SasView Documentation

Release 4.2.1

The SasView Project

Feb 10, 2019
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### 1.1 Model Functions

#### 1.1.1 Cylinder Functions

**barbell**

Cylinder with spherical end caps

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
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<tr>
<td>phi</td>
<td>Rotation about beam</td>
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The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition**

Calculates the scattering from a barbell-shaped cylinder. Like *capped_cylinder*, this is a spherocylinder with spherical end caps that have a radius larger than that of the cylinder, but with the center of the end cap radius lying outside of the cylinder. See the diagram for the details of the geometry and restrictions on parameter values.

The scattered intensity \( I(q) \) is calculated as

\[
I(q) = \frac{\Delta \rho^2}{V} \langle A^2(q, \alpha) \sin(\alpha) \rangle
\]

where the amplitude \( A(q, \alpha) \) with the rod axis at angle \( \alpha \) to \( q \) is given as

\[
A(q) = \pi r^2 L \sin \left( \frac{1}{2} qL \cos \alpha \right) \frac{2 J_1(qr \sin \alpha)}{qr \sin \alpha} \\
+ 4\pi R^3 \int_{-h/R}^{1} dt \cos \left( q \cos \alpha \left( R t + h + \frac{1}{2} L \right) \right) \times (1 - t^2) \frac{J_1 \left[ qR \sin \alpha \left( 1 - t^2 \right)^{1/2} \right]}{qR \sin \alpha \left( 1 - t^2 \right)^{1/2}}
\]
Fig. 1.1: Barbell geometry, where $r$ is radius, $R$ is radius_bell and $L$ is length. Since the end cap radius $R \geq r$ and by definition for this geometry $h < 0$, $h$ is then defined by $r$ and $R$ as $h = -\sqrt{R^2 - r^2}$.

The $\langle \ldots \rangle$ brackets denote an average of the structure over all orientations. $\langle A^2(q, \alpha) \rangle$ is then the form factor, $P(q)$. The scale factor is equivalent to the volume fraction of cylinders, each of volume, $V$. Contrast $\Delta \rho$ is the difference of scattering length densities of the cylinder and the surrounding solvent.

The volume of the barbell is

$$ V = \pi r^2 L + 2\pi \left( \frac{3}{2} R^3 + R^2 h - \frac{1}{2} h^3 \right) $$

and its radius of gyration is

$$ R_g^2 = \left[ \frac{12}{5} R^5 + R^4 (6h + \frac{3}{2} L) + R^2 (4h^2 + L^2 + 4Lh) + R^2 (3Lh^2 + \frac{3}{2} L^2 h) + \frac{2}{5} h^5 - \frac{1}{2} Lh^4 - \frac{1}{2} L^2 h^3 + \frac{1}{4} L^3 r^2 + \frac{3}{8} Lr^4 \right] \left( 4R^3 6R^2 h - 2h^3 + 3r^2 L \right)^{-1} $$

**Note:** The requirement that $R \geq r$ is not enforced in the model! It is up to you to restrict this during analysis.

The 2D scattering intensity is calculated similar to the 2D cylinder model.

Fig. 1.2: Definition of the angles for oriented 2D barbells.
Fig. 1.3: 1D and 2D plots corresponding to the default parameters of the model.

References

Authorship and Verification

• Author: NIST IGOR/DANSE Date: pre 2010
• Last Modified by: Paul Butler Date: March 20, 2016
• Last Reviewed by: Richard Heenan Date: January 4, 2017

capped_cylinder

Right circular cylinder with spherical end caps and uniform SLD

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
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</thead>
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</tr>
<tr>
<td>background</td>
<td>Source background</td>
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</tr>
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<td>Cylinder scattering length density</td>
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</tr>
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<td>Solvent scattering length density</td>
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<td>1</td>
</tr>
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<td>Cylinder radius</td>
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<td>60</td>
</tr>
<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
<td>60</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

Definitions

Calculates the scattering from a cylinder with spherical section end-caps. Like barbell, this is a sphereocylinder with end caps that have a radius larger than that of the cylinder, but with the center of the end cap radius lying within the cylinder. This model simply becomes a convex lens when the length of the cylinder $L = 0$. See the diagram for the details of the geometry and restrictions on parameter values.

The scattered intensity $I(q)$ is calculated as

$$I(q) = \frac{\Delta \rho^2}{V} \langle A^2(q, \alpha), \sin(\alpha) \rangle$$
where the amplitude $A(q, \alpha)$ with the rod axis at angle $\alpha$ to $q$ is given as

$$A(q) = \pi r^2 L \frac{\sin \left( \frac{1}{2} q L \cos \alpha \right)}{q L \cos \alpha} \frac{2 J_1(qr \sin \alpha)}{qr \sin \alpha}$$

$$+ 4\pi R^3 \int_{-h/R}^1 dt \cos \left[ q \cos \alpha \left( Rt + h + \frac{1}{2} L \right) \right] \times (1 - t^2) \frac{J_1 \left[ q R \sin \alpha \left( 1 - t^2 \right)^{1/2} \right]}{q R \sin \alpha \left( 1 - t^2 \right)^{1/2}}$$

The $\langle \ldots \rangle$ brackets denote an average of the structure over all orientations. $\langle A^2(q) \rangle$ is then the form factor, $P(q)$. The scale factor is equivalent to the volume fraction of cylinders, each of volume, $V$. Contrast $\Delta \rho$ is the difference of scattering length densities of the cylinder and the surrounding solvent.

The volume of the capped cylinder is (with $h$ as a positive value here)

$$V = \pi r^2 L + \frac{2\pi}{3} (R - h)^2 (2R + h)$$

and its radius of gyration is

$$R_g^2 = \left[ \frac{13}{5} R^5 + R^4 \left( 6h + \frac{3}{2} L \right) + R^2 \left( 4h^2 + L^2 + 4Lh \right) + R^2 \left( 3Lh^2 + \frac{3}{2} L^2 h \right) \right. + \frac{1}{2} h^5 - \frac{1}{2} L^2 h^3 + \frac{1}{2} L^3 r^2 + \frac{3}{2} L r^4 \right] \left( 4R^4 6 R^2 h - 2h^3 + 3r^2 L \right)^{-1}$$

Note: The requirement that $R \geq r$ is not enforced in the model! It is up to you to restrict this during analysis.

The 2D scattering intensity is calculated similar to the 2D cylinder model.

References

Authorship and Verification

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
- **Last Modified by:** Paul Butler **Date:** September 30, 2016
- **Last Reviewed by:** Richard Heenan **Date:** January 4, 2017

core_shell_bicelle

Circular cylinder with a core-shell scattering length density profile.
Fig. 1.5: Definition of the angles for oriented 2D cylinders.

Fig. 1.6: 1D and 2D plots corresponding to the default parameters of the model.
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<thead>
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<td>Cylinder axis to beam angle</td>
<td>degree</td>
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<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
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The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

Definition

This model provides the form factor for a circular cylinder with a core-shell scattering length density profile. Thus this is a variation of a core-shell cylinder or disc where the shell on the walls and ends may be of different thicknesses and scattering length densities. The form factor is normalized by the particle volume.

Given the scattering length densities (sld) \( \rho_c \), the core sld, \( \rho_f \), the face sld, \( \rho_r \), the rim sld and \( \rho_s \) the solvent sld, the scattering length density variation along the cylinder axis is:

\[
\rho(r) = \begin{cases} 
\rho_c & \text{for } 0 < r < R; -L < z < L \\
\rho_f & \text{for } 0 < r < R; -(L + 2t) < z < -L; L < z < (L + 2t) \\
\rho_r & \text{for } 0 < r < R; -(L + 2t) < z < -L; L < z < (L + 2t) 
\end{cases}
\]

Fig. 1.7: Schematic cross-section of bicelle. Note however that the model here calculates for rectangular, not curved, rims as shown below.
Fig. 1.8: Cross section of cylindrical symmetry model used here. Users will have to decide how to distribute “heads” and “tails” between the rim, face and core regions in order to estimate appropriate starting parameters.

The form factor for the bicelle is calculated in cylindrical coordinates, where \( \alpha \) is the angle between the \( Q \) vector and the cylinder axis, to give:

\[
I(Q, \alpha) = \frac{\text{scale}}{V_t} \cdot F(Q, \alpha)^2 \cdot \sin(\alpha) + \text{background}
\]

where

\[
F(Q, \alpha) = \left[ (\rho_c - \rho_f) V_c \frac{2J_1(Q R \sin(\alpha)) \sin(Q L \cos(\alpha)/2)}{Q R \sin(\alpha) \cdot Q (L/2) \cos(\alpha)} 
+ (\rho_f - \rho_r) V_{c+f} \frac{2J_1(Q R \sin(\alpha)) \sin(Q (L/2 + t_f) \cos(\alpha))}{Q R \sin(\alpha) \cdot Q (L/2 + t_f) \cos(\alpha)} 
+ (\rho_r - \rho_s) V_t \frac{2J_1(Q (R + t_r) \sin(\alpha)) \sin(Q (L/2 + t_f) \cos(\alpha))}{Q (R + t_r) \sin(\alpha) \cdot Q (L/2 + t_f) \cos(\alpha)} \right]
\]

where \( V_t \) is the total volume of the bicelle, \( V_c \) the volume of the core, \( V_{c+f} \) the volume of the core plus the volume of the faces, \( R \) is the radius of the core, \( L \) the length of the core, \( t_f \) the thickness of the face, \( t_r \) the thickness of the rim and \( J_1 \) the usual first order bessel function.

The output of the 1D scattering intensity function for randomly oriented cylinders is then given by integrating over all possible \( \theta \) and \( \phi \).

For oriented bicelles the \( \theta \) and \( \phi \) orientation parameters will appear when fitting 2D data, see the cylinder model for further information. Our implementation of the scattering kernel and the 1D scattering intensity use the c-library from NIST.

References

Authorship and Verification

- **Author**: NIST IGOR/DANSE **Date**: pre 2010
- **Last Modified by**: Paul Butler **Date**: September 30, 2016
- **Last Reviewed by**: Richard Heenan **Date**: January 4, 2017
Fig. 1.9: Definition of the angles for the oriented core shell bicelle model, note that the cylinder axis of the bicelle starts along the beam direction when $\theta = \phi = 0$.

Fig. 1.10: 1D and 2D plots corresponding to the default parameters of the model.
core_shell_bicelle_elliptical

Elliptical cylinder with a core-shell scattering length density profile.

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The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

This model provides the form factor for an elliptical cylinder with a core-shell scattering length density profile. Thus this is a variation of the core-shell bicelle model, but with an elliptical cylinder for the core. Outer shells on the rims and flat ends may be of different thicknesses and scattering length densities. The form factor is normalized by the total particle volume.

![Fig. 1.11: Schematic cross-section of bicelle. Note however that the model here calculates for rectangular, not curved, rims as shown below.](image)

Given the scattering length densities (sld) $\rho_c$, the core sld, $\rho_f$, the face sld, $\rho_r$, the rim sld and $\rho_s$ the solvent sld,
Fig. 1.12: Cross section of model used here. Users will have to decide how to distribute “heads” and “tails” between the rim, face and core regions in order to estimate appropriate starting parameters.

The scattering length density variation along the bicelle axis is:

\[ \rho(r) = \begin{cases} 
\rho_c & \text{for } 0 < r < R; -L < z < L \\
\rho_f & \text{for } 0 < r < R; -(L + 2t) < z < -L; L < z < (L + 2t) \\
\rho_r & \text{for } 0 < r < R; -(L + 2t) < z < -L; L < z < (L + 2t)
\end{cases} \]

The form factor for the bicelle is calculated in cylindrical coordinates, where \( \alpha \) is the angle between the \( Q \) vector and the cylinder axis, and \( \psi \) is the angle for the ellipsoidal cross section core, to give:

\[ I(Q, \alpha, \psi) = \text{scale} \cdot \frac{V_t}{V_c} \cdot F(Q, \alpha, \psi)^2 \cdot \sin(\alpha) + \text{background} \]

where a numerical integration of \( F(Q, \alpha, \psi)^2 \cdot \sin(\alpha) \) is carried out over alpha and psi for:

\[
F(Q, \alpha, \psi) = \left[ (\rho_c - \rho_f)V_c \frac{2J_1(QR'sina)\sin(QL\cos\alpha/2)}{QR'sina} \frac{Q(L/2)\cos\alpha}{Q(L/2)} \\
+ (\rho_f - \rho_r)V_{c+f} \frac{2J_1(QR'\sin(\alpha))\sin(Q(L/2+t_f)\cos\alpha)}{QR'\sin(\alpha)} \frac{Q(L/2+t_f)\cos\alpha}{Q(L/2+t_f)\cos\alpha} \\
+ (\rho_r - \rho_s)V_t \frac{2J_1(Q(R' + t_r)\sin(\alpha))\sin(Q(L/2+t_f)\cos\alpha)}{Q(R' + t_r)\sin(\alpha)} \frac{Q(L/2+t_f)\cos\alpha}{Q(L/2+t_f)\cos\alpha} \right]
\]

where

\[ R' = \frac{R}{\sqrt{2}} \sqrt{(1 + X_{core}^2) + (1 - X_{core}^2)\cos(\psi)} \]

and \( V_t = \pi.(R + t_r)(X_{core}.R + t_r)^2.(L + 2t_f) \) is the total volume of the bicelle, \( V_c = \pi.X_{core}.R^2.L \) the volume of the core, \( V_{c+f} = \pi.X_{core}.R^2.(L + 2t_f) \) the volume of the core plus the volume of the faces, \( R \) is the radius of the core, \( X_{core} \) is the axial ratio of the core, \( L \) the length of the core, \( t_f \) the thickness of the face, \( t_r \) the thickness of the rim and \( J_1 \) the usual first order bessel function. The core has radii \( R \) and \( X_{core} \) so is circular, as for the core_shell_bicelle model, for \( X_{core} = 1.0 \). Note that you may need to limit the range of \( X_{core} \), especially if using the Monte-Carlo algorithm, as setting radius to \( R/X_{core} \) and axial ratio to \( 1/X_{core} \) gives an equivalent solution.
The output of the 1D scattering intensity function for randomly oriented bicelles is then given by integrating over all possible $\alpha$ and $\psi$.

For oriented bicelles the $\theta$, $\phi$ and $\psi$ orientation parameters will appear when fitting 2D data, see the *elliptical_cylinder* model for further information.

Model verified using Monte Carlo simulation for 1D and 2D scattering.

References

**Authorship and Verification**

- **Author**: Richard Heenan **Date**: December 14, 2016
- **Last Modified by**: Richard Heenan **Date**: December 14, 2016
- **Last Reviewed by**: Paul Kienzle **Date**: Feb 28, 2018

**core_shell_bicelle_elliptical_belt_rough**

Elliptical cylinder with a core-shell scattering length density profile.
The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition**

This model provides the form factor for an elliptical cylinder with a core-shell scattering length density profile. Thus this is a variation of the core-shell bicelle model, but with an elliptical cylinder for the core. In this version the "rim" or "belt" does NOT extend the full length of the particle, but has the same length as the core. Outer shells on the rims and flat ends may be of different thicknesses and scattering length densities. The form factor is normalized by the total particle volume. This version includes an approximate “interfacial roughness”.

Given the scattering length densities (sld) \(\rho_c\), the core sld, \(\rho_f\), the face sld, \(\rho_r\), the rim sld and \(\rho_s\) the solvent sld, the scattering length density variation along the bicelle axis is:

\[
\rho(r) = \begin{cases} 
\rho_c & \text{for } 0 < r < R; -L/2 < z < L/2 \\
\rho_f & \text{for } 0 < r < R; -(L/2 + t_{face}) < z < -L/2; L/2 < z < (L/2 + t_{face}) \\
\rho_r & \text{for } R < r < R + t_{rim}; -L/2 < z < L/2
\end{cases}
\]

The form factor for the bicelle is calculated in cylindrical coordinates, where \(\alpha\) is the angle between the \(Q\) vector
Fig. 1.15: Schematic cross-section of bicelle with belt. Note however that the model here calculates for rectangular, not curved, rims as shown below.
Fig. 1.16: Cross section of model used here. Users will have to decide how to distribute “heads” and “tails” between the rim, face and core regions in order to estimate appropriate starting parameters.

and the cylinder axis, and $\psi$ is the angle for the ellipsoidal cross section core, to give:

$$ I(Q, \alpha, \psi) = \frac{\text{scale}}{V_t} \cdot F(Q, \alpha, \psi)^2 \cdot \sin(\alpha) \cdot \exp \left\{ -\frac{1}{2} Q^2 \sigma^2 \right\} + \text{background} $$

where a numerical integration of $F(Q, \alpha, \psi)^2 \sin(\alpha)$ is carried out over $\alpha$ and $\psi$ for:

$$ F(Q, \alpha, \psi) = \left[ (\rho_c - \rho_r - \rho_f + \rho_s) V_c \frac{2 J_1(Q R' \sin \alpha) \sin(Q L \cos \alpha/2)}{Q R' \sin \alpha} \frac{Q(L/2) \cos \alpha}{Q(L/2 + t_f) \cos \alpha} \right. $$

$$ + (\rho_f - \rho_s) V_{c+f} \frac{2 J_1(Q R' \sin \alpha) \sin(Q(L/2 + t_f) \cos \alpha)}{Q R' \sin \alpha} \frac{Q(L/2) \cos \alpha}{Q(L/2 + t_f) \cos \alpha} $$

$$ \left. + (\rho_r - \rho_s) V_{c+r} \frac{2 J_1(Q(R' + t_r) \sin \alpha) \sin(Q(L/2) \cos \alpha)}{Q(R' + t_r) \sin \alpha} \frac{Q(L/2) \cos \alpha}{Q(L/2) \cos \alpha} \right] $$

where

$$ R' = \frac{R}{\sqrt{2}} \sqrt{(1 + X_{core}^2) + (1 - X_{core}^2) \cos(\psi)} $$

and $V_t = \pi (R + t_r)(X_{core} R + t_r)L + 2 \pi X_{core} R^2 t_f$ is the total volume of the bicelle, $V_c = \pi X_{core} R^2 L$ the volume of the core, $V_{c+f} = \pi X_{core} R^2 (L + 2t_f)$ the volume of the core plus the volume of the faces, $V_{c+r} = \pi (R + t_r)(X_{core} R + t_r)L$ the volume of the core plus the rim, $R$ is the radius of the core, $X_{core}$ is the axial ratio of the core, $L$ the length of the core, $t_f$ the thickness of the face, $t_r$ the thickness of the rim and $J_1$ the usual first order bessel function. The core has radii $R$ and $X_{core} R$ so is circular, as for the core_shell_bicelle model, for $X_{core} = 1$. Note that you may need to limit the range of $X_{core}$, especially if using the Monte-Carlo algorithm, as setting radius to $R/X_{core}$ and axial ratio to $1/X_{core}$ gives an equivalent solution!

An approximation for the effects of “Gaussian interfacial roughness” $\sigma$ is included, by multiplying $I(Q)$ by

$$ \exp \left\{ -\frac{1}{2} Q^2 \sigma^2 \right\}. $$

This applies, in some way, to all interfaces in the model not just the external ones. (Note that
for a one dimensional system convolution of the scattering length density profile with a Gaussian of standard deviation $\sigma$ does exactly this multiplication.) Leave $\sigma$ set to zero for the usual sharp interfaces.

The output of the 1D scattering intensity function for randomly oriented bicelles is then given by integrating over all possible $\alpha$ and $\psi$.

For oriented bicelles the $\theta$, $\phi$ and $\psi$ orientation parameters will appear when fitting 2D data, for further details of the calculation and angular dispersions see Oriented particles.

![Diagram of oriented core_shell_bicelle_elliptical particles](image)

Fig. 1.17: Definition of the angles for the oriented core_shell_bicelle_elliptical particles.

References

Authorship and Verification

- **Author**: Richard Heenan  **Date**: October 5, 2017
- **Last Modified by**: Richard Heenan new 2d orientation  **Date**: October 5, 2017
- **Last Reviewed by**: Richard Heenan 2d calc seems agree with 1d  **Date**: Nov 2, 2017

**core_shell_cylinder**

Right circular cylinder with a core-shell scattering length density profile.
Fig. 1.18: 1D and 2D plots corresponding to the default parameters of the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
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<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
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<td>Source intensity</td>
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<td>background</td>
<td>Source background</td>
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</tr>
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<td>sld_shell</td>
<td>Cylinder shell scattering length density</td>
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</tr>
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<td>sld_solvent</td>
<td>Solvent scattering length density</td>
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<td>1</td>
</tr>
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<td>Cylinder core radius</td>
<td>Å</td>
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</tr>
<tr>
<td>thickness</td>
<td>Cylinder shell thickness</td>
<td>Å</td>
<td>20</td>
</tr>
<tr>
<td>length</td>
<td>Cylinder length</td>
<td>Å</td>
<td>400</td>
</tr>
<tr>
<td>theta</td>
<td>Cylinder axis to beam angle</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
<td>60</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

The output of the 2D scattering intensity function for oriented core-shell cylinders is given by (Kline, 2006²). The form factor is normalized by the particle volume. Note that in this model the shell envelops the entire core so that besides a “sleeve” around the core, the shell also provides two flat end caps of thickness = shell thickness. In other words the length of the total cylinder is the length of the core cylinder plus twice the thickness of the shell. If no end caps are desired one should use the `core_shell_bicelle` and set the thickness of the end caps (in this case the “thick_face”) to zero.

\[
I(q, \alpha) = \frac{\text{scale}}{V_s} F^2(q, \alpha) \sin(\alpha) + \text{background}
\]

where

\[
F(q, \alpha) = (\rho_c - \rho_s)V_c \frac{\sin \left( q \frac{1}{2} L \cos \alpha \right)}{q \frac{1}{2} L \cos \alpha} \frac{2J_1 \left( q R \sin \alpha \right)}{q R \sin \alpha} + (\rho_s - \rho_{solv})V_s \frac{\sin \left( q \left( \frac{1}{2} L + T \right) \cos \alpha \right)}{q \left( \frac{1}{2} L + T \right) \cos \alpha} \frac{2J_1 \left( q(R + T) \sin \alpha \right)}{q(R + T) \sin \alpha}
\]

and

\[
V_s = \pi(R + T)^2(L + 2T)
\]

and $\alpha$ is the angle between the axis of the cylinder and $\vec{q}$, $V_s$ is the total volume (i.e. including both the core and the outer shell), $V_c$ is the volume of the core, $L$ is the length of the core, $R$ is the radius of the core, $T$ is the thickness of the shell, $\rho_c$ is the scattering length density of the core, $\rho_s$ is the scattering length density of the shell, $\rho_{\text{solv}}$ is the scattering length density of the solvent, and background is the background level. The outer radius of the shell is given by $R + T$ and the total length of the outer shell is given by $L + 2T$. $J_1$ is the first order Bessel function.

