Preface for Users of SasView 4.n.x

SasView is in a constant state of development by an international team of developers.

Whilst we strive to ensure that we always provide you with the most functional, user-friendly, and bug-free application that we can, our limited resources mean that we are constantly having to make compromises. One of those compromises is always the balance between what we code and what we document.

This tutorial was written for SasView 2.1.x, and you are now using SasView 4.n.x. Rather than spending time updating this tutorial, we have instead been overhauling the SasView help guide (select 'Help' in the program menu bar) and initiating a new suite of tutorials. Indeed, we hope that members of the SAS Community, like yourself, will contribute some of these tutorials! If you want to know more, then please visit: **http://trac.sasview.org/wiki/TutorialsTNGForAuthors** .

Whilst this tutorial is still sufficiently useful that it continues to warrant inclusion in current releases of SasView, be aware that some functionality may have been added, changed, or even removed. So use this tutorial in concert with the help guide.

Thank you for your patience, and we hope you enjoy using SasView!

The SasView Developers

SasView
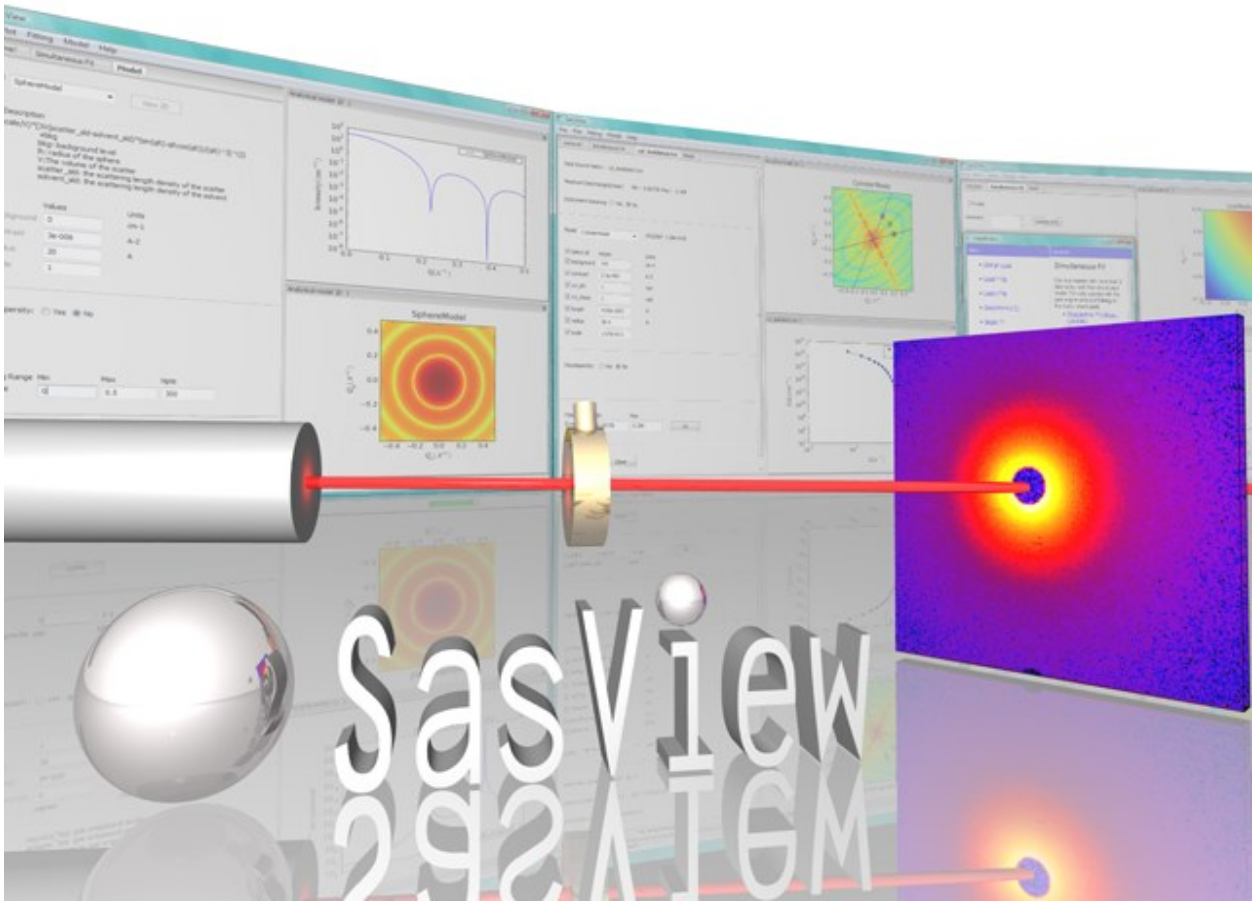
This software was originally developed by the University of Tennessee as part of the Distributed Data Analysis of Neutron Scattering Experiments (DANSE) project funded by the US National Science Foundation and is currently being developed as an open source project hosted at SourceForge and managed by a consortium of scattering facilities. Participating facilities include: The European Spallation Source, ISIS, The Institut Laue Langevin, The National Institute of Standards and Technology Center for Neutron Research and the Oak Ridge National Laboratory Neutron Sciences Directorate.

Table of Contents

Introduction

An application for SAS oriented system modeling and data analysis.

Roadmap:
SasView is a new application provided to the community to generate feedback. It is part of a broader effort to provide analysis tools to the SANS community. In providing this application, we hope to learn about the analysis needs of the users. We are interested in suggestions in two areas:

• Functionality: what functionality would you like to see in an analysis application for SANS/SAXS
• Ease-of-use: how would you improve the user interface

Main Features:
• Polarization and magnetic models.
•Generic SANS calculator/ pdb reader & atomic scattering calculator.
•Easy custom model writer/editor.
• Data operating tool.
• 3D (surface plot) view for 2d data/results.
• Python shell/editor.
• Simultaneous fit with the constraints.
• Loading and displaying 1D and 2D data in various formats.
• Batch fitting.
• Support P(r) inversion (via. indirect Fourier transform).
• Supporting polydispersity and /or orientational distribution for virtually all built-in model functions.
• Supporting pinhole or slit smearing for 1d and pinhole smearing for 2d.
• Supporting various 2D averaging methods : Circular, Sectorslicer, Annulus, Boxsum, BoxQx and BoxQy.
• Supporting a number of standard models and model-independent functions including form factor and structure factor functions and their multiplications as well as reflectivity models.
• Supporting the invariant calculation.
• User sets Qrange (Qmin and Qmax) for both 1D and 2D data for fitting and modeling.
• User sets a mask for 2d so that fitting takes account only unmasked data into the calculation.
Installation and Usage:
Currently the installer is supported only on the Windows : Windows , and Mac were tested.

Contact us:
You can visit the SasView web page at: **http://www.sasview.org**
Comments? Bugs? Requests? Help?
Write to us at: *sansviewproject-developers@lists.sourceforge.net*

How to install

1. Go to our Small Angle Neutron Scattering Project web page, http://www.sasview.org/ or check the Sourceforge download site at http://sourceforge.net/projects/sasview/files/.

2. Once "setupSasView-#.#.#.exe is downloaded, open the installer and follow the steps
as directed.
Note: If you are not an administrator for that PC/MAC, select the destination folder where you have permission to write (like your home Desktop). Otherwise, the installation will simply fail.
If you have the previous version installed, we recommend to uninstall it using the uninstaller in its sasview folder before installing the newer version.
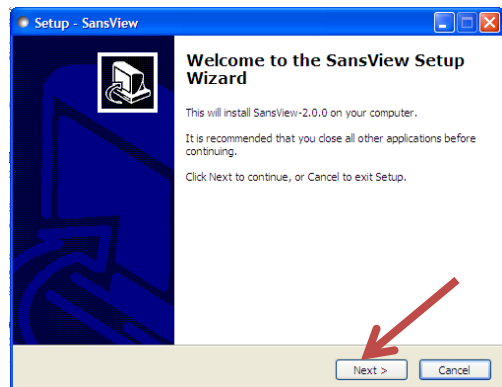
3. Once the SasView is installed, some samples of 1D and 2D data files can be found inside the "test" folder in the SasView folder (/Content/Resources/test/ for Mac). This allows you to follow this tutorial session without having your own data set.
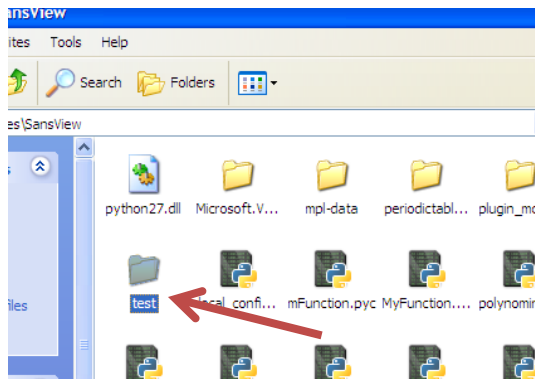
4. The "plugin_models" ("plugins" for SasView < 2.1) folder also includes some example python so that users can rewrite their own model function. This folder can be found in USERHOMEDir /.sasview/. One can edit a model file directly or using the custom model editor that we provided in the menu bar (Fitting/EditCustomModel).
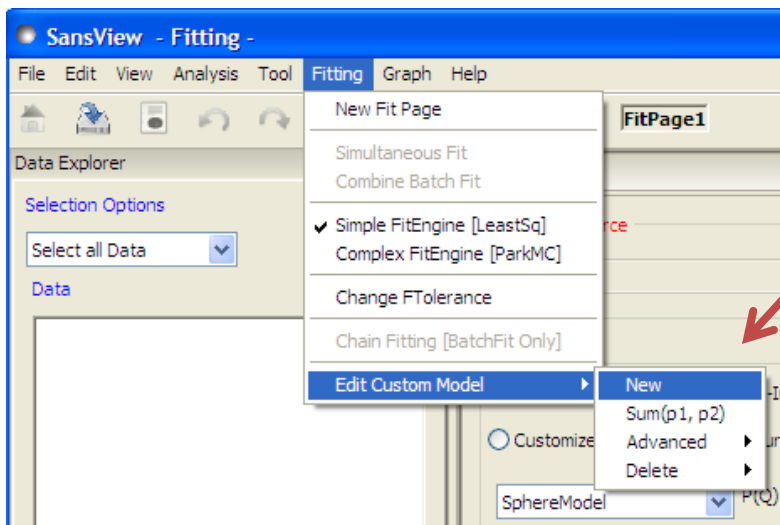
I. Loading 1D, 2D data, and SasView project

I-1. Click on "Load Data" from the File menu (Fig. I-1).

Note: If the data contains a q=0 point, the point will be excluded.

I-2. Locate your data file and click on the "Load Data" button (Fig. I-2)

(You can choose either 1D or 2D data in this way).

File extension types that can be loaded are:

i)   for 1d data: txt, asc, dat , CANSASxml or w/o extension,
ii) for 2d data: ASC and DAT in NIST 2D format, and sans files.

The format of txt 1d files should consist of 2 to 4 columns of Q, I, (dI, dQ) in order, where dQ is the instrumental resolution in Q and assumed to be originated by pinhole geometry.

For 2D data, NIST q-map format is currently standard but most of the header lines can be removed except the last line, and also only first three columns (Qx, Qy, and I) are required as shown in an example data file, SILIC010_noheader_3col.DAT in test folder.

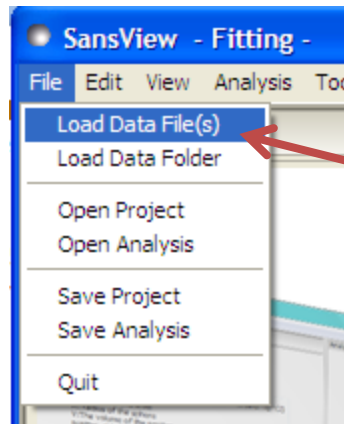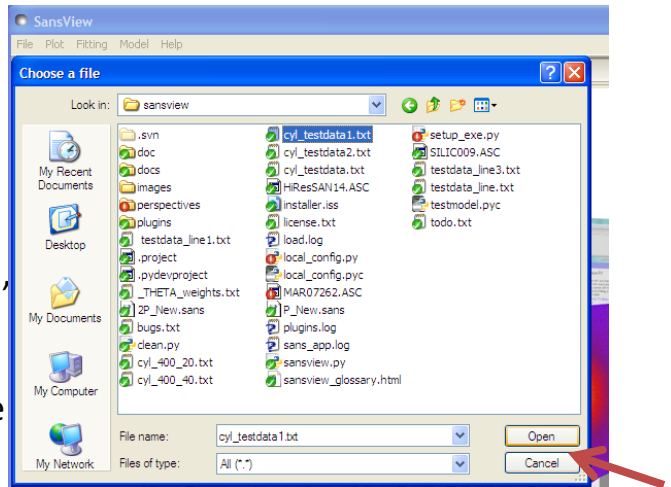I-3. Fig. I-3 shows an example of 1 D and 2D plots of the loaded data.

Fig. I-1

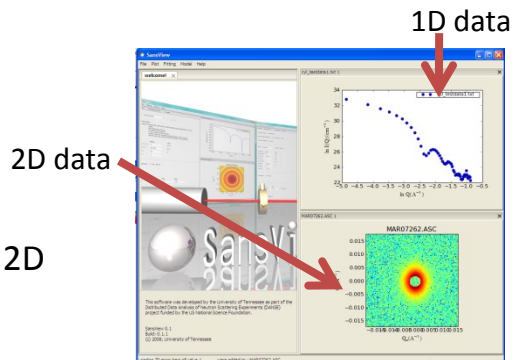Fig. I-2 Mutiple data files can be chosen by pressing Ctrl key and clicking pointer on the files.

