PrView

version 0.2

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PrView is an application to perform P(r) inversion of SANS data. The technique used is based on P. Moore, J. Appl. Cryst. (1980) 13, 168-175.

What's new in version 0.2:

- Improved user interface.
- Automated estimate of the number of terms.
- I(q=0) and Rg are now outputs of the inversion.
- Slit smearing has been added.
- Constant background estimation.
- Functionality to compare p(r) output with data from a file.
- Functionality to change the number of p(r) points of the output dsitribution.

Roadmap:

PrView is a prototype application provided to the community to generate feedback. It is intentionally limited in scope and functionality, and 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

Contact us:

You can visit the PrView web page at: **http://danse.chem.utk.edu/prview.html**

For comments, feature requests and bug reports, you can write to us at **sansdanse@gmail.com**

The technique used is a modified version of the technique described in P. Moore, J. Appl. Cryst. (1980) 13, 168-175.

I(q) can be written in terms of p(r) as follows:

$$I(q) = \int p(r) \frac{\sin 2\pi rq}{2\pi rq} dr$$

To evaluate p(r), we write is as an expansion of in terms of base functions:

$$p(r) = \sum_{i=1}^{N} c_i \varphi_i(r) \qquad \text{where} \qquad \varphi_n(r) = 2r \sin(\pi rn/D_{max})$$

We can then re-write I(q) as

$$I(q) = \sum_{i=q}^{N} c_i \Phi_i(q) \qquad \text{where} \qquad \Phi_i(q) = \int \varphi_i(r) \frac{\sin 2\pi rq}{2\pi rq} dr$$

The coefficient of each base function is found by minimizing the following:

$$\chi^2 = \sum_{i=1}^{Npts} \left(I_i^{obs} - I(q_i)\right)^2 / \sigma_i^2 + \alpha \int \frac{d^2 p(r)}{dr^2} dr$$

The second term is a regularization term to ensure that the output is smooth. It is estimated numerically. The minimization is done with a simple linear least square fit.

Each panel except the 1D plot can be closed by clicking the "X" mark on the upper right corner.

You can rearrange your workspace by clicking on the title bar of a panel and dragging it outside the interface
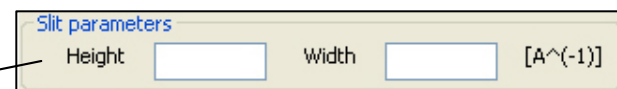
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Selecting I(Q) data
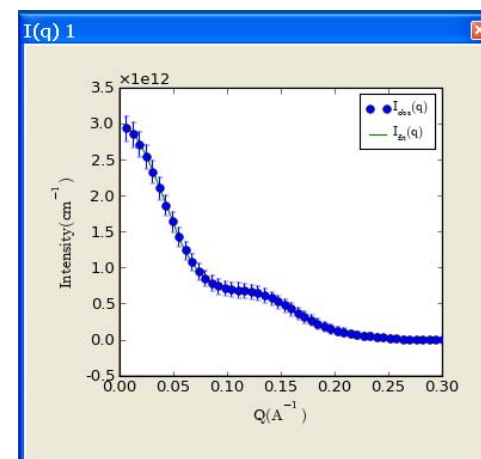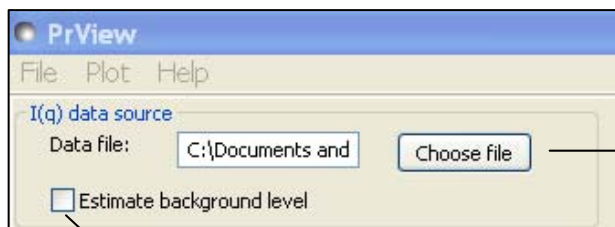
Data source

I(Q) data files can be loaded from the File menu or by clicking on the "Choose file" button. Once a parameter is changed, the plots will update automatically

Background estimate

By checking the background estimate box, you can let the application fit a constant background value for your I(q) data.

Slit smearing

By entering smearing height and/or smearing width, you can include slit smearing in the inversion calculations. Leaving the boxes empty will skip the smearing procedure. When smearing is used, the I(Q) distribution resulting from the inversion will be displayed both with and without smearing and compared to the original I(Q) data. The height and width are entered in units of Å^{-1}.

The smearing procedure is described in J. Lake, Acta Cryst. (1967) 23, 191.

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Q range
Q min   0.0061   Q max   0.3   [A^(-1)]

Parameters

P(r) is found by fitting a set of base functions to I(Q). The minimization involves a regularization term to ensure a smooth P(r). The alpha parameter gives the size of that term. The suggested value is the value above which the output P(r) will have only one peak.

		Suggested value
Number of terms	14	14
Regularization constant	5e-018	4e-018
Max distance [A]	100.0	

Slit smearing

When a file is loaded, the Q range is displayed. The minimum and maximum Q can be modified before doing the computation.

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.

Input parameters

Number of terms: number of terms in the expansion.
Regularization constant: α parameter of the regularization term (see page 2).
Max distance: Maximum distance between any two points in the system.

Starting the inversion

There are two ways of starting the inversion process: using the "Compute" button or hovering over the I(q) curve and choosing the "Compute P(r)" menu item.

Starting the inversion from the context menu will automatically make use of the suggested value for the number of terms and the regularization constant.

