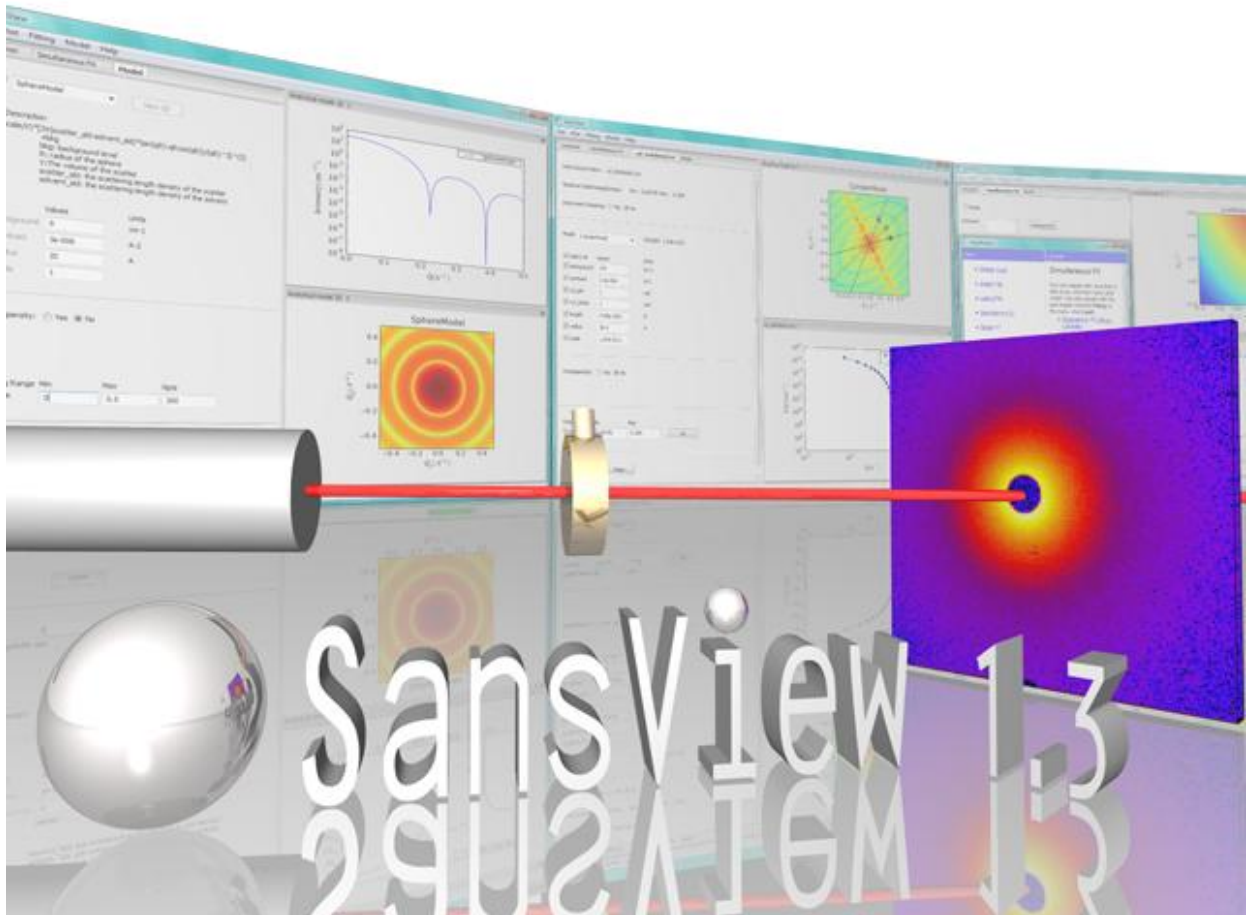**SansView 1.3**

DANSE/SANS Group
University of Tennessee

This software was developed by the University of Tennessee as part of the Distributed Data Analysis of Neutron Scattering Experiments (DANSE) project funded by the US National Foundation.

SansView 1.3
Build: 1.3
(c) 2009, University of Tennessee

*G. Alina, P. Butler, J. Cho, M. Doucet, and P. Kienzle,
"SANS analysis software", to be published.*

Table of Contents

New application for SANS oriented system modeling and data analysis.
Apr. , 2010: version 1.3 is released.

Roadmap:
SansView 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 our users. We are interested in suggestions in two areas:

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

The functionality provided by SansView will be incorporated in a more complete analysis application scheduled for late 2009. SansView will continue to be supported and updates will mostly focus on both feature adding and bug fixing. See our Mission page for more details on the plans for future developments.

Main Features:
• Simultaneous fit of a number of different sets of SANS data with/without the constraints.
• Loading and displaying 1D and 2D data in various formats.
• 1D and 2D data fitting using Scipy (L-M algorithm) or Park (a MC fitting optimizer) fitting engine.
• 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.
• 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.
• 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.
• The user can toggle between a number of different scales on all plots.

Installation and Usage:
Currently the installer is supported only on the Windows : Windows XP (PC), Vista (PC), and VMware (with Windows XP) on Mac were tested.

Contact us:
You can visit the SansView web page at: **http://danse.chem.utk.edu/sansview.html**
Comments? Bugs? Requests? Write to us at **sansdanse@gmail.com**

1. Go to our DANSE Small Angle Neutron Scattering Project web page,
   http://danse.chem.utk.edu/index.html
   and clicking on the "SansView 1.3" will point to the release page
   where the windows installer can be downloaded.
   Also, SansView tutorial can be
   found at the same site.

2. Once "setupSansView-1.3.exe is downloaded, open the installer and
   follow the steps
   as directed.
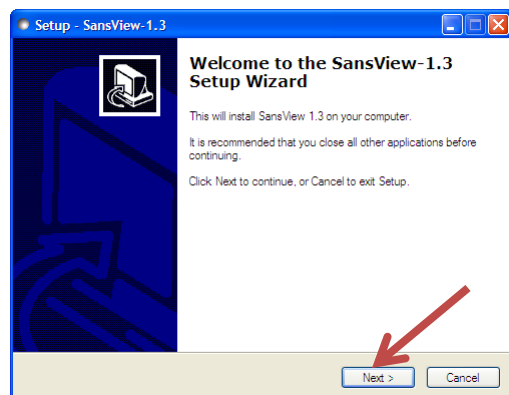
How to install (continued)

3. Once the SansView is installed, some sample 1D and 2D data can be found inside the "test" folder in the SansView-1.3 folder (/Content/Resources/test/ for Mac). This allows you to follow this tutorial session without having your own data set.
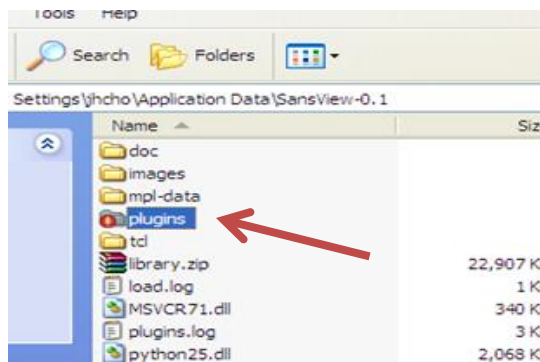
4. The "plugins" folder also includes two example python files (testmodel_2.py and testmodel.py) for users so that they can write their own model function. The file should be modified and saved as a different file name before running the SansView application in order for the functions to work. Modify the arrowed lines for your own functions. Each file can hold one model function and more than one functions can be added in this way. See Appendix or the example files in the plugins folder of the SansView folder for more details.

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

import math


# Your model HAS to be called Model
class Model(Model1DPlugin):
    """ Class that evaluates a cos(x) model.
    """

    ## Name of the model
    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'] = 0.0
        self.params['B'] = 1.0
        self.params['C'] = 0.0

        ## Parameter details [units, min, max]
        self.details = {}
        self.details['A'] = ['', -1e16, 1e16]
        self.details['B'] = ['', -1e16, 1e16]
        self.details['C'] = ['', -1e16, 1e16]