1D data

2D data

Fig. I-3

I-4. Example data files: Use a text editor such as WordPad to look at the
supporting data formats .

    i)   1-D data: testdata_line*.txt, circular_test*.txt, cyl_400_*.txt,
        cyl_testdata*.txt, PolySheres.txt, sphere_*.txt, and latex_smeared.xml
        ← Even if existed, the headers are ignored except CANSASxml files.

    ii) 2-D data: MAR07262.ASC, SILIC010_*.DAT, P_New.sans, and HiResSANS14.ASC.
        ← The dI is assumed to be sqrt(I) for the 2d data from **.DAT files (NIST
            2d qmap data).

    iii) Orientational distribution (custom) 'array' data: _phi_weights.txt.

    iv) Polydispersity (custom) 'array' data: _radius_dist.txt.

    v) Beam profile data for 'Slit Size Calculator': beam profile.DAT.

I-5. SasView has its own file formats to save and open either a whole project
(.svs) or a subproject (i.e., one analysis; for example, .fitv for fitting, .inv for
invariant, and .prv for pr-inversion computation). Use the open/save
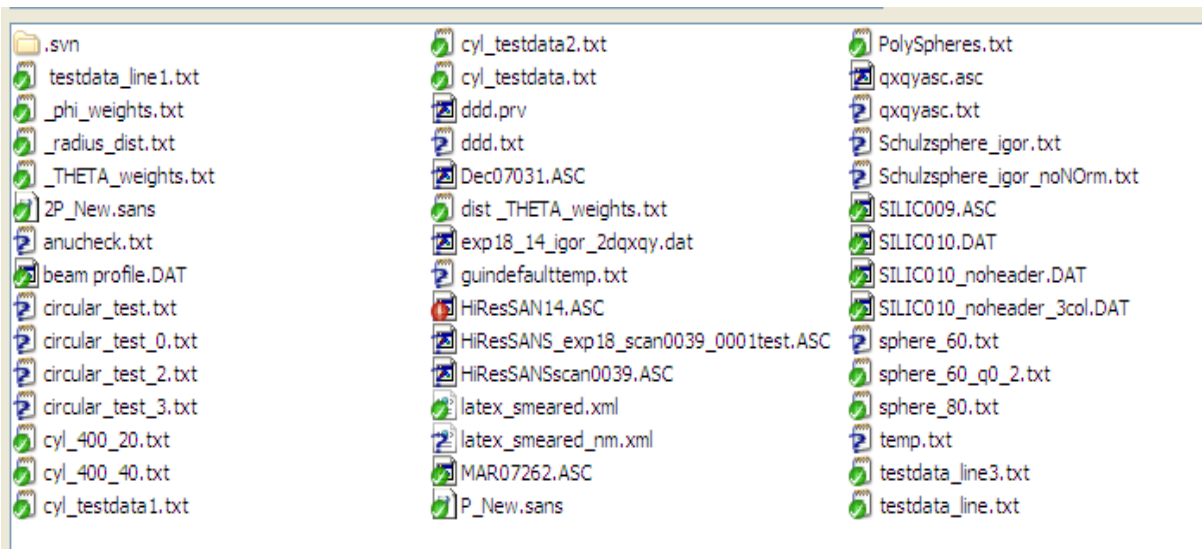project/analysis in the File menu.

Fig. I-4. Example data files in a test folder

II. Analysis and tool

II-1. Analysis:

Currently, the SasView provides **model fitting**, **invariant computation**, and **P(r) inversion**. Each of the control panels can be switched and accessible via. switching the item in the 'Analysis' menu in the menu bar. With the Data Explorer ON, use the 'Send to button to set a data set to a analysis panel after a data set is loaded. With the Data Explorer OFF, it will automatically set the data into the current Analysis panel.

II-2. Tool:

i) **SLD Calculator**: To calculate the neutron (and X-ray) scattering length density (SLD) of a molecule. The method is provided via 'Help' menu.

ii) Slit Length Calculator: This tool is generally for X-ray users to calculate the slit size (FWHM/2) for smearing data using their half beam profile data (*SAXSess: For example, see I-4 v.*). We assume that the slit size given is FWHM/2 in the slit smear calculation.

iii) Kiessig Calculator: a simple tool to convert a q value to a real space value (i.e., thickness or size).

iv) **SANS Resolution calculator**: to estimate dQ (instrumental resolution at a givven q value(s)). See 'Calculator Help' in the menu bar for details.
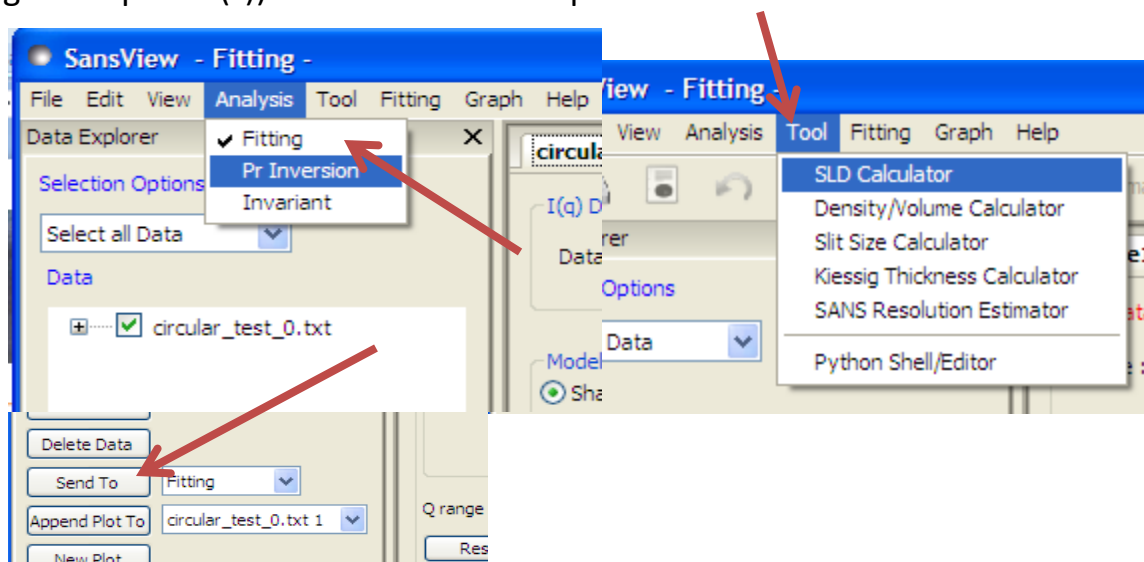

Fig. II-1. Analysis and Tool menu

III-1. Method I] If a data is already plotted, highlight the data symbols by locating your mouse pointer to it (Fig. III-1). (For 2D, just right -click on 2D data image plot.) Then, select "Select data for fitting" (Fig. III-2).
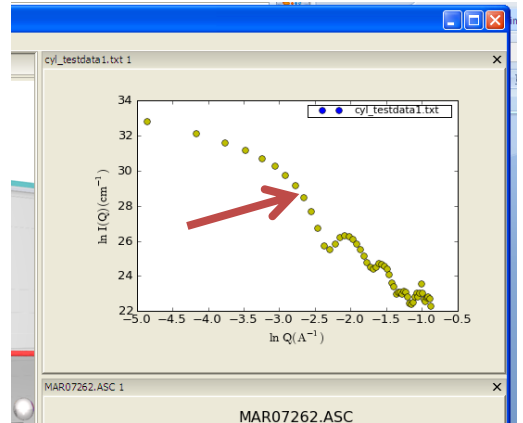

Fig. III-1

III-2. Mehod II] With Data Explorer ON, select a data set by checking it from the data tree. And press the 'Send to' button (Fig. III-3).
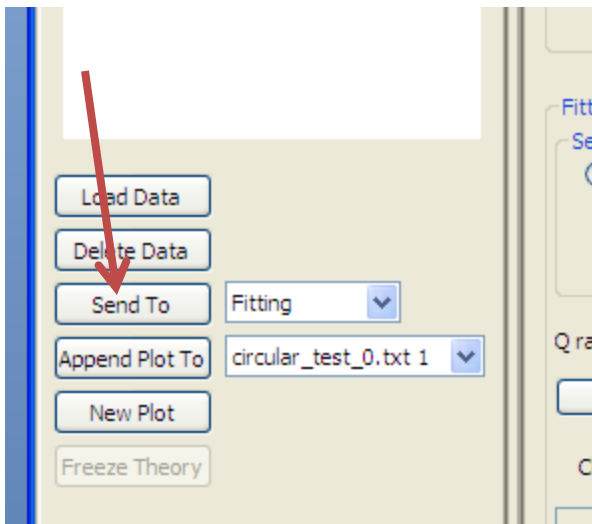

Fig. III-2
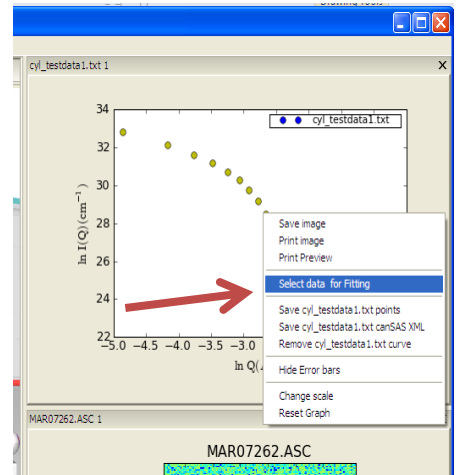
Fig. III-3

III-3. Method III) Turn the Explorer OFF, and load a data from the File menu. It will automatically set the data into a control panel in the current analysis.

III-4. Select a model type of interest.
Right click on the arrow of the model drop box, and choose the model function to fit(Fig. III-4)

Fig. III-4

III-5. Adjust the parameter values so that you have a model calculated (green) curve as closed to the data as possible (Fig. III-5).

Fig. III- 5

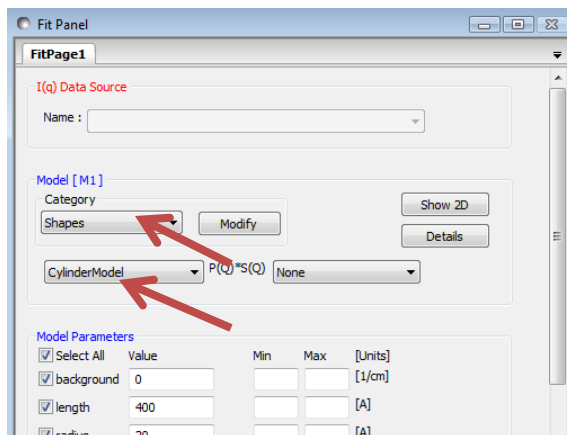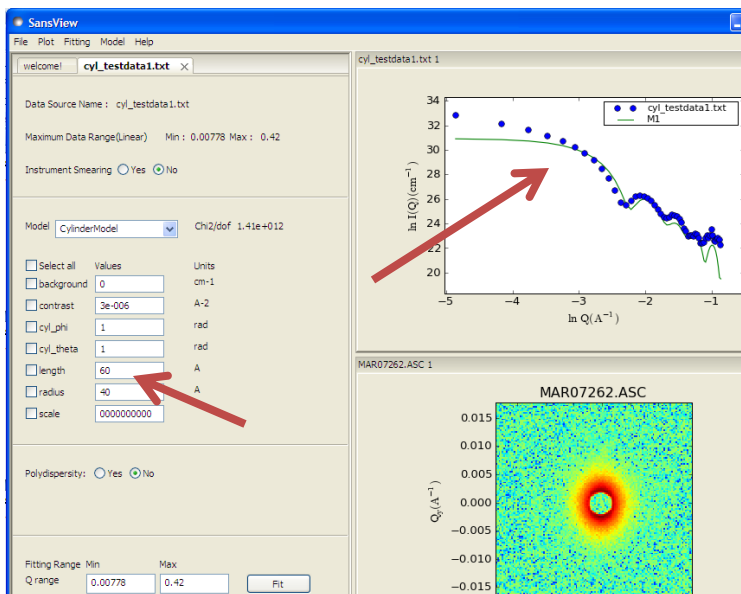III-6. Select parameters to fit by checking the box. (Fig. III-6).

III-7. Setting custom smearing w/o dQ data is available in the panel. The pinhole or slit smear can be set. Note: If pinhole smear is set, temp. increasing dQ data will be generated by linear interpolation from the min to the max value as Q increases.
: 2D smear is extremely time consuming (NOT recommended to use it for fitting.)

III-8. Select an option of how to weight the each data points for fitting (Fig. III-6).

