

SansView 1.0



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 1.0 Build: 1.0 (c) 2009, University of Tennessee

*If you use this program to do productive scientific research that leads to publication, we ask that you acknowledge use of the program by citing the following paper in your publication: "This work benefited from DANSE software developed under NSF award DMR-0520547."

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





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Introduction

New application for SANS oriented system modeling and data analysis. Oct. 1, 2009: version 0.1 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.

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 all the data with dQ (or dQl, dQw) data given.
- 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.
- Plug-in mechanism for data readers.
- User sets Qrange (Qmin and Qmax) for both 1D and 2D data for fitting and modeling.
- 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





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How to install

Go to our DANSE Small Angle Neutron Scattering Project web page, 1. http://danse.chem.utk.edu/index.html and clicking on the "SansView 1.0" will point to the release page

where the windows installer can be downloaded.

- Also, SansView tutorial can be http://danse.chem.utk.edu/index.html found at the same site. itarted 脑 Latest Headlines 📄 Customize Links **DANSE Small Angle Neutron S** University of Tennessee home mission links / downloads contacts Currently supported only on Windows : Windows 2 (Notes for Wile (Linux/Mac) user.) Download links: The Department of Chemistry at UT is involved in a five-year s data reduction, data analysis, modeling and simulation. Windows installer SansView-1.0 Tutorial: SansView 1.0 tutorial (pdf format) News: · Documentation: Description of the model functions (Oct 09: SansView 1.0 is now available. Previous versions: July 09: PrView 0.3 is now available. SansView-0.9.0
 - Once "setupSansView-1.0.exe is downloaded, open the installer and 2. follow the steps Setup - SansView-1.0 as directed.







How to install (continued)

- 4
- Once the SansView is installed, some sample 1D and 2D data can be found inside the "test" folder in the SansView-1.0 folder. This allows you to follow this tutorial session without having your own data





4. The "plugins" folder also includes two example python files (testmodel_2.py and testmodel.py) for users to 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 (page 31) or the example files in the plugins folder of the SansView folder for more details.

-	
10	
2	Test plug-in model
3	
4	from sans.models.pluginmodel import Model1DPlugin
5	
6	import math
7	
8	
9	# Your model HAS to be called Model
109	class Model (Model1DPlugin):
110	""" Class that evaluates a $\cos(x)$ [3].
12	"""
13	
14	ii Name of the model
15	name = "AltBone (2011/Cein(201"
16	
176	def init (colf).
10	Uti(STI).
10	
20	Modelibridgininit(Sell, name- Sell, name)
20	
21	** Parameters definition and definits
22	seir.params = ()
23	self.params['A'] = 0.0
24	seif.params['B'] = 1.0
25	self.params['C'] = 0.0
26	
27	## Parameter details [units, man, max]
28	self.details = {}
29	self.details['A'] = ['', -1e16, 1e16]
30	<pre>self.details['B'] = ['', -le16, le16]</pre>
31	<pre>self.details['C'] = ['', -1e16, 1e16]</pre>
32	
336	<pre>def function(self, x = 0.0):</pre>
340	""" Evaluate the model
35	<pre>@param x: input x</pre>
36	Greturn: function value
37	
38	return self.params['A']+self.params['B']*math. s(2.0*x)+self.params['C']*math.sin(2_0*x)
39	



I. Loading 1D and 2D data

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



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

(You can choose either 1D or 2D data in this way). File extension types that can be loaded are ASCII (text), CANSASxml, ASC (2D), sans, pr files.

The format of ASCII files should consist of 2 to 4 columns of Q, Intensity, (dI, dQ) in order where dQ is the instrumental uncertainty of Q and assumed to be originated by pinhole geometry.



Fig. 2













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

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II-1. Highlight the data in the plot by locating your mouse pointer to the plot symbols (Fig. 4). (For 2D, right click on 2D data image plot.)



II-2. After right clicking on the highlighted data, you select "Select data for fitting" (Fig. 5).*Same for 2D from now.



II-3. Then, you have a fitting panel for the data you have chosen, on the left side (Fig. 6).







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II. Data fitting : 1D and 2D data; Single fit (continued)

II-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. 7)



Fig. 7

II-5. Play with the parameter values so that you have a model calculated (green) curve as closed to the data as possible (Fig. 8).