    def function(self, x = 0.0):
        """ Evaluate the model
            @param x: input x
            @return: function value
        """
        return self.params['A']+self.params['B']*math.cos(2.0*x)+self.params['C']*math.sin(2.0*x)
```

I. Loading 1D and 2D data

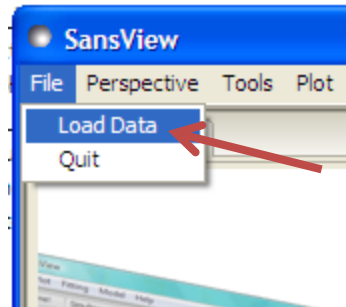I-1. Click on "Load Data" from the File menu (Fig. I-1).

Fig. I-1

I-2. Locate your data file and click on the "Open" 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 , pr, 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, Intensity, (dI, dQ) in order where dQ is the instrumental uncertainty in Q and assumed to be originated by pinhole geometry.

For 2D data, NIST qmap format is currently standard but most of the header 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.
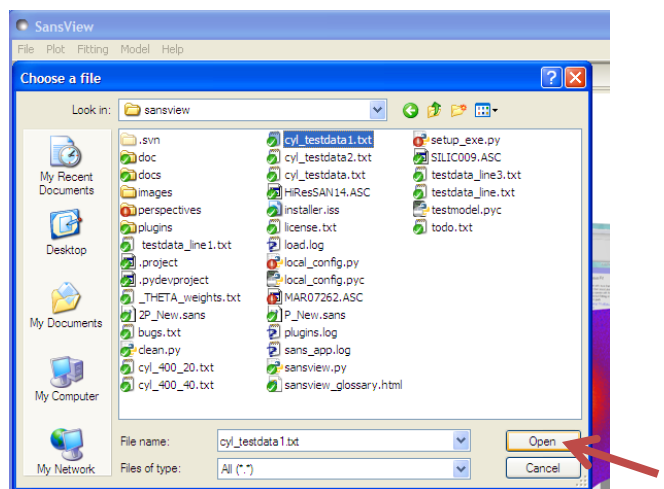

Fig. I-2

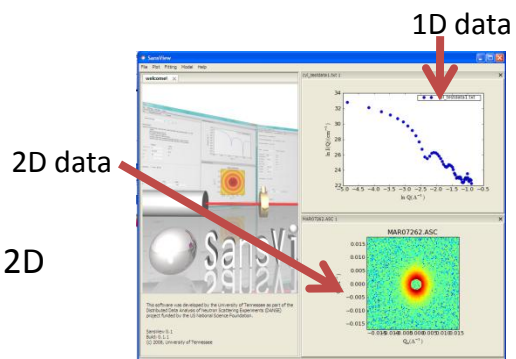I-3. Fig. I-3 shows an example of 1 D and 2D plots of the loaded data.

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.

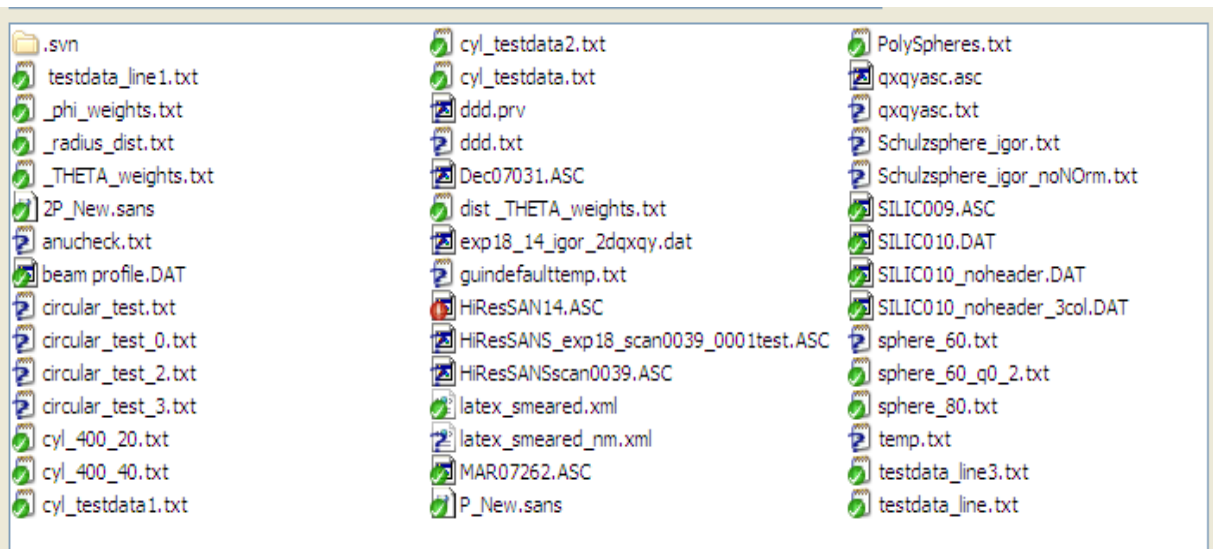- v) Beam profile data for 'Slit Size Calculator': beam profile.DAT.

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

II-1. Perspective:

Currently, the SansView provides model fitting, invariant computation, and P(r) inversion. Each control panels can be switched and accessible via. the 'Perspective' menu in the menu bar, while loading a data to the panels should be done by a right-clicking method (see Sec. III-5) on data plot after a data file is open. A 'Theory' is also provided in the 'Perspective' menu only for investigating a model function without loading a data file.

II-2. Tools:

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) for smearing data using their half beam profile data (*SAXSess: For example, see I-4 v.*).
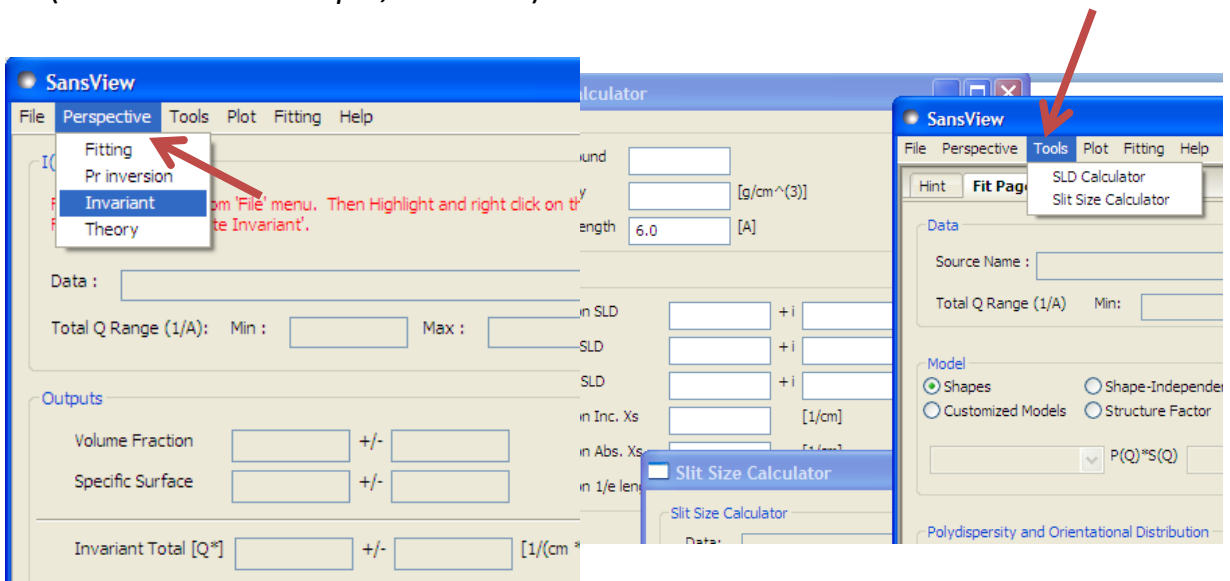

Fig. II-1. Perspective and Tools menu

III. Data fitting: 1D and 2D data; Single fit

III-1. Highlight the data in the plot by locating your mouse pointer to the plot symbols (Fig. III-1). (For 2D, right just click on 2D data image plot.)