III-9. Adjust Q range of data for fitting (optional) (Fig. III-6).
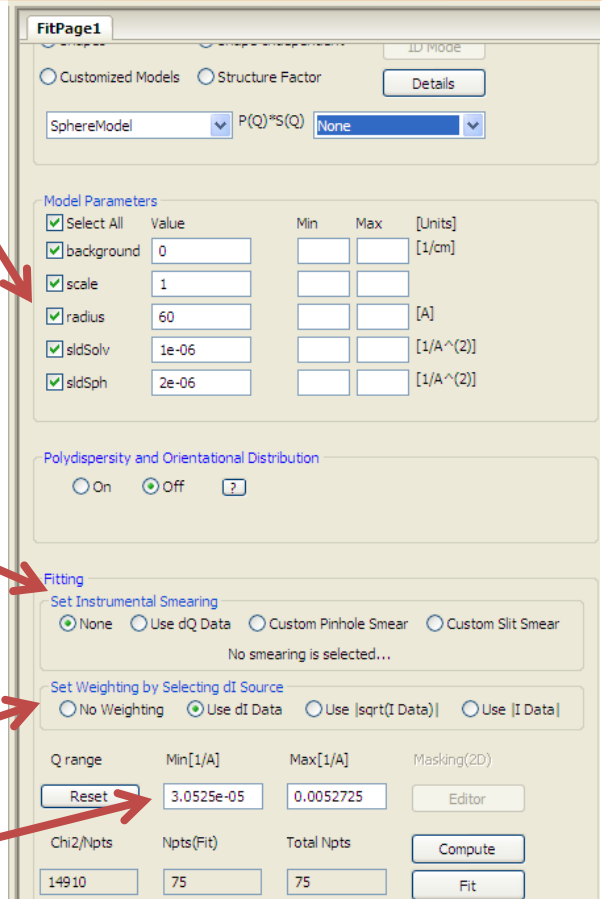
Fig. III-6

III-10. (Optional) You can switch Simple Fit (Leastsq from Scipy) or Complex Fit (ParkMC) fitting engine by selecting or deselecting "Park" in the Fitting menu (Fig. III-7).
*Note that the simple fit uses Levenberg–Marquardt algorithm, and the complex fit employs ParkMC to find a global minimum in chi2 space (longer run time).
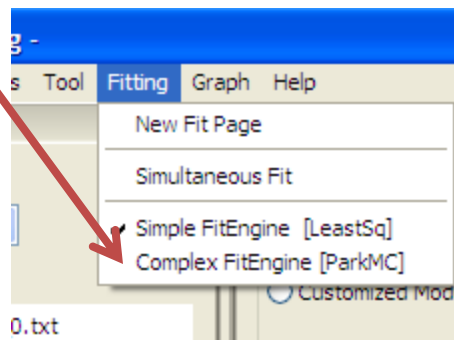
III-11. Click on the "Fit" button (Fig. III-6) at the bottom of the control panel.

Fig. III-7

III-12. If the fitting is successful, the fitting errors and chi2 will show up in the panel, and there will be nice consistency between the fitted curve and your data. ((Fig. III-8).
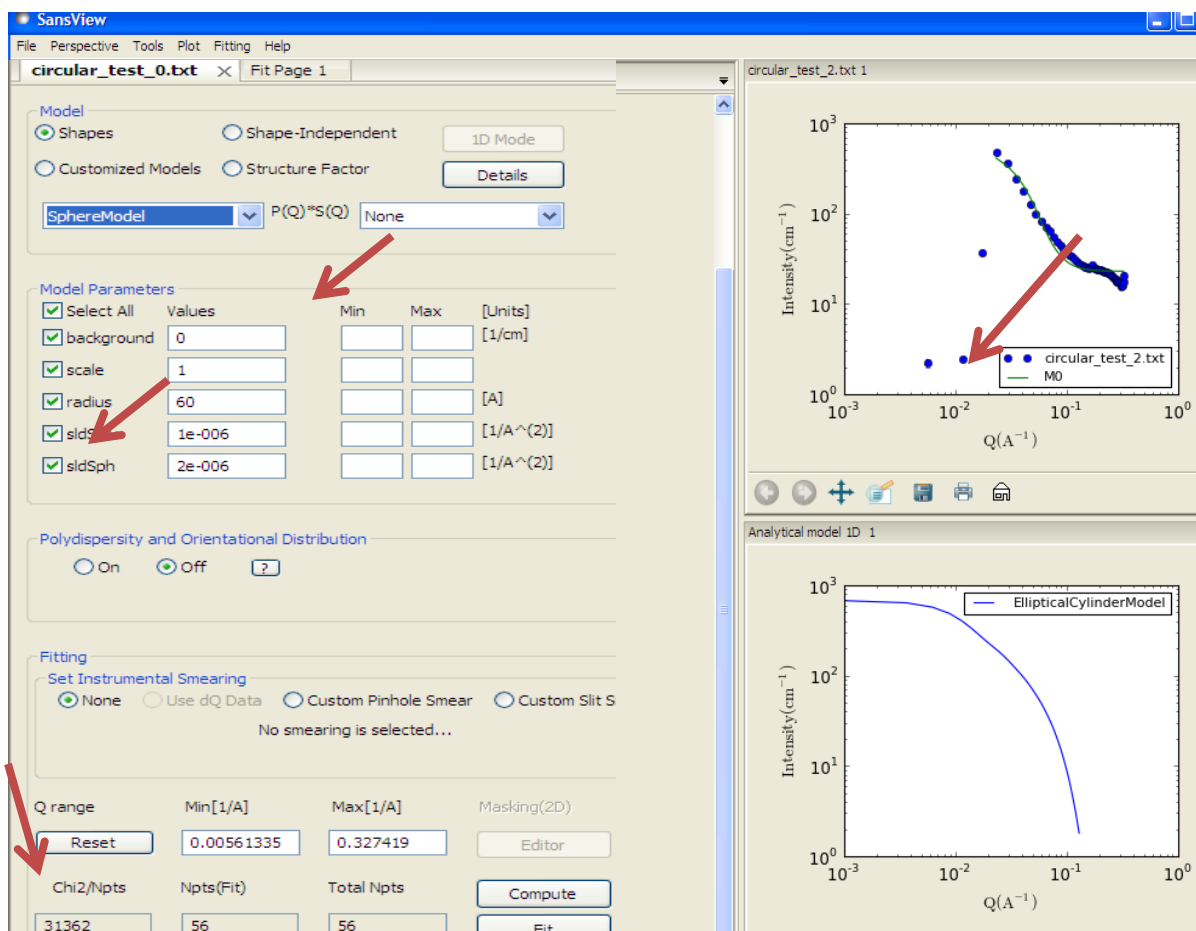
Fig. III-8

III-13. If the fitting is not successful, you can play more with other model functions by choosing another model function (see Step III-4), or polydispersity parameters which will show up by clicking on "polydispersity" "yes" check box . (Fig. III-8): For polydispersity parameters, a good value of Nsigmas is between 2.5 and 5, where Nsigmas tells how much portion of the function from the center is taken account for the polydispersion averaging (2 times sigma, 3 times, etc). Npts is the number of points taken for the averaging. The PD = Sig/mean. And Sig is the STD of the distribution function (also see Sect. X-12).

III-14. The fitting panel (and model panel) can be bookmarked by right-clicking on the panel and choosing bookmark in the popup menu (or from bookmark icon in the toolbar. Once the panel is bookmarked, it can be recalled later by right-clicking on the panel and choosing the model name in the popup menu (Fig. III-9). (Note that once the bookmark is recalled, you may loose the previous panel that you were working on unless it was already bookmarked.)
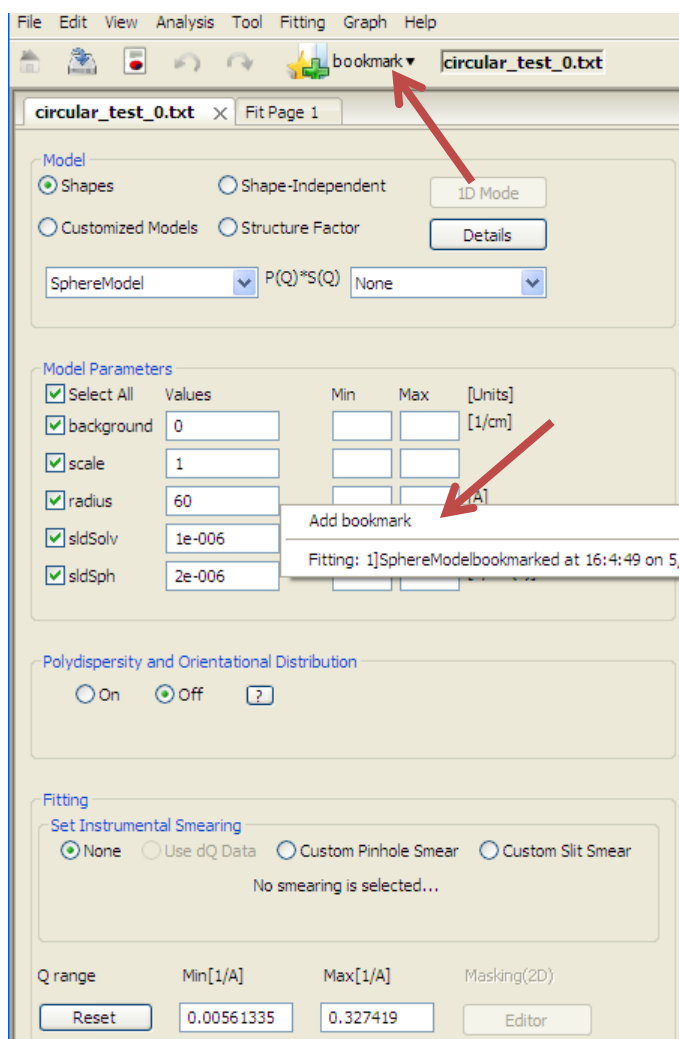

Fig. III-9

III-15. It is possible that the fitting results return with an error, especially when the initial model parameters do not work with your data. This case, some functionalities of the panel may not work. You can delete the fitting panel by clicking on the "x" mark beside of the panel title, and always make a new fitting panel by (Step III-1 - 3) (Fig. III-10).
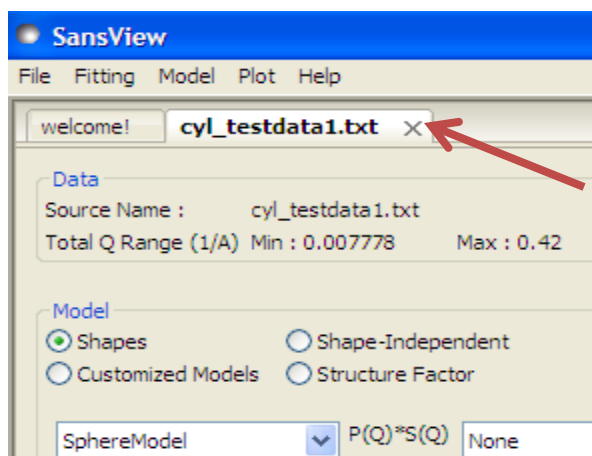
Fig. III-10

III-16. **2D mask editor**: Mask editor for2D data is available by clicking Editor button in the panel (Fig. III-11). Select the shape of mask , move the slicer lines where the mask should be placed, and then push the button 'Add' or 'Erase' to finish the masking. You also can reset/clear the mask you had using the corresponding button. After done, simply close the window by clicking X mark at the top-corner (Fig.III-12). Then, the model fitting/calculation (and the model plot) will be masked.

Fig. III-11

Fig. III-12

III-17 A geometry of the cylinder model (2D) is shown in (Fig. III-13). See model functions in the Help menu (of the SasView Application) for other models.

Only with 2D view in theory perspective or with 2D data, the orientational angle parameters will be displayed in the panel if they are available in the model function but used only for 2D calculations.
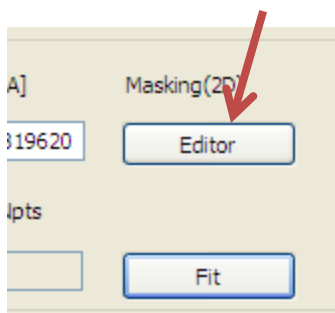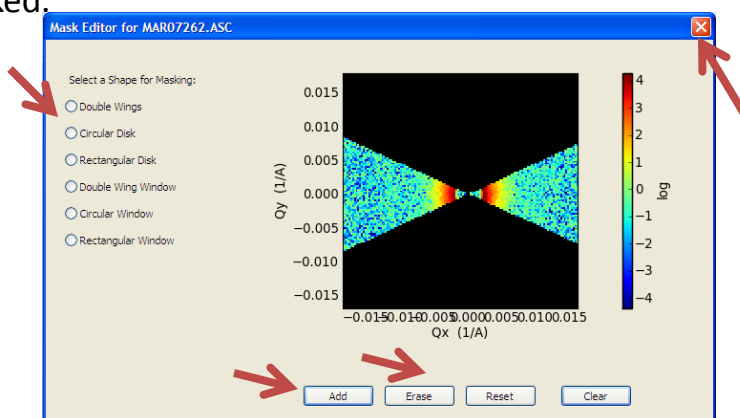
Fig. III-13

IV. Data fitting; Simultaneous fit

IV-1. The simultaneous fit uses the complex fit engine (Park).

IV-2. Repeat Step III-1 to III-6 to load the data set(s). Make sure that all adjustable parameters are checked including the parameters you want to constrain for the simultaneous fitting.