Fig. 8





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II-6. Select parameters to fit by clicking on the check box. (Fig. 9).	SansView File Perspective Plot Fitting Model Help cyl_testdata1.txt × Data Source Name : cyl_testdata1.txt Total Q Range (1/A) Min : 0.007778 Max : 0.42 Model Shapes Customized Models Shape-Independent Details Customized Model V P(Q)*S(Q) Marco V
II-7. Adjust Q range of data for fitting (optional) (Fig. 9).	Model Parameters [Units] Select all Values [Units] background 0 [1/cm] contrast 3e-006 [1/A ²] V length 400 [A] radius 20 scale 1
II-8. Q range can be reset to the default values by clicking the reset button (Fig. 9).	Polydispersity and Orientational Distribution On Off Fitting Instrument Smealing? Yes No Chi2/dof 7.55e+012 Q range Min Max Reset 0.007778 0.42 Fit Fig. 9

- II-9. (Optional) You can switch Simple Fit (Scipy) or Complex Fit (Park) fitting engine by selecting or deselecting "Park" in the Fitting menu (Fig. 10).
 - *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).
 - II-10. Click on the "Fit" button (Fig. 9).

Kile	Fitting	Model	Plot	Help		
	Simp Com	le Fit [S plex Fit	cipy] [Park]	2	1D Fit	×
C Sc	Simu	ltaneous	Page		del	
То	tal Q Ra	nge (1/A) Min	: 0.0		Μ





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II-10. 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. 11).



- Fig. 11
- II-11. If the fitting is not successful, you can play more with other model functions by choosing another model function (see Step II-4), or polydispersity parameters which will show up by clicking on "polydispersity" "yes" check box . (Fig. 11): For polydispersity parameters, good values of Nsigmas are between 3 and 5, where Nsigma refers to x-distance of Gaussian distribution to be considered in the unit of sigma (See VII-10 for more details).





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II-12. 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. 12). (Note that once the bookmark is recalled, you may loose the previous panel that you were working on unless it was already bookmarked.)

SansView	
File Perspective Plot Fitting Model Help	
cyl_testdata1.txt ×	
Data Source Name : cyl_testdata1.txt Total Q Range (1/A) Min : 0.007778 Max : 0.42 Model Shapes Shape-Independent Ocustomized Models Structure Factor CylinderModel P(Q)*S(Q) None	
Model Parameters Select all Values background 0 contrast 3e-006 [1/A ²] length 400 Y radius 20 scale 1	Bookmark M0[1]
Polydispersity and Orientational Distribution	
Fitting Instrument Smearing? Yes No Chi2/dof 7.55e+012	
Q range Min Max	
Reset 0.007778 0.42 Fit	





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II-12. You can also try instrumental smearing by clicking on "On" button only if users provide dQ (, dQl, or dQw) in the forth column of their data (Fig. 13).

🕑 length	400	[A]	
🗸 radius	20	[A]	
scale	1		
Polydisperarty	and Orientational Distrib	ution	
On	⊙ Off		



II-13. It is possible that the fitting results return with an error, especially when the model does 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 open a new fitting panel by (Step II-2) (Fig. 14).

SansView	
File Fitting Model Plot Help	
welcome! cyl_testdata1.txt X	
Data	
Source Name : cyl_testdata1.txt	
Total Q Range (1/A) Min : 0.007778 Max : 0.42	
Model	
 Shapes Shape-Independent 	
O Customized Models O Structure Factor	
	F '. 4
SphereModel V P(Q)*S(Q) None	⊦ıg. 1





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II-14 A geometry of the cylinder model (2D) is shown in (Fig. 15). See model functions in the Help menu (of the SansView Application) for other models.







III. Data fitting; Simultaneous fit

- III-1. The simultaneous fit uses the complex fit engine (Park).
- III-2. Repeat Step II-1 to II-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.
- III-3. Open the simultaneous fit panel by clicking on "Simultaneous" in the Fitting menu (Fig. 16). The complex fitting engine will be set automatically.



Fig. 16

III-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,...)







III. Data fitting; Simultaneous fit (continued)

III-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. 18).