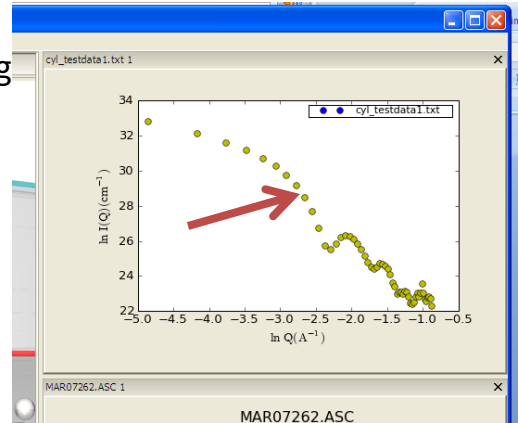

Fig. III-1

III-2. After right clicking on the highlighted data, you select "Select data for fitting" (Fig. III-2). *Same for 2D from now.
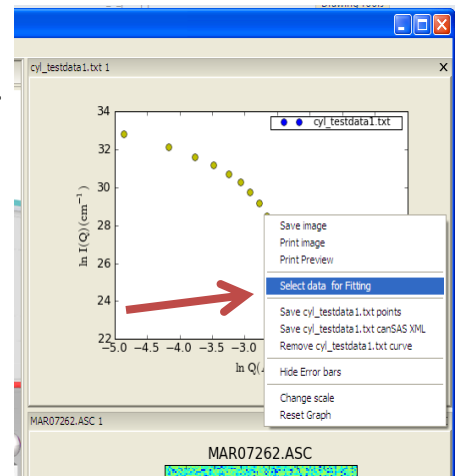
Fig. III-2

III-3. Then, you will have a fitting panel for the data you have chosen, on the left side (Fig. III-3).

Fig. III-3

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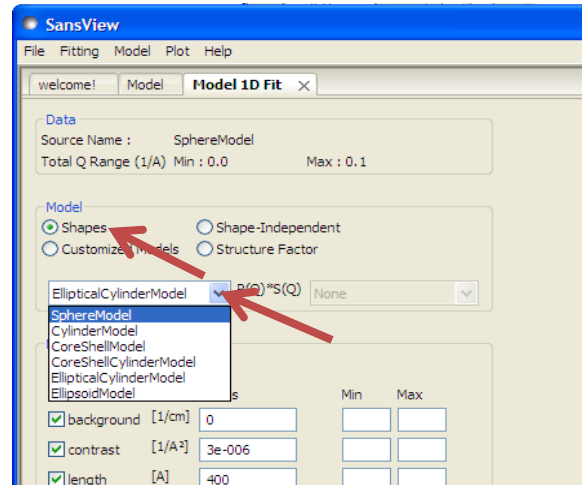Right click on the arrow of the model drop box, and choose the model function to fit(Fig. III-4)

Fig. III-4

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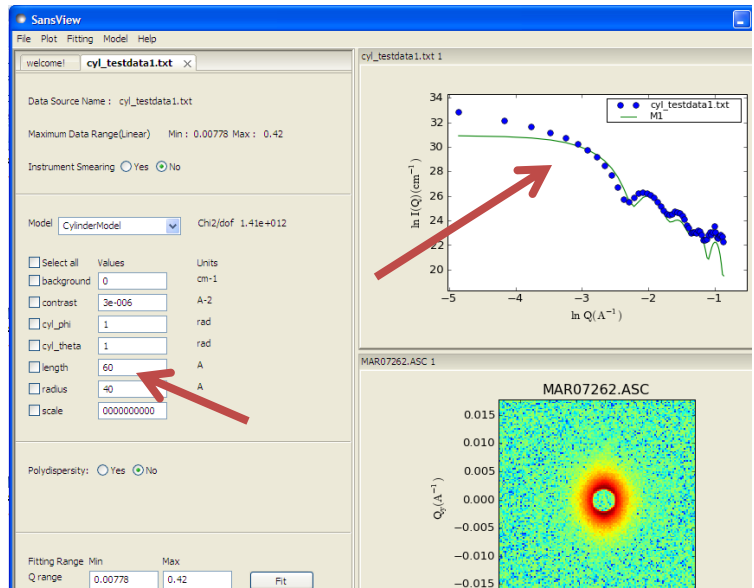

Fig. III- 5

III-6. Select parameters to fit by marking on the check 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.

III-8. Adjust Q range of data for fitting (optional) (Fig. III-6).

III-9. Q range can be reset to the default values by clicking the reset button (Fig. III-6).
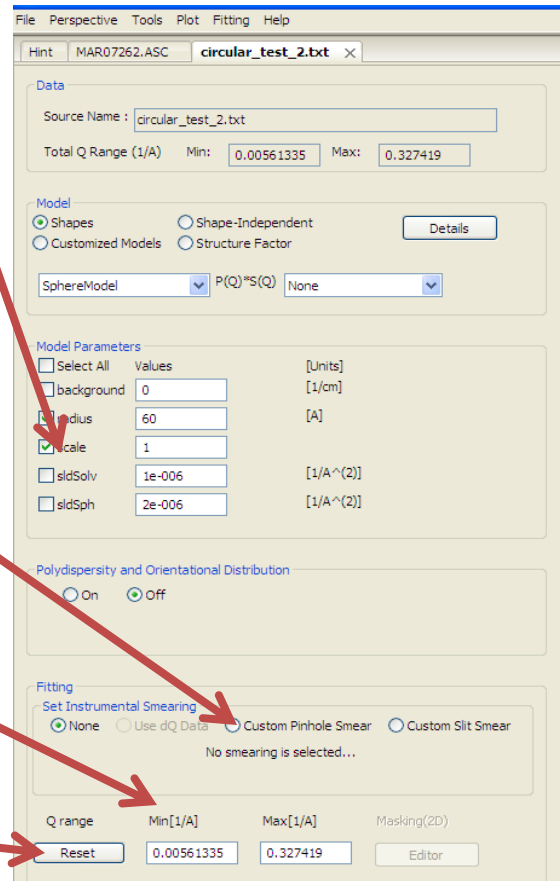

Fig. III-6

III-10. (Optional) You can switch Simple Fit (Scipy) or Complex Fit (Park) fitting engine by selecting or deselecting "Park" in the Fitting menu (Fig. III-7).

   *Note that the simple fit uses Levenberg–Marquardt algorithm, while the complex fit employs MC to find a global minimum in chi2 space (longer run time).
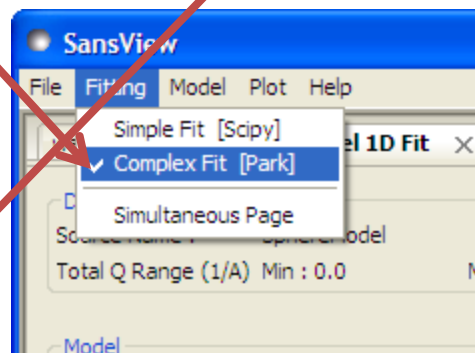
III-11. Click on the "Fit" button (Fig. III-6).

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).
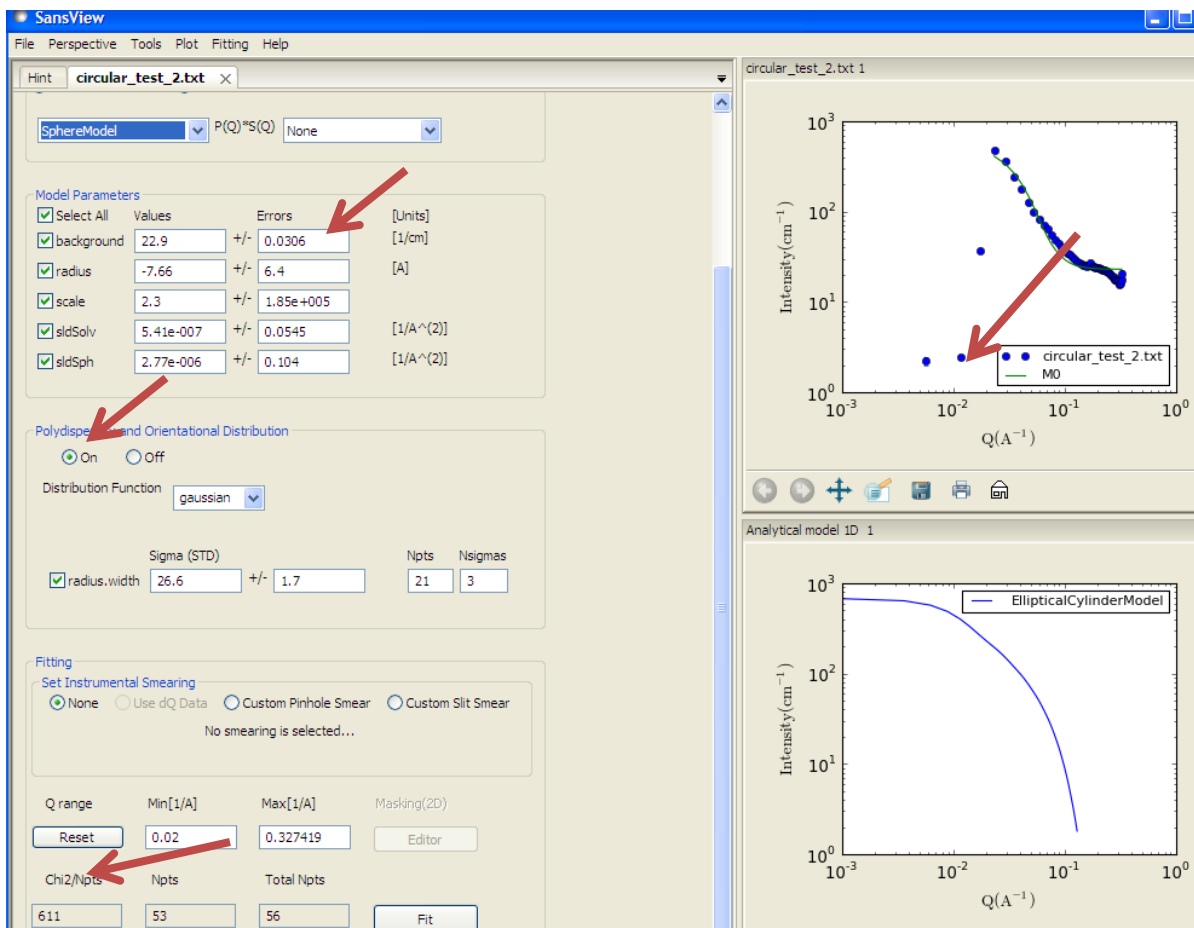
Fig. III-8

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. And Sigma is the STD of the distribution function which is fittable (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. 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.)
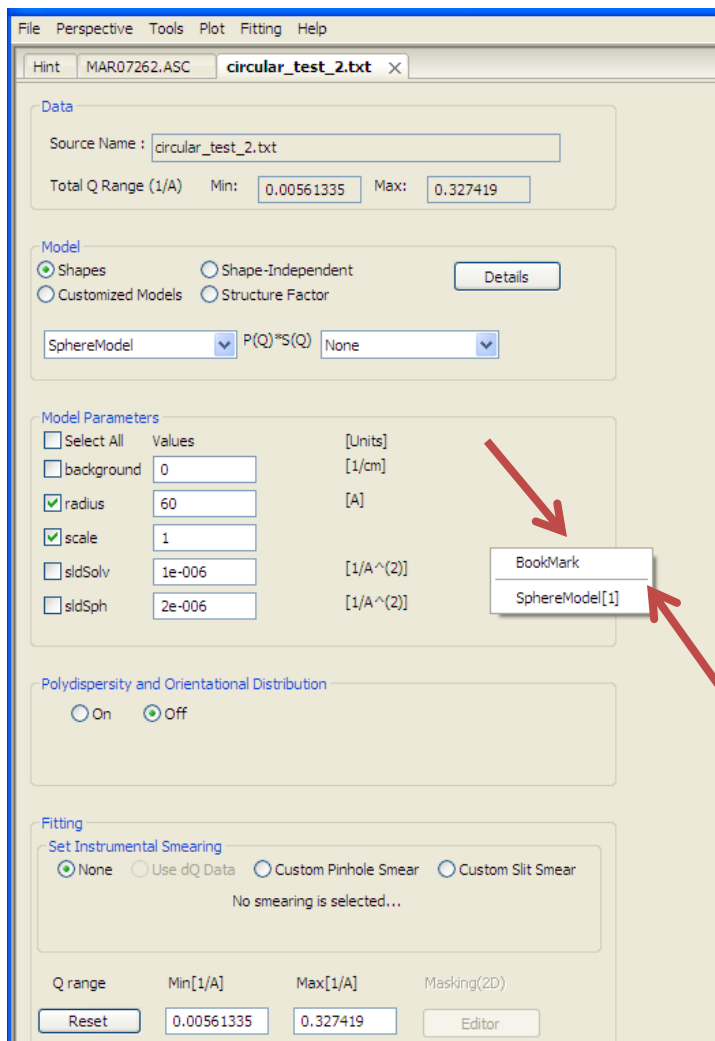

Fig. III-9

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-2) (Fig. III-10).
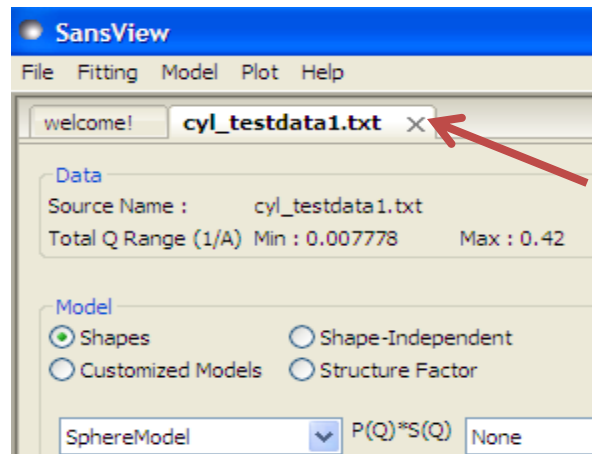
Fig. III-10

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, 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, simple 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.