IV-3. Open the simultaneous fit panel by clicking on "Simultaneous Fit" in the Fitting menu (Fig. IV-1). The complex FitEngine will be set automatically.
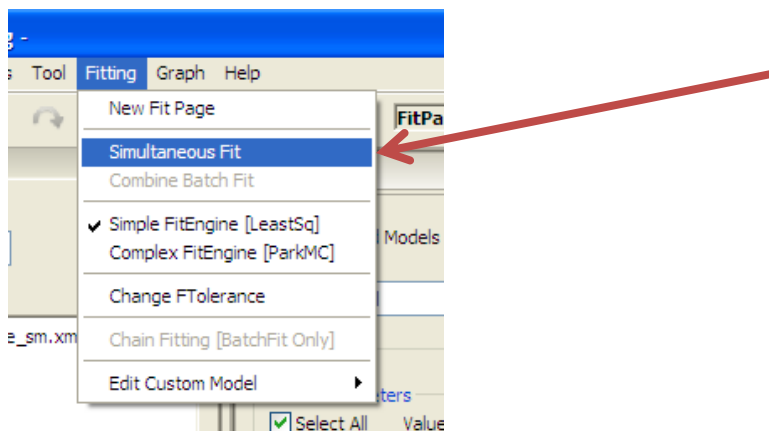

Fig. IV-1

IV-4. Make sure that you know the model fitting function name labeled in your data plot (green curve): It is automatically named as M0, M1, M2,…)
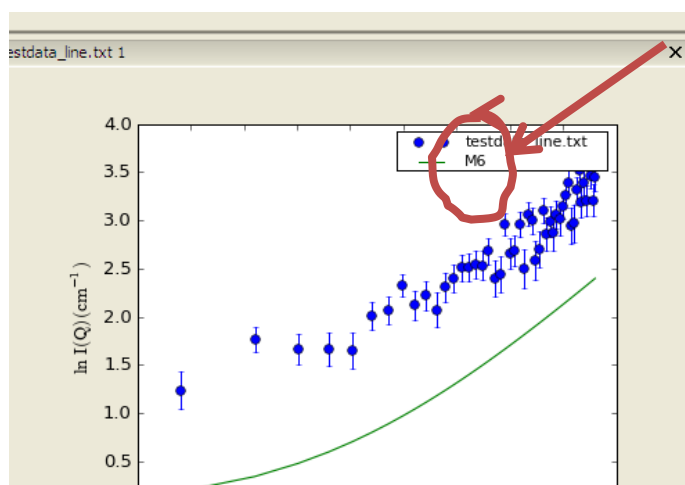

Fig. IV-2

IV-5. Assuming your model describes your data well, in the Simultaneous Fit panel, click on the check box on your models corresponding to your data to fit or click on the Models check box to select all of them (Fig. IV-3).

(The easy setup option is useful when one wants to fit a USANS data and a SANS data simultaneously with one model. For example, select M1 and M2 in the dropdown boxes and click the 'Set All' button. It will generate a number of constraints that equalize all the fittable parameter values of M1 to those of M2 (see IV-6 for another method).)
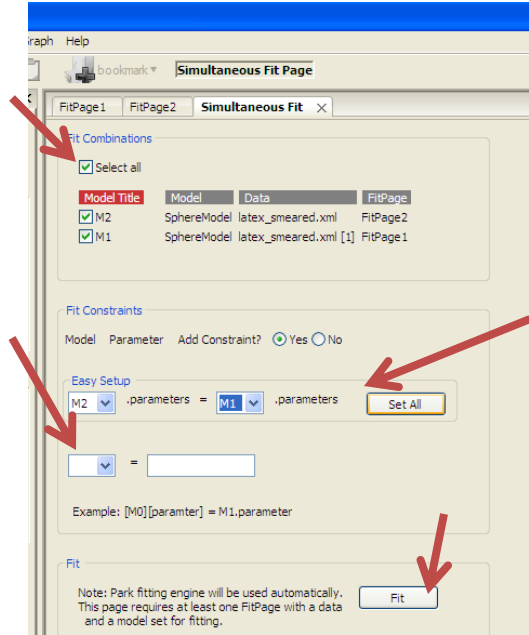
Fig. IV-3

IV-6. Click "Yes" to " Add constraints".
Select and type the constraints between two sets of fitting parameters (Fig. 18); eg., [M0][radius] =M1.radius , or [M0][radius] =2*M1.radius +M1.length For more constraint box ,click on Add button. Or click on Remove button when it is not applicable.

IV-7 Once all constraint setups are done, click the Fit button to perform fit.

IV-8. When the fitting is finished, the progress bar at the bottom of window will disappear (Fig. IV-4).

Fig. IV-4

IV-9. Go back to the Fit panel, and inspect the results (Fig. IV-5).
    Note: Currently the errors of constrained parameters will not be displayed
    well, but can be calculated by applying the equation of your constraints.
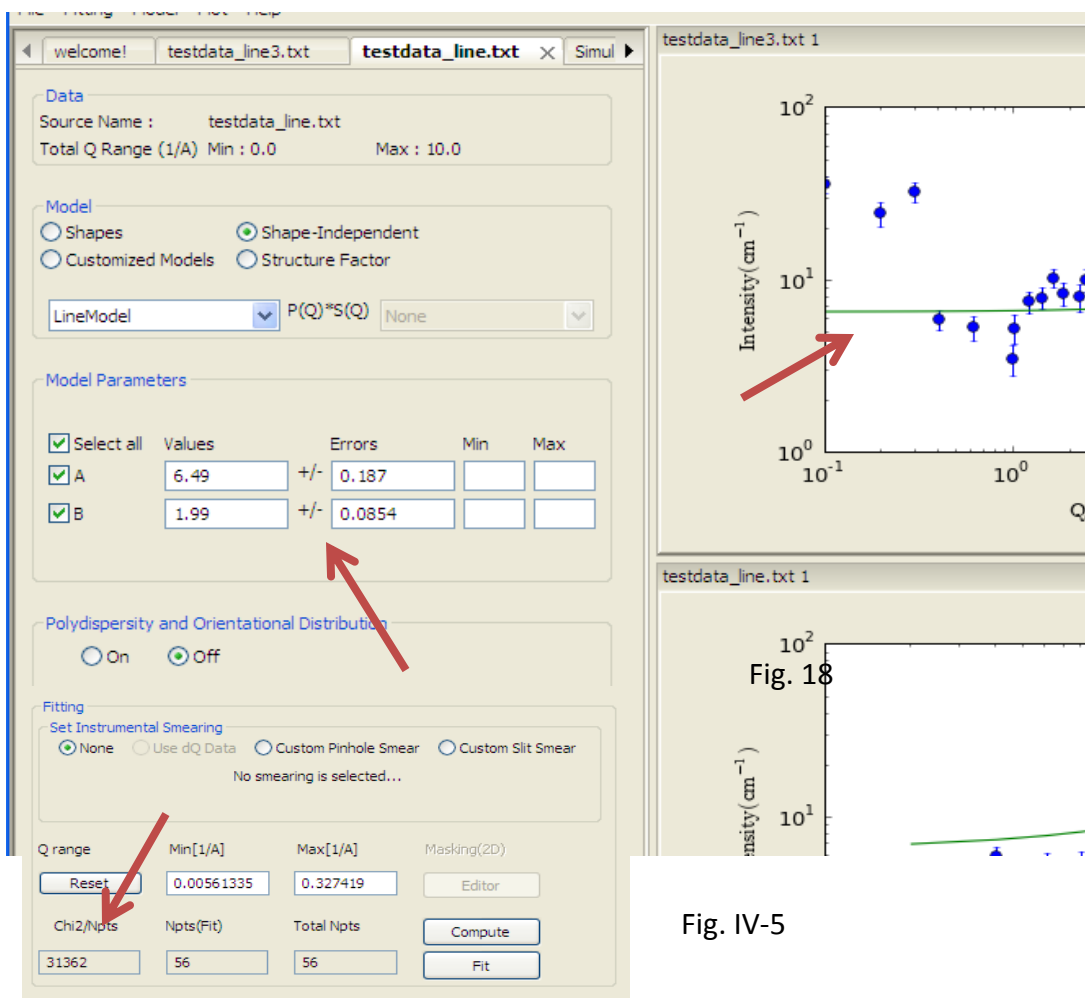
Fig. IV-5

IV-10. If the fitting results return with an error at the bottom of the control
    panel, close the Simultaneous Fit panel (in the same way shown in Step IV-
    3), and repeat it again with different initial values of your parameters.

V. Data fitting; Batch fit

V-1. Load multiple data sets (see Fig. I-2).

V-2. Click the batch mode and click the "send to (Fitting)". It will make a plot of only one of data and a BatchPage. Adjust the parameter values with the best guess.

Those values (if checked for fit) will be used as initial values when fitting each data set as a default. If one wants them to be propagated from the previous results (of another data if any), one can select "Chain Fitting" option under the 'Fitting' menu in the menu bar. Otherwise, just make sure that the menu is unchecked.
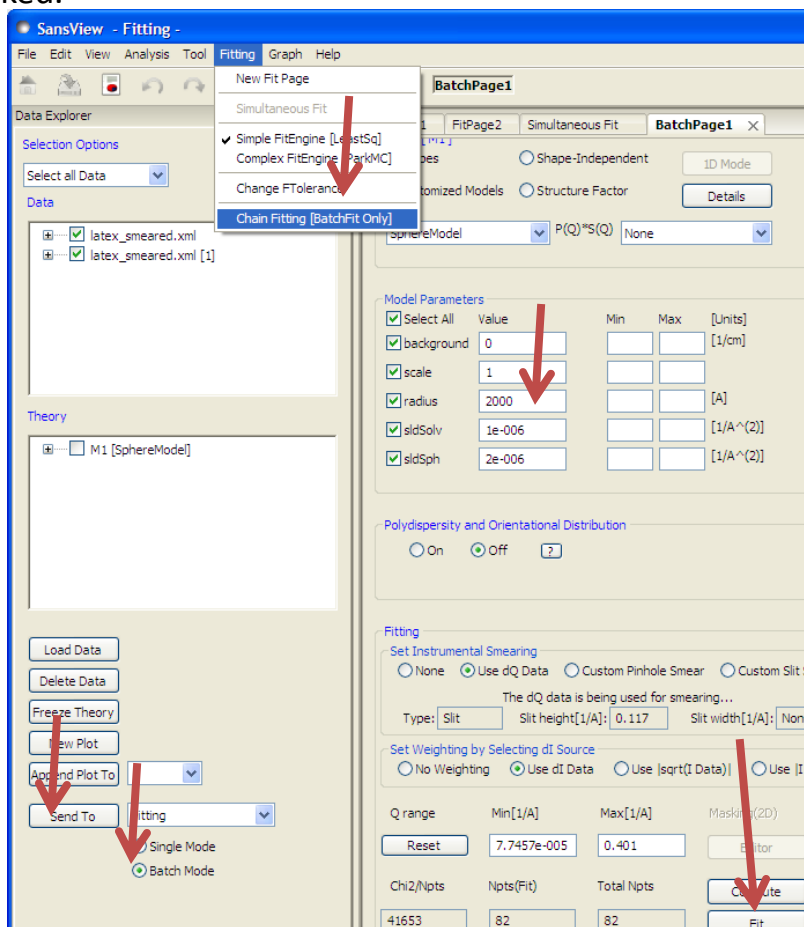
Fig. V-1

V-3. Once ready, simply click the 'Fit' button in the Batch page. The results will show up in the Grid Window. More details about the Batch fit can be found in the 'Help'/ 'Fitting Help' in the menu bar of the SasView window.

VI-1. Without a data set, one can use a default 'Fit Page' or an additional 'Fit Page just for modeling. A new Fit Page can be created by selecting the 'New Fit Page' from the 'Fitting' menu (Fig. VI-1).
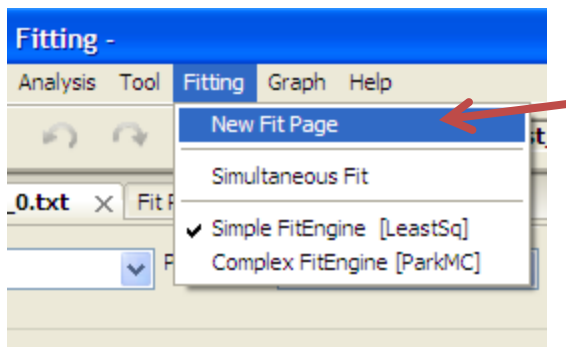
Fig. VI-1

VI-2. In the Fit Page, one can select a model function by selecting another from "Model" combo-box. Also, Q range and the number of points of the calculation can be adjusted by users. the model description and parameter inputs are also provided (Fig. VI-2).
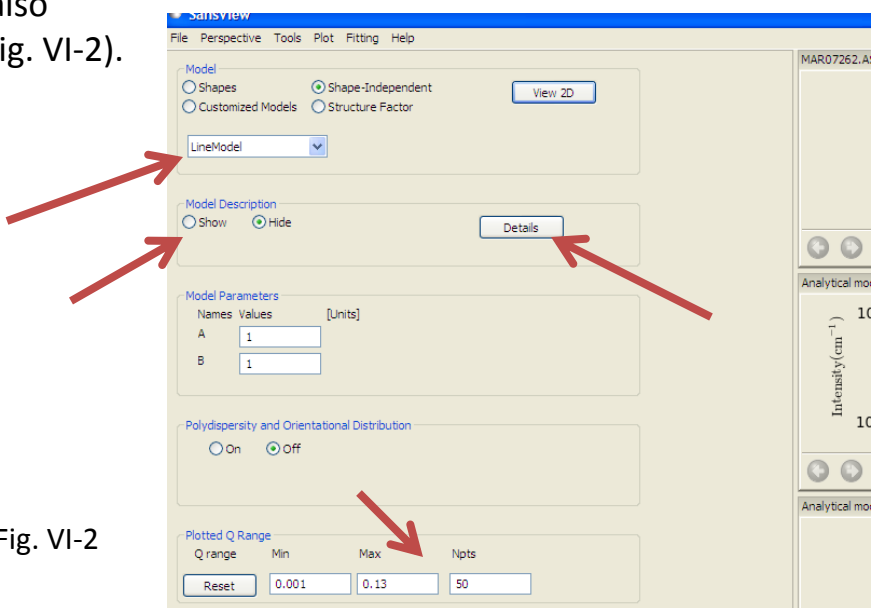
Fig. VI-2