![Core shell cylinder schematic](image)

Fig. 1.19: Core shell cylinder schematic.

To provide easy access to the orientation of the core-shell cylinder, we define the axis of the cylinder using two angles $\theta$ and $\phi$. (see cylinder model)

NB: The 2nd virial coefficient of the cylinder is calculated based on the radius and 2 length values, and used as the effective radius for $S(q)$ when $P(q) \cdot S(q)$ is applied.

The $\theta$ and $\phi$ parameters are not used for the 1D output.

![1D and 2D plots](image)

Fig. 1.20: 1D and 2D plots corresponding to the default parameters of the model.

**Reference**

**Authorship and Verification**

- **Author**: NIST IGOR/DANSE **Date**: pre 2010
- **Last Modified by**: Paul Kienzle **Date**: Aug 8, 2016
cylinder

Right circular cylinder with uniform scattering length density.

<table>
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<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
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<td>Source intensity</td>
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</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
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</tr>
<tr>
<td>sld</td>
<td>Cylinder scattering length density</td>
<td>10(^6)Å(^{-2})</td>
<td>4</td>
</tr>
<tr>
<td>sld_solute</td>
<td>Solvent scattering length density</td>
<td>10(^6)Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>radius</td>
<td>Cylinder radius</td>
<td>Å</td>
<td>20</td>
</tr>
<tr>
<td>length</td>
<td>Cylinder length</td>
<td>Å</td>
<td>400</td>
</tr>
<tr>
<td>theta</td>
<td>Cylinder axis to beam angle</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
<td>60</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

For information about polarised and magnetic scattering, see the Polarisation/Magnetic Scattering documentation.

Definition

The output of the 2D scattering intensity function for oriented cylinders is given by (Guinier, 1955)

\[
P(q, \alpha) = \frac{\text{scale}}{V} F^2(q, \alpha) \sin(\alpha) + \text{background}
\]

where

\[
F(q, \alpha) = 2(|\Delta \rho|) V \frac{\sin \left( \frac{1}{2} q L \cos \alpha \right) J_1(q R \sin \alpha)}{q R \sin \alpha}
\]

and \(\alpha\) is the angle between the axis of the cylinder and \(\vec{q}\), \(V = \pi R^2 L\) is the volume of the cylinder, \(L\) is the length of the cylinder, \(R\) is the radius of the cylinder, and \(|\Delta \rho|\) (contrast) is the scattering length density difference between the scatterer and the solvent. \(J_1\) is the first order Bessel function.

For randomly oriented particles:

\[
F^2(q) = \int_0^{\pi/2} F^2(q, \alpha) \sin(\alpha) d\alpha = \int_0^1 F^2(q, u) du
\]

Numerical integration is simplified by a change of variable to \(u = \cos(\alpha)\) with \(\sin(\alpha) = \sqrt{1 - u^2}\).

The output of the 1D scattering intensity function for randomly oriented cylinders is thus given by

\[
P(q) = \frac{\text{scale}}{V} \int_0^{\pi/2} F^2(q, \alpha) \sin \alpha d\alpha + \text{background}
\]

NB: The 2nd virial coefficient of the cylinder is calculated based on the radius and length values, and used as the effective radius for \(S(q)\) when \(P(q) \cdot S(q)\) is applied.

For 2d scattering from oriented cylinders, we define the direction of the axis of the cylinder using two angles \(\theta\) (note this is not the same as the scattering angle used in \(q\)) and \(\phi\). Those angles are defined in Fig. 1.21, for further details see Oriented particles.

The \(\theta\) and \(\phi\) parameters to orient the cylinder only appear in the model when fitting 2d data.

Validation

Validation of the code was done by comparing the output of the 1D model to the output of the software provided by the NIST (Kline, 2006). The implementation of the intensity for fully oriented cylinders was done by averaging over a uniform distribution of orientations using

\[
P(q) = \int_0^{\pi/2} d\phi \int_0^\pi p(\theta) P_0(q, \theta) \sin \theta d\theta
\]
Fig. 1.21: Angles $\theta$ and $\phi$ orient the cylinder relative to the beam line coordinates, where the beam is along the $z$ axis. Rotation $\theta$, initially in the $xz$ plane, is carried out first, then rotation $\phi$ about the $z$ axis. Orientation distributions are described as rotations about two perpendicular axes $\delta_1$ and $\delta_2$ in the frame of the cylinder itself, which when $\theta = \phi = 0$ are parallel to the $Y$ and $X$ axes.

Fig. 1.22: Examples for oriented cylinders.
where \( p(\theta, \phi) = 1 \) is the probability distribution for the orientation and \( P_0(q, \theta) \) is the scattering intensity for the fully oriented system, and then comparing to the 1D result.

Fig. 1.23: 1D and 2D plots corresponding to the default parameters of the model.

References

**elliptical_cylinder**

Form factor for an elliptical cylinder.

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<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
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<td>Ellipse minor radius</td>
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<td>20</td>
</tr>
<tr>
<td>axis_ratio</td>
<td>Ratio of major radius over minor radius</td>
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<tr>
<td>length</td>
<td>Length of the cylinder</td>
<td>Å</td>
<td>400</td>
</tr>
<tr>
<td>sld</td>
<td>Cylinder scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>4</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>theta</td>
<td>Cylinder axis to beam angle</td>
<td>degree</td>
<td>90</td>
</tr>
<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
<td>0</td>
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<tr>
<td>psi</td>
<td>Rotation about cylinder axis</td>
<td>degree</td>
<td>0</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

The function calculated is

\[
I(q) = \frac{1}{V_{\text{cyl}}} \int d\psi \int d\phi \int p(\theta, \phi, \psi) F^2(q, \alpha, \psi) \sin(\alpha) d\alpha
\]

with the functions

\[
F(q, \alpha, \psi) = 2 \frac{J_1(a) \sin(b)}{ab}
\]
Fig. 1.24: Elliptical cylinder geometry $a = r_{\text{minor}}$ and $\nu = r_{\text{major}} / r_{\text{minor}}$ is the axis_ratio.

where

\[
a = qr' \sin(\alpha)
\]
\[
b = q \frac{L}{2} \cos(\alpha)
\]
\[
r' = \frac{r_{\text{minor}}}{\sqrt{2}} \sqrt{(1 + \nu^2) + (1 - \nu^2)\cos(\psi)}
\]

and the angle $\psi$ is defined as the orientation of the major axis of the ellipse with respect to the vector $\vec{q}$. The angle $\alpha$ is the angle between the axis of the cylinder and $\vec{q}$.

For 1D scattering, with no preferred orientation, the form factor is averaged over all possible orientations and normalized by the particle volume

\[P(q) = \text{scale} < F^2 > /V\]

For 2D data the orientation of the particle is required, described using a different set of angles as in the diagrams below, for further details of the calculation and angular dispersions see Oriented particles.

The $\theta$ and $\phi$ parameters to orient the cylinder only appear in the model when fitting 2d data.

NB: The 2nd virial coefficient of the cylinder is calculated based on the averaged radius ($= \sqrt{r_{\text{minor}}^2 * \text{axis ratio}}$) and length values, and used as the effective radius for $S(Q)$ when $P(Q) * S(Q)$ is applied.

Validation

Validation of our code was done by comparing the output of the 1D calculation to the angular average of the output of the 2D calculation over all possible angles.

In the 2D average, more binning in the angle $\phi$ is necessary to get the proper result. The following figure shows the results of the averaging by varying the number of angular bins.

References


Authorship and Verification

- **Author:**
- **Last Modified by:**
- **Last Reviewed by:** Richard Heenan - corrected equation in docs **Date:** December 21, 2016
Fig. 1.25: Note that the angles here are not the same as in the equations for the scattering function. Rotation $\theta$, initially in the $xz$ plane, is carried out first, then rotation $\phi$ about the $z$ axis, finally rotation $\Psi$ is now around the axis of the cylinder. The neutron or X-ray beam is along the $z$ axis.
Fig. 1.26: Examples of the angles for oriented elliptical cylinders against the detector plane, with $\Psi = 0$.

Fig. 1.27: The intensities averaged from 2D over different numbers of bins and angles.
Fig. 1.28: 1D and 2D plots corresponding to the default parameters of the model.

flexible_cylinder

Flexible cylinder where the form factor is normalized by the volume of the cylinder.

<table>
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<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
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<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<td>background</td>
<td>Source background</td>
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<td>Length of the flexible cylinder</td>
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</tr>
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<td>Kuhn length of the flexible cylinder</td>
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</tr>
<tr>
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<td>Radius of the flexible cylinder</td>
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<tr>
<td>sld</td>
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<td>Solvent scattering length density</td>
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<td>6.3</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model provides the form factor, \(P(q)\), for a flexible cylinder where the form factor is normalized by the volume of the cylinder. **Inter-cylinder interactions are NOT provided for.**

\[
P(q) = \text{scale } \langle F^2 \rangle / V + \text{background}
\]

where the averaging \(\langle \ldots \rangle\) is applied only for the 1D calculation.

The 2D scattering intensity is the same as 1D, regardless of the orientation of the q vector which is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

**Definitions**

The chain of contour length, \(L\), (the total length) can be described as a chain of some number of locally stiff segments of length \(l_p\), the persistence length (the length along the cylinder over which the flexible cylinder can be considered a rigid rod). The Kuhn length \((b = 2 * l_p)\) is also used to describe the stiffness of a chain.

The returned value is in units of cm\(^{-1}\), on absolute scale.

In the parameters, the sld and sld_solvent represent the SLD of the cylinder and solvent respectively.

Our model uses the form factor calculations implemented in a c-library provided by the NIST Center for Neutron Research (Kline, 2006).

From the reference:
‘Method 3 With Excluded Volume’ is used. The model is a parametrization of simulations of a discrete representation of the worm-like chain model of Kratky and Porod applied in the pseudocontinuous limit. See equations (13,26-27) in the original reference for the details.

References


Correction of the formula can be found in


**flexible_cylinder_elliptical**

Flexible cylinder with an elliptical cross section and a uniform scattering length density.
<table>
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<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
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</thead>
<tbody>
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<td>scale</td>
<td>Source intensity</td>
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<tr>
<td>background</td>
<td>Source background</td>
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</tr>
<tr>
<td>length</td>
<td>Length of the flexible cylinder</td>
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</tr>
<tr>
<td>kuhn_length</td>
<td>Kuhn length of the flexible cylinder</td>
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</tr>
<tr>
<td>radius</td>
<td>Radius of the flexible cylinder</td>
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<td>20</td>
</tr>
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</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10(^{6})Å(^{-2})</td>
<td>6.3</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model calculates the form factor for a flexible cylinder with an elliptical cross section and a uniform scattering length density. The non-negligible diameter of the cylinder is included by accounting for excluded volume interactions within the walk of a single cylinder. The form factor is normalized by the particle volume such that

\[
P(q) = \text{scale} \langle F^2 \rangle / V + \text{background}
\]

where the averaging \( \langle \ldots \rangle \) is over all possible orientations of the flexible cylinder.

The 2D scattering intensity is the same as 1D, regardless of the orientation of the q vector which is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

**Definitions**

The function calculated in a similar way to that for the flexible_cylinder model from the reference given below using the author’s “Method 3 With Excluded Volume”. The model is a parameterization of simulations of a discrete representation of the worm-like chain model of Kratky and Porod applied in the pseudo-continuous limit. See equations (13, 26-27) in the original reference for the details.

**Note:** There are several typos in the original reference that have been corrected by WRC. Details of the corrections are in the reference below. Most notably

- Equation (13): the term \((1 - w(QR))\) should swap position with \(w(QR)\)
- Equations (23) and (24) are incorrect; WRC has entered these into Mathematica and solved analytically. The results were then converted to code.
- Equation (27) should be \(q_0 = \max(a3/sqrt(RgSquare), 3)\) instead of \(\max(a3 * b/sqrt(RgSquare), 3)\)
- The scattering function is negative for a range of parameter values and q-values that are experimentally accessible. A correction function has been added to give the proper behavior.
The chain of contour length, $L$, (the total length) can be described as a chain of some number of locally stiff segments of length $l_p$, the persistence length (the length along the cylinder over which the flexible cylinder can be considered a rigid rod). The Kuhn length ($b = 2 \times l_p$) is also used to describe the stiffness of a chain.

The cross section of the cylinder is elliptical, with minor radius $a$. The major radius is larger, so of course, the axis ratio (parameter 5) must be greater than one. Simple constraints should be applied during curve fitting to maintain this inequality.

The returned value is in units of $cm^{-1}$, on absolute scale.

In the parameters, the sld and sld.solvent represent the SLD of the chain/cylinder and solvent respectively. The scale, and the contrast are both multiplicative factors in the model and are perfectly correlated. One or both of these parameters must be held fixed during model fitting.

No inter-cylinder interference effects are included in this calculation.

![Fig. 1.30: 1D plot corresponding to the default parameters of the model.](image)

**References**


Correction of the formula can be found in

hollow_cylinder

<table>
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<tr>
<th>Parameter</th>
<th>Description</th>
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<tbody>
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<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>radius</td>
<td>Cylinder core radius</td>
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<tr>
<td>thickness</td>
<td>Cylinder wall thickness</td>
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<tr>
<td>length</td>
<td>Cylinder total length</td>
<td>Å</td>
<td>400</td>
</tr>
<tr>
<td>sld</td>
<td>Cylinder sld</td>
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<td>6.3</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent sld</td>
<td>10⁶Å⁻²</td>
<td>1</td>
</tr>
<tr>
<td>theta</td>
<td>Cylinder axis to beam angle</td>
<td>degree</td>
<td>90</td>
</tr>
<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
<td>0</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

This model provides the form factor, \( P(q) \), for a monodisperse hollow right angle circular cylinder (rigid tube) where the inside and outside of the hollow cylinder are assumed to have the same SLD and the form factor is thus normalized by the volume of the tube (i.e. not by the total cylinder volume).

\[
P(q) = \text{scale} \langle F^2 \rangle / V_{shell} + \text{background}
\]

where the averaging \( \langle \ldots \rangle \) is applied only for the 1D calculation. If Intensity is given on an absolute scale, the scale factor here is the volume fraction of the shell. This differs from the core_shell_cylinder in that, in that case, scale is the volume fraction of the entire cylinder (core+shell). The application might be for a bilayer which wraps into a hollow tube and the volume fraction of material is all in the shell, whereas the core_shell_cylinder model might be used for a cylindrical micelle where the tails in the core have a different SLD than the headgroups (in the shell) and the volume fraction of material comes from the whole cylinder. NOTE: the hollow_cylinder represents a tube whereas the core_shell_cylinder includes a shell layer covering the ends (end caps) as well.

The 1D scattering intensity is calculated in the following way (Guinier, 1955)

\[
P(q) = (\text{scale})V_{shell} \Delta \rho^2 \int_0^1 \Psi^2 [q_z, R_{outer}(1 - x^2)^{1/2}, R_{core}(1 - x^2)^{1/2}] \left( \frac{\sin(qHx)}{qHx} \right)^2 dx \\
\Psi[q, y, z] = \frac{1}{1 - \gamma^2} [\Lambda(qy) - \gamma^2 \Lambda(qz)] \\
\Lambda(a) = 2J_1(a)/a \\
\gamma = R_{core}/R_{outer} \\
V_{shell} = \pi \left( R_{outer}^2 - R_{core}^2 \right) L \\
J_1(x) = (\sin(x) - x \cdot \cos(x))/x^2
\]

where \( \text{scale} \) is a scale factor, \( H = L/2 \) and \( J_1 \) is the 1st order Bessel function.

**NB:** The 2nd virial coefficient of the cylinder is calculated based on the outer radius and full length, which give an the effective radius for structure factor \( S(q) \) when \( P(q) \cdot S(q) \) is applied.

In the parameters, the **radius** is \( R_{core} \) while **thickness** is \( R_{outer} - R_{core} \).

To provide easy access to the orientation of the core-shell cylinder, we define the axis of the cylinder using two angles \( \theta \) and \( \phi \) (see cylinder model).

**References**

**Authorship and Verification**

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
- **Last Modified by:** Paul Butler **Date:** September 06, 2018 (corrected VR calculation)
- **Last Reviewed by:** Paul Butler **Date:** September 06, 2018
pearl_necklace

Colloidal spheres chained together with no preferential orientation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>radius</td>
<td>Mean radius of the chained spheres</td>
<td>Å</td>
<td>80</td>
</tr>
<tr>
<td>edge_sep</td>
<td>Mean separation of chained particles</td>
<td>Å</td>
<td>350</td>
</tr>
<tr>
<td>thick_string</td>
<td>Thickness of the chain linkage</td>
<td>Å</td>
<td>2.5</td>
</tr>
<tr>
<td>num_pearls</td>
<td>Number of pearls in the necklace (must be integer)</td>
<td>none</td>
<td>3</td>
</tr>
<tr>
<td>sld</td>
<td>Scattering length density of the chained spheres</td>
<td>10(^{6})Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>sld_string</td>
<td>Scattering length density of the chain linkage</td>
<td>10(^{6})Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Scattering length density of the solvent</td>
<td>10(^{6})Å(^{-2})</td>
<td>6.3</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model provides the form factor for a pearl necklace composed of two elements: \(N\) pearls (homogeneous spheres of radius \(R\)) freely jointed by \(M\) rods (like strings - with a total mass \(M_w = M \ast m_f + N \ast m_s\), and the string segment length (or edge separation) \(l = A - 2R\)). \(A\) is the center-to-center pearl separation distance.

**Definition**

The output of the scattering intensity function for the pearl_necklace is given by (Schweins, 2004)

\[
I(q) = \frac{\text{scale}}{\mathcal{V}} \cdot \frac{(S_{ss}(q) + S_{ff}(q) + S_{fs}(q))}{(M \cdot m_f + N \cdot m_s)^2} + \text{bkg}
\]
where

\[ S_{ss}(q) = \sin^2 \psi^2(q) \left[ \frac{N}{1 - \sin(qA)/qA} - \frac{N}{2} \cdot \frac{1 - (\sin(qA)/qA)^N}{1 - \sin(qA)/qA} \cdot \frac{\sin(qA)}{qA} \right] \]

\[ S_{ff}(q) = \sin^2 \theta \left[ 2\Lambda(\theta) - \frac{\sin(q/2)}{q/2} \right] + \frac{2M\beta^2(q)}{1 - \sin(qA)/qA} - 2\beta^2(q) \cdot \frac{1 - (\sin(qA)/qA)^M}{1 - \sin(qA)/qA} \]

\[ S_{fs}(q) = m_r\beta(q) \cdot m_s \psi(q) \cdot 4 \left[ \frac{N - 1}{1 - \sin(qA)/qA} - \frac{1 - (\sin(qA)/qA)^{N-1}}{1 - \sin(qA)/qA} \cdot \frac{\sin(qA)}{qA} \right] \]

\[ \psi(q) = 3 \cdot \frac{\sin(qR) - (qR) \cdot \cos(qR)}{(qR)^3} \]

\[ \Lambda(q) = \int_0^{qL} \frac{\sin(t)}{t} \frac{dt}{qL} \]

\[ \beta(q) = \int_{qR}^{qR(A-R)} \frac{\sin(t)}{qR} \frac{dt}{t} \]

where the mass \( m_i \) is (SLD\(_i\) - SLD\(_{solvent}\)) * (volume of the \( N \) pearls/rods). \( V \) is the total volume of the necklace.

The 2D scattering intensity is the same as \( P(q) \) above, regardless of the orientation of the \( q \) vector.

The returned value is scaled to units of cm\(^{-1}\) and the parameters of the pearl_necklace model are the following

NB: num_pearls must be an integer.

References


**pringle**

The Pringle model provides the form factor, \( P(q) \), for a ‘pringle’ or ‘saddle-shaped’ disc that is bent in two directions.
Fig. 1.33: 1D plot corresponding to the default parameters of the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>radius</td>
<td>Pringle radius</td>
<td>Å</td>
<td>60</td>
</tr>
<tr>
<td>thickness</td>
<td>Thickness of pringle</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>alpha</td>
<td>Curvature parameter alpha</td>
<td>None</td>
<td>0.001</td>
</tr>
<tr>
<td>beta</td>
<td>Curvature parameter beta</td>
<td>None</td>
<td>0.02</td>
</tr>
<tr>
<td>sld</td>
<td>Pringle sld</td>
<td>Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent sld</td>
<td>Å(^{-2})</td>
<td>6.3</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition**

The form factor for this bent disc is essentially that of a hyperbolic paraboloid and calculated as

\[
P(q) = (\Delta \rho)^2 V \int_0^{\pi/2} d\psi \sin \psi \sin^2 \left( \frac{qd \cos \psi}{2} \right) \left[ \left( S_0^2 + C_0^2 \right) + 2 \sum_{n=1}^{\infty} \left( S_n^2 + C_n^2 \right) \right]
\]

where

\[
C_n = \frac{1}{r^2} \int_0^R rdr \cos(qr^2 \alpha \cos \psi) J_n(qr^2 \alpha \cos \psi) J_{2n}(qr \sin \psi)
\]

and

\[
S_n = \frac{1}{r^2} \int_0^R rdr \sin(qr^2 \alpha \cos \psi) J_n(qr^2 \alpha \cos \psi) J_{2n}(qr \sin \psi)
\]

and \(\Delta \rho = \rho_{\text{pringle}} - \rho_{\text{solvent}}\), \(V\) is the volume of the disc, \(\psi\) is the angle between the normal to the disc and the q vector, \(d\) and \(R\) are the “pringle” thickness and radius respectively, \(\alpha\) and \(\beta\) are the two curvature parameters, and \(J_n\) is the \(n^{th}\) order Bessel function of the first kind.