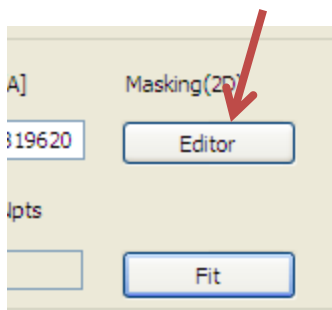
Fig. III-11
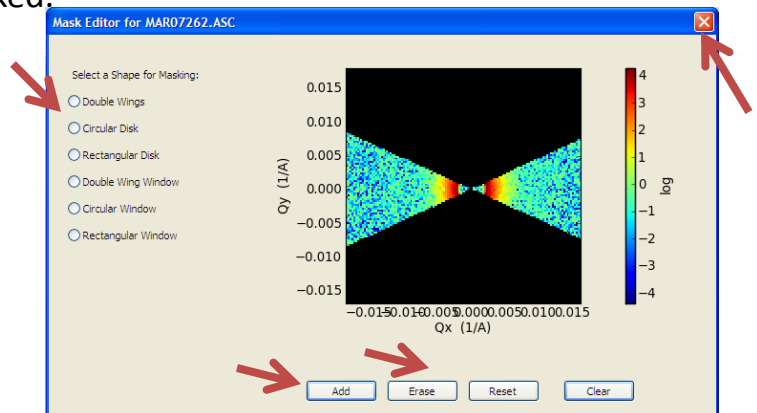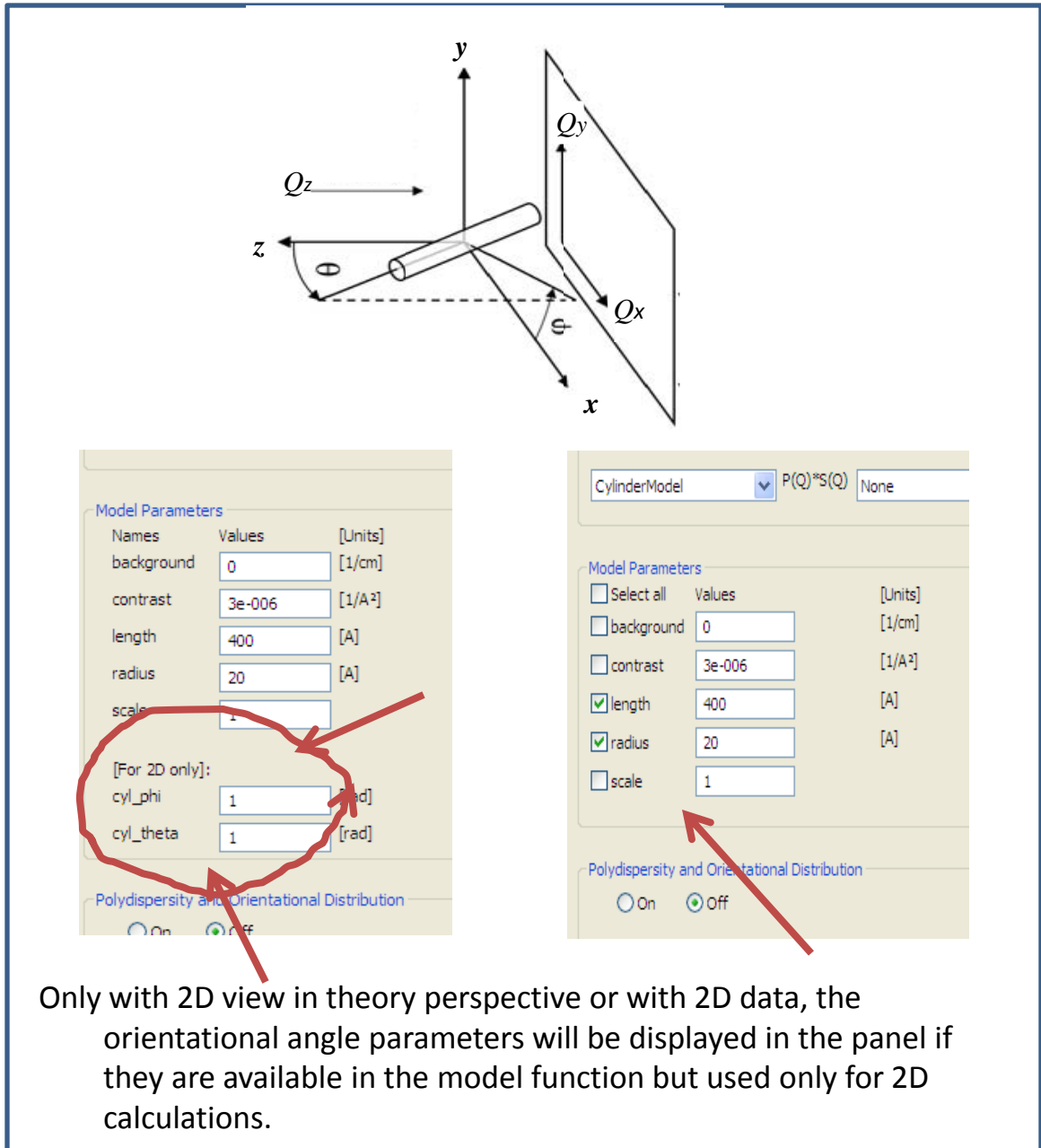
Fig. III-12

III-17 A geometry of the cylinder model (2D) is shown in (Fig. III-13). See model functions in the Help menu (of the SansView 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-1. The simultaneous fit uses the complex fit engine (Park).

IV-2. Repeat Step III-1 to III-6 to load at least two data set. Make sure that all adjustable parameters were checked including the parameters you want to constrain for the simultaneous fitting.

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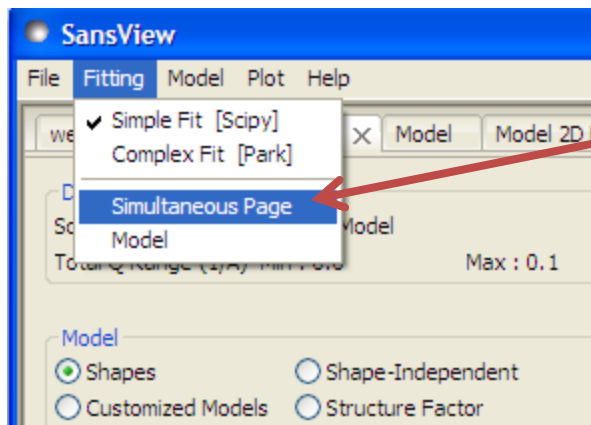
Fig. IV-1

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,...)
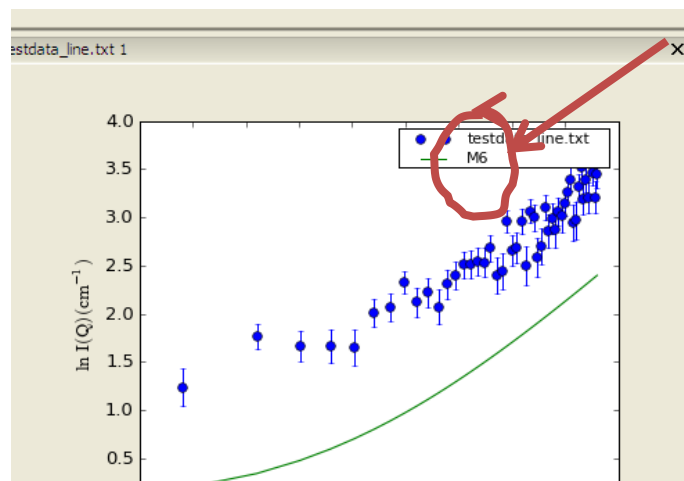
Fig. IV-2

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).

Fig. IV-3
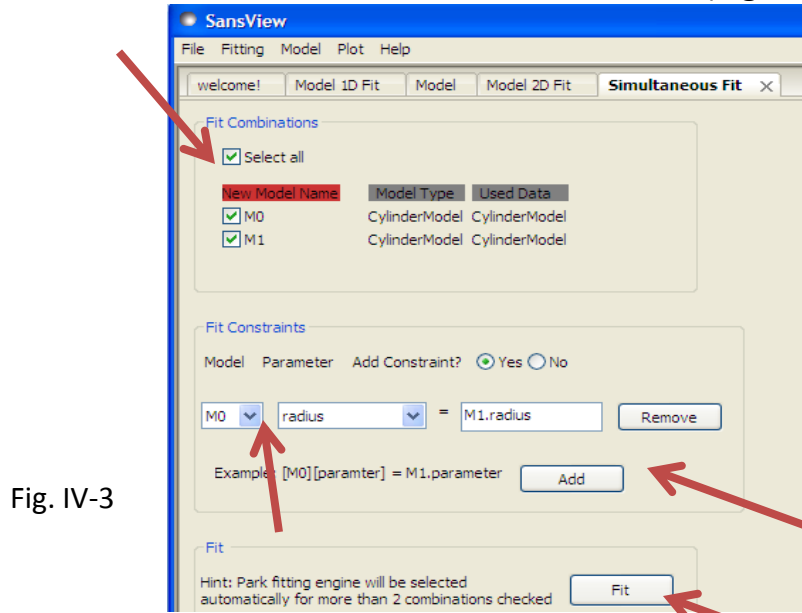
IV-6. Click on "Yes" to " Add constraints".

Select and type the constraints between two sets of fitting parmeters (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 on 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).
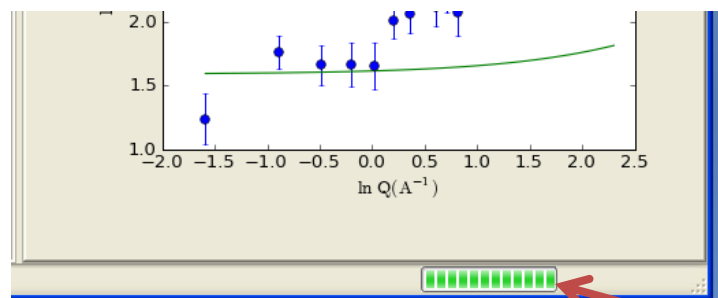
Fig. IV-4

IV-9. Then, go back to the Fit panels of the data, 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.
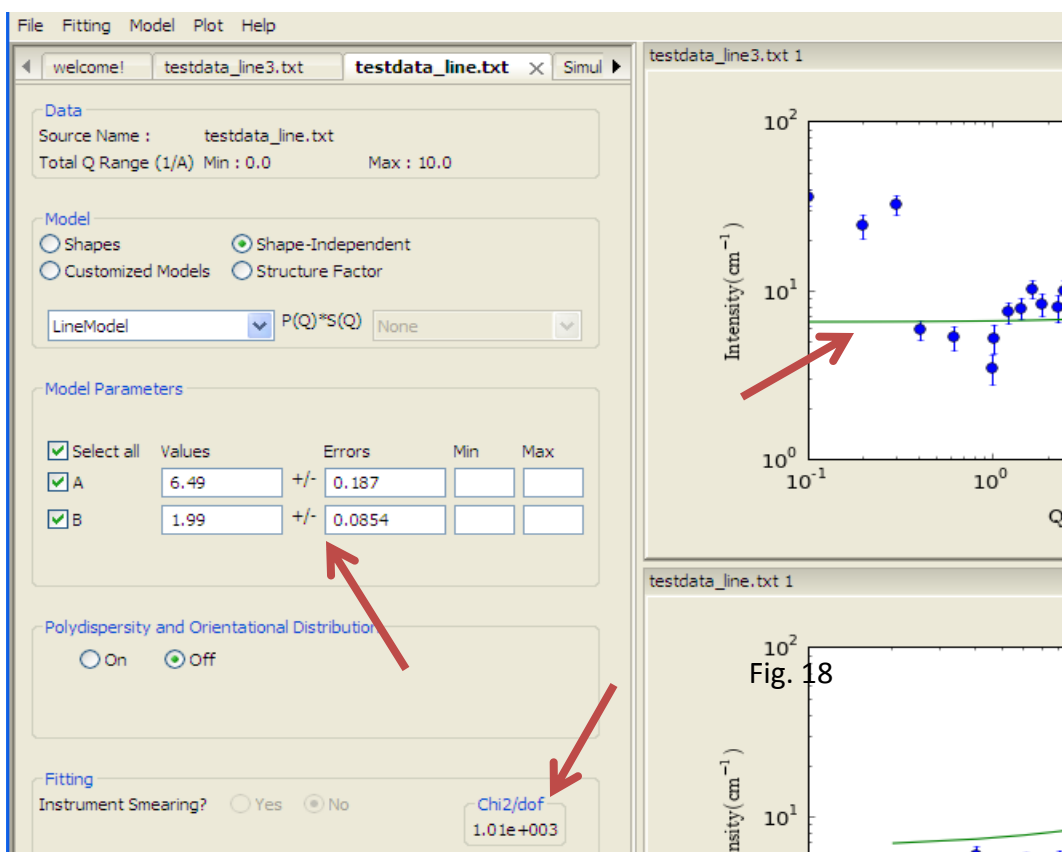
Fig. IV-5

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. Model calculation w/o data (Theory)

V-1. Click on 'Theory' in the 'Perspectives' menu (Fig. V-1). It will open a new panel where a model can be selected (Fig. V-2).
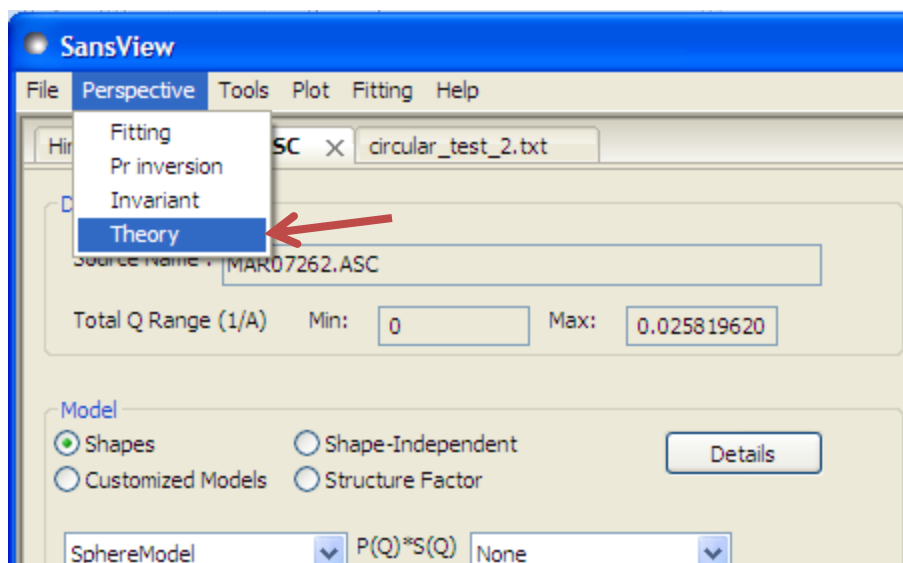
Fig. V-1

V-2. In the model panel, user 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. V-2).
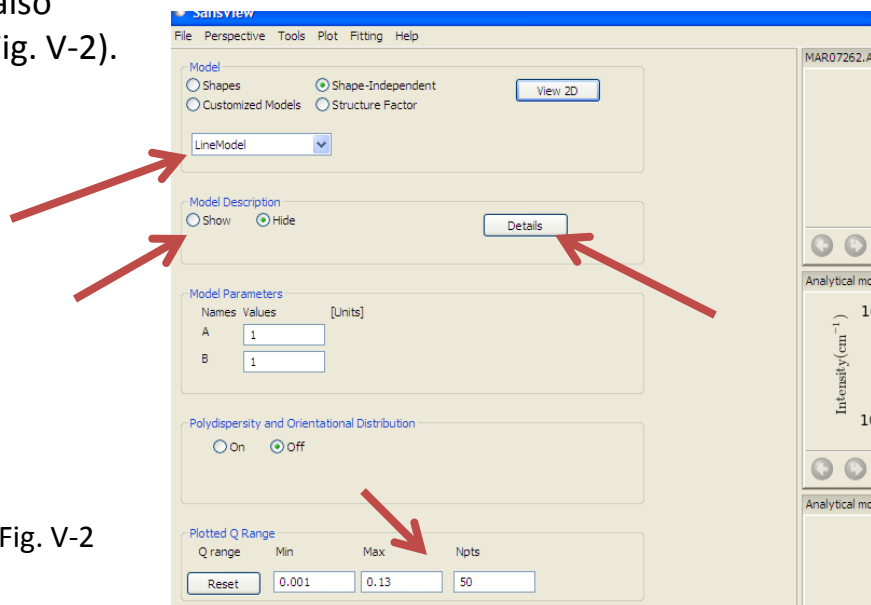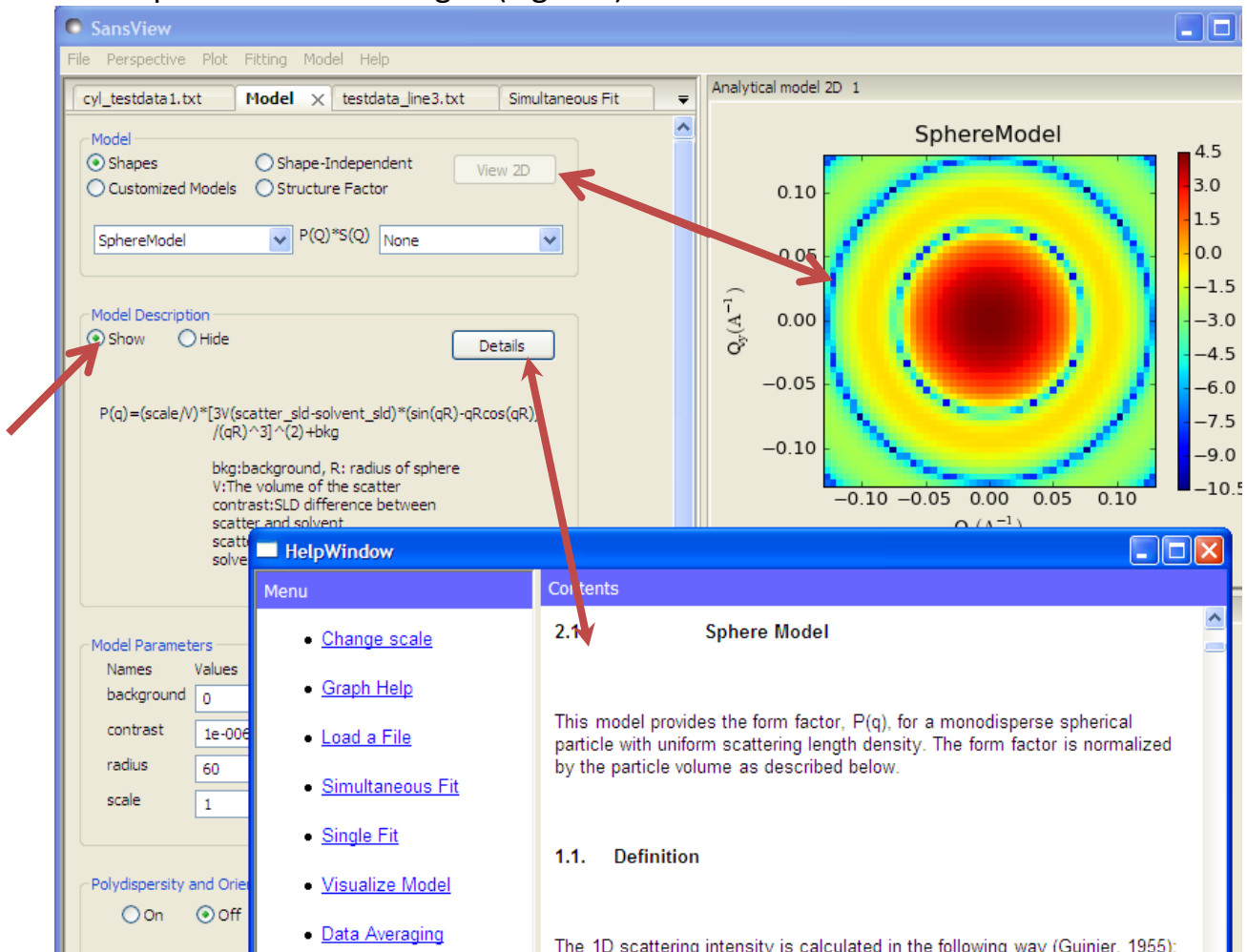
Fig. V-2

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

Fig. V-3

V-4. User can reset 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 also can be saved and open later from the Fitting
    menu in the menu bar or by right-clicking and selecting it from the panel.

VI. 2D averaging