VI-3. 2D model plot panel can be open by clicking the "1D Mode" button, and it will automatically be updated afterward together with 1D plot as the input values are changed (Fig. VI-3).
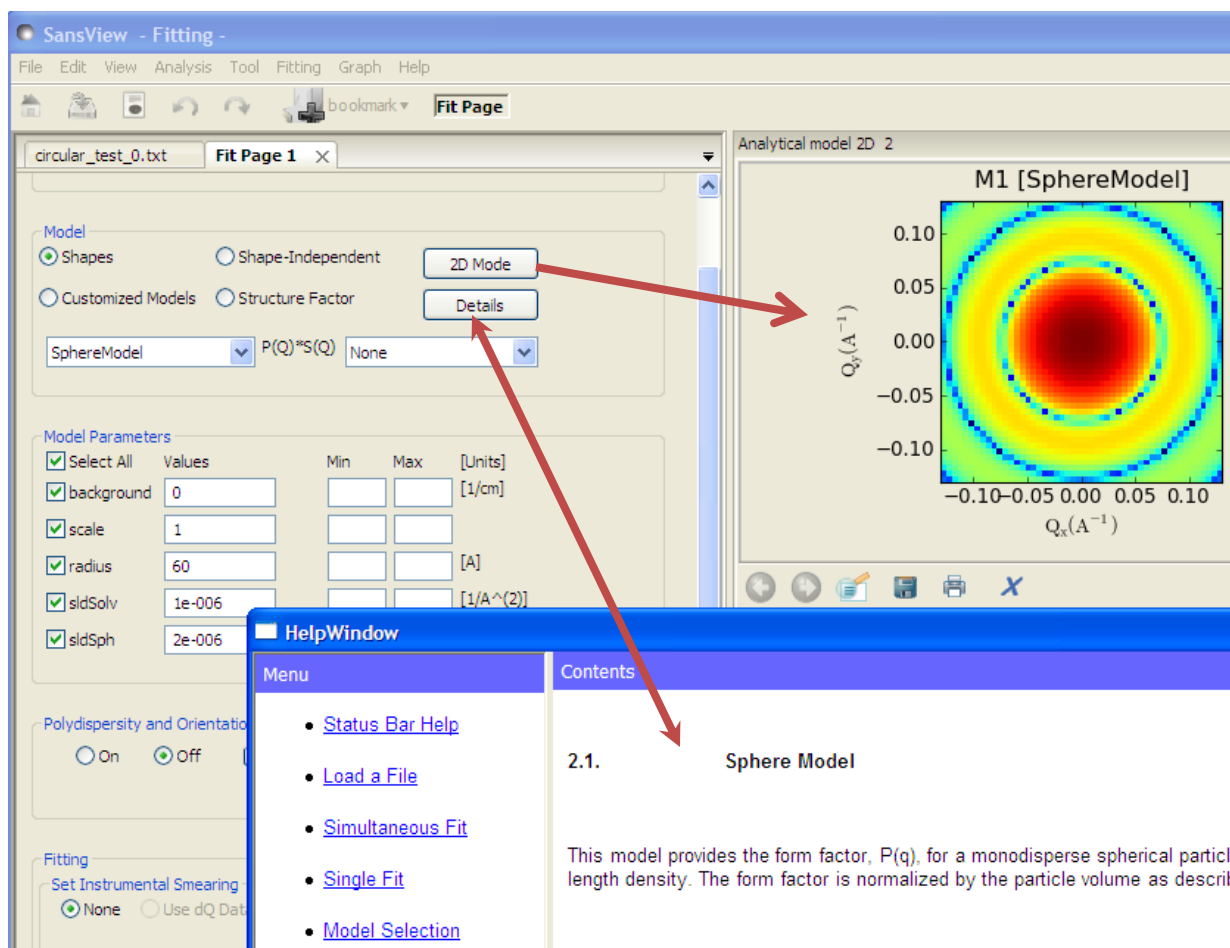
Fig. VI-3

VI-4. User resets the model panel by selecting a new model from the "Model" menu, and also can delete any control panel by clicking on "x" mark beside of the panel name at the top right side corner. By clicking the Save button, the panel can also be saved and open later from the Fitting menu in the menu bar or by right-clicking and selecting it from the panel.

VII. 2D averaging

VII-1. Once user has a 2D plot, 2D averaging is ready to go.

VII-2. Locate the mouse pointer anywhere in the 2D image, and select one of averaging methods (Sector, Annulus, Boxsum or Box average) by right-click-holding the mouse and by locating the pointer.
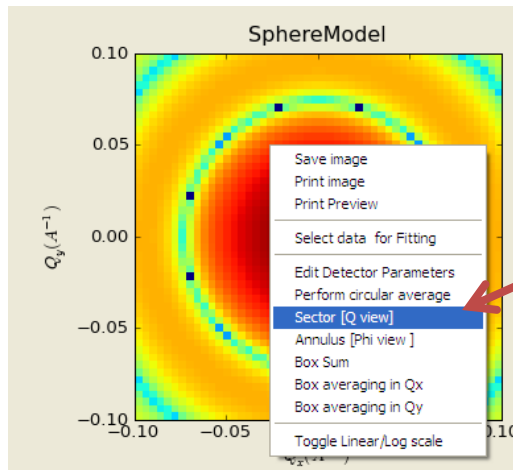
Fig. VII-1

VII-3. Use your mouse to hold and to drag the small cursor in the line to perform an average the area between lines or inside lines (except the circular average). Depending on the kinds of averaging features, the cursor movement is restricted to fit the geometry of the area to perform the averaging.

VII-4. If the error bars block the averaged 1D plot, right-click on the highlighted 1D plot and choose "hide error bars".
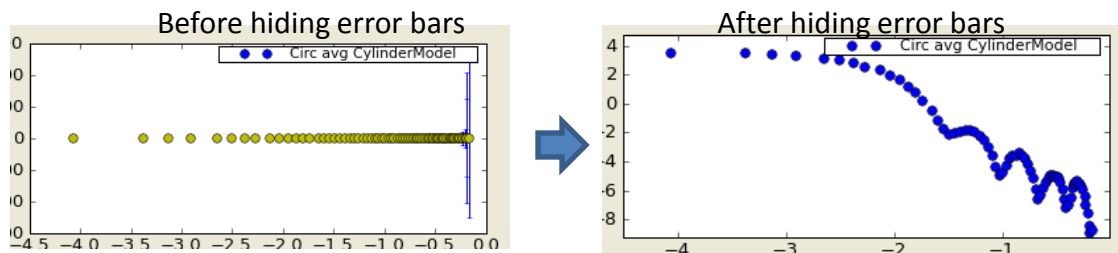
Fig. VII-2

VII-5. Some screen shots below show the shape of averaging area that we
support.

Fig. VII-3

VIII. Save data and print plots
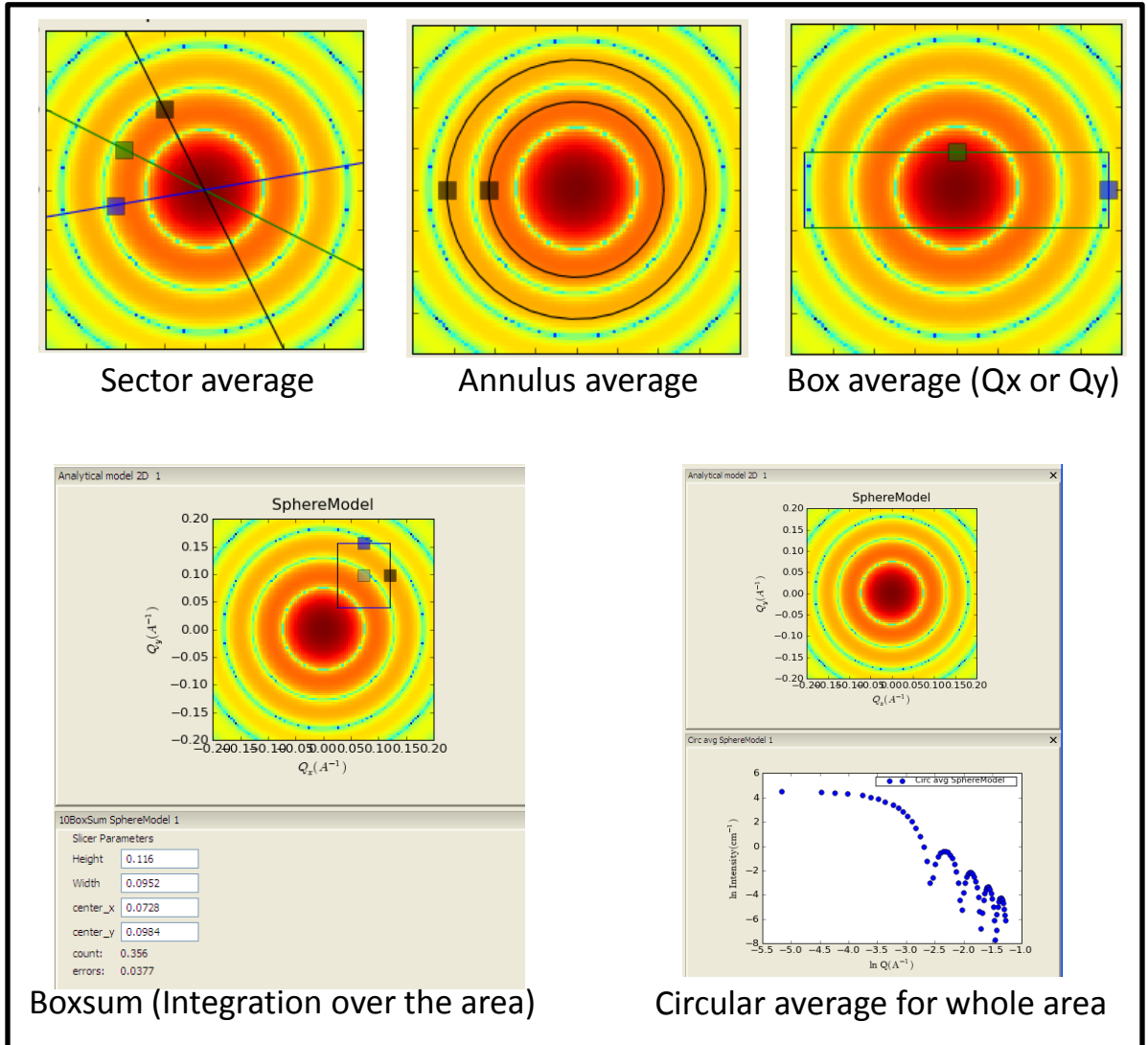
VIII-1. Currently saving a plot panel snapshot is supported in png, pdf, ps, and eps formats. Method 1: Right-clicking on anywhere inside 1D and 2D plot will bring the context menu box. Select "Save image", "Print image", or "Print Preview" of interest (Fig. VIII-1). Method 2: Click on the icon at the bottom of the plots.
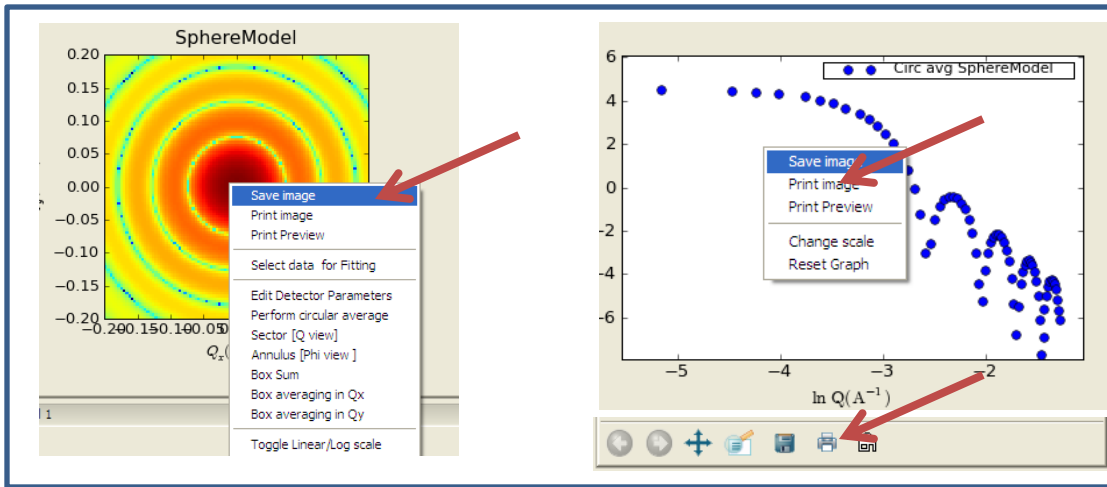
Fig.VIII-1