**Reference**


- **Author:** Andrew Jackson  **Date:** 2008
Fig. 1.34: Schematic of model shape (Graphic from Matt Henderson, matt@matthen.com)

Fig. 1.35: 1D plot corresponding to the default parameters of the model.
**stacked_disks**

Form factor for a stacked set of non exfoliated core/shell disks

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>thick_core</td>
<td>Thickness of the core disk</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>thick_layer</td>
<td>Thickness of layer each side of core</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>radius</td>
<td>Radius of the stacked disk</td>
<td>Å</td>
<td>15</td>
</tr>
<tr>
<td>n_stacking</td>
<td>Number of stacked layer/core/layer disks</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>sigma_d</td>
<td>Sigma of nearest neighbor spacing</td>
<td>Å</td>
<td>0</td>
</tr>
<tr>
<td>sld_core</td>
<td>Core scattering length density</td>
<td>10⁶Å⁻²</td>
<td>4</td>
</tr>
<tr>
<td>sld_layer</td>
<td>Layer scattering length density</td>
<td>10⁶Å⁻²</td>
<td>0</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10⁶Å⁻²</td>
<td>5</td>
</tr>
<tr>
<td>theta</td>
<td>Orientation of the stacked disk axis w/respect incoming beam</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
<td>0</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

This model provides the form factor, $P(q)$, for stacked discs (tactoids) with a core/layer structure which is constructed itself as $P(q)S(Q)$ multiplying a $P(q)$ for individual core/layer disks by a structure factor $S(q)$ proposed by Kratky and Porod in 1949¹ assuming the next neighbor distance (d-spacing) in the stack of parallel discs obeys a Gaussian distribution. As such the normalization of this “composite” form factor is relative to the individual disk volume, not the volume of the stack of disks. This model is appropriate for example for non non exfoliated clay particles such as Laponite.

![Fig. 1.36: Geometry of a single core[layer disk](image)

The scattered intensity $I(q)$ is calculated as

$$I(q) = N \int_0^{\pi/2} [\Delta \rho_t (V_t f_t(q, \alpha) - V_c f_c(q, \alpha)) + \Delta \rho_c V_c f_c(q, \alpha)]^2 S(q, \alpha) \sin \alpha \, d\alpha + \text{background}$$

where the contrast

$$\Delta \rho_t = \rho_t - \rho_{\text{solvent}}$$

and $N$ is the number of individual (single) discs per unit volume, $\alpha$ is the angle between the axis of the disc and

¹ O Kratky and G Porod, J. Colloid Science, 4, (1949) 35
\( q \), and \( V_t \) and \( V_c \) are the total volume and the core volume of a single disc, respectively, and

\[
\begin{align*}
  f_t(q, \alpha) &= \left( \frac{\sin(q(d + h) \cos \alpha)}{q(d + h) \cos \alpha} \right) \left( \frac{2J_1(qR \sin \alpha)}{qR \sin \alpha} \right) \\
  f_c(q, \alpha) &= \left( \frac{\sin(qh \cos \alpha)}{qh \cos \alpha} \right) \left( \frac{2J_1(qR \sin \alpha)}{qR \sin \alpha} \right)
\end{align*}
\]

where \( d = \) thickness of the layer (\textit{thick} \_\textit{layer}), \( 2h = \) core thickness (\textit{thick} \_\textit{core}), and \( R = \) radius of the disc (\textit{radius}).

\[
S(q, \alpha) = 1 + \frac{1}{2} \sum_{k=1}^{n} (n - k) \cos (kDq \cos \alpha) \exp \left[ -k(q)^2 (D \cos \alpha \sigma_d)^2 / 2 \right]
\]

where \( n \) is the total number of the disc stacked (\textit{n} \_\textit{stacking}), \( D = 2(d + h) \) is the next neighbor center-to-center distance (d-spacing), and \( \sigma_d = \) the Gaussian standard deviation of the d-spacing (\textit{sigma} \_\textit{d}). Note that \( D \cos(\alpha) \) is the component of \( D \) parallel to \( q \) and the last term in the equation above is effectively a Debye-Waller factor term.

**Note:** 1. Each assembly in the stack is layer/core/layer, so the spacing of the cores is core plus two layers. The 2nd virial coefficient of the cylinder is calculated based on the \textit{radius} and \textit{length} = \textit{n} \_\textit{stacking} * \textit{thick} \_\textit{core} + 2 * \textit{thick} \_\textit{layer} values, and used as the effective radius for \( S(Q) \) when \( P(Q) \times S(Q) \) is applied.

2. The resolution smearing calculation uses 76 Gaussian quadrature points to properly smear the model since the function is HIGHLY oscillatory, especially around the \( q \)-values that correspond to the repeat distance of the layers.

2d scattering from oriented stacks is calculated in the same way as for cylinders, for further details of the calculation and angular dispersions see **Oriented particles**.

---

**Fig. 1.37:** Angles \( \theta \) and \( \phi \) orient the stack of discs relative to the beam line coordinates, where the beam is along the \( z \) axis. Rotation \( \theta \), initially in the \( xz \) plane, is carried out first, then rotation \( \phi \) about the \( z \) axis. Orientation distributions are described as rotations about two perpendicular axes \( \delta_1 \) and \( \delta_2 \) in the frame of the cylinder itself, which when \( \theta = \phi = 0 \) are parallel to the \( Y \) and \( X \) axes.

Our model is derived from the form factor calculations implemented in a c-library provided by the NIST Center for Neutron Research.\(^2\)

## 1.1.2 Ellipsoid Functions

**core_shell_ellipsoid**

Form factor for an spheroid ellipsoid particle with a core shell structure.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>radius_equat_core</td>
<td>Equatorial radius of core</td>
<td>Å</td>
<td>20</td>
</tr>
<tr>
<td>x_core</td>
<td>Axial ratio of core, X = r_polar/r_equatorial</td>
<td>None</td>
<td>3</td>
</tr>
<tr>
<td>thick_shell</td>
<td>Thickness of shell at equator</td>
<td>Å</td>
<td>30</td>
</tr>
<tr>
<td>x_polar_shell</td>
<td>Ratio of thickness of shell at pole to that at equator</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>sld_core</td>
<td>Core scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>2</td>
</tr>
<tr>
<td>sld_shell</td>
<td>Shell scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>6.3</td>
</tr>
<tr>
<td>theta</td>
<td>Ellipsoid axis to beam angle</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
<td>0</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition**

Parameters for this model are the core axial ratio X and a shell thickness, which are more often what we would like to determine and makes the model better behaved, particularly when polydispersity is applied than the four independent radii used in the original parameterization of this model.
The geometric parameters of this model are shown in the diagram above, which shows (a) a cut through at the circular equator and (b) a cross section through the poles, of a prolate ellipsoid.

When $X_{core} < 1$ the core is oblate; when $X_{core} > 1$ it is prolate. $X_{core} = 1$ is a spherical core.

For a fixed shell thickness $X_{polarShell} = 1$, to scale the shell thickness pro-rata with the radius set or constrain $X_{polarShell} = X_{core}$.

When including an $S(q)$, the radius in $S(q)$ is calculated to be that of a sphere with the same 2nd virial coefficient of the outer surface of the ellipsoid. This may have some undesirable effects if the aspect ratio of the ellipsoid is large (ie, if $X << 1$ or $X >> 1$), when the $S(q)$ - which assumes spheres - will not in any case be valid. Generating a custom product model will enable separate effective volume fraction and effective radius in the $S(q)$.

If SAS data are in absolute units, and the SLDs are correct, then scale should be the total volume fraction of the “outer particle”. When $S(q)$ is introduced this moves to the $S(q)$ volume fraction, and scale should then be 1.0, or contain some other units conversion factor (for example, if you have SAXS data).

The calculation of intensity follows that for the solid ellipsoid, but with separate terms for the core-shell and shell-solvent boundaries.

$$P(q, \alpha) = \frac{\text{scale}}{V} F^2(q, \alpha) + \text{background}$$

where

$$F(q, \alpha) = f(q, \text{radius\_equat\_core}, \text{radius\_equat\_core\_x\_core}, \alpha)$$

$$+ f(q, \text{radius\_equat\_core} + \text{thick\_shell}, \text{radius\_equat\_core\_x\_core} + \text{thick\_shell\_x\_polar\_shell}, \alpha)$$

where

$$f(q, R_e, R_p, \alpha) = \frac{3\Delta p V [\sin(qr(R_p, R_e, \alpha)) - \cos(qr(R_p, R_e, \alpha))]}{[qr(R_p, R_e, \alpha)]^3}$$

and

$$r(R_e, R_p, \alpha) = \left[ R_e^2 \sin^2 \alpha + R_p^2 \cos^2 \alpha \right]^{1/2}$$

$\alpha$ is the angle between the axis of the ellipsoid and $\vec{q}$, $V = (4/3)\pi R_p R_e^2$ is the volume of the ellipsoid, $R_p$ is the polar radius along the rotational axis of the ellipsoid, $R_e$ is the equatorial radius perpendicular to the rotational
axis of the ellipsoid and \( \Delta \rho \) (contrast) is the scattering length density difference, either \((\text{sld\_core} - \text{sld\_shell})\) or \((\text{sld\_shell} - \text{sld\_solvent})\).

For randomly oriented particles:

\[
F^2(q) = \int_{0}^{\pi/2} F^2(q, \alpha) \sin(\alpha) d\alpha
\]

For oriented ellipsoids the \( \theta, \phi \) and \( \psi \) orientation parameters will appear when fitting 2D data, see the \textit{elliptical\_cylinder} model for further information.

Fig. 1.39: 1D and 2D plots corresponding to the default parameters of the model.


**Authorship and Verification**

- **Author**: NIST IGOR/DANSE Date: pre 2010
- **Last Modified by**: Richard Heenan (reparametrised model) Date: 2015
- **Last Reviewed by**: Richard Heenan Date: October 6, 2016

**ellipsoid**

Ellipsoid of revolution with uniform scattering length density.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>sld</td>
<td>Ellipsoid scattering length density</td>
<td>(10^6) Å(^{-2})</td>
<td>4</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>(10^6) Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>radius_polar</td>
<td>Polar radius</td>
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<tr>
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<td>Equatorial radius</td>
<td>Å</td>
<td>400</td>
</tr>
<tr>
<td>theta</td>
<td>ellipsoid axis to beam angle</td>
<td>degree</td>
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</tr>
<tr>
<td>phi</td>
<td>rotation axis to beam</td>
<td>degree</td>
<td>60</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

The form factor is normalized by the particle volume

1.1. Model Functions
Definition

The output of the 2D scattering intensity function for oriented ellipsoids is given by (Feigin, 1987)

\[ P(q, \alpha) = \frac{\text{scale}}{V} F^2(q, \alpha) + \text{background} \]

where

\[ F(q, \alpha) = \Delta \rho V \frac{3(\sin qr - qr \cos qr)}{(qr)^3} \]

for

\[ r = \left[ R_e^2 \sin^2 \alpha + R_p^2 \cos^2 \alpha \right]^{1/2} \]

\( \alpha \) is the angle between the axis of the ellipsoid and \( \vec{q} \), \( V = \frac{4}{3} \pi R_p R_e^2 \) is the volume of the ellipsoid, \( R_p \) is the polar radius along the rotational axis of the ellipsoid, \( R_e \) is the equatorial radius perpendicular to the rotational axis of the ellipsoid and \( \Delta \rho \) (contrast) is the scattering length density difference between the scatterer and the solvent.

For randomly oriented particles use the orientational average,

\[ \langle F^2(q) \rangle = \int_0^{\pi/2} F^2(q, \alpha) \sin(\alpha) \, d\alpha \]

computed via substitution of \( u = \sin(\alpha) \), \( du = \cos(\alpha) \, d\alpha \) as

\[ \langle F^2(q) \rangle = \int_0^1 F^2(q, u) \, du \]

with

\[ r = R_e \left[ 1 + u^2 \left( R_p^2/R_e^2 - 1 \right) \right]^{1/2} \]

For 2d data from oriented ellipsoids the direction of the rotation axis of the ellipsoid is defined using two angles \( \theta \) and \( \phi \) as for the cylinder orientation figure. For the ellipsoid, \( \theta \) is the angle between the rotational axis and the \( z \)-axis in the \( xz \) plane followed by a rotation by \( \phi \) in the \( xy \) plane, for further details of the calculation and angular dispersions see Oriented particles.

NB: The 2nd virial coefficient of the solid ellipsoid is calculated based on the \( R_p \) and \( R_e \) values, and used as the effective radius for \( S(q) \) when \( P(q) \cdot S(q) \) is applied.

The \( \theta \) and \( \phi \) parameters are not used for the 1D output.

Validation

Validation of the code was done by comparing the output of the 1D model to the output of the software provided by the NIST (Kline, 2006).

The implementation of the intensity for fully oriented ellipsoids was validated by averaging the 2D output using a uniform distribution \( p(\theta, \phi) = 1.0 \) and comparing with the output of the 1D calculation.

The discrepancy above \( q = 0.3 \text{ cm}^{-1} \) is due to the way the form factors are calculated in the c-library provided by NIST. A numerical integration has to be performed to obtain \( P(q) \) for randomly oriented particles. The NIST software performs that integration with a 76-point Gaussian quadrature rule, which will become imprecise at high \( q \) where the amplitude varies quickly as a function of \( q \). The SasView result shown has been obtained by summing over 501 equidistant points. Our result was found to be stable over the range of \( q \) shown for a number of points higher than 500.

Model was also tested against the triaxial ellipsoid model with equal major and minor equatorial radii. It is also consistent with the cyclinder model with polar radius equal to length and equatorial radius equal to radius.

References

Fig. 1.40: Comparison of the intensity for uniformly distributed ellipsoids calculated from our 2D model and the intensity from the NIST SANS analysis software. The parameters used were: scale = 1.0, radius_polar = 20 Å, radius_equatorial = 400 Å, contrast = 3e-6 Å⁻², and background = 0.0 cm⁻¹.

Fig. 1.41: 1D and 2D plots corresponding to the default parameters of the model.
triaxial_ellipsoid

Ellipsoid of uniform scattering length density with three independent axes.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>sld</td>
<td>Ellipsoid scattering length density</td>
<td>10⁻⁶ Å⁻²</td>
<td>4</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10⁻⁶ Å⁻²</td>
<td>1</td>
</tr>
<tr>
<td>radius_equat_minor</td>
<td>Minor equatorial radius, Ra</td>
<td>Å</td>
<td>20</td>
</tr>
<tr>
<td>radius_equat_major</td>
<td>Major equatorial radius, Rb</td>
<td>Å</td>
<td>400</td>
</tr>
<tr>
<td>radius_polar</td>
<td>Polar radius, Rc</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>theta</td>
<td>polar axis to beam angle</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>phi</td>
<td>rotation about beam</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>psi</td>
<td>rotation about polar axis</td>
<td>degree</td>
<td>60</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

Given an ellipsoid

\[
\frac{X^2}{R_a^2} + \frac{Y^2}{R_b^2} + \frac{Z^2}{R_c^2} = 1
\]

the scattering for randomly oriented particles is defined by the average over all orientations \(\Omega\) of:

\[
P(q) = \text{scale}(\Delta \rho)^2 \frac{V}{4\pi} \int_{\Omega} \Phi(qr) \, d\Omega + \text{background}
\]

where

\[
\Phi(qr) = 3j_1(qr)/qr = 3(sin qr - qr \cos qr)/(qr)^3
\]

\[
r^2 = R_a^2 e^2 + R_b^2 f^2 + R_c^2 g^2
\]

\[
V = \frac{4}{3} \pi R_a R_b R_c
\]

Fig. 1.42: Ellipsoid with \(R_a\) as radius_equat_minor, \(R_b\) as radius_equat_major and \(R_c\) as radius_polar.
The $e$, $f$ and $g$ terms are the projections of the orientation vector on $X$, $Y$ and $Z$ respectively. Keeping the orientation fixed at the canonical axes, we can integrate over the incident direction using polar angle $-\pi/2 \leq \gamma \leq \pi/2$ and equatorial angle $0 \leq \phi \leq 2\pi$ (as defined in ref [1]),

$$\langle \Phi^2 \rangle = \int_{-\pi/2}^{\pi/2} \int_{0}^{2\pi} \Phi^2(qr) \cos \gamma \, d\gamma \, d\phi$$

with $e = \cos \gamma \sin \phi$, $f = \cos \gamma \cos \phi$ and $g = \sin \gamma$. A little algebra yields

$$r^2 = b^2(p_a \sin^2 \phi \cos^2 \gamma + 1 + p_c \sin^2 \gamma)$$

for

$$p_a = \frac{a^2}{b^2} - 1 \text{ and } p_c = \frac{c^2}{b^2} - 1$$

Due to symmetry, the ranges can be restricted to a single quadrant $0 \leq \gamma \leq \pi/2$ and $0 \leq \phi \leq \pi/2$, scaling the resulting integral by 8. The computation is done using the substitution $u = \sin \gamma$, $du = \cos \gamma \, d\gamma$, giving

$$\langle \Phi^2 \rangle = 8 \int_{0}^{\pi/2} \int_{0}^{1} \Phi^2(qr) \, du \, d\phi$$

$$r^2 = b^2(p_a \sin^2(\phi)(1 - u^2) + 1 + p_c u^2)$$

Though for convenience we describe the three radii of the ellipsoid as equatorial and polar, they may be given in any size order. To avoid multiple solutions, especially with Monte-Carlo fit methods, it may be advisable to restrict their ranges. For typical small angle diffraction situations there may be a number of closely similar “best fits”, so some trial and error, or fixing of some radii at expected values, may help.

To provide easy access to the orientation of the triaxial ellipsoid, we define the axis of the cylinder using the angles $\theta$, $\phi$ and $\psi$. These angles are defined analogously to the elliptical_cylinder below, note that angle $\phi$ is now NOT the same as in the equations above.

For oriented ellipsoids the $\text{theta}$, $\text{phi}$ and $\text{psi}$ orientation parameters will appear when fitting 2D data, see the elliptical_cylinder model for further information.

The radius-of-gyration for this system is $R_g^2 = (R_a R_b R_c)^2 / 5$.

The contrast $\Delta \rho$ is defined as $\text{SLD(ellipsoid)} - \text{SLD(solvent)}$. In the parameters, $R_a$ is the minor equatorial radius, $R_b$ is the major equatorial radius, and $R_c$ is the polar radius of the ellipsoid.

NB: The 2nd virial coefficient of the triaxial solid ellipsoid is calculated after sorting the three radii to give the most appropriate prolate or oblate form, from the new polar radius $R_p = R_c$ and effective equatorial radius, $R_e = \sqrt{R_a R_b}$, to then be used as the effective radius for $S(q)$ when $P(q) \cdot S(q)$ is applied.

Validation

Validation of our code was done by comparing the output of the 1D calculation to the angular average of the output of 2D calculation over all possible angles.

References


Authorship and Verification

- **Author:** NIST IGOR/DANSE Date: pre 2010
- **Last Modified by:** Paul Kienzle (improved calculation) Date: April 4, 2017
- **Last Reviewed by:** Paul Kienzle & Richard Heenan Date: April 4, 2017
Fig. 1.43: Definition of angles for oriented triaxial ellipsoid, where radii are for illustration here $a < b << c$ and angle $\Psi$ is a rotation around the axis of the particle.
Fig. 1.44: Some examples for an oriented triaxial ellipsoid.

Fig. 1.45: 1D and 2D plots corresponding to the default parameters of the model.
1.1.3 Lamellae Functions

**lamellar**

Lyotropic lamellar phase with uniform SLD and random distribution

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
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<tr>
<td>thickness</td>
<td>total layer thickness</td>
<td>Å</td>
<td>50</td>
</tr>
<tr>
<td>sld</td>
<td>Layer scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>1</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>6</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

Polydispersity in the bilayer thickness can be applied from the GUI.

**Definition**

The scattering intensity \( I(q) \) for dilute, randomly oriented, “infinitely large” sheets or lamellae is

\[
I(q) = \text{scale} \frac{2\pi P(q)}{q^2 \delta} + \text{background}
\]

The form factor is

\[
P(q) = \frac{2\Delta \rho^2}{q^2} (1 - \cos(q\delta)) = \frac{4\Delta \rho^2}{q^2} \sin^2 \left( \frac{q\delta}{2} \right)
\]

where \( \delta \) is the total layer thickness and \( \Delta \rho \) is the scattering length density difference.

This is the limiting form for a spherical shell of infinitely large radius. Note that the division by \( \delta \) means that \textit{scale} in sasview is the volume fraction of sheet, \( \phi = S \delta \) where \( S \) is the area of sheet per unit volume. \( S \) is half the Porod surface area per unit volume of a thicker layer (as that would include both faces of the sheet).

The 2D scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

**References**


**lamellar_hg**

Random lamellar phase with Head and Tail Groups

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>length_tail</td>
<td>Tail thickness ( total = H+T+T+H)</td>
<td>Å</td>
<td>15</td>
</tr>
<tr>
<td>length_head</td>
<td>Head thickness</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>sld</td>
<td>Tail scattering length density</td>
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</tr>
<tr>
<td>sld_head</td>
<td>Head scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>3</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>6</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.
This model provides the scattering intensity, $I(q)$, for a lyotropic lamellar phase where a random distribution in solution are assumed. The SLD of the head region is taken to be different from the SLD of the tail region.

**Definition**

The scattering intensity $I(q)$ is

$$I(q) = 2\pi \frac{\text{scale}}{2(\delta_H + \delta_T)} P(q) \frac{1}{q^2}$$

The form factor $P(q)$ is

$$P(q) = \frac{4}{q^2} \left\{ \Delta \rho_H \left[ \sin[q(\delta_H + \delta_T)] - \sin(q\delta_T)] \right] + \Delta \rho_T \sin(q\delta_T) \right\}^2$$

where $\delta_T$ is $\text{length}_\text{tail}$, $\delta_H$ is $\text{length}_\text{head}$, $\Delta \rho_H$ is the head contrast ($\text{sld}_\text{head} - \text{sld}_\text{solvent}$), and $\Delta \rho_T$ is tail contrast ($\text{sld} - \text{sld}_\text{solvent}$).