VI-1. Once user loaded a 2D data or 2D model plot panel, 2D averaging is ready to go.

VI-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.
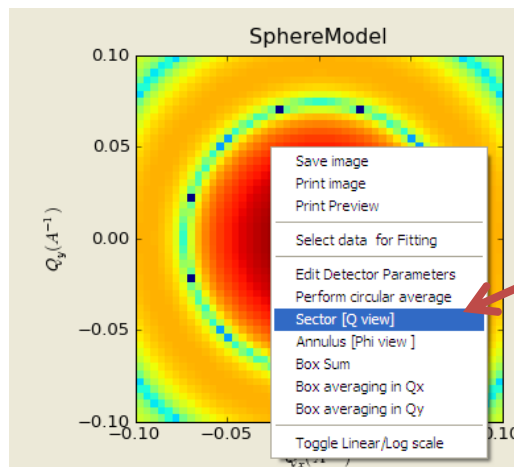
Fig. VI-1

VI-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.

VI-4. In some case, the error may interrupt to see the pattern of the averaged 1D plot. Right-click on the highlighted 1D plot and choose "hide error bars".
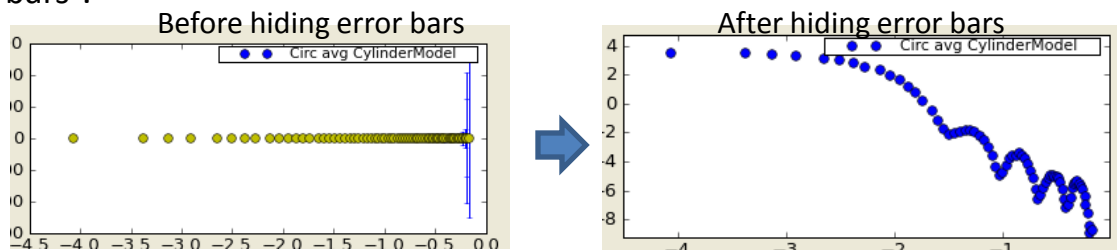
Fig. VI-2

VI. 2D average (continued)

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

Sector average   Annulus average   Box average (Qx or Qy)

Boxsum (Integration over the area)   Circular average for whole area
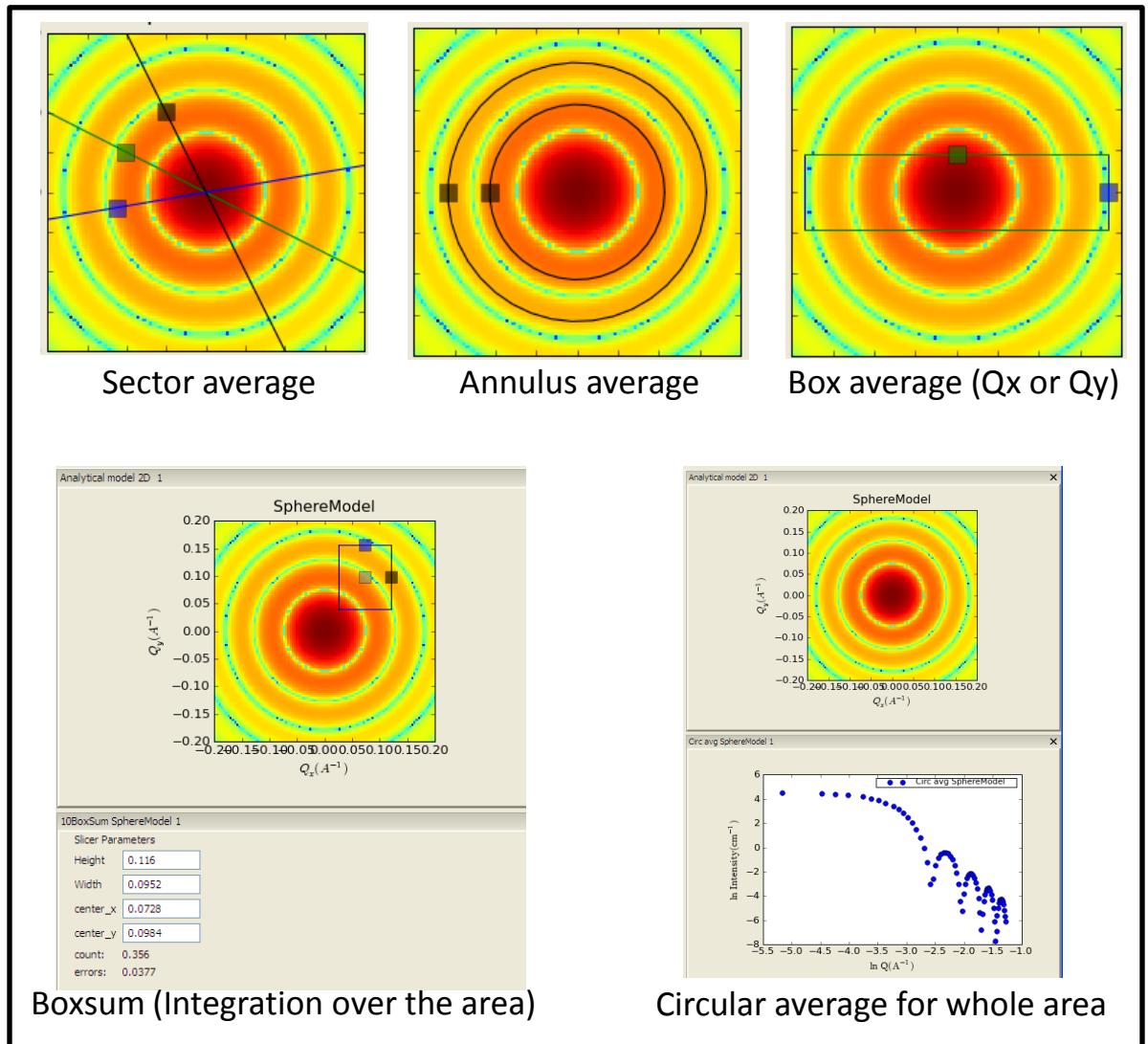
Fig. VI-3

VII. Save data and print images and plots

VII-1. Currently saving an image or a plot panel 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. VII-1). Method 2: Click on the icon at the bottom of the plots.
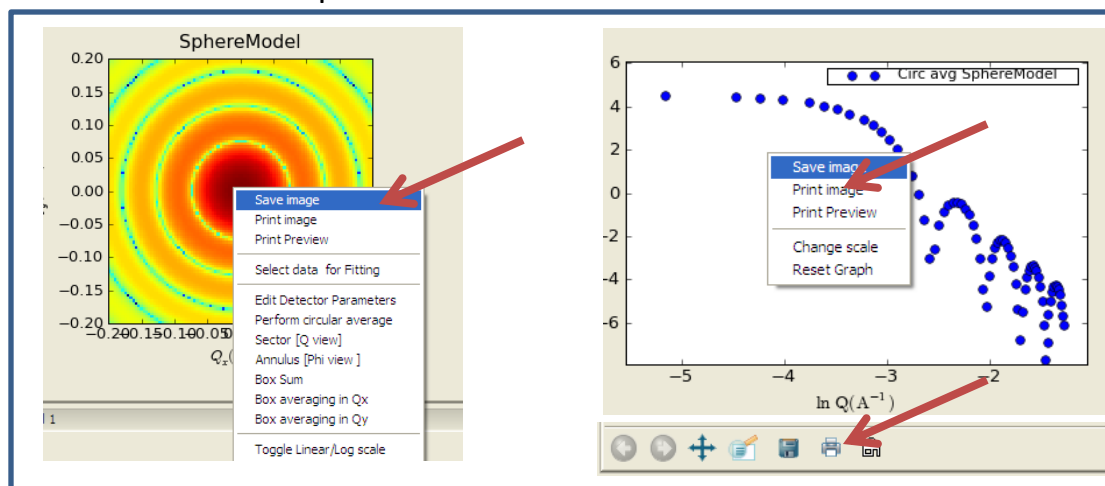
Fig.VII-1

VII-2. 1 D data in the plot can be saved in the formats of txt and CanSAS xml. 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" (Fig. VII-2).
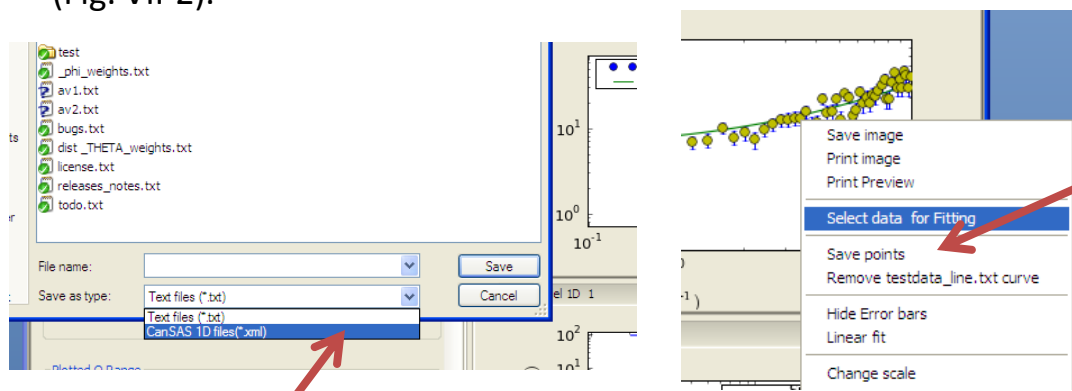
Fig. VII-2

VIII. 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 show how to switch between Fitting (or model
calculations) and Pr inversion.**

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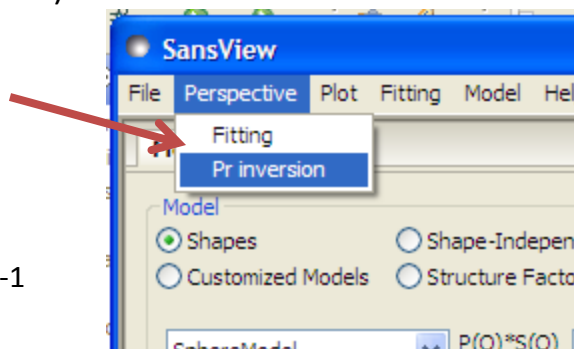
Fig. VIII-1

VIII-2. If you have a data plot open, locate your mouse to the plot to
highlight (yellow). On right-clicking, choose 'compute P(r)' **to load the data**
for Pr inversion. Once the data loaded for Pr inversion, the data file name
will be displayed in the text box named 'Data'. If you don't have data
open, follow the steps in Sec. I-1 and I-2 to open your data first.
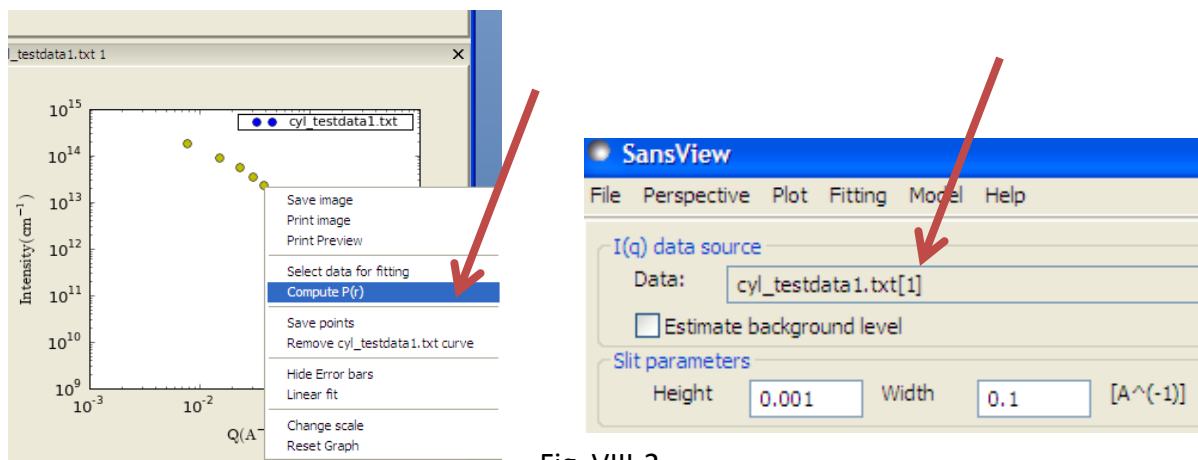
Fig. VIII-2

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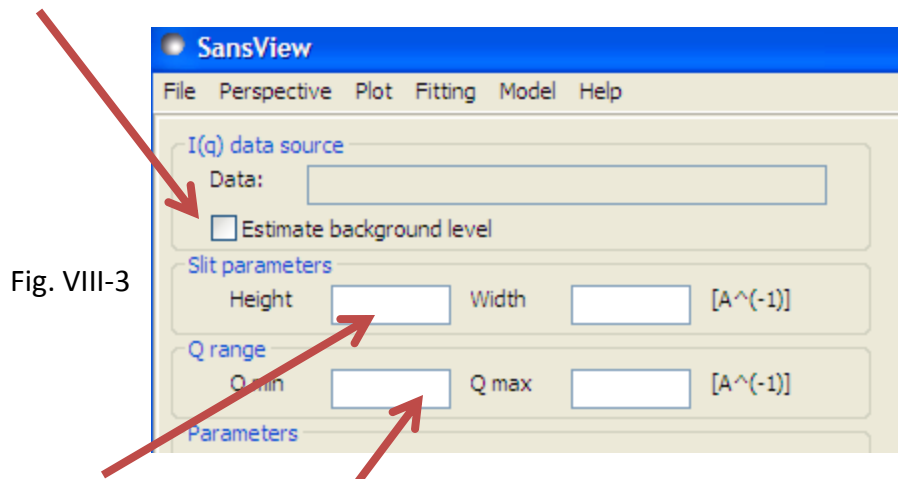
Fig. VIII-3