VIII-2. The data points in the plot can be saved in the txt and CanSAS xml (DAT for 2D) formats. Move mouse to the data points to highlight the symbols. Then, right-click on the highlighted data points. In the context menu, select "Save Points as a FIle" (Fig. VIII-2).
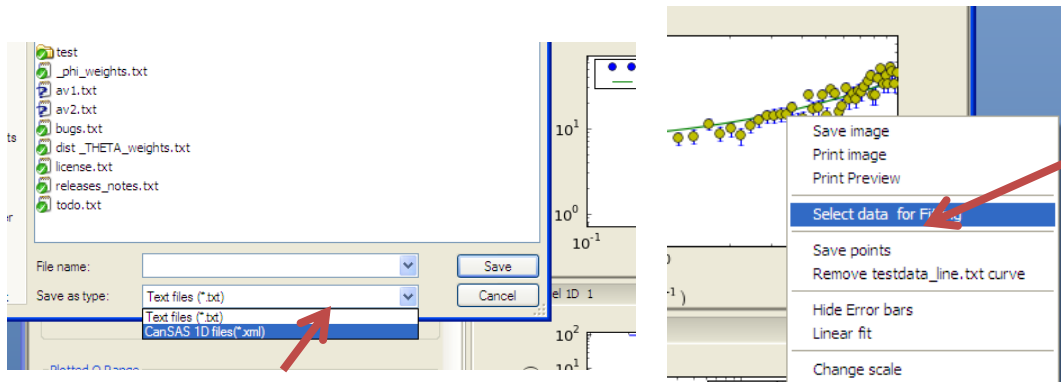
Fig. VIII-2

IX. Pr inversion

Pr inversion is based on P. Moore, J. Appl. Cryst. (1980) 13, 168-175.
**This calculation method is available in a stand alone application (PrView).
Please see details at**
http://danse.chem.utk.edu/downloads/PrView0.2_tutorial.pdf

**In this tutorial, we will show how to switch between Fitting (or model
calculations) and Pr inversion.**

IX-1. Choose 'Pr inversion' from 'Analysis' in the menu (cf. , choose 'Fitting'
to go back to model fitting panels).
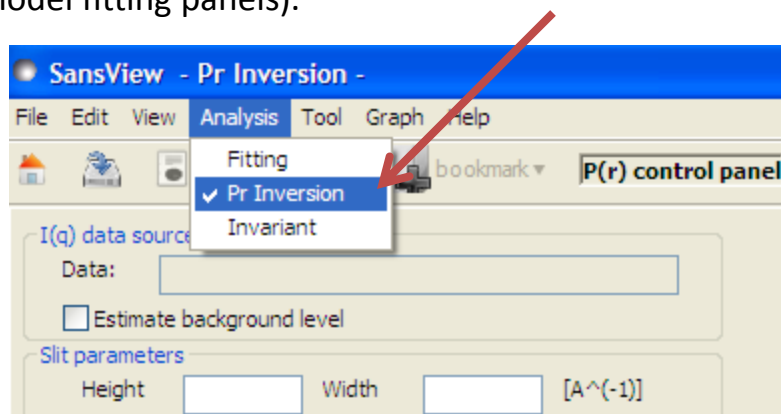
Fig. IX-1

IX-2. Use III-1, III-2, or III-3 step to load a data to the Pr control panel. And
make sure the data name is shown in the panel.
Note that unlike Fitting, Pr Inversion allows only one control panel.

To save this
analysis
panel status
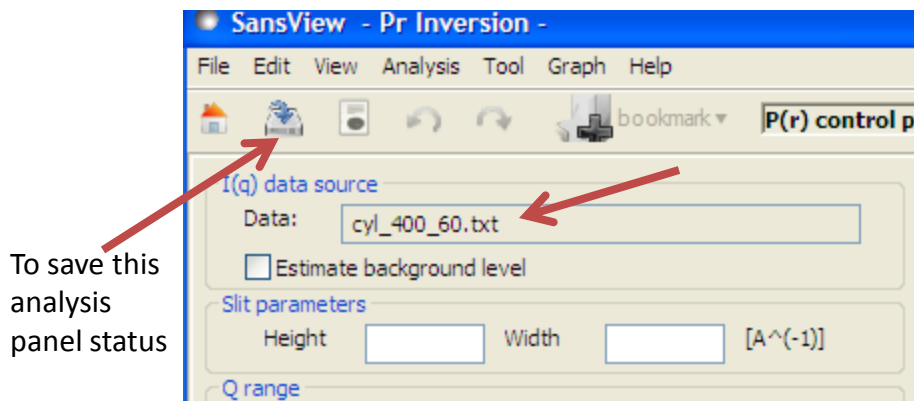
Fig. IX-2

IX-3. **Background estimate:** By checking the background estimate box, you can let the application fit a constant background value for your I(q) data.

Fig. IX-3
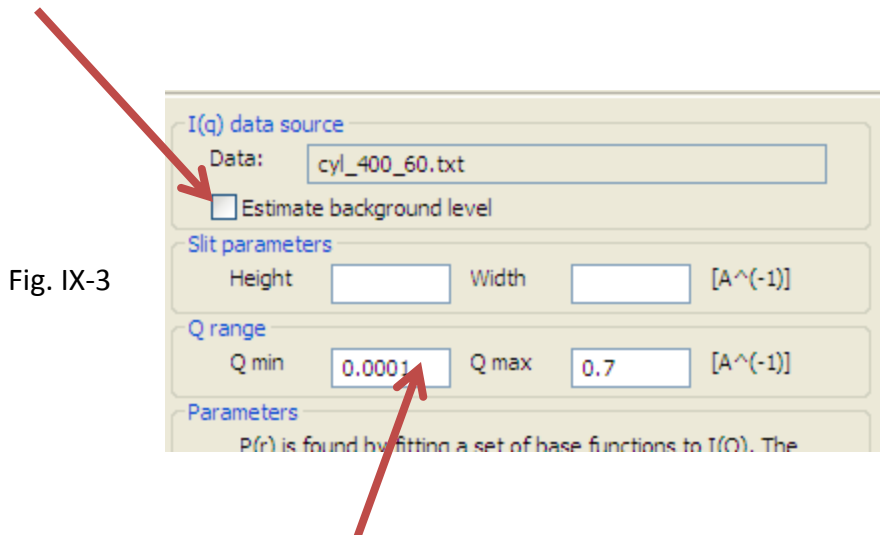
IX-4. **Q range:** Q range for the I(q) may be specify in the Q min and Q max text boxes.

IX-5. **Suggested values:** Estimates for the number of terms and the regularization constant are computed when the maximum distance or Q range is changed. When an estimate is available, a button with the value will be enabled. Click the button to accept the value.

IX-6. **Input parameters:**
1) Number of terms: number of terms in the expansion.
2) Regularization constant: α parameter of the regularization term.
3) Max distance: maximum distance between any two points in the system.

Fig. IX-4
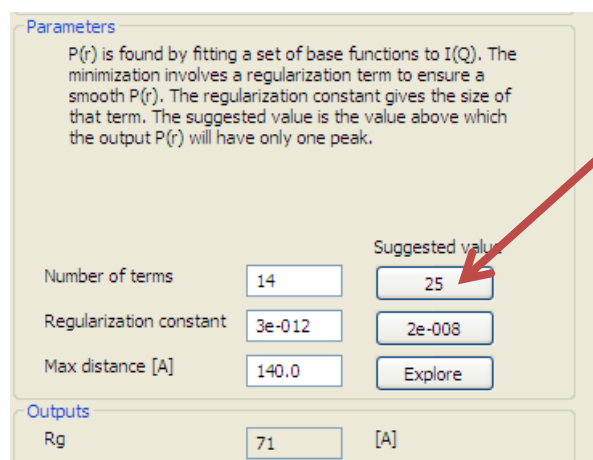
IX-7. **Output parameters:** Several output parameters are provided as figures of merit of the inversion process.
1) Rg and I(Q=0) are computed from the P(r) distribution.
2) Positive fraction: The fraction of the integral of the absolute value of p(r) that is positive.
3) 1-sigma positive fraction: The fraction of the integral of the absolute value of p(r) that is at least one standard deviation above zero.
4) Oscillations: The oscillation parameter is defined as

$$integral(dp(r)/dp)^2/integral((p(r))^2)dr$$

Its value is 1.1 for a spherical system.

IX-8. **Buttons:**
1) Save: To save the information and results in the panel into a file so that later it can be reloaded.
2) Reset: To reset the panel to the default.
3) Compute: To perform the Pr calculations.

Fig. IX-5

Outputs		
Rg	71	[A]
I(Q=0)	1e+0/4	[A^(-1)]
Background	0	[A^(-1)]
Computation time	0.34	secs
Chi2/dof	1.8e+014	
Oscillations	2.5	
Positive fraction	1	
1-sigma positive fraction	0.52	

Save   Reset   Compute

IX-9. **P(r) plot:** Right clicking on the highlighted data points on locating mouse pointer to the data points in the P(r) plot panel, will provides a popup (context) menu. Then:
1) another set of P(r) data can be added into the plot by selecting 'Add P(r) data' from the menu
2) the number of the calculation points can be changed by selecting 'Change number of P(r) points' from the menu
3) scaling and normalization can be also done by choosing a proper menu in the same way.

IX-10. **Results:** Once the p(r) distribution has be computed, the I(Q) corresponding to the Fourier transform of that distribution is shown and compared with the input data.

IX-11. **Explore Dmax:** Maximum distance (Dmax) can be examined by clicking the 'Explore' button next to the Max distance input box. New popup window will be open displaying Chi^2 vs. Dmax as defaults. Exploring Dmax with other parameter spaces can be done by choosing the parameter in the combobox named 'Select a dependent variable' at the top of the window.
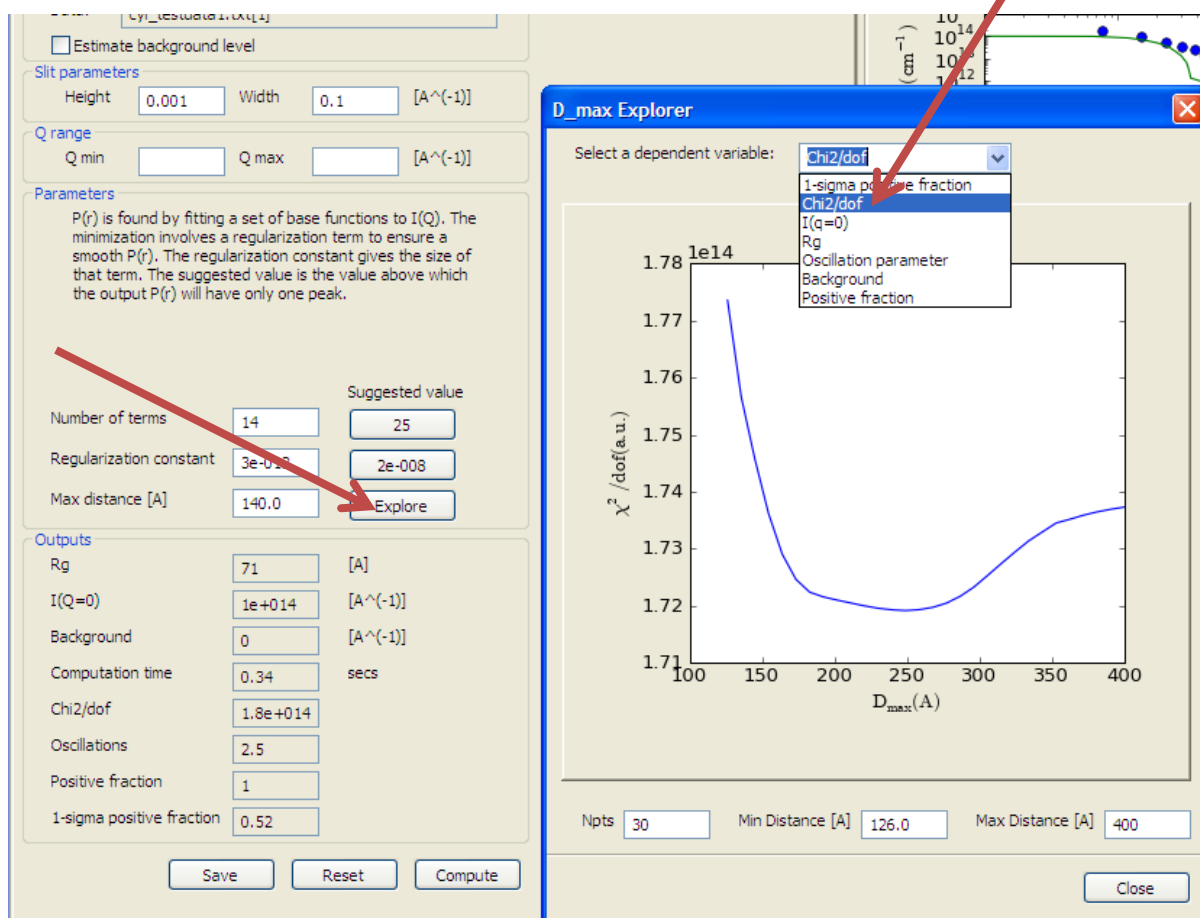

Fig. IX-6

X-1. Theory

The scattering invariant (Q*)

The scattering invariant (Q*) is a model-independent quantity that can be easily calculated from scattering data. For two phase systems, the scattering invariant, Q*, is defined as the integral of the square of the wave transfer (q) multiplied by the scattering cross section over the full range of q. Q* is given by the following equation,

$$Q^* = \int_0^\infty (qg)I(q)dq$$

This model independent quantity (Q*) is calculated from the scattering data that can be used to determine the volume fraction and the specific area of the sample under consideration. These quantities are useful in their own right and can be used in further analysis. With this scattering invariant module users will also be able to determine the consistency of those properties between data. There is no real data defined from zero to infinity because they usually have a limited range. Q* is not really computed from zero to infinity. Our maximum q range is 1e-5 ~ 10 (1/A). The lower and/or higher q range than data given can be extrapolated by fitting some data nearby.

