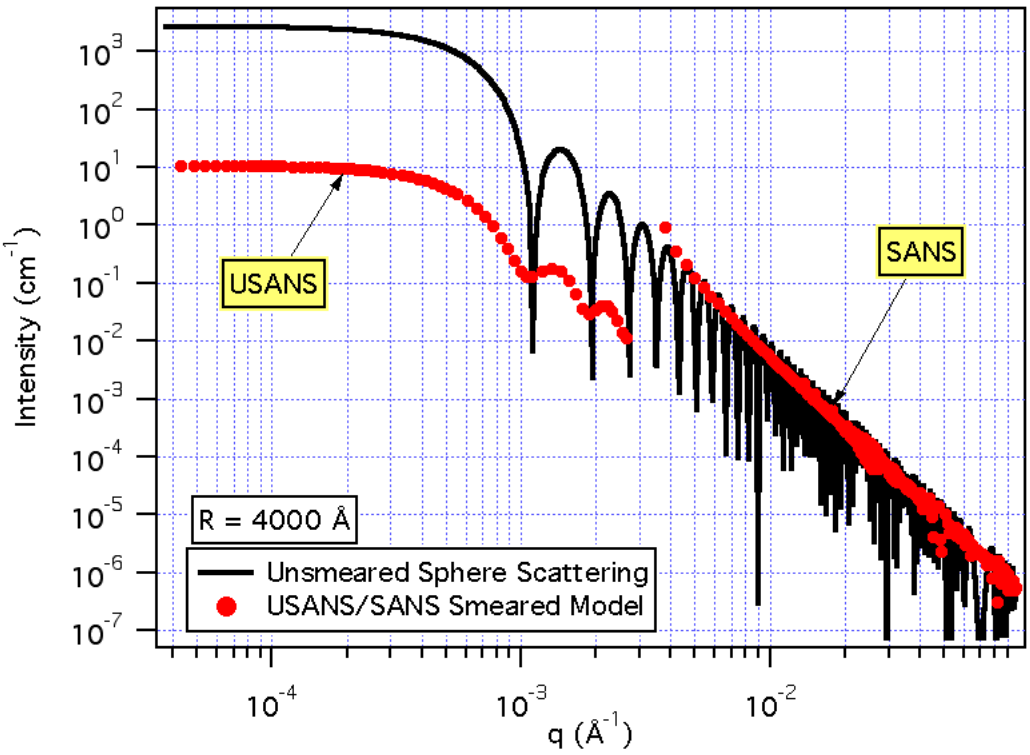
(2) is monodisperse spheres with a radius in the USANS range. The USANS-smeared model is again orders of magnitude lower than the unsmeared model, and the slit-smeared form factor oscillations are now quite significantly blurred. In the SANS range, the form factor oscillations are so closely spaced in q for such a large sphere that the pinhole smeared data is essentially

smooth with a Porod slope of -4.

(1)



(2)



5) What is the input file format for 1-D data?

As of 2010, the default 1-D output format of the NCNR Reduction packages is canSAS-XML. It contains all of the same information as our previous ASCII format, but is now in a format that is standardized across a number of scattering facilities to provide better portability of your reduced data. It is fully supported read/write in all of the packages at the NCNR and its implementation is essentially invisible to you. If you do not want to use the XML format, but would rahter use the old ASCII style output, then un-check the XML preference in the SANS Preferences panel. If you want to convert XML data to ASCII, there is a conversion tool available in the Data Management panel.

The old NCNR-ASCII 1-D data files of I(q) are 6-columns of ASCII data. There have from 4 to 14 header lines (depending on the reduction process used) that are automatically skipped by the file loader. The 6 columns in SANS data files are:

q = q
I(q) = intensity
σI = standard deviation of the intensity
σq = standard deviation of the Gaussian approximation to the q-resolution
q(mean) = mean q-value
fs = beamstop shadowing factor (= 0 behind beamstop, =1 away from beamstop)

The resolution columns are calculated based on the geometry and optics of the instrument configuration and the resolution equations in Barker & Pedersen, *J. Appl. Cryst.*, (1995) **28**, 105-114.

USANS data is slit-smeared, and can be characterized by a single value, the slit height, Δqv. USANS data files are still 6 columns, where the three columns that represent the resolution function are filled with a constant value -Δqv = -0.117 (1/A). The negative value is a flag for the smearing code to use slit smearing, as explained above, and in the USANS reduction manual. If the USANS data has been desmeared, the resolution columns are set to "perfect" values (σq = q/100) so that model fits are effectively not smeared.

If you do not have resolution information, you can still use the analysis models with 3 column data, (q -I -σI), but you will not be able to do any smeared model fits.

6) What are some good references to learn about SANS?

- NIST SANS Summer School, information at: <http://www.ncnr.nist.gov/summerschool/index.html>
- Tutorials on the SANS Web pages: <http://www.ncnr.nist.gov/programs/sans/tutorials/index.html>
- R-J. Roe, "Methods of X-Ray and Neutron Scattering in Polymer Science", Oxford Press, New York, 2000. This book is easy to read and covers static and dynamic scattering, applies to more than just polymers, and is currently in print.
- O. Glatter and O. Kratky, "Small Angle X-Ray Scattering", Academic Press, New York, 1982. A classic. The notation is geared towards x-ray scattering, but it still applies. It has been out-of-print for many years and is somewhat hard (darn near impossible) to find a bound copy. It is currently available as a free PDF download from Otto's web page.
- S-H. Chen and T-L. Lin, "Colloidal Solutions", in Methods of Experimental Physics, Vol. 23 Part B, (1987), pp. 489-543. A book chapter that covers a lot of basic theory,

geared towards soft matter. Lots of references and examples.

- J. S. Pedersen, "Analysis of small-angle scattering data from colloids and polymer solutions: modeling and least squares fitting", Adv. Coll. Interface Sci., 70(1997) 171-210. This is a review article with detailed description of the mathematics of analysis techniques and a large listing of form factors for various structures.

- And the disclaimer... This is not an all inclusive list of sources of information about scattering and analysis of scattering data. Mention of any product or reference here does not imply any endorsement by NIST, nor does it imply that the named item is necessarily the best item for the stated purpose.