VIII-4. **Slit smearing:** By typing slit height and/or width (in 1/A), you can include the smearing effect to the calculations. When smearing is included, both of the results with and without the smearing effect will be displayed.

VIII-5. **Q range:** Q range for the I(q) may be specify in the Q min and Q max text boxes.

VIII-6. **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.

VIII-7. **Input parameters:**
1) number of terms: number of terms in the expansion.
2) Regularization constant: α parameter of the regularization term.
3) Max distance: maxmum distance in the any two points in the system.

Fig. VIII-4

VIII-8. **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 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.

VIII-9. **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. VIII-5

VIII-10. **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.

VIII-11. **Results:** Once the p(r) distribution has be computed, the I(Q) corresponding to the Fourier transform of that distribution is shown and compared to the input data.

VIII. Pr inversion (continued)

VIII-12. **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.
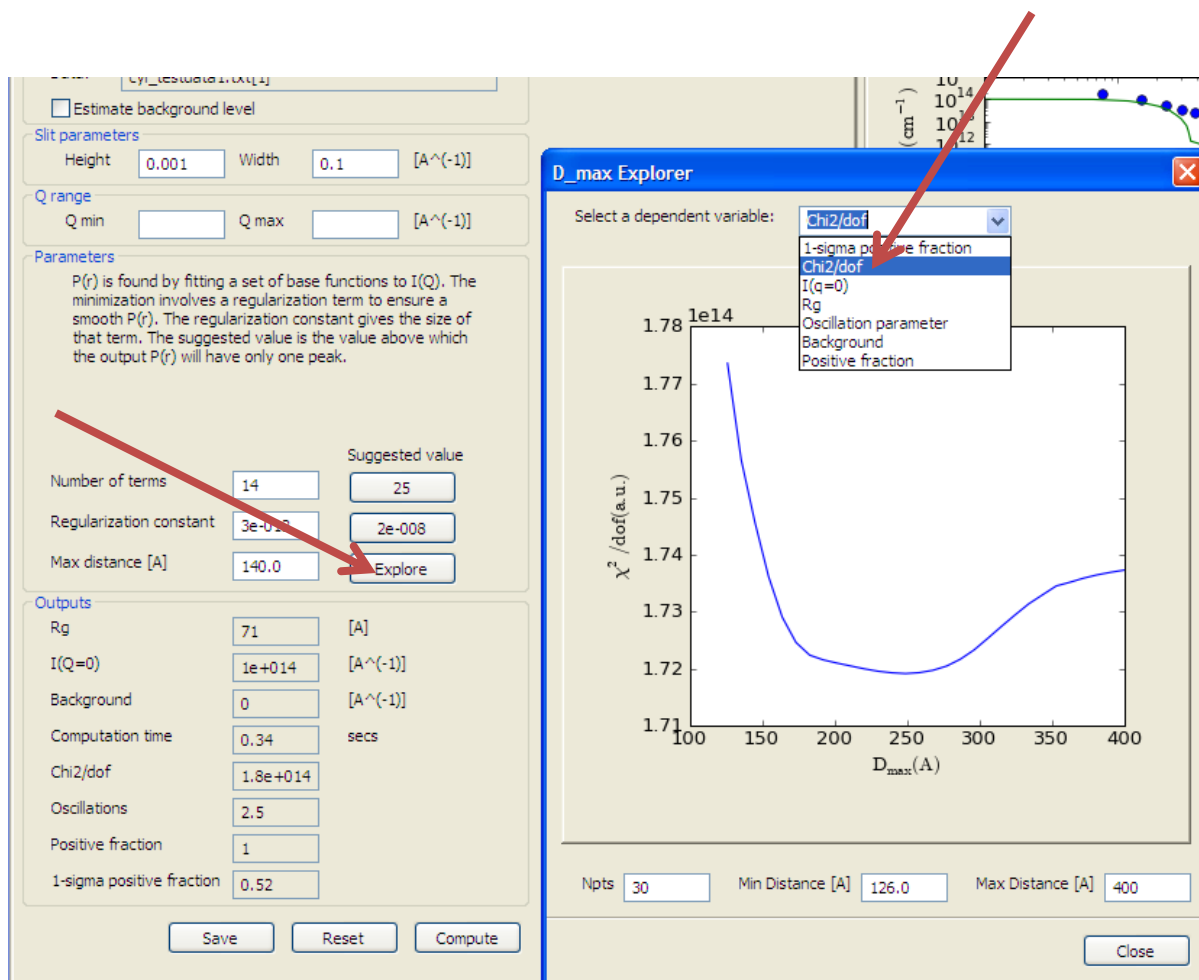
Fig. VIII-6

IX-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, there usually have 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 low q range and at 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/

IX -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 be 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.
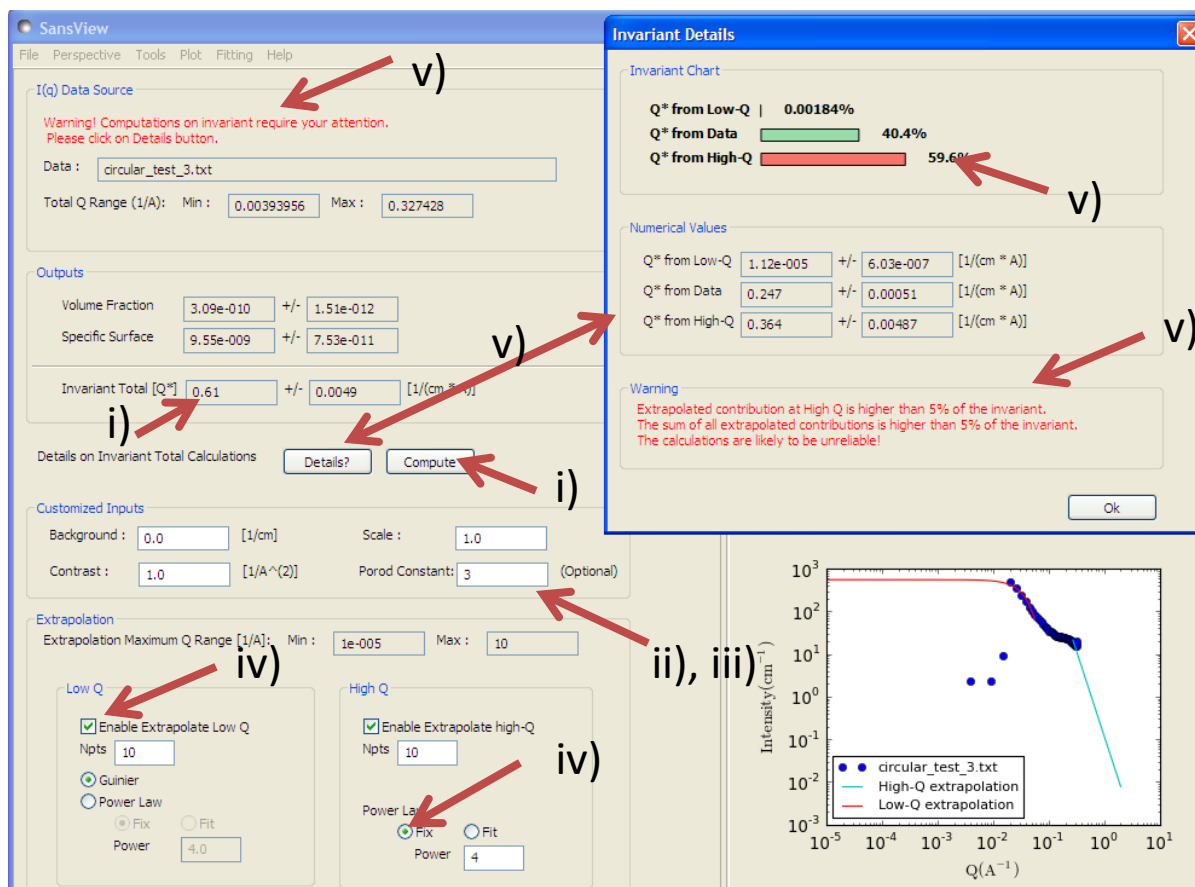
Fig. IX-1

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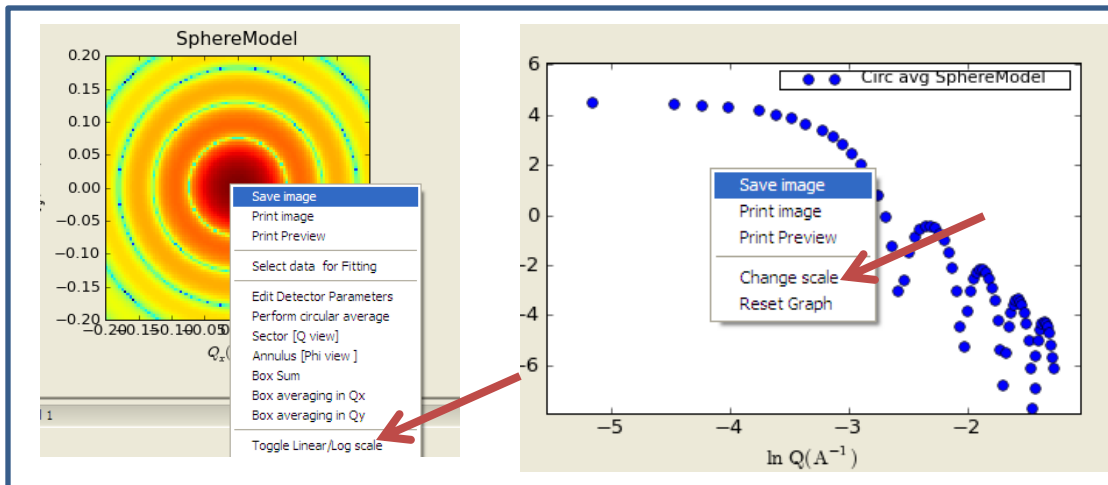
Fig. X-1

X-2. Close an open plot panels: All plot panels can be closed by clicking on 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. X-2).
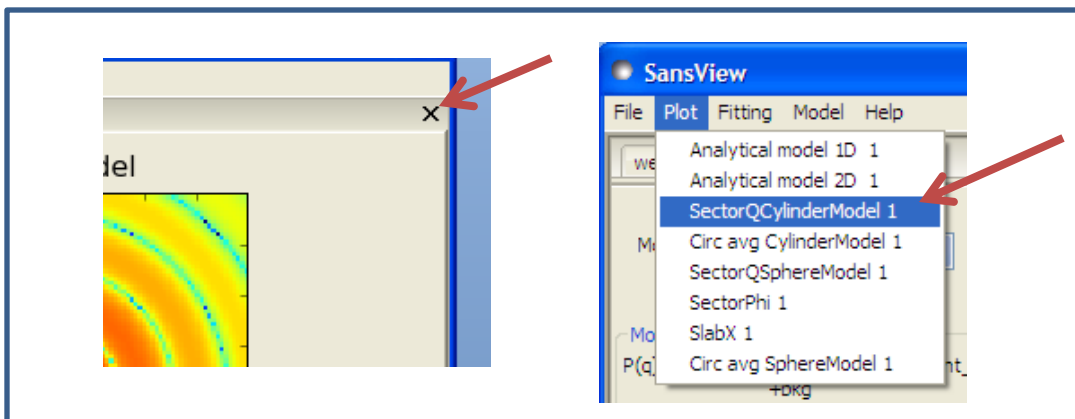
Fig. X-2

X. Miscellaneous (Continued)

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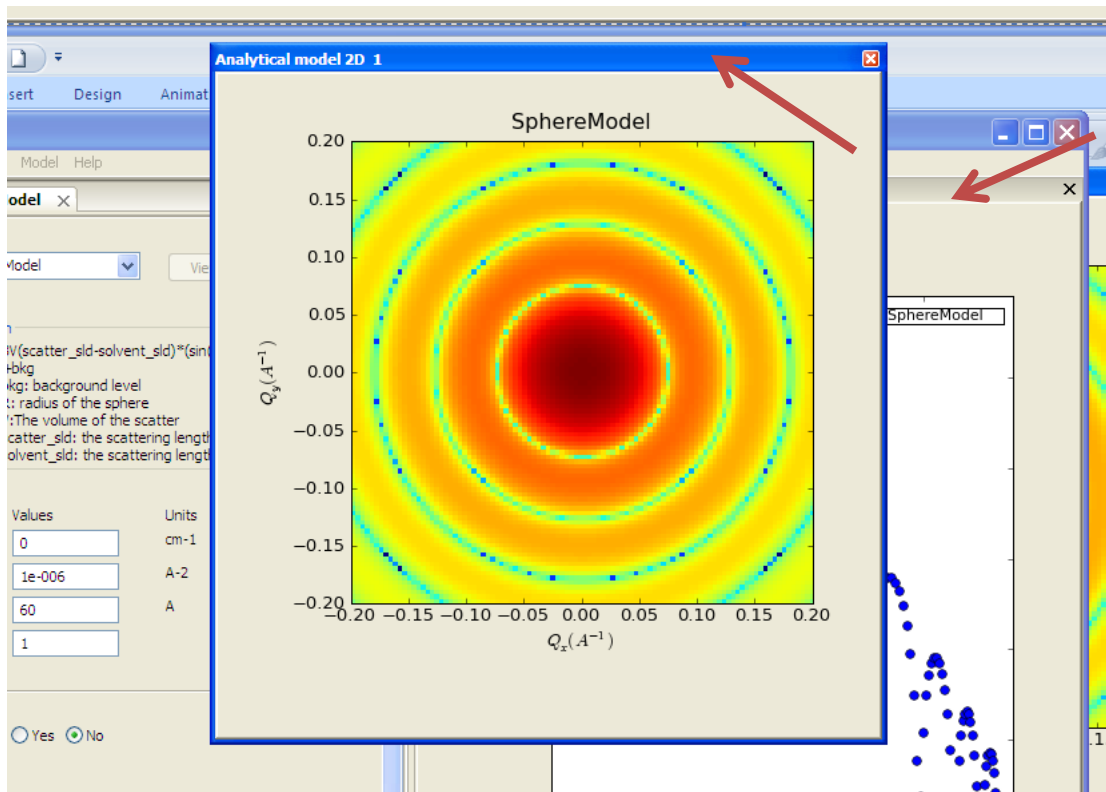
Fig.X-3

X-4. Changing color map of a 2D image (Fig. X-4); Open the context menu by right-clicking on the image plot. Select "Edit detector parameters ". Type integer numbers (non zero) in the box. If no number (no space) is 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. X-4).