The scattering invariant is computed as follow:
- $I(q) = I(q)$ w/o background : If the data includes a background, user sets the value to subtract the background for the Q* computation.

- *Reset $I(q) = I(q)*$ scaling factor , $\delta I(q) = \delta I(q)*$scaling factor* : If non-zero scaling factor is given, it will be considered.

- Invariant: $Q^* = \int_0^\infty (qg)I(q)dq$

    where, g =q for the pinhole geometry and g = q_v(the slit height) for the slit geometry which can be given in data or as a value.

- Higher q-region (>= qmax in data):
    Power law (w/o background term) function = C/q^4 will be used
    where the constant C(=$2\pi\Delta\rho\, S_v$) is to be found by fitting part of data with the range of q_{N-m} to q_N (m<N).

- Lower q-region (<= qmin in data):
    Guinier function = $I_0 exp(-R_g^2 q^2/3)$ where I_0 and R_g are obtained by fitting, similarly to the high q region above.
    Power law can also be used.

The volume fraction ϕ:

$$\phi(1-\phi) = \frac{Q^*}{2\pi^2(\Delta\rho)^2} \equiv A$$

where $\Delta\rho$ is the SLD contrast of which value is given by users.

Thus,

$$\phi = \frac{1 \pm \sqrt{1-4A}}{2}$$

where 0 =< A =<1/4 in order for these values to be physically valid.

The specific surface area :

$$S_v = \frac{2\pi\phi(1-\phi)C_p}{Q^*} = \frac{2\pi A C_p}{Q^*}$$

where A and Q^* are obtained from previous sections, and the Porod constant C_p is given by users.

Definitions:

Q : the magnitude of neutron (or X-ray) momentum transfer vector.

I(Q): the scattering intensity as a function of the momentum transfer Q.

Invariant total is the sum of the invariant calculated from data's q range and the invariant resulting from extrapolation at a low q range and at a high q range if considered.

Reference:

Porod's chapter (2) from O. Glatter and O. Kratky, "Small Angle X-Ray Scattering", Academic Press, New York, 1982

Otto's web page: http://physchem.kfunigraz.ac.at/sm/

XI -2. GUI:

i)   Loading data to the panel: See Chapter III-1 and -2 but select 'Compute invariant' in the pop-up menu.
ii) To subtract a background or/and to rescale the data, type the values in Customized Input box.
iii) If you want to calculate the volume fraction and the specific surface area, type the optional inputs in the customized input box, and then press 'Compute' button.
iv) The invariant can also be calculated including the outside of the data Q range: To include the lower Q and/or the higher Q range, check in the enable extrapolation check box in 'Extrapolation 'box. If the power low is chosen, the power (exponent) can be either held or fitted by checking the corresponding radio button. The Npts for fitting the data that is used for the extrapolation can be specified.
v)   If the invariant calculated from the extrapolated region is too large , it will warn in red at the top of the panel, which means that your data is not proper to calculate the invariant.
vi) The details of the calculation is available by clicking the 'Details' button in the middle of the panel.

Fig. IX-1

XII. Miscellaneous

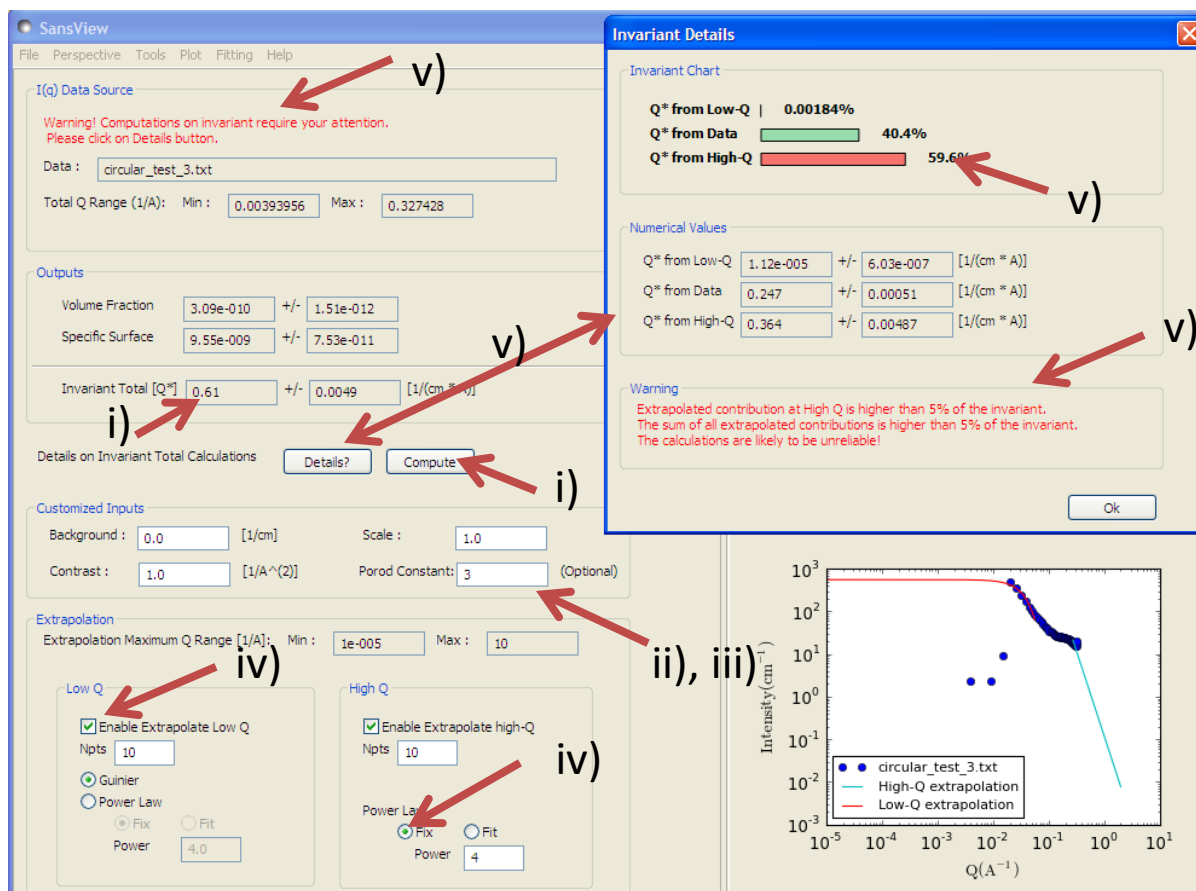XII-1. Change scales or toggle Linear/ Log.
   Right-click on 1D, 2D plot. Select "Change scale" or "Toggle Linear/Log scale" (Fig. XII-1).
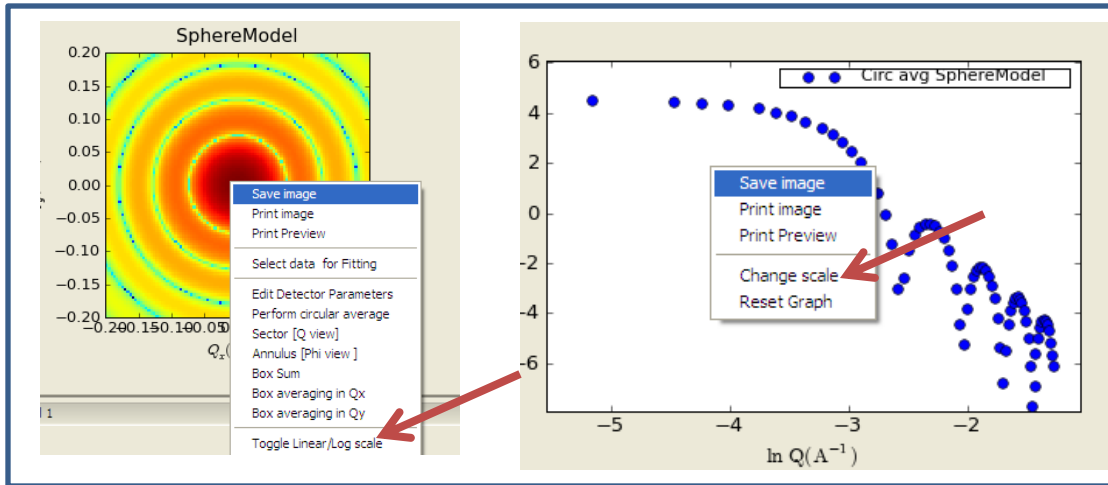

Fig. XII-1

XII-2. Close an open plot panels (below v2.2): All plot panels can be closed by clicking the "x" mark at the top of window. In order to bring that panel back, go to the menu bar and select the panel to open under "Plot" menu (Fig. XII-2).
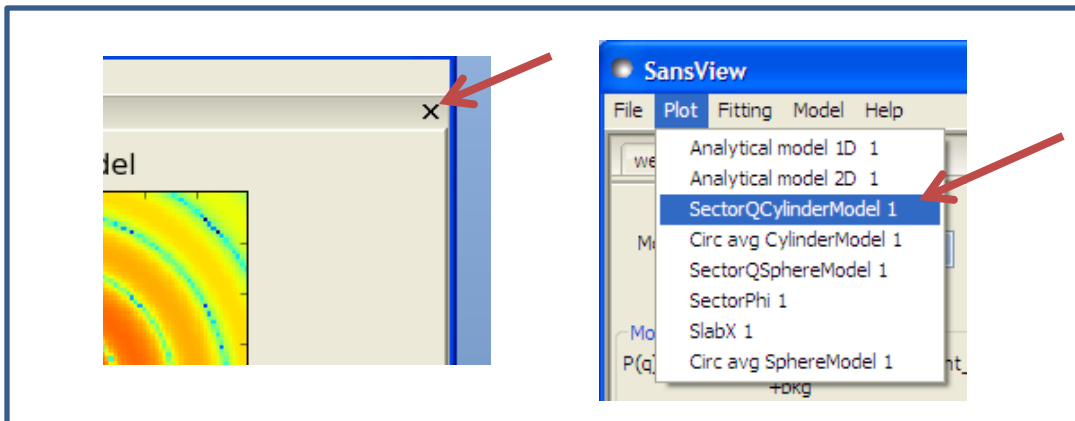
Fig. XII-2

XII-3. Your workspace can be re-arranged by clicking and dragging the title bar outside or back to inside of the SasView interface (Fig. XII-3).
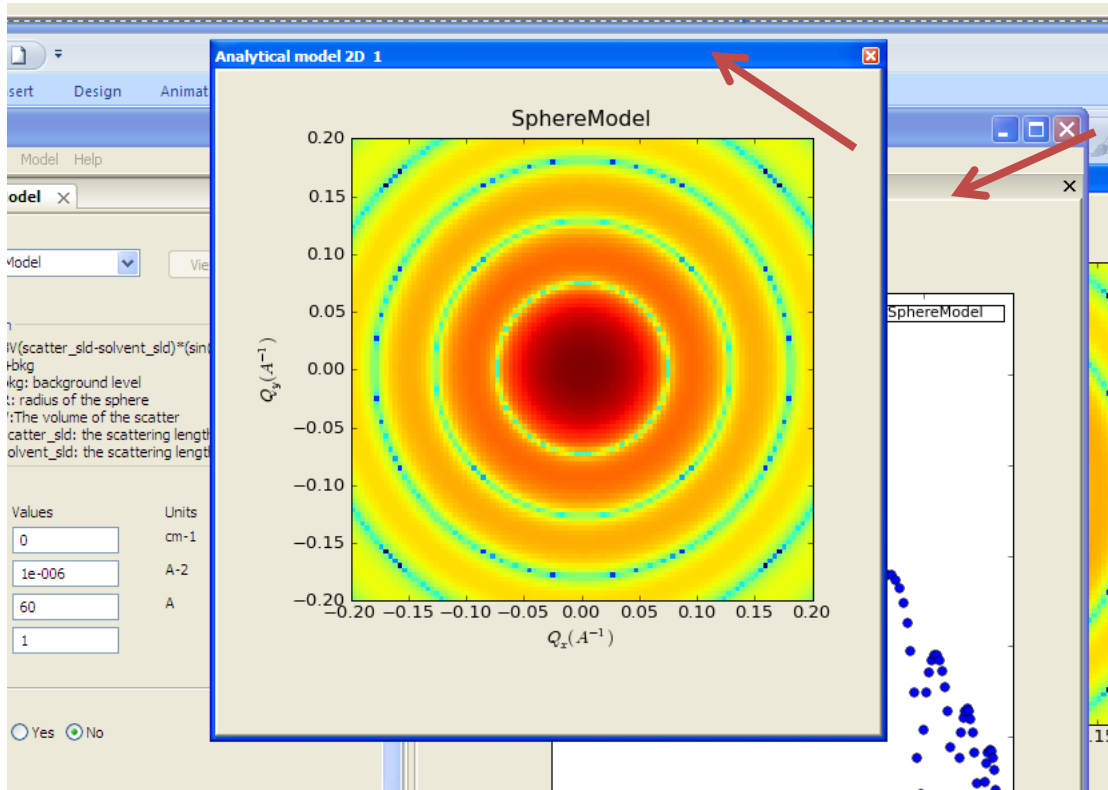
Fig.XII-3