The total thickness of the lamellar sheet is $\delta_H + \delta_T + \delta_T + \delta_H$. Note that in a non aqueous solvent the chemical “head” group may be the “Tail region” and vice-versa.

The 2D scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

**References**


2014/04/17 - Description reviewed by S King and P Butler.

**lamellar_hg_stack_caille**

Random lamellar head/tail/tail/head sheet with Caille structure factor
Fig. 1.47: 1D plot corresponding to the default parameters of the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>length_tail</td>
<td>Tail thickness</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>length_head</td>
<td>head thickness</td>
<td>Å</td>
<td>2</td>
</tr>
<tr>
<td>Nlayers</td>
<td>Number of layers</td>
<td>None</td>
<td>30</td>
</tr>
<tr>
<td>d_spacing</td>
<td>lamellar d-spacing of Caille S(Q)</td>
<td>Å</td>
<td>40</td>
</tr>
<tr>
<td>Caille_parameter</td>
<td>Caille parameter</td>
<td>None</td>
<td>0.001</td>
</tr>
<tr>
<td>sld</td>
<td>Tail scattering length density</td>
<td>10⁶Å⁻²</td>
<td>0.4</td>
</tr>
<tr>
<td>sld_head</td>
<td>Head scattering length density</td>
<td>10⁶Å⁻²</td>
<td>2</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10⁶Å⁻²</td>
<td>6</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

This model provides the scattering intensity, \( I(q) = P(q)S(q) \), for a lamellar phase where a random distribution in solution are assumed. Here a Caille \( S(q) \) is used for the lamellar stacks.

The scattering intensity \( I(q) \) is

\[
I(q) = 2\pi \frac{P(q)S(q)}{q^2\delta}
\]

The form factor \( P(q) \) is

\[
P(q) = \frac{4}{q^2} \left\{ \Delta \rho_H [\sin[q(\delta_H + \delta_T)] - \sin(q\delta_T)] + \Delta \rho_T \sin(q\delta_T) \right\}^2
\]

and the structure factor \( S(q) \) is

\[
S(q) = 1 + 2 \sum_{n}^{N-1} \left(1 - \frac{n}{N}\right) \cos(qdn) \exp \left(-\frac{2q^2d^2\alpha(n)}{2}\right)
\]
where

\[ \alpha(n) = \frac{\eta_{cp}}{4\pi^2} (\ln(\pi n) + \gamma_E) \]

\[ \gamma_E = 0.5772156649 \quad \text{Euler’s constant} \]

\[ \eta_{cp} = \frac{q^2 k_B T}{8\pi \sqrt{K B}} \quad \text{Caille constant} \]

\[ \delta_T \text{ is the tail length (or length\_tail)}, \delta_H \text{ is the head thickness (or length\_head)}, \Delta\rho_H \text{ is SLD(headgroup) - SLD(solvent)}, \text{and } \Delta\rho_T \text{ is SLD(tail) - SLD(headgroup)\. Here } d \text{ is (repeat) spacing, } K \text{ is smectic bending elasticity, } B \text{ is compression modulus, and } N \text{ is the number of lamellar plates (Nlayers).} \]

**NB:** **When the Caille parameter is greater than approximately 0.8 to 1.0, the assumptions of the model are incorrect.** And due to a complication of the model function, users are responsible for making sure that all the assumptions are handled accurately (see the original reference below for more details).

Non-integer numbers of stacks are calculated as a linear combination of results for the next lower and higher values.

Be aware that the computations may be very slow.

The 2D scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[ q = \sqrt{q_x^2 + q_y^2} \]

![Fig. 1.48: 1D plot corresponding to the default parameters of the model.](image)

**References**


**lamellar_stack_caille**

Random lamellar sheet with Caille structure factor
The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model provides the scattering intensity, \(I(q) = P(q)S(q)\), for a lamellar phase where a random distribution in solution are assumed. Here a Caille \(S(q)\) is used for the lamellar stacks.

**Definition**

The scattering intensity \(I(q)\) is

\[
I(q) = 2\pi \frac{P(q)S(q)}{q^2 \delta}
\]

The form factor is

\[
P(q) = \frac{2\Delta \rho^2}{q^2} (1 - \cos q\delta)
\]

and the structure factor is

\[
S(q) = 1 + 2 \sum_{n=1}^{N-1} \left(1 - \frac{n}{N}\right) \cos(qdn) \exp\left(-\frac{2q^2d^2\alpha(n)}{2}\right)
\]

where

\[
\alpha(n) = \frac{\eta_cp}{4\pi^2} (\ln(n\pi) + \gamma_E)
\]

\[
\gamma_E = 0.5772156649 \quad \text{Euler’s constant}
\]

\[
\eta_cp = \frac{q_x^2k_BT}{8\pi\sqrt{KB}} \quad \text{Caille constant}
\]

Here \(d\) = (repeat) \(d\_spacing\), \(\delta\) = bilayer thickness, the contrast \(\Delta \rho = \text{SLD(headgroup)} - \text{SLD(solvent)}\), \(K = \text{smectic bending elasticity}\), \(B = \text{compression modulus}\), and \(N = \text{number of lamellar plates (n\_plates)}\).

**NB:** When the Caille parameter is greater than approximately 0.8 to 1.0, the assumptions of the model are incorrect. And due to a complication of the model function, users are responsible for making sure that all the assumptions are handled accurately (see the original reference below for more details).

Non-integer numbers of stacks are calculated as a linear combination of results for the next lower and higher values.

The 2D scattering intensity is calculated in the same way as 1D, where the \(q\) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

**References**


Fig. 1.49: 1D plot corresponding to the default parameters of the model.

**lamellar_stack_paracrystal**

Random lamellar sheet with paracrystal structure factor

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>thickness</td>
<td>sheet thickness</td>
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<td>33</td>
</tr>
<tr>
<td>Nlayers</td>
<td>Number of layers</td>
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<td>20</td>
</tr>
<tr>
<td>d_spacing</td>
<td>lamellar spacing of paracrystal stack</td>
<td>Å</td>
<td>250</td>
</tr>
<tr>
<td>sigma_d</td>
<td>Sigma (polydispersity) of the lamellar spacing</td>
<td>Å</td>
<td>0</td>
</tr>
<tr>
<td>sdl</td>
<td>layer scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>sdl_solvent</td>
<td>Solvent scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>6.34</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model calculates the scattering from a stack of repeating lamellar structures. The stacks of lamellae (infinite in lateral dimension) are treated as a paracrystal to account for the repeating spacing. The repeat distance is further characterized by a Gaussian polydispersity. **This model can be used for large multilamellar vesicles.**

**Definition**

In the equations below,

- *scale* is used instead of the mass per area of the bilayer \(\Gamma_m\) (this corresponds to the volume fraction of the material in the bilayer, *not* the total excluded volume of the paracrystal),
- *sld* – *sld_solvent* is the contrast \(\Delta \rho\),
- *thickness* is the layer thickness \(t\),
- *Nlayers* is the number of layers \(N\),
- *d_spacing* is the average distance between adjacent layers \(\langle D \rangle\), and
- *sigma_d* is the relative standard deviation of the Gaussian layer distance distribution \(\sigma_D/\langle D \rangle\).
The scattering intensity $I(q)$ is calculated as

$$I(q) = 2\pi\Delta\rho^2\Gamma_m \frac{P_{\text{bil}}(q)}{q^2} Z_N(q)$$

The form factor of the bilayer is approximated as the cross section of an infinite, planar bilayer of thickness $t$ (compare the equations for the lamellar model).

$$P_{\text{bil}}(q) = \left( \frac{\sin(qt/2)}{qt/2} \right)^2$$

$Z_N(q)$ describes the interference effects for aggregates consisting of more than one bilayer. The equations used are (3-5) from the Bergstrom reference:

$$Z_N(q) = \frac{1 - w^2}{1 + w^2 - 2w \cos(q\langle D \rangle)} + x_N S_N + (1 - x_N) S_{N+1}$$

where

$$S_N(q) = \frac{a_N}{N} [1 + w^2 - 2w \cos(q\langle D \rangle)]^2$$

and

$$a_N = 4w^2 - 2(w^3 + w) \cos(q\langle D \rangle) - 4w^{N+2} \cos(Nq\langle D \rangle) + 2w^{N+3} \cos[(N-1)q\langle D \rangle] + 2w^{N+1} \cos[(N+1)q\langle D \rangle]$$

for the layer spacing distribution $w = \exp(-\sigma^2 q^2/2)$.

Non-integer numbers of stacks are calculated as a linear combination of the lower and higher values

$$N_L = x_N N + (1 - x_N)(N + 1)$$

The 2D scattering intensity is the same as 1D, regardless of the orientation of the $q$ vector which is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

Fig. 1.50: 1D plot corresponding to the default parameters of the model.

Reference

1.1.4 Paracrystal Functions

**bcc_paracrystal**

Body-centred cubic lattice with paracrystalline distortion

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
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</tr>
<tr>
<td>dnn</td>
<td>Nearest neighbour distance</td>
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<td>220</td>
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<td>d_factor</td>
<td>Paracrystal distortion factor</td>
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<td>Particle radius</td>
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</tr>
<tr>
<td>sld</td>
<td>Particle scattering length density</td>
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<td>4</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10⁻⁶ Å⁻²</td>
<td>1</td>
</tr>
<tr>
<td>theta</td>
<td>c axis to beam angle</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>psi</td>
<td>rotation about beam</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>psi</td>
<td>rotation about c axis</td>
<td>degree</td>
<td>60</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Warning:** This model and this model description are under review following concerns raised by SasView users. If you need to use this model, please email help@sasview.org for the latest situation. The SasView Developers. September 2018.

**Definition**

Calculates the scattering from a body-centered cubic lattice with paracrystalline distortion. Thermal vibrations are considered to be negligible, and the size of the paracrystal is infinitely large. Paracrystalline distortion is assumed to be isotropic and characterized by a Gaussian distribution.

The scattering intensity $I(q)$ is calculated as

$$I(q) = \frac{\text{scale}}{V_p} V_{lattice} P(q) Z(q)$$

where *scale* is the volume fraction of spheres, $V_p$ is the volume of the primary particle, $V_{lattice}$ is a volume correction for the crystal structure, $P(q)$ is the form factor of the sphere (normalized), and $Z(q)$ is the paracrystalline structure factor for a body-centered cubic structure.

Equation (1) of the 1990 reference² is used to calculate $Z(q)$, using equations (29)-(31) from the 1987 paper¹ for $Z_1$, $Z_2$, and $Z_3$.

The lattice correction (the occupied volume of the lattice) for a body-centered cubic structure of particles of radius $R$ and nearest neighbor separation $D$ is

$$V_{lattice} = \frac{16\pi}{3} \frac{R^3}{(D\sqrt{2})^3}$$

The distortion factor (one standard deviation) of the paracrystal is included in the calculation of $Z(q)$

$$\Delta a = gD$$

where $g$ is a fractional distortion based on the nearest neighbor distance.

For a crystal, diffraction peaks appear at reduced q-values given by

$$\frac{qD}{2\pi} = \sqrt{h^2 + k^2 + l^2}$$

---

where for a body-centered cubic lattice, only reflections where \((h + k + l) = \text{even}\) are allowed and reflections where \((h + k + l) = \text{odd}\) are forbidden. Thus the peak positions correspond to (just the first 5):

\[
\begin{array}{cccccc}
q/q_0 & 1 & \sqrt{2} & \sqrt{3} & \sqrt{4} & \sqrt{5} \\
Indices & (110) & (200) & (211) & (220) & (310)
\end{array}
\]

**Note:** The calculation of \(Z(q)\) is a double numerical integral that must be carried out with a high density of points to properly capture the sharp peaks of the paracrystalline scattering. So be warned that the calculation is slow. Fitting of any experimental data must be resolution smeared for any meaningful fit. This makes a triple integral which may be very slow.

This example dataset is produced using 200 data points, \(q_{\text{min}} = 0.001 \text{ Å}^{-1}, q_{\text{max}} = 0.1 \text{ Å}^{-1}\) and the above default values.

The 2D (Anisotropic model) is based on the reference below where \(I(q)\) is approximated for 1d scattering. Thus the scattering pattern for 2D may not be accurate, particularly at low \(q\). For general details of the calculation and angular dispersions for oriented particles see Oriented particles. Note that we are not responsible for any incorrectness of the 2D model computation.

**References**

**Authorship and Verification**

- **Author:** NIST IGOR/DANSE  **Date:** pre 2010
- **Last Modified by:** Paul Butler  **Date:** September 29, 2016
- **Last Reviewed by:** Richard Heenan  **Date:** March 21, 2016

**fcc_paracrystal**

Face-centred cubic lattice with paracrystalline distortion
Fig. 1.52: Orientation of the crystal with respect to the scattering plane, when $\theta = \phi = 0$ the $c$ axis is along the beam direction (the $z$ axis).

Fig. 1.53: 1D and 2D plots corresponding to the default parameters of the model.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>dnn</td>
<td>Nearest neighbour distance</td>
<td>Å</td>
<td>220</td>
</tr>
<tr>
<td>d_factor</td>
<td>Paracrystal distortion factor</td>
<td>None</td>
<td>0.06</td>
</tr>
<tr>
<td>radius</td>
<td>Particle radius</td>
<td>Å</td>
<td>40</td>
</tr>
<tr>
<td>sld</td>
<td>Particle scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>4</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>1</td>
</tr>
<tr>
<td>theta</td>
<td>c axis to beam angle</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>phi</td>
<td>rotation about beam</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>psi</td>
<td>rotation about c axis</td>
<td>degree</td>
<td>60</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Warning:** This model and this model description are under review following concerns raised by SasView users. If you need to use this model, please email help@sasview.org for the latest situation. *The SasView Developers. September 2018.*

**Definition**

Calculates the scattering from a **face-centered cubic lattice** with paracrystalline distortion. Thermal vibrations are considered to be negligible, and the size of the paracrystal is infinitely large. Paracrystalline distortion is assumed to be isotropic and characterized by a Gaussian distribution.

The scattering intensity $I(q)$ is calculated as

$$I(q) = \frac{\text{scale}}{V_p} V_{\text{lattice}} P(q) Z(q)$$

where `scale` is the volume fraction of spheres, $V_p$ is the volume of the primary particle, $V_{\text{lattice}}$ is a volume correction for the crystal structure, $P(q)$ is the form factor of the sphere (normalized), and $Z(q)$ is the paracrystalline structure factor for a face-centered cubic structure.

Equation (1) of the 1990 reference² is used to calculate $Z(q)$, using equations (23)-(25) from the 1987 paper¹ for $Z_1$, $Z_2$, and $Z_3$.

The lattice correction (the occupied volume of the lattice) for a face-centered cubic structure of particles of radius $R$ and nearest neighbor separation $D$ is

$$V_{\text{lattice}} = \frac{16\pi}{3} \frac{R^3}{(D\sqrt{2})^3}$$

The distortion factor (one standard deviation) of the paracrystal is included in the calculation of $Z(q)$

$$\Delta a = gD$$

where $g$ is a fractional distortion based on the nearest neighbor distance.

For a crystal, diffraction peaks appear at reduced q-values given by

$$\frac{qD}{2\pi} = \sqrt{h^2 + k^2 + l^2}$$

where for a face-centered cubic lattice $h, k, l$ all odd or all even are allowed and reflections where $h, k, l$ are mixed odd/even are forbidden. Thus the peak positions correspond to (just the first 5)

<table>
<thead>
<tr>
<th>Indices (111) (200) (220) (311) (222)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q/q_0$ 1 $\sqrt{4/3}$ $\sqrt{8/3}$ $\sqrt{11/3}$ $\sqrt{7}$</td>
</tr>
</tbody>
</table>


Note: The calculation of \( Z(q) \) is a double numerical integral that must be carried out with a high density of points to properly capture the sharp peaks of the paracrystalline scattering. So be warned that the calculation is slow. Fitting of any experimental data must be resolution smeared for any meaningful fit. This makes a triple integral which may be very slow.

The 2D (Anisotropic model) is based on the reference below where \( I(q) \) is approximated for 1d scattering. Thus the scattering pattern for 2D may not be accurate particularly at low \( q \). For general details of the calculation and angular dispersions for oriented particles see Oriented particles. Note that we are not responsible for any incorrectness of the 2D model computation.

References

Authorship and Verification

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
- **Last Modified by:** Paul Butler **Date:** September 29, 2016
- **Last Reviewed by:** Richard Heenan **Date:** March 21, 2016

**sc_paracrystal**

Simple cubic lattice with paracrystalline distorton

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-2})</td>
<td>0.001</td>
</tr>
<tr>
<td>dnn</td>
<td>Nearest neighbor distance</td>
<td>Å</td>
<td>220</td>
</tr>
<tr>
<td>d_factor</td>
<td>Paracrystal distortion factor</td>
<td>None</td>
<td>0.06</td>
</tr>
<tr>
<td>radius</td>
<td>Radius of sphere</td>
<td>Å</td>
<td>40</td>
</tr>
<tr>
<td>sld</td>
<td>Sphere scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>3</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>6.3</td>
</tr>
<tr>
<td>theta</td>
<td>c axis to beam angle</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>phi</td>
<td>rotation about beam</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>psi</td>
<td>rotation about c axis</td>
<td>degree</td>
<td>0</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

1.1. Model Functions
Fig. 1.55: Orientation of the crystal with respect to the scattering plane, when $\theta = \phi = 0$ the $c$ axis is along the beam direction (the $z$ axis).

Fig. 1.56: 1D and 2D plots corresponding to the default parameters of the model.
Warning: This model and this model description are under review following concerns raised by SasView users. If you need to use this model, please email help@sasview.org for the latest situation. The SasView Developers. September 2018.

Definition

Calculates the scattering from a simple cubic lattice with paracrystalline distortion. Thermal vibrations are considered to be negligible, and the size of the paracrystal is infinitely large. Paracrystalline distortion is assumed to be isotropic and characterized by a Gaussian distribution.

The scattering intensity $I(q)$ is calculated as

$$I(q) = \text{scale} \frac{V_{\text{lattice}} P(q) Z(q)}{V_p} + \text{background}$$

where scale is the volume fraction of spheres, $V_p$ is the volume of the primary particle, $V_{\text{lattice}}$ is a volume correction for the crystal structure, $P(q)$ is the form factor of the sphere (normalized), and $Z(q)$ is the paracrystalline structure factor for a simple cubic structure.

Equation (16) of the 1987 reference\(^1\) is used to calculate $Z(q)$, using equations (13)-(15) from the 1987 paper\(^1\) for $Z_1$, $Z_2$, and $Z_3$.

The lattice correction (the occupied volume of the lattice) for a simple cubic structure of particles of radius $R$ and nearest neighbor separation $D$ is

$$V_{\text{lattice}} = \frac{4\pi}{3} R^3 D^3$$

The distortion factor (one standard deviation) of the paracrystal is included in the calculation of $Z(q)$

$$\Delta a = gD$$

where $g$ is a fractional distortion based on the nearest neighbor distance.

The simple cubic lattice is

For a crystal, diffraction peaks appear at reduced q-values given by

$$\frac{qD}{2\pi} = \sqrt{h^2 + k^2 + l^2}$$

where for a simple cubic lattice any $h$, $k$, $l$ are allowed and none are forbidden. Thus the peak positions correspond to (just the first 5)

<table>
<thead>
<tr>
<th>Indices</th>
<th>$q/q_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>(100)</td>
<td>(110)</td>
</tr>
</tbody>
</table>

Note: The calculation of $Z(q)$ is a double numerical integral that must be carried out with a high density of points to properly capture the sharp peaks of the paracrystalline scattering. So be warned that the calculation is slow. Fitting of any experimental data must be resolution smeared for any meaningful fit. This makes a triple integral which may be very slow.

The 2D (Anisotropic model) is based on the reference below where $I(q)$ is approximated for 1d scattering. Thus the scattering pattern for 2D may not be accurate particularly at low $q$. For general details of the calculation and angular dispersions for oriented particles see Oriented particles. Note that we are not responsible for any incorrectness of the 2D model computation.

Reference

Authorship and Verification

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
- **Last Modified by:** Paul Butler **Date:** September 29, 2016
- **Last Reviewed by:** Richard Heenan **Date:** March 21, 2016

1.1.5 Parallelepiped Functions

**core_shell_parallelepiped**

Rectangular solid with a core-shell structure.
Fig. 1.58: 1D and 2D plots corresponding to the default parameters of the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm$^{-1}$</td>
<td>0.001</td>
</tr>
<tr>
<td>sld_core</td>
<td>Parallelepiped core scattering length density</td>
<td>$10^8$Å$^{-2}$</td>
<td>1</td>
</tr>
<tr>
<td>sld_a</td>
<td>Parallelepiped A rim scattering length density</td>
<td>$10^8$Å$^{-2}$</td>
<td>2</td>
</tr>
<tr>
<td>sld_b</td>
<td>Parallelepiped B rim scattering length density</td>
<td>$10^8$Å$^{-2}$</td>
<td>4</td>
</tr>
<tr>
<td>sld_c</td>
<td>Parallelepiped C rim scattering length density</td>
<td>$10^8$Å$^{-2}$</td>
<td>2</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>$10^8$Å$^{-2}$</td>
<td>6</td>
</tr>
<tr>
<td>length_a</td>
<td>Shorter side of the parallelepiped</td>
<td>Å</td>
<td>35</td>
</tr>
<tr>
<td>length_b</td>
<td>Second side of the parallelepiped</td>
<td>Å</td>
<td>75</td>
</tr>
<tr>
<td>length_c</td>
<td>Larger side of the parallelepiped</td>
<td>Å</td>
<td>400</td>
</tr>
<tr>
<td>thick_rim_a</td>
<td>Thickness of A rim</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>thick_rim_b</td>
<td>Thickness of B rim</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>thick_rim_c</td>
<td>Thickness of C rim</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>theta</td>
<td>$c$ axis to beam angle</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>phi</td>
<td>Rotation about beam</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>psi</td>
<td>Rotation about $c$ axis</td>
<td>degree</td>
<td>0</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

**Definition**

Calculates the form factor for a rectangular solid with a core-shell structure. The thickness and the scattering length density of the shell or “rim” can be different on each (pair) of faces. The three dimensions of the core of the parallelepiped (strictly here a cuboid) may be given in any size order as long as the particles are randomly oriented (i.e. take on all possible orientations see notes on 2D below). To avoid multiple fit solutions, especially with Monte-Carlo fit methods, it may be advisable to restrict their ranges. There may be a number of closely similar “best fits”, so some trial and error, or fixing of some dimensions at expected values, may help.