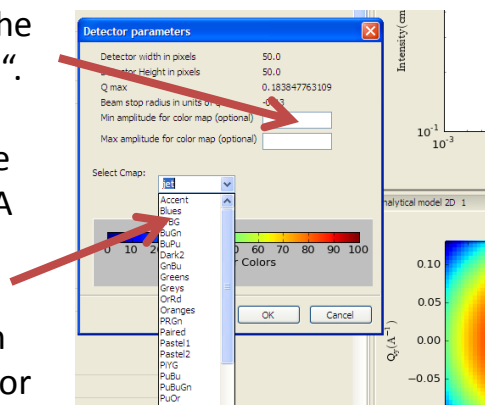
Fig.X-4

X. Miscellaneous (Continued)

X-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. X-5).
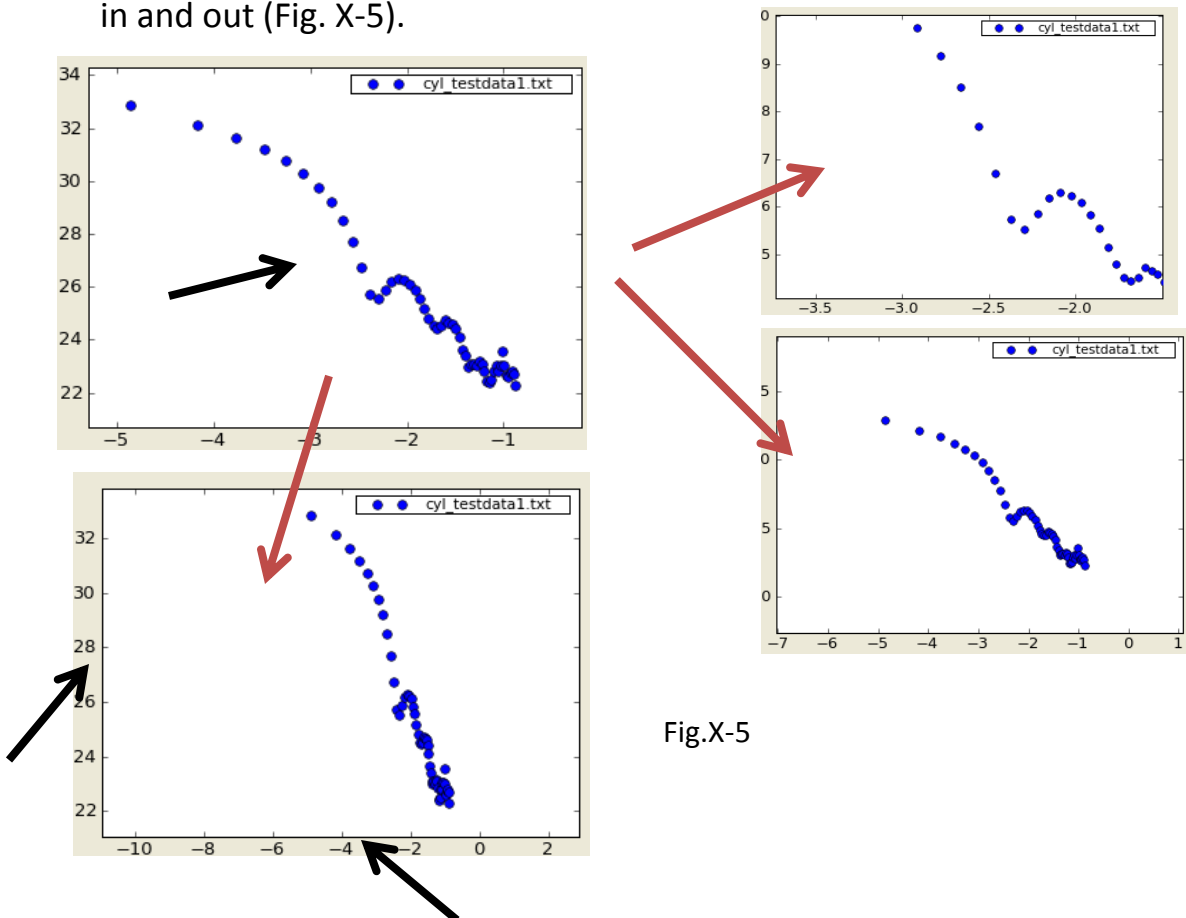
Fig.X-5

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

X-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.

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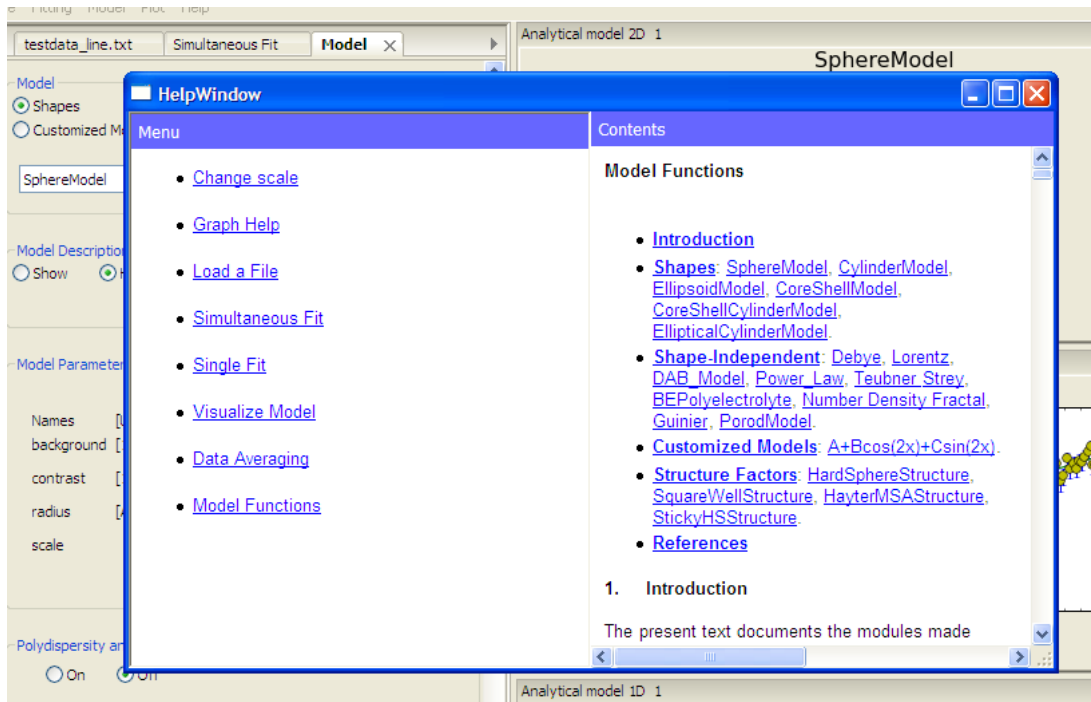
Fig.X-6

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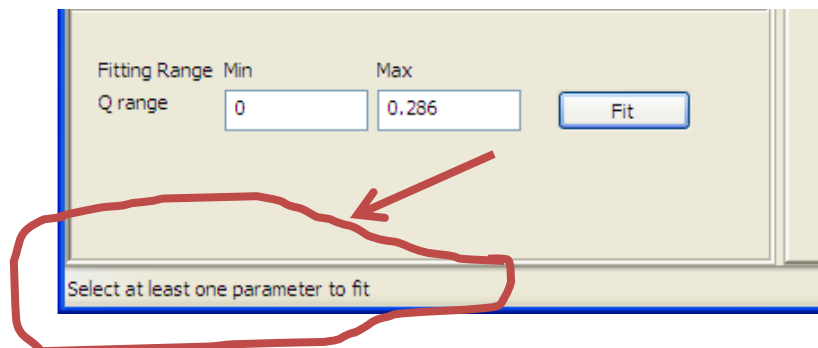
Fig.X-7

X-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.
   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 SansView folder (See page 4 and Appendix: User model documentation).

X-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: Users can define their own model functions by modifying an example pyhton file in the "plugins" folder inside of the SansView 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.

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

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

A) We use the *Gaussian, Lognormal, or Schulz* distribution function (where width =Sigma (STD), 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. The sigma is fittable and its unit is the same as the host parameter while others are unitless. Another way of defining the sigma is " the polydispersity multiplied by the value of the parameter for the dispersion".

B) Using a customized model:

Users can make two columns of a distribution function, and open the functional data file from a fitting panel with polydispersity ON. The file should includes two columns of data where the first column is consistent with the values of the parameter and the 2nd column is for weighting factors. (Note that this user data will override the corresponding parameter value (eg., radius) so that the parameter will become no longer fittable.) An example of the user function is;

radian	weight
0.707	0.4
1.14	1
1.414	0.4