XII-4. Changing color map of a 2D image (Fig. XII-4); Open the context menu by right-clicking the image plot. Select "2D Color Map". Type integer numbers (non zero) in the box. If no numbers (no space) are entered, the image will be displayed in the default color depth. A different color map can be selected by choosing one from the combobox named Cmap. This feature is one time feature, which means it will not be updated when updating or changing the image plot. Note: This feature is still under construction, so use it with care. (Fig. XII-4).
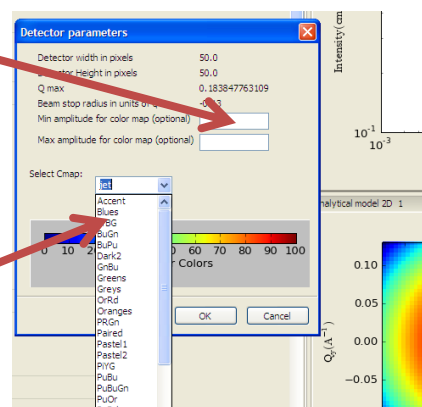
Fig.XII-4

XII-5. Zooming: 1D data plot can be zoomed out and in:

 A) for both x- and y-axis; one-click in the plot panel , locate your pointer inside the axes then rotate the roller at the center of your mouse to zoom in and out (Fig. XII-5).
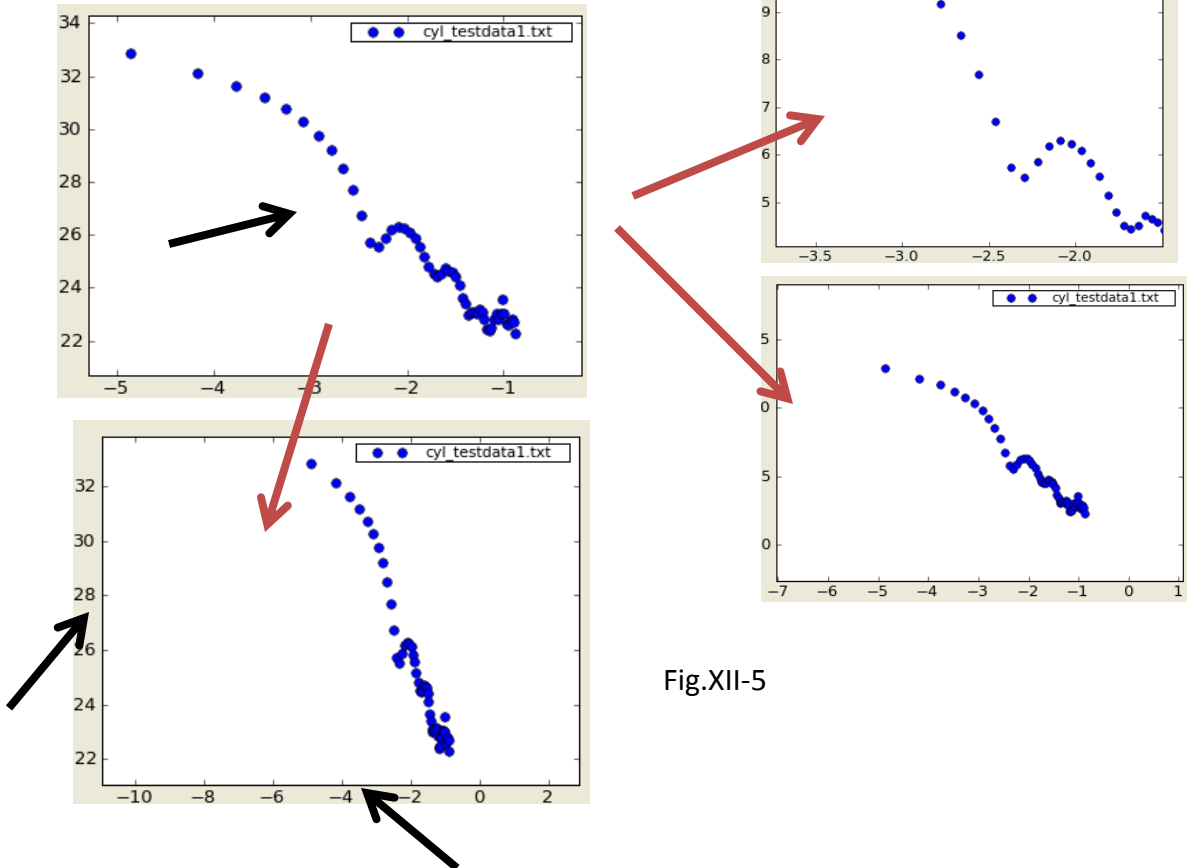
Fig.XII-5

 B) The x- or y- axis separately; click once in the plot panel , locate your pointer (black arrows in Fig. XII-5) somewhere between the axis line and label, and use the mouse roller to zoom in and out the axis as desired.

XII-6. The data points or curve can also be dragged around by selecting the arrow icon in the toolbar then by clicking-holding-dragging the plot.

XII-7. Some Helps and tips are available within the SasView application. Select "Fitting help" or others in the "Help" menu. This will provide you an instant help (Fig. XII-6).

Fig.XII-6

XII-8. Simple tips will be displayed at the bottom line of the application whenever necessary (Fig. XII-7).

Fig.XII-7

XII-9. Loadable data formats (Also, see I-4):

    A) 1D data:

        a) File extensions that can be loaded: .txt, .dat, .abs, .xml, or w/o extension (ASC format).

        b) 2 to 4 columns of data are required in order of Q, I, (dI, dQ).

        c) The meta data (header) will be ignored unless in a standard xml format.

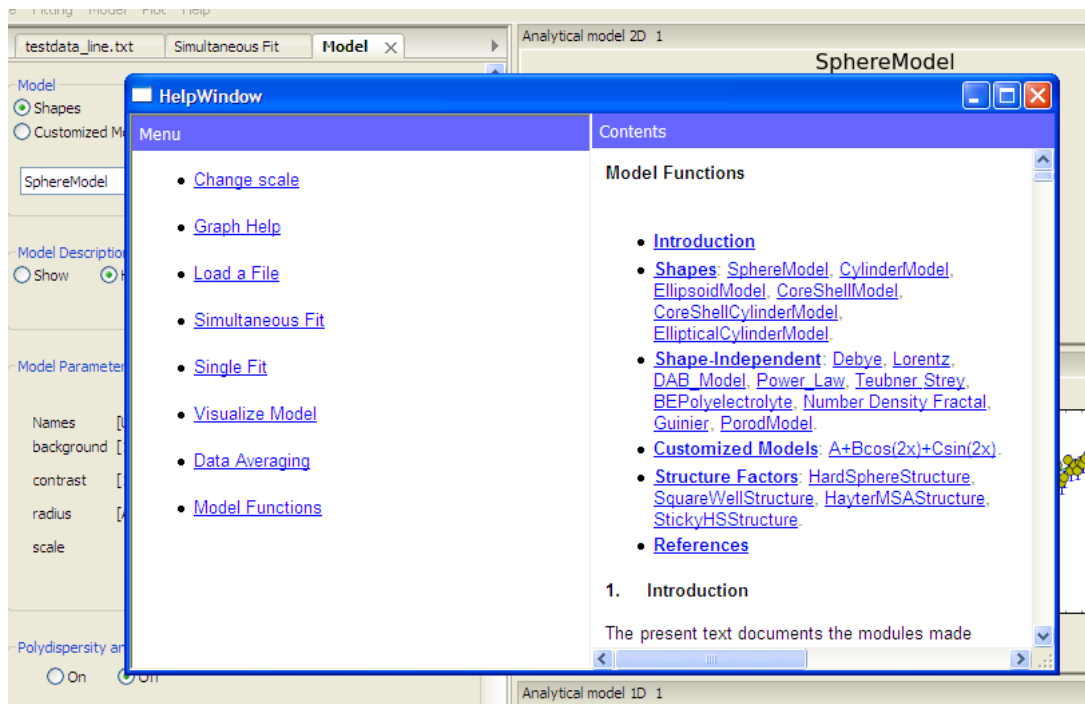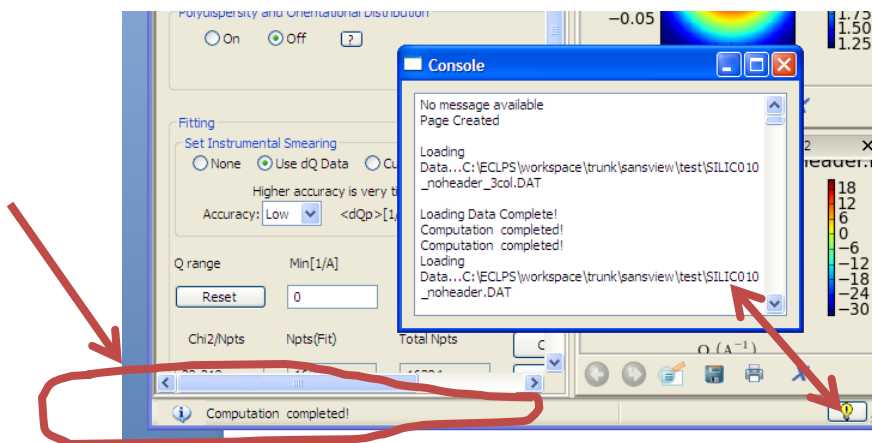   B) 2D data:

        a) File extensions that can be loaded: .ASC, .DAT, .sans

        b) 2D ASCII file should be from NIST IgorPro SANS reduction package and saved to the detector coordinates (*.ASC).

        c) 2D NIST reduced q map file (*.DAT).

        d) Examples of data files are available in "test" folder inside the SasView folder (See page 4 and Appendix: User model documentation).

XII-10. Supporting model functions: The descriptions are available in the help menu.

    A) Shape models (form factors): sphere, cylinder, coreshell cylinder, coreshell sphere, ellipsoid, elliptical cylinder, and many more.

    B) Shape independent models: DAB, BEPolyelectrolyte, Guinier, Debye, Porod, line, number density fractal, Lorentz, power law, etc.

    C) Structure factors: SquareWell, HardSphere, StickyHS, HayterMSA.

    D) Customized models: Refelectivety, ReflectivityII, and example models. Users can define their own model functions by modifying an example pyhton file in the "plugins" folder inside of the SasView folder. See Appendix or the example files in the plugins folder.

    E) P(Q)*S(Q): Form factor times structure factor supports for some shape based models (with 4 structure factors above). For cylinder and ellipsoid based models, the 2nd virial coefficient will be calculated automatically and applied to the structure factors.

XII-11. Instrumental smearing is supported in fitting when your data includes dQ in its forth column.

XII-12. Polydispersity (1D and 2D) and orientational distribution (2D only) can be taken account for modeling and fitting.

A) The SasView provides *Gaussian, flat, Lognormal, or Schulz* distribution function (where PD =Sigma (STD)/mean, Sig=Sigma (for angles), Npts = number of points to average over the distribution, Nsigma = number (of which times sigma is the distance from the center over the distribution function). Proper values for Npts and Nsigmas may be 10 to 30 and 2.5 to 5, respectively depending on the distribution function chosen. The PD/Sig is fittable but frequently it becomes saturated

B) Using a customized function:

Users can make two columns of a distribution function, and open the file from 'array' function option. The file should include two columns of data where the first column is the values of the parameter and the 2nd column is the weighting factors. (Note that this values will override the corresponding mean value (eg., radius) so that the parameter will become no longer active.) An example of the distribution functions is;

degree	weight
0.707	0.4
1.14	1
1.414	0.4

XII-13. Customized models: Users can define their own SANS model function in the plugin_models folder of the SasView folder. Modify the sample files in the folder, or create a new one. If it compiled OK, the model function will be show up under "Customized model" menu in the menu bar. See Appendix or the example files in the plugin_models folder of SasView folder for more details. For SasView > 2.1. use the easy editor provided in the menu bar of the application.

XII-14. Startup Setting: A 'StartupSetting' is found under the 'View' in the menu. With the current option selected, the default View will be changed after restarting the SasView; for example, if you don't want the DataExplorer panel shown, select the current option after the DataExplorer closed, etc.

The SasView will try to remember as much as close to the View you current have.

User Model Documentation

SasView has a plug-in mechanism that allows users to write their own models in python. Each user model is placed in the *plugin_models* folder of the SasView installation. For instance, on the default Windows installation, the user model files will be placed in
\user's home directory\.sasview\plugin_models

Note that the user may thus define any number of such special models. The structure of each model plugin is the following:

```python
"""
    Test plug-in model
"""
from sans.models.pluginmodel import Model1DPlugin

import math


# ALL Your models MUST  HAVE  the class name Model as listed below (i.e.
#DO NOT MODIFY this next line).
# The unique name that appears in the menu for each of your models comes
#next (Name of the model)
class Model(Model1DPlugin):
    """ Class that evaluates a user model.
    """
```

```python
## Name of the model  -- this is where you put the uniqe name
        ##for the model that will appear in the menu
name = "A+Bcos(2x)+Csin(2x)"

def __init__(self):
    """ Initialization """
    Model1DPlugin.__init__(self, name= self.name)

    ## Parameters definition and defaults
    self.params = {}
    self.params['A'] = 1.0
    self.params['B'] = 1.0
    self.params['C'] = 10.0

    ## Parameter details [units, minimum value, maximum value]
    self.details = {}
    self.details['A'] = ['', -1e16, 1e16]
    self.details['B'] = ['', -1e16, 1e16]
    self.details['C'] = ['', -1e16, 1e16]
    self.description = "F(x)=A+Bcos(2x)+Csin(2x) "

def function(self, x = 0.0):
    """ Evaluate the model
        @param x: input x
        @return: function value
    """
    # For convenience, use local variables for the parameters
    A = self.params['A']
    B = self.params['B']
    C = self.params['C']

    return A+B*math.cos(2.0*x)+C*math.sin(2.0*x)
```