The form factor is normalized by the particle volume $V$ such that

$$I(q) = \frac{\text{scale}}{V} \langle P(q, \alpha, \beta) \rangle + \text{background}$$

where $\langle \ldots \rangle$ is an average over all possible orientations of the rectangular solid, and the usual $\Delta \rho^2 V^2$ term cannot be pulled out of the form factor term due to the multiple slds in the model.

1.1. Model Functions
The core of the solid is defined by the dimensions $A$, $B$, $C$ here shown such that $A < B < C$.

![Diagram of core of core shell parallelepiped with corresponding definition of sides.](image)

**Fig. 1.59:** Core of the core shell parallelepiped with the corresponding definition of sides.

There are rectangular “slabs” of thickness $t_A$ that add to the $A$ dimension (on the $BC$ faces). There are similar slabs on the $AC$ ($= t_B$) and $AB$ ($= t_C$) faces. The projection in the $AB$ plane is

![Diagram of AB cut through the core-shell parallelepiped showing the cross section of four of the six shell slabs.](image)

**Fig. 1.60:** AB cut through the core-shell parallelepiped showing the cross section of four of the six shell slabs. As can be seen, this model leaves “gaps” at the corners of the solid.

The total volume of the solid is thus given as

$$V = ABC + 2t_A BC + 2t_B AC + 2t_C AB$$

The intensity calculated follows the parallelepiped model, with the core-shell intensity being calculated as the square of the sum of the amplitudes of the core and the slabs on the edges. The scattering amplitude is computed for a particular orientation of the core-shell parallelepiped with respect to the scattering vector and then averaged over all possible orientations, where $\alpha$ is the angle between the $z$ axis and the $C$ axis of the parallelepiped, and $\beta$ is the angle between the projection of the particle in the $xy$ detector plane and the $y$ axis.

$$P(q) = \frac{\int_{\alpha=0}^{\pi/2} \int_{\beta=0}^{\pi/2} F^2(q, \alpha, \beta) \sin \alpha \, d\alpha \, d\beta}{\int_{\alpha=0}^{\pi/2} \sin \alpha \, d\alpha \, d\beta}$$
and
\[
F(q, \alpha, \beta) = (\rho_{\text{core}} - \rho_{\text{solvent}})S(Q_A, A)S(Q_B, B)S(Q_C, C)
+ (\rho_A - \rho_{\text{solvent}}) [S(Q_A, A + 2t_A) - S(Q_A, A)] S(Q_B, B)S(Q_C, C)
+ (\rho_B - \rho_{\text{solvent}}) [S(Q_B, A + 2t_B) - S(Q_B, A)] S(Q_B, B)S(Q_C, C)
+ (\rho_C - \rho_{\text{solvent}}) S(Q_A, A)S(Q_B, B) [S(Q_C, A + 2t_C) - S(Q_C, C)]
\]

with
\[
S(Q_X, L) = L \frac{\sin(\frac{1}{2}Q_X L)}{\frac{1}{2}Q_X L}
\]

and
\[
Q_A = q \sin \alpha \sin \beta \\
Q_B = q \sin \alpha \cos \beta \\
Q_C = q \cos \alpha
\]

where \(\rho_{\text{core}}\), \(\rho_A\), \(\rho_B\) and \(\rho_C\) are the scattering lengths of the parallelepiped core, and the rectangular slabs of thickness \(t_A\), \(t_B\) and \(t_C\), respectively. \(\rho_{\text{solvent}}\) is the scattering length of the solvent.

**Note:** the code actually implements two substitutions: \(d(\cos \alpha)\) is substituted for \(-\sin \alpha \, d\alpha\) (note that in the parallelepiped code this is explicitly implemented with \(\sigma = \cos \alpha\)), and \(\beta\) is set to \(\beta = \arctan(2)\) so that \(du = \pi/2 \, d\beta\). Thus both integrals go from 0 to 1 rather than 0 to \(\pi/2\).

---

**FITTING NOTES**

1. There are many parameters in this model. Hold as many fixed as possible with known values, or you will certainly end up at a solution that is unphysical.

2. The 2nd virial coefficient of the core_shell_parallelepiped is calculated based on the the averaged effective radius \((= \sqrt{(A + 2t_A)(B + 2t_B)/\pi})\) and length \((C + 2t_C)\) values, after appropriately sorting the three dimensions to give an oblate or prolate particle, to give an effective radius for \(S(q)\) when \(P(q) \ast S(q)\) is applied.

3. For 2d data the orientation of the particle is required, described using angles \(\theta\), \(\phi\) and \(\Psi\) as in the diagrams below, where \(\theta\) and \(\phi\) define the orientation of the director in the laboratory reference frame of the beam direction (z) and detector plane (x - y plane), while the angle \(\Psi\) is effectively the rotational angle around the particle C axis. For \(\theta = 0\) and \(\phi = 0\), \(\Psi = 0\) corresponds to the B axis oriented parallel to the y-axis of the detector with A along the x-axis. For other \(\theta\), \(\phi\) values, the order of rotations matters. In particular, the parallelepiped must first be rotated \(\theta\) degrees in the \(x - z\) plane before rotating \(\phi\) degrees around the \(z\) axis (in the \(x - y\) plane). Applying orientational distribution to the particle orientation (i.e jitter to one or more of these angles) can get more confusing as jitter is defined **NOT** with respect to the laboratory frame but the particle reference frame. It is thus highly recommended to read **Oriented particles** for further details of the calculation and angular dispersions.

**Note:** For 2d, constraints must be applied during fitting to ensure that the order of sides chosen is not altered, and hence that the correct definition of angles is preserved. For the default choice shown here, that means ensuring that the inequality \(A < B < C\) is not violated, The calculation will not report an error, but the results may be not correct.

---

**Validation**

Cross-checked against hollow rectangular prism and rectangular prism for equal thickness overlapping sides, and by Monte Carlo sampling of points within the shape for non-uniform, non-overlapping sides.

**References**

**Authorship and Verification**

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
Fig. 1.61: Definition of the angles for oriented core-shell parallelepipeds. Note that rotation $\theta$, initially in the $x - z$ plane, is carried out first, then rotation $\phi$ about the $z$ axis, finally rotation $\Psi$ is now around the $C$ axis of the particle. The neutron or X-ray beam is along the $z$ axis and the detector defines the $x - y$ plane.
Fig. 1.62: Examples of the angles for oriented core-shell parallelepipeds against the detector plane.

Fig. 1.63: 1D and 2D plots corresponding to the default parameters of the model.
hollow_rectangular_prism

Hollow rectangular parallelepiped with uniform scattering length density.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>sld</td>
<td>Parallelepiped scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>6.3</td>
</tr>
<tr>
<td>sld_solute</td>
<td>Solvent scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>1</td>
</tr>
<tr>
<td>length_a</td>
<td>Shorter side of the parallelepiped</td>
<td>Å</td>
<td>35</td>
</tr>
<tr>
<td>b2a_ratio</td>
<td>Ratio sides b/a</td>
<td>Å</td>
<td>1</td>
</tr>
<tr>
<td>c2a_ratio</td>
<td>Ratio sides c/a</td>
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<td>1</td>
</tr>
<tr>
<td>thickness</td>
<td>Thickness of parallelepiped</td>
<td>Å</td>
<td>1</td>
</tr>
<tr>
<td>theta</td>
<td>c axis to beam angle</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>phi</td>
<td>rotation about beam</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>psi</td>
<td>rotation about c axis</td>
<td>degree</td>
<td>0</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹sr⁻¹, absolute scale.

**Definition**

This model provides the form factor, \( P(q) \), for a hollow rectangular parallelepiped with a wall of thickness \( \Delta \). The 1D scattering intensity for this model is calculated by forming the difference of the amplitudes of two massive parallelepipeds differing in their outermost dimensions in each direction by the same length increment \( 2\Delta \) (Nayuk, 2012).

As in the case of the massive parallelepiped model (rectangular_prism), the scattering amplitude is computed for a particular orientation of the parallelepiped with respect to the scattering vector and then averaged over all possible orientations, giving

\[
P(q) = \frac{1}{\sqrt{2}\pi} \frac{2}{q} \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} A_P(q) \sin \theta \, d\theta \, d\phi
\]

where \( \theta \) is the angle between the \( z \) axis and the longest axis of the parallelepiped, \( \phi \) is the angle between the scattering vector (lying in the \( xy \) plane) and the \( y \) axis, and

\[
A_P(q) = ABC \left[ \frac{\sin \left( \frac{qC}{2} \cos \theta \right)}{\left( \frac{qC}{2} \cos \theta \right)} \right] \left[ \frac{\sin \left( \frac{qB}{2} \sin \theta \sin \phi \right)}{\left( \frac{qB}{2} \sin \theta \sin \phi \right)} \right] \left[ \frac{\sin \left( \frac{qA}{2} \sin \theta \cos \phi \right)}{\left( \frac{qA}{2} \sin \theta \cos \phi \right)} \right] - 8 \left( \frac{A}{2} - \Delta \right) \left( \frac{B}{2} - \Delta \right) \left( \frac{C}{2} - \Delta \right) \left[ \frac{\sin \left[ q \left( \frac{C}{2} - \Delta \right) \cos \theta \right]}{q \left( \frac{C}{2} - \Delta \right) \cos \theta} \right] \left[ \frac{\sin \left[ q \left( \frac{B}{2} - \Delta \right) \sin \theta \sin \phi \right]}{q \left( \frac{B}{2} - \Delta \right) \sin \theta \sin \phi} \right] \left[ \frac{\sin \left[ q \left( \frac{A}{2} - \Delta \right) \sin \theta \cos \phi \right]}{q \left( \frac{A}{2} - \Delta \right) \sin \theta \cos \phi} \right]
\]

where \( A, B \) and \( C \) are the external sides of the parallelepiped fulfilling \( A \leq B \leq C \), and the volume \( V \) of the parallelepiped is

\[
V = ABC - (A - 2\Delta)(B - 2\Delta)(C - 2\Delta)
\]

The 1D scattering intensity is then calculated as

\[
I(q) = \text{scale} \times V \times (\rho_p - \rho_{\text{solvent}})^2 \times P(q) + \text{background}
\]

where \( \rho_p \) is the scattering length density of the parallelepiped, \( \rho_{\text{solvent}} \) is the scattering length density of the solvent, and (if the data are in absolute units) \( \text{scale} \) represents the volume fraction (which is unitless) of the rectangular shell of material (i.e. not including the volume of the solvent filled core).

For 2D data the orientation of the particle is required, described using angles $\theta$, $\phi$ and $\Psi$ as in the diagrams below, for further details of the calculation and angular dispersions see Oriented particles. The angle $\Psi$ is the rotational angle around the long $C$ axis. For example, $\Psi = 0$ when the $B$ axis is parallel to the $x$-axis of the detector.

For 2D, constraints must be applied during fitting to ensure that the inequality $A < B < C$ is not violated, and hence the correct definition of angles is preserved. The calculation will not report an error if the inequality is not preserved, but the results may be not correct.

Fig. 1.64: Definition of the angles for oriented hollow rectangular prism. Note that rotation $\theta$, initially in the $xz$ plane, is carried out first, then rotation $\phi$ about the $z$ axis, finally rotation $\Psi$ is now around the axis of the prism. The neutron or X-ray beam is along the $z$ axis.

Validation
Validation of the code was conducted by qualitatively comparing the output of the 1D model to the curves shown in (Nayuk, 2012).

References

Authorship and Verification
- **Author:** Miguel Gonzales **Date:** February 26, 2016
- **Last Modified by:** Paul Kienzle **Date:** December 14, 2017
- **Last Reviewed by:** Paul Butler **Date:** September 06, 2018

**hollow_rectangular_prism_thin_walls**

Hollow rectangular parallelepiped with thin walls.
Fig. 1.65: Examples of the angles for oriented hollow rectangular prisms against the detector plane.

Fig. 1.66: 1D and 2D plots corresponding to the default parameters of the model.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
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<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
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<td>sld</td>
<td>Parallelepiped scattering length density</td>
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<td>sld_solvent</td>
<td>Solvent scattering length density</td>
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<td>Shorter side of the parallelepiped</td>
<td>Å</td>
<td>35</td>
</tr>
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<td>b2a_ratio</td>
<td>Ratio sides b/a</td>
<td>Å</td>
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</tr>
<tr>
<td>c2a_ratio</td>
<td>Ratio sides c/a</td>
<td>Å</td>
<td>1</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

This model provides the form factor, \( P(q) \), for a hollow rectangular prism with infinitely thin walls. It computes only the 1D scattering, not the 2D. The 1D scattering intensity for this model is calculated according to the equations given by Nayuk and Huber⁴.

Assuming a hollow parallelepiped with infinitely thin walls, edge lengths \( A \leq B \leq C \) and presenting an orientation with respect to the scattering vector given by \( \theta \) and \( \phi \), where \( \theta \) is the angle between the \( z \) axis and the longest axis of the parallelepiped \( C \), and \( \phi \) is the angle between the scattering vector (lying in the \( xy \) plane) and the \( y \) axis, the form factor is given by

\[
P(q) = \frac{1}{V^2} \frac{2}{\pi} \int_0^\frac{\pi}{2} \int_0^\frac{\pi}{2} [A_L(q) + A_T(q)]^2 \sin \theta \, d\theta \, d\phi
\]

where

\[
V = 2AB + 2AC + 2BC
\]

\[
A_L(q) = 8 \times \frac{\sin \left(\frac{1}{2}QA \sin \phi \sin \theta\right) \sin \left(\frac{1}{2}QB \cos \phi \sin \theta\right) \cos \left(\frac{1}{2}QC \cos \theta\right)}{q^2 \sin^2 \theta \sin \phi \cos \phi}
\]

\[
A_T(q) = A_F(q) \times \frac{2 \sin \left(\frac{1}{2}QC \cos \theta\right)}{q \cos \theta}
\]

and

\[
A_F(q) = 4 \times \frac{\cos \left(\frac{1}{2}QA \sin \phi \sin \theta\right) \sin \left(\frac{1}{2}QB \cos \phi \sin \theta\right)}{q \cos \phi \sin \theta} + \frac{4 \sin \left(\frac{1}{2}QA \sin \phi \sin \theta\right) \cos \left(\frac{1}{2}QB \cos \phi \sin \theta\right)}{q \sin \phi \sin \theta}
\]

The 1D scattering intensity is then calculated as

\[
I(q) = \text{scale} \times V \times (\rho_p - \rho_{\text{solvent}})^2 \times P(q)
\]

where \( V \) is the surface area of the rectangular prism, \( \rho_p \) is the scattering length density of the parallelepiped, \( \rho_{\text{solvent}} \) is the scattering length density of the solvent, and (if the data are in absolute units) \( \text{scale} \) is related to the total surface area.

The 2D scattering intensity is not computed by this model.

**Validation**

Validation of the code was conducted by qualitatively comparing the output of the 1D model to the curves shown in (Nayuk, 2012⁴).

**References**

Authorship and Verification

- **Author:** Miguel Gonzales **Date:** February 26, 2016
- **Last Modified by:** Paul Kienzle **Date:** October 15, 2016
- **Last Reviewed by:** Paul Butler **Date:** September 07, 2018

---

Fig. 1.67: 1D plot corresponding to the default parameters of the model.

**parallelepiped**

Rectangular parallelepiped with uniform scattering length density.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>sld</td>
<td>Parallelepiped scattering length density</td>
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<td>4</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>(10^6)Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>length_a</td>
<td>Shorter side of the parallelepiped</td>
<td>Å</td>
<td>35</td>
</tr>
<tr>
<td>length_b</td>
<td>Second side of the parallelepiped</td>
<td>Å</td>
<td>75</td>
</tr>
<tr>
<td>length_c</td>
<td>Larger side of the parallelepiped</td>
<td>Å</td>
<td>400</td>
</tr>
<tr>
<td>theta</td>
<td>c axis to beam angle</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>phi</td>
<td>rotation about beam</td>
<td>degree</td>
<td>60</td>
</tr>
<tr>
<td>psi</td>
<td>rotation about c axis</td>
<td>degree</td>
<td>60</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition**

This model calculates the scattering from a rectangular solid (Fig. 1.68). If you need to apply polydispersity, see also *rectangular_prism*. For information about polarised and magnetic scattering, see the *Polarisation/Magnetic Scattering* documentation.

The three dimensions of the parallelepiped (strictly here a cuboid) may be given in *any* size order as long as the particles are randomly oriented (i.e. take on all possible orientations see notes on 2D below). To avoid multiple fit solutions, especially with Monte-Carlo fit methods, it may be advisable to restrict their ranges. There may be a number of closely similar “best fits”, so some trial and error, or fixing of some dimensions at expected values, may help.

The form factor is normalized by the particle volume and the 1D scattering intensity \(I(q)\) is then calculated as:

\[
I(q) = \frac{\text{scale}}{V} (\Delta \rho \cdot V)^2 \langle P(q, \alpha, \beta) \rangle + \text{background}
\]

where the volume \(V = ABC\), the contrast is defined as \(\Delta \rho = \rho_p - \rho_{\text{solvent}}\). \(P(q, \alpha, \beta)\) is the form factor corresponding to a parallelepiped oriented at an angle \(\alpha\) (angle between the long axis C and \(\vec{q}\)), and \(\beta\) (the angle...
between the projection of the particle in the \( xy \) detector plane and the \( y \) axis) and the averaging \( \langle \ldots \rangle \) is applied over all orientations.

Assuming \( a = A/B < 1 \), \( b = B/B = 1 \), and \( c = C/B > 1 \), the form factor is given by (Mittelbach and Porod, 1961)

\[
P(q, \alpha) = \int_0^1 \phi_Q \left( \mu \sqrt{1 - \sigma^2}, \alpha \right) \left| S(\mu \sigma/2) \right|^2 d\sigma
\]

with

\[
\phi_Q(\mu, \alpha) = \int_0^1 \left\{ S \left[ \frac{\mu}{2} \cos \left( \frac{\pi u}{2} \right) \right] S \left[ \frac{\mu a}{2} \sin \left( \frac{\pi u}{2} \right) \right] \right\}^2 \, du
\]

\[
S(x) = \frac{\sin x}{x}
\]

\[
\mu = qB
\]

where substitution of \( \sigma = \cos \alpha \) and \( \beta = \pi/2 \) have been applied.

For \textit{oriented} particles, the 2D scattering intensity, \( I(q_x, q_y) \), is given as:

\[
I(q_x, q_y) = \text{scale} \cdot V \cdot (\Delta \rho \cdot V)^2 P(q_x, q_y) + \text{background}
\]

Where \( P(q_x, q_y) \) for a given orientation of the form factor is calculated as

\[
P(q_x, q_y) = \left[ \sin \left( \frac{1}{2} qA \cos \alpha \right) \right]^2 \left[ \sin \left( \frac{1}{2} qB \cos \beta \right) \right]^2 \left[ \sin \left( \frac{1}{2} qC \cos \gamma \right) \right]^2
\]

with

\[
\cos \alpha = \hat{A} \cdot \hat{q},
\]

\[
\cos \beta = \hat{B} \cdot \hat{q},
\]

\[
\cos \gamma = \hat{C} \cdot \hat{q}
\]

\textbf{FITTING NOTES}

1. The 2nd virial coefficient of the parallelepiped is calculated based on the averaged effective radius, after appropriately sorting the three dimensions, to give an oblate or prolate particle, \((= \sqrt{AB}/\pi)\) and length \((= C)\) values, and used as the effective radius for \( S(q) \) when \( P(q) \cdot S(q) \) is applied.

---

\footnote{P Mittelbach and G Porod, \textit{Acta Physica Austriaca}, 14 (1961) 185-211}
2. For 2D data the orientation of the particle is required, described using angles $\theta$, $\phi$ and $\Psi$ as in the diagrams below, where $\theta$ and $\phi$ define the orientation of the director in the laboratory reference frame of the beam direction ($z$) and detector plane ($x-y$ plane), while the angle $\Psi$ is effectively the rotational angle around the particle $C$ axis. For $\theta = 0$ and $\phi = 0$, $\Psi = 0$ corresponds to the $B$ axis oriented parallel to the $y$-axis of the detector with $A$ along the $x$-axis. For other $\theta$, $\phi$ values, the order of rotations matters. In particular, the parallelepiped must first be rotated $\theta$ degrees in the $x-z$ plane before rotating $\phi$ degrees around the $z$ axis (in the $x-y$ plane). Applying orientational distribution to the particle orientation (i.e. jitter to one or more of these angles) can get more confusing as jitter is defined NOT with respect to the laboratory frame but the particle reference frame. It is thus highly recommended to read Oriented particles for further details of the calculation and angular dispersions.

Note: For 2D, constraints must be applied during fitting to ensure that the order of sides chosen is not altered, and hence that the correct definition of angles is preserved. For the default choice shown here, that means ensuring that the inequality $A < B < C$ is not violated. The calculation will not report an error, but the results may be not correct.

Fig. 1.69: Definition of the angles for oriented parallelepiped, shown with $A < B < C$.

Validation

Validation of the code was done by comparing the output of the 1D calculation to the angular average of the output of a 2D calculation over all possible angles.

References

Authorship and Verification

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
- **Last Modified by:** Paul Kienzle **Date:** April 05, 2017
Fig. 1.70: Examples of the angles for an oriented parallelepiped against the detector plane.

Fig. 1.71: 1D and 2D plots corresponding to the default parameters of the model.
rectangular_prism

Rectangular parallelepiped with uniform scattering length density.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>sld</td>
<td>Parallelepiped scattering length density</td>
<td>(10^6)Å(^{-2})</td>
<td>6.3</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>(10^6)Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>length_a</td>
<td>Shorter side of the parallelepiped</td>
<td>Å</td>
<td>35</td>
</tr>
<tr>
<td>b2a_ratio</td>
<td>Ratio sides b/a</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>c2a_ratio</td>
<td>Ratio sides c/a</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>theta</td>
<td>c axis to beam angle</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>phi</td>
<td>rotation about beam</td>
<td>degree</td>
<td>0</td>
</tr>
<tr>
<td>psi</td>
<td>rotation about c axis</td>
<td>degree</td>
<td>0</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model provides the form factor, \(P(q)\), for a rectangular prism.