File Fitting Model Plot Help
welcome! Model 1D Fit Model Model 2D Fit Simultaneous Fit ×
Fit Combinations Select all Mew Model Name Model Type Used Data Mo CylinderModel Cy
Fit Constraints Model Parameter Add Constraint? • Yes No
M0 v radius v = M1.radius Remove Example [M0][paramter] = M1.parameter Add
Fit Hint: Park fitting engine will be selected automatically for more than 2 combinations checked Fit

III-6. Click on "Yes" to "Add constraints".

Fig.

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.

- III-7 Once all constraint setups are done, click on the Fit button to perform fit.
- III-8. When the fitting is finished, the progress bar at the bottom of window will disappear (Fig.19).







III. Data fitting; Simultaneous fit (continued)

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III-9. Then, go back to the Fit panels of the data, and inspect the results (Fig. 20). Note: Currently the errors of constrained parameters will not be displayed well, but can be calculated by applying the equation of your constraints.

ile Fitting Model Plo	t Help				
welcome! testdat	ta_line3.txt tes	stdata_line.txt	× Simul ►	testdata_line3.txt 1	
Data Source Name : te Total Q Range (1/A) M	estdata_line.txt in : 0.0 M	lax: 10.0		10 ²	
Model Shapes Customized Models	Shape-Independ Structure Factor P(Q)*S(Q)	dent r None	•	$\ln (cm^{-1})$	* * ++** * * *
Model Parameters Select all Values A 6.49 B 1.99	Errors +/- 0.187 +/- 0.085	Min	Max	10 ⁰	10 ⁰
Polydispersity and Orie	entational Distribution			testdata_line.txt 1	
Fitting Instrument Smearing?	⊖Yes ⑧No	Chi2/ 1.01e	dof +003	Fig. 18	A .

Fig. 20

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





IV. Model calculation

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IV-1. Click on the model in the "Model" menu bar (Fig. 21). It will open a model panel as well as a plot panel (Fig. 22).

SansVie	w		
File Fitting	Model Plot Help		
welcome Data Source Nar Total Q Ra Model	Shapes Shape-Independent Structure Factors Customized Models P(Q)*S(Q)	 SphereModel CylinderModel CoreShellModel CoreShellCylinderModel EllipticalCylinderModel EllipsoidModel 	te
Custom Custom LineMode	Shape-In ized Models Structur P(Q) ameters	ndependent e Factor *S(Q) None	
Select	ali values	Errors Min Max	

Fig. 21

IV-2. In the model panel, the model description and parameter inputs are provided. User can also change model function by selecting another from "Model" combo-box. Also, Q range and the number of points of the

calculation can be	SansView	
	File Fitting Model Plot Help	
adjusted by users	testdata_line.txt Simultaneous Fit Model ×	▶ testdata_line3.txt 1
(Fig.22).	Model Shapes Shape-Independent O Customized Models Structure Factor LineModel ♥ P(Q) *S(Q) Model Description Show Hide Details	10 ²
	Model Parameters Names Values A 1 B 1	Analytical model 1D 1 10 ¹ (
	Polydispersity and Orientational Distribution	10 ⁰
Fig. 22	Plotted Q Range Min Max Npts Q range 0 0.1 50	10 ²





IV. Model calculation (continued)

IV-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. 23).



IV-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.





V. 2D averaging

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



- V-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.
- V-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".







V. 2D average (continued)

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









VI. Save data and print images and plots

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VI-1. Currently saving an image or a plot panel is supported in png format. 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. 27).



- Fig. 27
- VI-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. 28).







VII. 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

http://danse.chem.utk.edu/downloads/PrView0.2_tutorial.pe or http://danse.chem.utk.edu/prview.html

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

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



VII-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 page 5 (Chapter I) to open your data first.



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VII. Pr inversion (continued)

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

	File Perspective Plot Fitting Model Help
	I(q) data source Data: Estimate background level
Fig. 31	Slit parameters Height Width [A^(-1)]
	Q range Q max [A^(-1)]

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

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

VII-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.