X-13. Customized models: Users can define their own model function in the plugin folder of the sansview folder. Take a look and modify the sample file in the folder, or create a new one. Then the model function will be show up under "Customized model" menu in the menu bar. See Appendix or the example files in the plugins folder of SansView folder for more details.

X-14. Append a data to graph (1d only): Follow the Chapter I-1 and -2, it will be asked that whether or not you want to append to the data. Say yes if you want to. (It will append the data in the highlighted (blue) plot). To highlight a plot just click on any where in the plot panel.
Note: Only one model plot per plot panel is currently available.

User Model Documentation

SansView has a plug-in mechanism that allows users to write their own models in python. Each user model is placed in the *plugins* folder of the SansView installation. For instance, on the default Windows installation, the user model files will be placed in
C:\Program Files\SansView-[version]\plugins

Note that the user may thus define any number of such special models. The content 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)
```

Notice the use of the *math* module in the function definition. The functions available through python's *math* module are documented in the python web site. Any number of user models can be defined. They will appear in the customized model list after restarting the SansView.

The user models in the current version of SansView have a number of limitations:

1) SansView has to be restarted in order to see a new model appear in the Model menu. Similarly, any change in the model will require restarting SansView to be effective. Work is currently planned to allow live changes of the models.

2) Polydispersity is not currently available for user models. This feature is currently under development.

3) Since they are coded in python, user models can be slower to use. Contact the DANSE team if you would like to incorporate your model in the DANSE framework. The DANSE team will be able to port your model to a faster implementation.