Note that this model is almost totally equivalent to the existing parallelepiped model. The only difference is that the way the relevant parameters are defined here (\(a, b/a, c/a\) instead of \(a, b, c\)) which allows use of polydispersity with this model while keeping the shape of the prism (e.g. setting \(b/a = 1\) and \(c/a = 1\) and applying polydispersity to \(a\) will generate a distribution of cubes of different sizes).

Definition

The 1D scattering intensity for this model was calculated by Mittelbach and Porod (Mittelbach, 1961), but the implementation here is closer to the equations given by Nayuk and Huber (Nayuk, 2012). Note also that the angle definitions used in the code and the present documentation correspond to those used in (Nayuk, 2012) (see Fig. 1 of that reference), with \(\theta\) corresponding to \(\alpha\) in that paper, and not to the usual convention used for example in the parallelepiped model.

In this model the scattering from a massive parallelepiped with an orientation with respect to the scattering vector given by \(\theta\) and \(\phi\)

\[
A_P(q) = \frac{\sin \left( \frac{1}{2} q C \cos \theta \right)}{\frac{1}{2} q C \cos \theta} \times \frac{\sin \left( \frac{1}{2} q A \cos \theta \right)}{\frac{1}{2} q A \cos \theta} \times \frac{\sin \left( \frac{1}{2} q B \cos \theta \right)}{\frac{1}{2} q B \cos \theta}
\]

where \(A, B, C\) are the sides of the parallelepiped and must fulfill \(A \leq B \leq C\), \(\theta\) is the angle between the \(z\) axis and the longest axis of the parallelepiped \(C\), and \(\phi\) is the angle between the scattering vector (lying in the \(xy\) plane) and the \(y\) axis.

The normalized form factor in 1D is obtained averaging over all possible orientations

\[
P(q) = \frac{2}{\pi} \int_0^\pi \int_0^{2\pi} A_P^2(q) \sin \theta \, d\theta \, d\phi
\]

And the 1D scattering intensity is calculated as

\[
I(q) = \text{scale} \times V \times (\rho_p - \rho_{solvent})^2 \times P(q)
\]

where \(V\) is the volume of the rectangular prism, \(\rho_p\) is the scattering length of the parallelepiped, \(\rho_{solvent}\) is the scattering length of the solvent, and (if the data are in absolute units) \text{scale} represents the volume fraction (which is unitless).

For 2d data the orientation of the particle is required, described using angles \(\theta, \phi\) and \(\Psi\) as in the diagrams below, for further details of the calculation and angular dispersions see Oriented particles. The angle \(\Psi\) is the rotational angle around the long \(C\) axis. For example, \(\Psi = 0\) when the \(B\) axis is parallel to the \(x\)-axis of the detector.
For 2d, constraints must be applied during fitting to ensure that the inequality $A < B < C$ is not violated, and hence the correct definition of angles is preserved. The calculation will not report an error, but the results may be not correct.

Fig. 1.72: Definition of the angles for oriented core-shell parallelepipeds. Note that rotation $\theta$, initially in the $xz$ plane, is carried out first, then rotation $\phi$ about the $z$ axis, finally rotation $\Psi$ is now around the axis of the cylinder. The neutron or X-ray beam is along the $z$ axis.

**Validation**

Validation of the code was conducted by comparing the output of the 1D model to the output of the existing parallelepiped model.

**References**


### 1.1.6 Sphere Functions

**adsorbed_layer**

Scattering from an adsorbed layer on particles
Fig. 1.73: Examples of the angles for oriented rectangular prisms against the detector plane.

Fig. 1.74: 1D and 2D plots corresponding to the default parameters of the model.
## Definition

This model describes the scattering from a layer of surfactant or polymer adsorbed on large, smooth, notionally spherical particles under the conditions that (i) the particles (cores) are contrast-matched to the dispersion medium, (ii) $S(Q) \sim 1$ (ie, the particle volume fraction is dilute), (iii) the particle radius is $>>$ layer thickness (ie, the interface is locally flat), and (iv) scattering from excess unadsorbed adsorbate in the bulk medium is absent or has been corrected for.

Unlike many other core-shell models, this model does not assume any form for the density distribution of the adsorbed species normal to the interface (cf, a core-shell model normally assumes the density distribution to be a homogeneous step-function). For comparison, if the thickness of a (traditional core-shell like) step function distribution is $t$, the second moment about the mean of the density distribution (ie, the distance of the centre-of-mass of the distribution from the interface), $\sigma = \sqrt{t^2/12}$.

$$I(q) = scale \cdot (\rho_{\text{poly}} - \rho_{\text{solv}})^2 \left[ \frac{6\pi \phi_{\text{core}}}{Q^2} \frac{\Gamma^2}{\delta_{\text{poly}}^2 R_{\text{core}}} \exp(-Q^2\sigma^2) \right] + \text{background}$$

where $scale$ is a scale factor, $\rho_{\text{poly}}$ is the sld of the polymer (or surfactant) layer, $\rho_{\text{solv}}$ is the sld of the solvent/medium and cores, $\phi_{\text{core}}$ is the volume fraction of the core particles, $\delta_{\text{poly}}$ is the bulk density of the polymer, $\Gamma$ is the adsorbed amount, and $\sigma$ is the second moment of the thickness distribution.

Note that all parameters except $\sigma$ are correlated so fitting more than one of these parameters will generally fail. Also note that unlike other shape models, no volume normalization is applied to this model (the calculation is exact).

The code for this model is based originally on a a fortran implementation by Steve King at ISIS in the SANDRA package c. 1990.

### References

**Authorship and Verification**

- **Author**: Jae-Hi Cho **Date**: pre 2010
- **Last Modified by**: Paul Kienzle **Date**: April 14, 2016
- **Last Reviewed by**: Steve King **Date**: March 18, 2016

### binary_hard_sphere

binary mixture of hard spheres with hard sphere interactions.
Fig. 1.75: 1D plot corresponding to the default parameters of the model.

<table>
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<th>Description</th>
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<td>background</td>
<td>Source background</td>
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</tr>
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</tr>
<tr>
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<tr>
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<td>Solvent scattering length density</td>
<td>10⁻⁶Å⁻²</td>
<td>6.36</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

The binary hard sphere model provides the scattering intensity, for binary mixture of hard spheres including hard sphere interaction between those particles, using rhw Percus-Yevick closure. The calculation is an exact multi-component solution that properly accounts for the 3 partial structure factors as follows:

\[ I(q) = (1 - x) f_1^2(q) S_{11}(q) + 2x(1 - x)^{1/2} f_1(q) f_2(q) S_{12}(q) + x f_2^2(q) S_{22}(q) \]

where \( S_{ij} \) are the partial structure factors and \( f_i \) are the scattering amplitudes of the particles. The subscript 1 is for the smaller particle and 2 is for the larger. The number fraction of the larger particle, \((x = n_2/(n_1 + n_2))\), where \( n \) is the number density) is internally calculated based on the diameter ratio and the volume fractions.

\[
x = \frac{(\phi_2/\phi)\alpha^3}{(1 - (\phi_2/\phi) + (\phi_2/\phi)\alpha^3)}
\]

\[
\phi = \phi_1 + \phi_2 = \text{total volume fraction}
\]

\[
\alpha = R_1/R_2 = \text{size ratio}
\]

The 2D scattering intensity is the same as 1D, regardless of the orientation of the \( q \) vector which is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]
NOTE 1: The volume fractions and the scattering contrasts are loosely correlated, so holding as many parameters fixed to known values during fitting will improve the robustness of the fit.

NOTE 2: Since the calculation uses the Percus-Yevick closure, all of the limitations of that closure relation apply here. Specifically, one should be wary of results for (total) volume fractions greater than approximately 40%. Depending on the size ratios or number fractions, the limit on total volume fraction may be lower.

NOTE 3: The heavy arithmetic operations also mean that at present the function is poorly behaved at very low qr. In some cases very large qr may also be poorly behaved. These should however be outside any useful region of qr.

The code for this model is based originally on a c-library implementation by the NIST Center for Neutron Research (Kline, 2006).

See the references for details.

Fig. 1.76: 1D plot corresponding to the default parameters of the model.

References

Authorship and Verification

- **Author**: NIST IGOR/DANSE **Date**: pre 2010
- **Last Modified by**: Paul Butler **Date**: March 20, 2016
- **Last Reviewed by**: Paul Butler **Date**: March 20, 2016

**core_multi_shell**

This model provides the scattering from a spherical core with 1 to 4 concentric shell structures. The SLDs of the core and each shell are individually specified.
### Parameter Description

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm^{-1}</td>
<td>0.001</td>
</tr>
<tr>
<td>sld_core</td>
<td>Core scattering length density</td>
<td>10^{-6} Å^{-2}</td>
<td>1</td>
</tr>
<tr>
<td>radius</td>
<td>Radius of the core</td>
<td>Å</td>
<td>200</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10^{-6} Å^{-2}</td>
<td>6.4</td>
</tr>
<tr>
<td>n</td>
<td>number of shells</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>sld[n]</td>
<td>scattering length density of shell k</td>
<td>10^{-6} Å^{-2}</td>
<td>1.7</td>
</tr>
<tr>
<td>thickness[n]</td>
<td>Thickness of shell k</td>
<td>Å</td>
<td>40</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm^{-1} sr^{-1}, absolute scale.

### Definition

This model is a trivial extension of the CoreShell function to a larger number of shells. The scattering length density profile for the default sld values (w/ 4 shells).

![SLD profile](image)

Fig. 1.77: SLD profile of the core_multi_shell object from the center of sphere out for the default SLDs.*

The 2D scattering intensity is the same as $P(q)$ above, regardless of the orientation of the $\vec{q}$ vector which is defined as

$$ q = \sqrt{q_x^2 + q_y^2} $$

**Note:** Be careful! The SLDs and scale can be highly correlated. Hold as many of these parameters fixed as possible.

**Note:** The outer most radius ($= radius + thickness$) is used as the effective radius for $S(Q)$ when $P(Q) \ast S(Q)$ is applied.

For information about polarised and magnetic scattering, see the Polarisation/Magnetic Scattering documentation.
Our model uses the form factor calculations implemented in a c-library provided by the NIST Center for Neutron Research (Kline, 2006)\textsuperscript{2}.

![1D plot corresponding to the default parameters of the model.](image)

References

Authorship and Verification

- **Author**: NIST IGOR/DANSE
- **Date**: pre 2010
- **Last Modified by**: Paul Kienzle
- **Date**: September 12, 2016
- **Last Reviewed by**: Paul Kienzle
- **Date**: September 12, 2016

**core_shell_sphere**

Form factor for a monodisperse spherical particle with particle with a core-shell structure.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>radius</td>
<td>Sphere core radius</td>
<td>Å</td>
<td>60</td>
</tr>
<tr>
<td>thickness</td>
<td>Sphere shell thickness</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>sld_core</td>
<td>core scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>sld_shell</td>
<td>shell scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>2</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>3</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model provides the form factor, \(P(q)\), for a spherical particle with a core-shell structure. The form factor is normalized by the particle volume.

For information about polarised and magnetic scattering, see the Polarisation/Magnetic Scattering documentation.

Definition

The 1D scattering intensity is calculated in the following way (Guinier, 1955)

\[ P(q) = \text{scale} \cdot F^2(q) + \text{background} \]

where

\[ F(q) = \frac{3}{V_s} \left[ V_c (\rho_c - \rho_s) \frac{\sin(qr_c) - qr_c \cos(qr_c)}{(qr_c)^3} + V_s (\rho_s - \rho_{\text{solv}}) \frac{\sin(qr_s) - qr_s \cos(qr_s)}{(qr_s)^3} \right] \]

where \( V_s \) is the volume of the whole particle, \( V_c \) is the volume of the core, \( r_s = \text{radius} + \text{thickness} \) is the radius of the particle, \( r_c \) is the radius of the core, \( \rho_c \) is the scattering length density of the core, \( \rho_s \) is the scattering length density of the shell, \( \rho_{\text{solv}} \) is the scattering length density of the solvent.

The 2D scattering intensity is the same as \( P(q) \) above, regardless of the orientation of the \( q \) vector.

NB: The outer most radius (ie, = radius + thickness) is used as the effective radius for \( S(Q) \) when \( P(Q) \cdot S(Q) \) is applied.

![Fig. 1.79: 1D plot corresponding to the default parameters of the model.](image)

**References**


**Validation**

Validation of our code was done by comparing the output of the 1D model to the output of the software provided by NIST (Kline, 2006). Figure 1 shows a comparison of the output of our model and the output of the NIST software.

**fuzzy_sphere**

Scattering from spherical particles with a fuzzy surface.
The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

For information about polarised and magnetic scattering, see the Polarisation/Magnetic Scattering documentation.

**Definition**

The scattering intensity $I(q)$ is calculated as:

$$I(q) = \frac{\text{scale}}{V}(\Delta \rho)^2 A^2(q) S(q) + \text{background}$$

where the amplitude $A(q)$ is given as the typical sphere scattering convoluted with a Gaussian to get a gradual drop-off in the scattering length density:

$$A(q) = \frac{3 [\sin(qR) - qR \cos(qR)]}{(qR)^3} \exp \left( -\left(\frac{\sigma_{\text{fuzzy}}q}{2}\right)^2 \right)$$

Here $A(q)^2$ is the form factor, $P(q)$. The scale is equivalent to the volume fraction of spheres, each of volume, $V$. Contrast $(\Delta \rho)$ is the difference of scattering length densities of the sphere and the surrounding solvent.

Poly-dispersion in radius and in fuzziness is provided for, though the fuzziness must be kept much smaller than the sphere radius for meaningful results.

From the reference:

The “fuzziness” of the interface is defined by the parameter $\sigma_{\text{fuzzy}}$. The particle radius $R$ represents the radius of the particle where the scattering length density profile decreased to 1/2 of the core density. $\sigma_{\text{fuzzy}}$ is the width of the smeared particle surface; i.e., the standard deviation from the average height of the fuzzy interface. The inner regions of the microgel that display a higher density are described by the radial box profile extending to a radius of approximately $R_{\text{box}} \sim R - 2\sigma$. The profile approaches zero as $R_{\text{ans}} \sim R + 2\sigma$.

For 2D data: The 2D scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

**References**


**linear_pears**

Linear pearls model of scattering from spherical pearls.
The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model provides the form factor for \(N\) spherical pearls of radius \(R\) linearly joined by short strings (or segment length or edge separation) \(l (= A - 2R)\). \(A\) is the center-to-center pearl separation distance. The thickness of each string is assumed to be negligible.

\[
P(Q) = \frac{\text{scale}}{V} \left[ m_p^2 \left( N + 2 \sum_{n=1}^{N-1} (N - n) \frac{\sin(nql)}{nql} \right) \left( \frac{3 \sin(qR) - qR \cos(qR)}{(qr)^3} \right)^2 \right]
\]

where the mass \(m_p\) is \((\text{SLD}_{\text{pearl}} - \text{SLD}_{\text{solvent}}) \times \) (volume of \(N\) pearls). \(V\) is the total volume.

---

**Parameter** | **Description** | **Units** | **Default value**
---|---|---|---
scale | Source intensity | None | 1
background | Source background | cm\(^{-1}\) | 0.001
radius | Radius of the pearls | Å | 80
edge_sep | Length of the string segment - surface to surface | Å | 350
num_pearls | Number of the pearls | None | 3
sld | SLD of the pearl spheres | \(10^6\) Å\(^{-2}\) | 1
sld_solvent | SLD of the solvent | \(10^6\) Å\(^{-2}\) | 6.3

**Definition**

The output of the scattering intensity function for the linear_pearls model is given by (Dobrynin, 1996)

\[
P(Q) = \frac{\text{scale}}{V} \left[ m_p^2 \left( N + 2 \sum_{n=1}^{N-1} (N - n) \frac{\sin(nql)}{nql} \right) \left( \frac{3 \sin(qR) - qR \cos(qR)}{(qr)^3} \right)^2 \right]
\]

where the mass \(m_p\) is \((\text{SLD}_{\text{pearl}} - \text{SLD}_{\text{solvent}}) \times \) (volume of \(N\) pearls). \(V\) is the total volume.
The 2D scattering intensity is the same as $P(q)$ above, regardless of the orientation of the $q$ vector.

![Graph showing 1D plot corresponding to the default parameters of the model.](image)

Fig. 1.81: 1D plot corresponding to the default parameters of the model.

**References**


**multilayer_vesicle**

$P(Q)$ for a Multi-lamellar vesicle

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm$^{-1}$</td>
<td>0.001</td>
</tr>
<tr>
<td>volfraction</td>
<td>volume fraction of vesicles</td>
<td>None</td>
<td>0.05</td>
</tr>
<tr>
<td>radius</td>
<td>radius of solvent filled core</td>
<td>Å</td>
<td>60</td>
</tr>
<tr>
<td>thick_shell</td>
<td>thickness of one shell</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>thick_solvent</td>
<td>solvent thickness between shells</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>solvent scattering length density</td>
<td>$10^6$ Å$^{-2}$</td>
<td>6.4</td>
</tr>
<tr>
<td>sld</td>
<td>Shell scattering length density</td>
<td>$10^6$ Å$^{-2}$</td>
<td>0.4</td>
</tr>
<tr>
<td>n_shells</td>
<td>Number of shell plus solvent layer pairs</td>
<td>None</td>
<td>2</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

**Definition**

This model is a trivial extension of the core_sphere function where the core is filled with solvent and is surrounded by $N$ shells of material (such as lipids) interleaved with $N-1$ layers of solvent. For $N = 1$, this returns the same as the vesicle model, except for the normalisation, which here is to outermost volume. The shell thicknesses and SLD are constant for all shells as expected for a multilayer vesicle.

See the [core_shell_sphere](#) model for more documentation.

The 1D scattering intensity is calculated in the following way (Guinier, 1955)

$$P(q) = \text{scale} \cdot \frac{\phi}{V(R_N)} F^2(q) + \text{background}$$

1.1. Model Functions
Multi-Shell Spherical Model
(e.g. multilamellar vesicles)

Fig. 1.82: Geometry of the multilayer_vesicle model.

where

\[ F(q) = (\rho_{\text{shell}} - \rho_{\text{solv}}) \sum_{i=1}^{N} \left[ 3V(r_i) \frac{\sin(qr_i) - qr_i \cos(qr_i)}{(qr_i)^3} - 3V(R_i) \frac{\sin(qR_i) - qR_i \cos(qR_i)}{(qR_i)^3} \right] \]

for

\[ r_i = r_c + (i-1)(t_s + t_w) \] solvent radius before shell \( i \)
\[ R_i = r_i + t_s \] shell radius for shell \( i \)

\( \phi \) is the volume fraction of particles, \( V(r) \) is the volume of a sphere of radius \( r \), \( r_c \) is the radius of the core, \( t_s \) is the thickness of the shell, \( t_w \) is the thickness of the solvent layer between the shells, \( \rho_{\text{shell}} \) is the scattering length density of a shell, and \( \rho_{\text{solv}} \) is the scattering length density of the solvent.

**USAGE NOTES**

- The outer-most shell radius \( R_N \) is used as the effective radius for \( P(Q) \) when \( P(Q) * S(Q) \) is applied. Calculations rather slow.
- The number of shells is always rounded to an integer value as a non integer number of layers is not physical.
- Thus Polydispersity should only be applied to number of shells **VERY CAREFULLY**. A possible legitimate use would be for mixed systems in which some vesicles have 1 shell, some have 2, etc. A polydispersity on \( N \) can be used to model the data by using the “array distribution” feature. First create a file such as `shell_dist.txt` containing the relative portion of each vesicle size:

<table>
<thead>
<tr>
<th>Shell</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20%</td>
</tr>
<tr>
<td>2</td>
<td>4%</td>
</tr>
<tr>
<td>3</td>
<td>1%</td>
</tr>
</tbody>
</table>

Turn on polydispersity and select an array distribution for the `n_shells` parameter. Choose the above `shell_dist.txt` file, and the model will be computed with 80% 1-shell vesicles, 16% 2-shell vesicles and 4% 3-shell vesicles.
• This is a highly non-linear, highly oscillatory (especially around the q-values that correspond to the repeat distance of the layers), model function complicated by the fact that the number of water/shell pairs must physically be an integer value, although the optimization treats it as a floating point value. Thus it may be that the resolution interpolation is not sufficiently fine grained in certain cases. Please report any such occurrences to the SasView team. Generally, for the best possible experience:
  • Start with the best possible guess
  • Using a priori knowledge, hold as many parameters fixed as possible
  • if N=1, tw (water thickness) must by definition be zero. Both N and tw should be fixed during fitting.
  • If N>1, use constraints to keep N > 1
  • Because N only really moves in integer steps, it may get “stuck” if the optimizer step size is too small so care should be taken If you experience problems with this please contact the SasView team and let them know the issue preferably with example data and model which fail to converge.

The 2D scattering intensity is the same as 1D, regardless of the orientation of the q vector which is defined as:

\[ q = \sqrt{q_x^2 + q_y^2} \]

For information about polarised and magnetic scattering, see the Polarisation/Magnetic Scattering documentation.

![Graph of 1D plot corresponding to the default parameters of the model.](image)

Fig. 1.83: 1D plot corresponding to the default parameters of the model.