VII-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. 32

Parameters P(r) is found by fitting minimization involves a	a set of base f regularization	unctions to I(Q). The term to ensure a
smooth P(r). The regu that term. The sugges the output P(r) will ha	larization const sted value is the ve only one pea	ant gives the size of e value above which ak.
		Suggested value
Number of terms	14	25
Regularization constant	3e-012	2e-008
Max distance [A]	140.0	Explore
Outputs		
Rg	71	[A]





VII. Pr inversion (continued)

VII-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

Outputs

Its value is 1.1 for a spherical system.

VII-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.



	Rg	71	[A]
n	I(Q=0)	1e+014	[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

VII-10. P(r) plot: Right clicking on the highlighted data points by 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.

VII-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.





VII. Pr inversion (continued)

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VII-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.

lit parameters			
Height 0.001 Width	0.1 [A^(-1)]	D_max Explorer	
2 range Q min Q max	[A^(-1)]	Select a dependent variable: Chi2/do	
arameters P(r) is found by fitting a set of minimization involves a regularization involves a regularization that term. The suggested value the output P(r) will have only of the output P(r) will hav	base functions to I(Q). The zation term to ensure a constant gives the size of e is the value above which ne peak. Suggested value 25 2e-008 Explore [A] 4 [A^(-1)] [A^(-1)] secs	1.78 1e14 1.78 1e14 1.77 - 1.76 - 1.75 - 1.75 - 1.75 - 1.74 - 1.73 - 1.72 - 1.71 - 1.72 - 1.72 - 1.72 - 1.72 - 1.72 - 1.73 - 1.72 - 1.72 - 1.72 - 1.73 - 1.72 - 1.72 - 1.72 - 1.72 - 1.73 - 1.72 - 1.72 - 1.72 - 1.73 - 1.72 - 1.72 - 1.73 - 1.75 -	prove fraction
Oscillations 2.5			
Positive fraction			
1-sigma positive fraction 0.52		Npts 30 Min Distance [A]	126.0 Max Distance [A] 400

Fig. 34



VIII. Miscellaneous

VII-1. Change scales or toggle Linear/ Log.

Right-click on 1D, 2D plot. Select "Change scale" or "Toggle Linear/Log scale" (Fig. 35).





VII-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. 36).









VII-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. 37).



VII-4. Changing color map of a 2D image (Fig. 38); Open the context menu by right-clicking on the

image plot. Select "Edit detector parameters ". Type integer numbers (not 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 change the image plot. Note: This feature is still under construction, so use it with care. (Fig. 38).



Fig.38





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VII-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. 39).



- B) x- or y- axis separately; one-click in the plot panel , locate your pointer (black arrows in Fig. 39) somewhere between the axis line and label, and use the mouse roller to zoom in and out the axis as desired.
- VII-7. The data points or curve can also be dragged around by click-andholding within the plot range.





VII-5. Some Helps and tips are available within the SansView application. Select "Fitting help" or others in the "Help" menu. This will provide you instant help (Fig. 40).



Fig.40

VII-6. Simple tips and information will be displayed at the bottom line of the application whenever it is necessary (Fig. 41).







VII-7. Loadable data formats:

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, .sans
- b) 2D ASCII file should be from NIST IgorPro SANS reduction package and saved to the detector coordinates.
- C) Examples of data files are available in "test" folder inside the SansView-1.0 folder (See page 4 and Appendix: User model documentation on page 27 -29).

VII-8. 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, Teubner Strey.

C) Structure factors: square well, 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-1.0 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.

VII-9. Instrumental smearing is supported in fitting when your data includes dQ in its forth column.





VII-10. Polydispersity (1D and 2D) and orientational distribution (2D only) can be taken account for modeling and fitting.

A) We use the *Gaussian* distribution function (where width =Sigma (STD), Npts = number of points over the distribution, Nsigma = number * sigma (distance from the center to be covered)). Good values for Npts and Nsigma may be 7 to 21 and 2.5 to 3, respectively.

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	0.1

VII-11. 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 (page 31) or the example files in the plugins folder of SansView folder for more details.





IX. Appendix

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:

.....

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.

.....





VIII. Appendix (Continued)

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)





VIII. Appendix (Continued)

Notice the use of the *math* module in the function definition. The functions available through python's *math* module are documented on the <u>python web site</u>. Any number of user models can be defined at one time. They will automatically appear in SansView in the Model menu, under "Customized Models".

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.