Context menus

Additional options to save the displayed data, images or change the scale are available through the context menu.
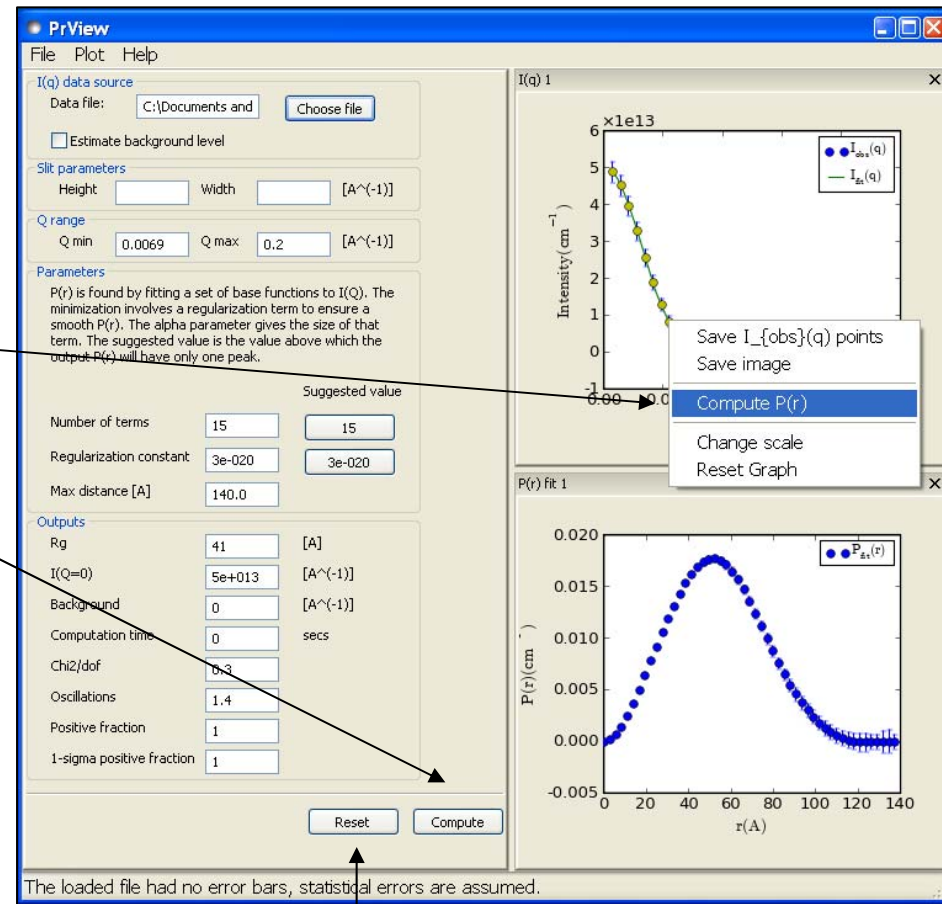
Reset button

A reset button is available to clear the output and reset the input parameters to their default values.

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Outputs

Rg	28	[A]
I(Q=0)	3e+012	[A^(-1)]
Background	0	[A^(-1)]
Computation time	0	secs
Chi2/dof	13	
Oscillations	2.8	
Positive fraction	0.99	
1-sigma positive fraction	0.98	

Output parameters

Several output parameters are provided as figures of merit of the inversion process.

Rg and I(Q=0) are computed from the p(r) distribution.

Oscillations

The oscillation parameter is defined as

$$Osc = \int \left(\frac{dp(r)}{dp} \right)^2 \bigg/ \int p^2(r) dr$$

Its value is 1.1 for a spherical system.

Positive fraction

The fraction of the integral of the absolute value of p(r) that is positive.

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.

Fit result and smeared result

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.

If slit smearing was used, both the I(Q) distributions with and without smearing are shown.
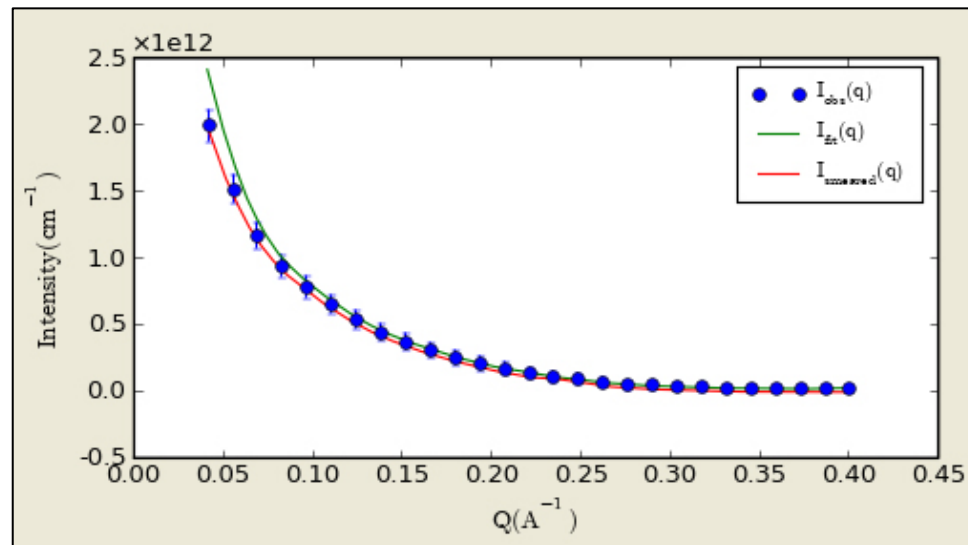
Adding data to the plot

By selecting "Add P(r) data", you can load a data file and plot it to compare it to the P(r) distribution.

Changing the number of p(r) points

A context menu item is provided to change the number of point on the p(r) distribution.

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