References

Authorship and Verification

• Author: NIST IGOR/DANSE Date: pre 2010
• Converted to sasmodels by: Piotr Rozyczko Date: Feb 24, 2016
• Last Modified by: Paul Kienzle Date: Feb 7, 2017
• Last Reviewed by: Paul Butler Date: March 12, 2017

onion

Onion shell model with constant, linear or exponential density

1.1. Model Functions
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm^{-1}</td>
<td>0.001</td>
</tr>
<tr>
<td>sld_core</td>
<td>Core scattering length density</td>
<td>10^6 Å^{-2}</td>
<td>1</td>
</tr>
<tr>
<td>radius_core</td>
<td>Radius of the core</td>
<td>A</td>
<td>200</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10^6 Å^{-2}</td>
<td>6.4</td>
</tr>
<tr>
<td>n_shells</td>
<td>number of shells</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>sld_in[n_shells]</td>
<td>scattering length density at the inner radius of shell k</td>
<td>10^6 Å^{-2}</td>
<td>1.7</td>
</tr>
<tr>
<td>sld_out[n_shells]</td>
<td>scattering length density at the outer radius of shell k</td>
<td>10^6 Å^{-2}</td>
<td>2</td>
</tr>
<tr>
<td>thickness[n_shells]</td>
<td>Thickness of shell k</td>
<td>Å</td>
<td>40</td>
</tr>
<tr>
<td>A[n_shells]</td>
<td>Decay rate of shell k</td>
<td>None</td>
<td>1</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm^{-1} sr^{-1}, absolute scale.

This model provides the form factor, $P(q)$, for a multi-shell sphere where the scattering length density (SLD) of each shell is described by an exponential, linear, or constant function. The form factor is normalized by the volume of the sphere where the SLD is not identical to the SLD of the solvent. We currently provide up to 9 shells with this model.

NB: $\text{radius}$ represents the core radius $r_0$ and $\text{thickness}[k]$ represents the thickness of the shell, $r_{k+1} - r_k$.

**Definition**

The 1D scattering intensity is calculated in the following way

$$P(q) = \left| f \right|^2 / V_{\text{particle}}$$

where

$$f = f_{\text{core}} + \left( \sum_{\text{shell}=1}^{N} f_{\text{shell}} \right) + f_{\text{solvent}}$$

The shells are spherically symmetric with particle density $\rho(r)$ and constant SLD within the core and solvent, so

$$f_{\text{core}} = 4\pi \int_0^{r_{\text{core}}} \rho_{\text{core}} \frac{\sin(qr)}{qr} r^2 \, dr = 3\rho_{\text{core}} V(r_{\text{core}}) \frac{j_1(qr_{\text{core}})}{qr_{\text{core}}}$$

$$f_{\text{shell}} = 4\pi \int_{r_{\text{shell}-1}}^{r_{\text{shell}}} \rho_{\text{shell}}(r) \frac{\sin(qr)}{qr} r^2 \, dr$$

$$f_{\text{solvent}} = 4\pi \int_{r_N}^{\infty} \rho_{\text{solvent}} \frac{\sin(qr)}{qr} r^2 \, dr = -3\rho_{\text{solvent}} V(r_N) \frac{j_1(qr_N)}{qr_N}$$

where the spherical bessel function $j_1$ is

$$j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}$$

and the volume is $V(r) = \frac{4\pi}{3} r^3$. The volume of the particle is determined by the radius of the outer shell, so $V_{\text{particle}} = V(r_N)$.

Now let’s consider the SLD of a shell defined by

$$\rho_{\text{shell}}(r) = \begin{cases} 
B \exp \left( A(r - r_{\text{shell}-1}) / \Delta t_{\text{shell}} \right) + C & \text{for } A \neq 0 \\
\rho_{\text{in}} = \text{constant} & \text{for } A = 0 
\end{cases}$$

An example of a possible SLD profile is shown below where $\rho_{\text{in}}$ and $\Delta t_{\text{shell}}$ stand for the SLD of the inner side of the $k$th shell and the thickness of the $k$th shell in the equation above, respectively.

For $A > 0$,

$$f_{\text{shell}} = 4\pi \int_{r_{\text{shell}-1}}^{r_{\text{shell}}} \left[ B \exp \left( A(r - r_{\text{shell}-1}) / \Delta t_{\text{shell}} \right) + C \right] \frac{\sin(qr)}{qr} r^2 \, dr$$

$$= 3BV(r_{\text{shell}}) e^A h(\alpha_{\text{out}}, \beta_{\text{out}}) - 3BV(r_{\text{shell}-1}) h(\alpha_{\text{in}}, \beta_{\text{in}}) + 3CV(r_{\text{shell}}) \frac{j_1(\beta_{\text{out}})}{\beta_{\text{out}}} - 3CV(r_{\text{shell}-1}) \frac{j_1(\beta_{\text{in}})}{\beta_{\text{in}}}$$
where $h$ is

$$h(x, y) = \frac{x \sin(y) - y \cos(y)}{(x^2 + y^2)^{3/2}} - \frac{(x^2 - y^2) \sin(y) - 2xy \cos(y)}{(x^2 + y^2)^{3/2}}$$

For $A \sim 0$, e.g., $A = -0.0001$, this function converges to that of the linear SLD profile with $\rho_{\text{shell}}(r) \approx A(r - r_{\text{shell}-1})/\Delta t_{\text{shell}} + B$, so this case is equivalent to

$$f_{\text{shell}} = 3V(r_{\text{shell}}) \Delta \rho_{\text{shell}} \left[ \frac{2 \cos(qr_{\text{out}}) + qr_{\text{out}} \sin(qr_{\text{out}})}{(qr_{\text{out}})^4} \right] - 3V(r_{\text{shell}}) \Delta \rho_{\text{shell}} \left[ \frac{2 \cos(qr_{\text{in}}) + qr_{\text{in}} \sin(qr_{\text{in}})}{(qr_{\text{in}})^4} \right] + 3\rho_{\text{out}} V(r_{\text{shell}}) \frac{j_1(qr_{\text{out}})}{qr_{\text{out}}} - 3\rho_{\text{in}} V(r_{\text{shell}-1}) \frac{j_1(qr_{\text{in}})}{qr_{\text{in}}}$$

For $A = 0$, the exponential function has no dependence on the radius (so that $\rho_{\text{out}}$ is ignored in this case) and becomes flat. We set the constant to $\rho_{\text{in}}$ for convenience, and thus the form factor contributed by the shells is

$$f_{\text{shell}} = 3\rho_{\text{in}} V(r_{\text{shell}}) \frac{j_1(qr_{\text{out}})}{qr_{\text{out}}} - 3\rho_{\text{in}} V(r_{\text{shell}-1}) \frac{j_1(qr_{\text{in}})}{qr_{\text{in}}}$$

The 2D scattering intensity is the same as $P(q)$ above, regardless of the orientation of the $q$ vector which is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

NB: The outer most radius is used as the effective radius for $S(q)$ when $P(q)S(q)$ is applied.

References


**polymer_micelle**

Polymer micelle model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>ndensity</td>
<td>Number density of micelles</td>
<td>10¹⁵ cm⁻¹</td>
<td>8.94</td>
</tr>
<tr>
<td>v_core</td>
<td>Core volume</td>
<td>Å³</td>
<td>62624</td>
</tr>
<tr>
<td>v_corona</td>
<td>Corona volume</td>
<td>Å³</td>
<td>61940</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10⁻⁶ Å⁻²</td>
<td>6.4</td>
</tr>
<tr>
<td>sld_core</td>
<td>Core scattering length density</td>
<td>10⁻⁶ Å⁻²</td>
<td>0.34</td>
</tr>
<tr>
<td>sld_corona</td>
<td>Corona scattering length density</td>
<td>10⁻⁶ Å⁻²</td>
<td>0.8</td>
</tr>
<tr>
<td>radius_core</td>
<td>Radius of core ( must be &gt;&gt; rg )</td>
<td>Å</td>
<td>45</td>
</tr>
<tr>
<td>rg</td>
<td>Radius of gyration of chains in corona</td>
<td>Å</td>
<td>20</td>
</tr>
<tr>
<td>d_penetration</td>
<td>Factor to mimic non-penetration of Gaussian chains</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>n_aggreg</td>
<td>Aggregation number of the micelle</td>
<td>None</td>
<td>6</td>
</tr>
</tbody>
</table>
Fig. 1.84: Example of an onion model profile.

Fig. 1.85: 1D plot corresponding to the default parameters of the model.
The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

This model provides the form factor, $P(q)$, for a micelle with a spherical core and Gaussian polymer chains attached to the surface, thus may be applied to block copolymer micelles. To work well the Gaussian chains must be much smaller than the core, which is often not the case. Please study the reference carefully.

**Definition**

The 1D scattering intensity for this model is calculated according to the equations given by Pedersen (Pedersen, 2000), summarised briefly here.

The micelle core is imagined as $N = n_{aggregate}$ polymer heads, each of volume $V_{core}$, which then defines a micelle core of radius $r = r_{core}$, which is a separate parameter even though it could be directly determined. The Gaussian random coil tails, of gyration radius $R_g$, are imagined uniformly distributed around the spherical core, centred at a distance $r + d \cdot R_g$ from the micelle centre, where $d = d_{penetration}$ is of order unity. A volume $V_{corona}$ is defined for each coil. The model in detail seems to separately parametrise the terms for the shape of $I(Q)$ and the relative intensity of each term, so use with caution and check parameters for consistency. The spherical core is monodisperse, so its intensity and the cross terms may have sharp oscillations (use $q$ resolution smearing if needed to help remove them).

\[
P(q) = N^2 \beta_s^2 \Phi(qr)^2 + N^2 \beta_s^2 P_c(q) + 2N^2 \beta_s \beta_c S_{sc}(q) + N(N-1)\beta_s^2 S_{cc}(q)
\]

\[
\beta_s = V_{core} (\rho_{core} - \rho_{solvent})
\]

\[
\beta_c = V_{corona} (\rho_{corona} - \rho_{solvent})
\]

where $\rho_{core}$, $\rho_{corona}$ and $\rho_{solvent}$ are the scattering length densities $sld_{core}$, $sld_{corona}$ and $sld_{solvent}$. For the spherical core of radius $r$

\[
\Phi(qr) = \frac{\sin(qr) - qr \cos(qr)}{(qr)^3}
\]

whilst for the Gaussian coils

\[
P_c(q) = 2[\exp(-Z) + Z - 1]/Z^2
\]

\[
Z = (qR_g)^2
\]

The sphere to coil (core to corona) and coil to coil (corona to corona) cross terms are approximated by:

\[
S_{sc}(q) = \Phi(qr) \psi(Z) \frac{\sin(q(r + d \cdot R_g))}{q(r + d \cdot R_g)}
\]

\[
S_{cc}(q) = \psi(Z)^2 \left[ \frac{\sin(q(r + d \cdot R_g))}{q(r + d \cdot R_g)} \right]^2
\]

\[
\psi(Z) = \frac{[1 - \exp^{-Z}]}{Z}
\]

**Validation**

$P(q)$ above is multiplied by $ndensity$, and a units conversion of $10^{-13}$, so $scale$ is likely 1.0 if the scattering data is in absolute units. This model has not yet been independently validated.

**References**


- **Modified by:** Richard Heenan **Date:** March 20, 2016
- **Verified by:** Paul Kienzle **Date:** November 29, 2017
- **Description modified by:** Paul Kienzle **Date:** November 29, 2017
- **Description reviewed by:** Steve King **Date:** November 30, 2017
Fig. 1.86: 1D plot corresponding to the default parameters of the model.

**raspberry**

Calculates the form factor, \( P(q) \), for a ‘Raspberry-like’ structure where there are smaller spheres at the surface of a larger sphere, such as the structure of a Pickering emulsion.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<tr>
<td>background</td>
<td>Source background</td>
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<td>sld_lg</td>
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<tr>
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<tr>
<td>sld_solvent</td>
<td>solvent scattering length density</td>
<td>(10^6)Å(^{-2})</td>
<td>6.36</td>
</tr>
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<td>vol_fraction_lg</td>
<td>volume fraction of large spheres</td>
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<td>0.05</td>
</tr>
<tr>
<td>vol_fraction_sm</td>
<td>volume fraction of small spheres</td>
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<td>0.005</td>
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<td>radius_lg</td>
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<td>radius_sm</td>
<td>radius of small spheres</td>
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<td>100</td>
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<td>penetration</td>
<td>fractional penetration depth of small spheres into large sphere</td>
<td>Å</td>
<td>0</td>
</tr>
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</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition**

The figure below shows a schematic of a large droplet surrounded by several smaller particles forming a structure similar to that of Pickering emulsions.

In order to calculate the form factor of the entire complex, the self-correlation of the large droplet, the self-correlation of the particles, the correlation terms between different particles and the cross terms between large droplet and small particles all need to be calculated.

Consider two infinitely thin shells of radii \( R_1 \) and \( R_2 \) separated by distance \( r \). The general structure of the equation is then the form factor of the two shells multiplied by the phase factor that accounts for the separation of their centers.

\[
S(q) = \frac{\sin(qR_1) \sin(qR_2) \sin(qr)}{qR_1 qR_2 qr}
\]
In this case, the large droplet and small particles are solid spheres rather than thin shells. Thus the two terms must be integrated over $R_L$ and $R_S$ respectively using the weighting function of a sphere. We then obtain the functions for the form of the two spheres:

$$
\Psi_L = \int_0^{R_L} \frac{1}{4\pi R_L^2} \frac{\sin(qR_L)}{qR_L} dR_L = \frac{3[\sin(qR_L) - qR_L \cos(qR_L)]}{(qR_L)^2}
$$

$$
\Psi_S = \int_0^{R_S} \frac{1}{4\pi R_S^2} \frac{\sin(qR_S)}{qR_S} dR_S = \frac{3[\sin(qR_S) - qR_L \cos(qR_S)]}{(qR_S)^2}
$$

The cross term between the large droplet and small particles is given by:

$$
S_{LS} = \Psi_L \Psi_S \frac{\sin(q(R_L + \delta R_S))}{q(R_L + \delta R_S)}
$$

and the self term between small particles is given by:

$$
S_{SS} = \Psi_S^2 \left[ \frac{\sin(q(R_L + \delta R_S))}{q(R_L + \delta R_S)} \right]^2
$$

The number of small particles per large droplet, $N_p$, is given by:

$$
N_p = \frac{\phi_S \phi_{\text{surface}} V_L}{\phi_L V_S}
$$

where $\phi_S$ is the volume fraction of small particles in the sample, $\phi_{\text{surface}}$ is the fraction of the small particles that are adsorbed to the large droplets, $\phi_L$ is the volume fraction of large droplets in the sample, and $V_S$ and $V_L$ are the volumes of individual small particles and large droplets respectively.

The form factor of the entire complex can now be calculated including the excess scattering length densities of the components $\Delta \rho_L$ and $\Delta \rho_S$, where $\Delta \rho_x = |\rho_x - \rho_{\text{solvent}}|:

$$
P_{LS} = \frac{1}{M^2} \left[ (\Delta \rho_L)^2 V_L^2 \Psi_L^2 + N_p (\Delta \rho_S)^2 V_S^2 \Psi_S^2 + N_p (1 - N_p) (\Delta \rho_S)^2 V_S^2 S_{SS} + 2 N_p \Delta \rho_L \Delta \rho_S V_L V_S S_{LS} \right]
$$
where $M$ is the total scattering length of the whole complex:

$$M = \Delta \rho_L V_L + N_p \Delta \rho_S V_S$$

In a real system, there will usually be an excess of small particles such that some fraction remain unbound. Therefore the overall scattering intensity is given by:

$$I(Q) = I_{LS}(Q) + I_S(Q) = (\phi_L (\Delta \rho_L)^2 V_L + \phi_S \phi_{surface} N_p (\Delta \rho_S)^2 V_S) P_{LS} + \phi_S (1 - \phi_{surface}) (\Delta \rho_S)^2 V_S \Psi_S^2$$

A useful parameter to extract is the fraction of the surface area of the large droplets that is covered by small particles. This can be calculated from the model parameters as:

$$\chi = \frac{4 \phi_L \phi_{surface} (R_L + \delta R_S)}{\phi_L R_S}$$

---

**Fig. 1.88:** 1D plot corresponding to the default parameters of the model.

**References**


- **Author:** Andrew Jackson  
  **Date:** 2008

- **Modified by:** Andrew Jackson  
  **Date:** March 20, 2016

- **Reviewed by:** Andrew Jackson  
  **Date:** March 20, 2016

**sphere**

Spheres with uniform scattering length density

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<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
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<th>Default value</th>
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<td>scale</td>
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<td>background</td>
<td>Source background</td>
<td>cm$^{-1}$</td>
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</tr>
<tr>
<td>sld</td>
<td>Layer scattering length density</td>
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</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
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<td>6</td>
</tr>
<tr>
<td>radius</td>
<td>Sphere radius</td>
<td>Å</td>
<td>50</td>
</tr>
</tbody>
</table>
The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

For information about polarised and magnetic scattering, see the Polarisation/Magnetic Scattering documentation.

**Definition**

The 1D scattering intensity is calculated in the following way (Guinier, 1955)

\[
I(q) = \frac{\text{scale}}{V} \cdot \left[ 3V(\Delta \rho) \cdot \frac{\sin(qr) - qr \cos(qr))}{(qr)^3} \right]^2 + \text{background}
\]

where \(\text{scale}\) is a volume fraction, \(V\) is the volume of the scatterer, \(r\) is the radius of the sphere and \(\text{background}\) is the background level. \(\text{sl}d\) and \(\text{sl}d\_\text{solvent}\) are the scattering length densities (SLDs) of the scatterer and the solvent respectively, whose difference is \(\Delta \rho\).

Note that if your data is in absolute scale, the \(\text{scale}\) should represent the volume fraction (which is unitless) if you have a good fit. If not, it should represent the volume fraction times a factor (by which your data might need to be rescaled).

The 2D scattering intensity is the same as above, regardless of the orientation of \(\vec{q}\).

**Validation**

Validation of our code was done by comparing the output of the 1D model to the output of the software provided by the NIST (Kline, 2006).

![1D plot corresponding to the default parameters of the model.](image)

Fig. 1.89: 1D plot corresponding to the default parameters of the model.

**References**


- **Last Reviewed by**: S King and P Parker **Date**: 2013/09/09 and 2014/01/06

**spherical_sld**

Spherical SLD intensity calculation
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
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<td>background</td>
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</tr>
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<td>solvent sld</td>
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<td>4.06</td>
</tr>
<tr>
<td>sld[n_shells]</td>
<td>sld of the shell</td>
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<td>1</td>
</tr>
<tr>
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<td>thickness shell</td>
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</tr>
<tr>
<td>interface[n_shells]</td>
<td>thickness of the interface</td>
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<td>shape[n_shells]</td>
<td>interface shape</td>
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<tr>
<td>nu[n_shells]</td>
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<tr>
<td>n_steps</td>
<td>number of steps in each interface (must be an odd integer)</td>
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<td>35</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition**

Similarly to the onion, this model provides the form factor, \(P(q)\), for a multi-shell sphere, where the interface between the each neighboring shells can be described by the error function, power-law, or exponential functions. The scattering intensity is computed by building a continuous custom SLD profile along the radius of the particle. The SLD profile is composed of a number of uniform shells with interfacial shells between them.

![An Example of a SLD Profile w/ n_shells = 2](image)

Fig. 1.90: Example SLD profile

Unlike the <onion> model (using an analytical integration), the interfacial shells here are sub-divided and numerically integrated assuming each sub-shell is described by a line function, with \(n\_steps\) sub-shells per interface. The form factor is normalized by the total volume of the sphere.

Interface shapes are as follows:
The form factor $P(q)$ in 1D is calculated by:

$$P(q) = \frac{f^2}{\rho_{\text{particle}}} = f = f_{\text{core}} + \sum_{\text{inter}=0}^N f_{\text{inter}} + \sum_{\text{flat}=0}^N f_{\text{flat}} + f_{\text{solvent}}$$

So that individual terms can be calculated as follows:

- Core: $f_{\text{core}} = 4\pi \int_0^{r_{\text{core}}} \rho_{\text{core}} \frac{\sin(qr)}{qr} r^2 dr = 3\rho_{\text{core}} V(r_{\text{core}}) \left[ \sin(qr_{\text{core}}) - qr_{\text{core}} \cos(qr_{\text{core}}) \right] / qr_{\text{core}}^3$
- INTER: $f_{\text{inter}} = 4\pi \int_{\Delta r_{\text{inter}}} \rho_{\text{inter}} \frac{\sin(qr)}{qr} r^2 dr$
- SHELL: $f_{\text{shell}} = 4\pi \int_{\Delta r_{\text{shell}}} \rho_{\text{shell}} \frac{\sin(qr)}{qr} r^2 dr = 3\rho_{\text{shell}} V(r_{\text{shell}} + \Delta r_{\text{shell}}) \left[ \sin(qr_{\text{shell}} + \Delta r_{\text{shell}}) - q(r_{\text{shell}} + \Delta r_{\text{shell}}) \cos(qr_{\text{shell}} + \Delta r_{\text{shell}}) \right] / qr_{\text{shell}}^3$
- SOLVENT: $f_{\text{solvent}} = 4\pi \int_{r_{\text{out}}}^{\infty} \rho_{\text{solvent}} \frac{\sin(qr)}{qr} r^2 dr = 3\rho_{\text{solvent}} V(r_{\text{solvent}}) \left[ \sin(qr_{\text{solvent}}) - qr_{\text{solvent}} \cos(qr_{\text{solvent}}) \right] / qr_{\text{solvent}}^3$

Here we assumed that the SLDs of the core and solvent are constant in $r$. The SLD at the interface between shells, $\rho_{\text{inter}}$, is calculated with a function chosen by an user, where the functions are:

**Exp:**

$$\rho_{\text{inter}}(r) = \begin{cases} \pm B \exp \left( \frac{\pm A(r-r_{\text{flat}})}{\Delta r_{\text{flat}}} \right) + C & \text{for } A \neq 0 \\ B \left( \frac{r-r_{\text{flat}}}{\Delta r_{\text{flat}}} \right) + C & \text{for } A = 0 \end{cases}$$

**Power-Law:**

$$\rho_{\text{inter}}(r) = \begin{cases} \pm B \left( \frac{r-r_{\text{flat}}}{\Delta r_{\text{flat}}} \right)^A + C & \text{for } A \neq 0 \\ \rho_{\text{flat}} & \text{for } A = 0 \end{cases}$$

**Erf:**

$$\rho_{\text{inter}}(r) = \begin{cases} B \text{Erf} \left( \frac{A(r-r_{\text{flat}})}{\sqrt{2}\Delta r_{\text{flat}}} \right) + C & \text{for } A \neq 0 \\ B \left( \frac{r-r_{\text{flat}}}{\Delta r_{\text{flat}}} \right) + C & \text{for } A = 0 \end{cases}$$

The functions are normalized so that they vary between 0 and 1, and they are constrained such that the SLD is continuous at the boundaries of the interface as well as each sub-shell. Thus B and C are determined.

Once $\rho_{\text{inter}}$ is found at the boundary of the sub-shell of the interface, we can find its contribution to the form factor $P(q)$

$$f_{\text{inter}} = 4\pi \int_{\Delta r_{\text{inter}}} \rho_{\text{inter}} \frac{\sin(qr)}{qr} r^2 dr = 4\pi \sum_{j=1}^{n_{\text{sub}}} \left[ 3(\rho_{\text{inter}}(r_{j+1}) - \rho_{\text{inter}}(r_j)) V(r_j) \left( \frac{r_j^2}{\beta_{\text{out}}^4} \sin(\beta_{\text{out}}) - \frac{(\beta_{\text{out}}^2 - 2) \cos(\beta_{\text{out}})}{\beta_{\text{out}}^4} \right) \\ - 3(\rho_{\text{inter}}(r_{j+1}) - \rho_{\text{inter}}(r_j)) V(r_{j-1}) \left( \frac{r_{j-1}^2}{\beta_{\text{in}}^4} \sin(\beta_{\text{in}}) - \frac{(\beta_{\text{in}}^2 - 2) \cos(\beta_{\text{in}})}{\beta_{\text{in}}^4} \right) \\ + 3\rho_{\text{inter}}(r_{j+1}) V(r_j) \left( \frac{\sin(\beta_{\text{out}}) - \cos(\beta_{\text{out}})}{\beta_{\text{out}}^4} \right) - 3\rho_{\text{inter}}(r_j) V(r_j) \left( \frac{\sin(\beta_{\text{in}}) - \cos(\beta_{\text{in}})}{\beta_{\text{in}}^4} \right) \right]$$
where

\[ V(a) = \frac{4\pi}{3} a^3 \]

\[ a_{in} \sim \frac{r_j}{r_{j+1} - r_j}, \quad a_{out} \sim \frac{r_{j+1}}{r_{j+1} - r_j} \]

\[ \beta_{in} = q r_j, \quad \beta_{out} = q r_{j+1} \]

We assume \( \rho_{inner}(r) \) is approximately linear within the sub-shell \( j \).

Finally the form factor can be calculated by

\[ P(q) = \frac{|f|^2}{V_{\text{particle}}} \text{ where } V_{\text{particle}} = V(r_{\text{shell},N}) \]

For 2D data the scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[ q = \sqrt{q_x^2 + q_y^2} \]

Note: The outer most radius is used as the effective radius for \( S(Q) \) when \( P(Q) * S(Q) \) is applied.

Fig. 1.91: 1D plot corresponding to the default parameters of the model.

References

Authorship and Verification

- **Author:** Jae-Hie Cho  **Date:** Nov 1, 2010
- **Last Modified by:** Paul Kienzle  **Date:** Dec 20, 2016
- **Last Reviewed by:** Paul Butler  **Date:** September 8, 2018

**vesicle**

Vesicle model representing a hollow sphere
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm$^{-1}$</td>
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</tr>
<tr>
<td>sld</td>
<td>vesicle shell scattering length density</td>
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<td>sld_solvent</td>
<td>solvent scattering length density</td>
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<td>radius</td>
<td>vesicle core radius</td>
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<td>vesicle shell thickness</td>
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The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

**Definition**

This model provides the form factor, $P(q)$, for an unilamellar vesicle and is effectively identical to the hollow sphere reparameterized to be more intuitive for a vesicle and normalizing the form factor by the volume of the shell. The 1D scattering intensity is calculated in the following way (Guinier, 1955):

$$P(q) = \frac{\phi V_{shell}}{3V_{core}(\rho_{solvent} - \rho_{shell})j_1(qR_{core})} + \frac{3V_{tot}(\rho_{shell} - \rho_{solvent})j_1(qR_{tot})}{qR_{tot}} + \text{background}$$

where $\phi$ is the volume fraction of shell material, $V_{shell}$ is the volume of the shell, $V_{core}$ is the volume of the core, $V_{tot}$ is the total volume, $R_{core}$ is the radius of the core, $R_{tot}$ is the outer radius of the shell, $\rho_{solvent}$ is the scattering length density of the solvent (which is the same as for the core in this case), $\rho_{scale}$ is the scattering length density of the shell, background is a flat background level (due for example to incoherent scattering in the case of neutrons), and $j_1$ is the spherical bessel function $j_1 = (\sin(x) - x \cos(x))/x^2$.

The functional form is identical to a “typical” core-shell structure, except that the scattering is normalized by the volume that is contributing to the scattering, namely the volume of the shell alone, the scattering length density of the core is fixed the same as that of the solvent, the scale factor when the data are on an absolute scale is equivalent to the volume fraction of material in the shell rather than the entire core+shell sphere, and the parameterization is done in terms of the core radius $= R_{core}$ and the shell thickness $= R_{tot} - R_{core}$.

![Fig. 1.92: Vesicle geometry.](image)

The 2D scattering intensity is the same as $P(q)$ above, regardless of the orientation of the $q$ vector which is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

NB: The outer most radius ($= \text{radius} + \text{thickness}$) is used as the effective radius for $S(Q)$ when $P(Q) * S(Q)$ is applied.

---

Fig. 1.93: 1D plot corresponding to the default parameters of the model.

References

Authorship and Verification

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
- **Last Modified by:** Paul Butler **Date:** March 20, 2016
- **Last Reviewed by:** Paul Butler **Date:** September 7, 2018

1.1.7 Shape-Independent Functions

**be_polyelectrolyte**

Polyelectrolyte with the RPA expression derived by Borue and Erukhimovich

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<th>Parameter</th>
<th>Description</th>
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<th>Default value</th>
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<td>background</td>
<td>Source background</td>
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<td>salt_concentration</td>
<td>Concentration of monovalent salt</td>
<td>mol/L</td>
<td>0</td>
</tr>
<tr>
<td>ionization_degree</td>
<td>Degree of ionization</td>
<td>None</td>
<td>0.05</td>
</tr>
<tr>
<td>polymer_concentration</td>
<td>Polymer molar concentration</td>
<td>mol/L</td>
<td>0.7</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Note:** Please read the Validation section below.

**Definition** This model calculates the structure factor of a polyelectrolyte solution with the RPA expression derived
by Borue and Erukhimovich\textsuperscript{1}. Note however that the fitting procedure here does not follow the notation in that reference as ‘s’ and ‘t’ are not decoupled. Instead the scattering intensity $I(q)$ is calculated as

$$I(q) = K \frac{q^2 + k^2}{4\pi L_b \alpha^2} \frac{1}{1 + r_0^4 (q^2 + k^2)(q^2 - 12hC_s/b^2) + \text{background}}$$

$$k^2 = 4\pi L_b (2C_s + \alpha C_a)$$

$$r_0^2 = \frac{b}{\alpha \sqrt{C_a} \sqrt{48\pi L_b}}$$

where

$K$ is the contrast factor for the polymer which is defined differently than in other models and is given in barns where 1 barn $= 10^{-24}$ cm$^2$. $K$ is defined as:

$$K = a^2$$

$$a = b_p - (v_p/v_s)b_s$$

where:

- $b_p$ and $b_s$ are \textit{sum of the scattering lengths of the atoms} constituting the polymer monomer and the solvent molecules, respectively.
- $v_p$ and $v_s$ are the partial molar volume of the polymer and the solvent, respectively.
- $L_b$ is the Bjerrum length (Å) - \textbf{Note:} This parameter needs to be kept constant for a given solvent and temperature!
- $h$ is the virial parameter (Å$^3$) - \textbf{Note:} See\textsuperscript{1} for the correct interpretation of this parameter. It incorporates second and third virial coefficients and can be negative.
- $b$ is the monomer length (Å).
- $C_s$ is the concentration of monovalent salt (1/Å$^3$ - internally converted from mol/L).
- $\alpha$ is the degree of ionization (the ratio of charged monomers to the total number of monomers)
- $C_a$ is the polymer molar concentration (1/Å$^3$ - internally converted from mol/L)
- \textit{background} is the incoherent background.

For 2D data the scattering intensity is calculated in the same way as 1D, where the $\vec{q}$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

\textbf{Validation}

As of the last revision, this code is believed to be correct. However it needs further validation and should be used with caution at this time. The history of this code goes back to a 1998 implementation. It was recently noted that in that implementation, while both the polymer concentration and salt concentration were converted from experimental units of mol/L to more dimensionally useful units of 1/Å$^3$, only the converted version of the polymer concentration was actually being used in the calculation while the unconverted salt concentration (still in apparent units of mol/L) was being used. This was carried through to Sasmodels as used for SasView 4.1 (though the line of code converting the salt concentration to the new units was removed somewhere along the line). Simple dimensional analysis of the calculation shows that the converted salt concentration should be used, which the original code suggests was the intention, so this has now been corrected (for SasView 4.2). Once better validation has been performed this note will be removed.

\textbf{References}

\textbf{Authorship and Verification}

- \textbf{Author:} NIST IGOR/DANSE \textbf{Date:} pre 2010
- \textbf{Last Modified by:} Paul Butler \textbf{Date:} September 25, 2018
- \textbf{Last Reviewed by:} Paul Butler \textbf{Date:} September 25, 2018

\textsuperscript{1} V Y Borue, I Y Erukhimovich, \textit{Macromolecules}, 21 (1988) 3240
Fig. 1.94: 1D plot corresponding to the default parameters of the model.

**broad_peak**

Broad Lorentzian type peak on top of a power law decay

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
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<tr>
<td>background</td>
<td>Source background</td>
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<td>0.001</td>
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<tr>
<td>porod_scale</td>
<td>Power law scale factor</td>
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<td>1e-05</td>
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<tr>
<td>porod_exp</td>
<td>Exponent of power law</td>
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<td>3</td>
</tr>
<tr>
<td>lorentz_scale</td>
<td>Scale factor for broad Lorentzian peak</td>
<td>None</td>
<td>10</td>
</tr>
<tr>
<td>lorentz_length</td>
<td>Lorentzian screening length</td>
<td>Å</td>
<td>50</td>
</tr>
<tr>
<td>peak_pos</td>
<td>Peak position in q</td>
<td>Å$^{-1}$</td>
<td>0.1</td>
</tr>
<tr>
<td>lorentz_exp</td>
<td>Exponent of Lorentz function</td>
<td>None</td>
<td>2</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

**Definition**

This model calculates an empirical functional form for SAS data characterized by a broad scattering peak. Many SAS spectra are characterized by a broad peak even though they are from amorphous soft materials. For example, soft systems that show a SAS peak include copolymers, polyelectrolytes, multiphase systems, layered structures, etc.

The d-spacing corresponding to the broad peak is a characteristic distance between the scattering inhomogeneities (such as in lamellar, cylindrical, or spherical morphologies, or for bicontinuous structures).

The scattering intensity $I(q)$ is calculated as

$$ I(q) = \frac{A}{q^n} + \frac{C}{1 + (|q - q_0|\xi)^m} + B $$

Here the peak position is related to the d-spacing as $q_0 = 2\pi/d_0$.

$A$ is the Porod law scale factor, $n$ the Porod exponent, $C$ is the Lorentzian scale factor, $m$ the exponent of $q$, $\xi$ the screening length, and $B$ the flat background.
For 2D data the scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$ q = \sqrt{q_x^2 + q_y^2} $$

Fig. 1.95: 1D plot corresponding to the default parameters of the model.

References
None.

Authorship and Verification
- **Author**: NIST IGOR/DANSE **Date**: pre 2010
- **Last Modified by**: Paul kienle **Date**: July 24, 2016
- **Last Reviewed by**: Richard Heenan **Date**: March 21, 2016

**correlation_length**

Calculates an empirical functional form for SAS data characterized by a low-Q signal and a high-Q signal.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm$^{-1}$</td>
<td>0.001</td>
</tr>
<tr>
<td>lorentz_scale</td>
<td>Lorentzian Scaling Factor</td>
<td>None</td>
<td>10</td>
</tr>
<tr>
<td>porod_scale</td>
<td>Porod Scaling Factor</td>
<td>None</td>
<td>1e-06</td>
</tr>
<tr>
<td>cor_length</td>
<td>Correlation length, $x_i$, in Lorentz</td>
<td>Å</td>
<td>50</td>
</tr>
<tr>
<td>porod_exp</td>
<td>Porod Exponent, n, in $q^n$-n</td>
<td>None</td>
<td>3</td>
</tr>
<tr>
<td>lorentz_exp</td>
<td>Lorentzian Exponent, m, in $1/(1+(q.xi)^m)$</td>
<td>Å$^{-2}$</td>
<td>2</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

**Definition**
The scattering intensity $I(q)$ is calculated as

$$I(Q) = \frac{A}{Q^n} + \frac{C}{1 + (Q\xi)^m} + \text{background}$$

The first term describes Porod scattering from clusters (exponent = $n$) and the second term is a Lorentzian function describing scattering from polymer chains (exponent = $m$). This second term characterizes the polymer/solvent interactions and therefore the thermodynamics. The two multiplicative factors $A$ and $C$, and the two exponents $n$ and $m$ are used as fitting parameters. (Respectively porod_scale, lorentz_scale, porod_exp and lorentz_exp in the parameter list.) The remaining parameter $\xi$ (cor_length in the parameter list) is a correlation length for the polymer chains. Note that when $m = 2$ this functional form becomes the familiar Lorentzian function. Some interpretation of the values of $A$ and $C$ may be possible depending on the values of $m$ and $n$.

For 2D data: The 2D scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

Fig. 1.96: 1D plot corresponding to the default parameters of the model.

References

B Hammouda, D L Ho and S R Kline, Insight into Clustering in Poly(ethylene oxide) Solutions, Macromolecules, 37 (2004) 6932-6937

**dab**

DAB (Debye Anderson Brumberger) Model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm$^{-1}$</td>
<td>0.001</td>
</tr>
<tr>
<td>cor_length</td>
<td>correlation length</td>
<td>Å</td>
<td>50</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.
Calculates the scattering from a randomly distributed, two-phase system based on the Debye-Anderson-Brumberger (DAB) model for such systems. The two-phase system is characterized by a single length scale, the correlation length, which is a measure of the average spacing between regions of phase 1 and phase 2. The model also assumes smooth interfaces between the phases and hence exhibits Porod behavior \( I \sim q^{-4} \) at large \( q \), \( (qL > 1) \).

The DAB model is ostensibly a development of the earlier Debye-Bueche model.

**Definition**

\[
I(q) = \text{scale} \cdot \frac{L^3}{(1 + (q \cdot L)^2)^2} + \text{background}
\]

where scale is

\[
\text{scale} = 8\pi\phi(1 - \phi)\Delta\rho^2
\]

and the parameter \( L \) is the correlation length.

For 2D data the scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

Fig. 1.97: 1D plot corresponding to the default parameters of the model.

**References**


2013/09/09 - Description reviewed by King, S and Parker, P.

**fractal**

Calculates the scattering from fractal-like aggregates of spheres following the Texiera reference.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
<td>0.001</td>
</tr>
<tr>
<td>vol fraction</td>
<td>volume fraction of blocks</td>
<td>None</td>
<td>0.05</td>
</tr>
<tr>
<td>radius</td>
<td>radius of particles</td>
<td>Å</td>
<td>5</td>
</tr>
<tr>
<td>fractal_dim</td>
<td>fractal dimension</td>
<td>None</td>
<td>2</td>
</tr>
<tr>
<td>cor_length</td>
<td>cluster correlation length</td>
<td>Å</td>
<td>100</td>
</tr>
<tr>
<td>sld_block</td>
<td>scattering length density of particles</td>
<td>10⁻⁶ Å⁻²</td>
<td>2</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>scattering length density of solvent</td>
<td>10⁻⁶ Å⁻²</td>
<td>6.4</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition** This model calculates the scattering from fractal-like aggregates of spherical building blocks according to the following equation:

\[
I(q) = \phi V_{\text{block}} (\rho_{\text{block}} - \rho_{\text{solvent}})^2 P(q) S(q) + \text{background}
\]

where \( \phi \) is the volume fraction of the spherical “building block” particles of radius \( R_0 \), \( V_{\text{block}} \) is the volume of a single building block, \( \rho_{\text{solvent}} \) is the scattering length density of the solvent, and \( \rho_{\text{block}} \) is the scattering length density of the building blocks, and \( P(q), S(q) \) are the scattering from randomly distributed spherical particles (the building blocks) and the interference from such building blocks organized in a fractal-like clusters. \( P(q) \) and \( S(q) \) are calculated as:

\[
P(q) = F(qR_0)^2
\]

\[
F(q) = \frac{3(\sin x - x \cos x)}{x^3}
\]

\[
V_{\text{particle}} = \frac{4}{3} \pi R_0^3
\]

\[
S(q) = 1 + \frac{D_f \Gamma(D_f - 1)}{[1 + 1/(q\xi)^2]^{(D_f - 1)/2}} \frac{\sin[(D_f - 1) \tan^{-1}(q\xi)]}{(qR_0)^D_f}
\]

where \( \xi \) is the correlation length representing the cluster size and \( D_f \) is the fractal dimension, representing the self similarity of the structure. Note that \( S(q) \) here goes negative if \( D_f \) is too large, and the Gamma function diverges at \( D_f = 0 \) and \( D_f = 1 \).

**Polydispersity on the radius is provided for.**

For 2D data: The 2D scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

**References**

**Authorship and Verification**

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
- **Converted to sasmodels by:** Paul Butler **Date:** March 19, 2016
- **Last Modified by:** Paul Butler **Date:** March 12, 2017
- **Last Reviewed by:** Paul Butler **Date:** March 12, 2017

**fractal_core_shell**

Scattering from a fractal structure formed from core shell spheres
Fig. 1.98: 1D plot corresponding to the default parameters of the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>radius</td>
<td>Sphere core radius</td>
<td>Å</td>
<td>60</td>
</tr>
<tr>
<td>thickness</td>
<td>Sphere shell thickness</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>sld_core</td>
<td>Sphere core scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>1</td>
</tr>
<tr>
<td>sld_shell</td>
<td>Sphere shell scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>2</td>
</tr>
<tr>
<td>sld_solvent</td>
<td>Solvent scattering length density</td>
<td>10(^{-6})Å(^{-2})</td>
<td>3</td>
</tr>
<tr>
<td>volfraction</td>
<td>Volume fraction of building block spheres</td>
<td>None</td>
<td>0.05</td>
</tr>
<tr>
<td>fractal_dim</td>
<td>Fractal dimension</td>
<td>None</td>
<td>2</td>
</tr>
<tr>
<td>cor_length</td>
<td>Correlation length of fractal-like aggregates</td>
<td>Å</td>
<td>100</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition** Calculates the scattering from a fractal structure with a primary building block of core-shell spheres, as opposed to just homogeneous spheres in the fractal model. It is an extension of the well known Teixeira\(^1\) fractal model replacing the \(P(q)\) of a solid sphere with that of a core-shell sphere. This model could find use for aggregates of coated particles, or aggregates of vesicles for example.

\[
I(q) = P(q)S(q) + \text{background}
\]

Where \(P(q)\) is the core-shell form factor and \(S(q)\) is the Teixeira\(^1\) fractal structure factor both of which are given again below:

\[
P(q) = \frac{\phi}{V_s} \left[ 3V_c(\rho_c - \rho_s) \frac{\sin(qr_c) - qr_c \cos(qr_c)}{(qr_c)^3} + 3V_s(\rho_s - \rho_{solvent}) \frac{\sin(qr_s) - qr_s \cos(qr_s)}{(qr_s)^3} \right]^2
\]

\[
S(q) = 1 + \frac{D_f \Gamma(D_f - 1)}{[1 + 1/(q\xi)^2]^{(D_f-1)/2}} \frac{\sin[(D_f - 1) \tan^{-1}(q\xi)]}{(qr_s)^{D_f}}
\]

where \(\phi\) is the volume fraction of particles, \(V_s\) is the volume of the whole particle, \(V_c\) is the volume of the core, \(\rho_c\), \(\rho_s\), and \(\rho_{solvent}\) are the scattering length densities of the core, shell, and solvent respectively, \(r_c\) and \(r_s\) are the radius of the core and the radius of the whole particle respectively, \(D_f\) is the fractal dimension, and \(\xi\) the correlation length.

Polydispersity of radius and thickness are also provided for.

This model does not allow for anisotropy and thus the 2D scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

Our model is derived from the form factor calculations implemented in IGOR macros by the NIST Center for Neutron Research.

![1D plot corresponding to the default parameters of the model.](image)

**Fig. 1.99:** 1D plot corresponding to the default parameters of the model.

**References**

**Authorship and Verification**

- **Author:** NIST IGOR/DANSE **Date:** pre 2010
- **Last Modified by:** Paul Butler and Paul Kienzle **Date:** November 27, 2016
- **Last Reviewed by:** Paul Butler and Paul Kienzle **Date:** November 27, 2016

**gauss_lorentz_gel**

Gauss Lorentz Gel model of scattering from a gel structure

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm$^{-1}$</td>
<td>0.001</td>
</tr>
<tr>
<td>gauss_scale</td>
<td>Gauss scale factor</td>
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<td>100</td>
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<tr>
<td>cor_length_static</td>
<td>Static correlation length</td>
<td>Å</td>
<td>100</td>
</tr>
<tr>
<td>lorentz_scale</td>
<td>Lorentzian scale factor</td>
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<td>50</td>
</tr>
<tr>
<td>cor_length_dynamic</td>
<td>Dynamic correlation length</td>
<td>Å</td>
<td>20</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

---

This model calculates the scattering from a gel structure, but typically a physical rather than chemical network. It is modeled as a sum of a low-q exponential decay (which happens to give a functional form similar to Guinier scattering, so interpret with care) plus a Lorentzian at higher-q values. See also the gel_fit model.

**Definition**

The scattering intensity $I(q)$ is calculated as (Eqn. 5 from the reference)

$$
I(q) = I_G(0) \exp(-q^2 \Xi^2/2) + I_L(0)/(1 + q^2 \xi^2)
$$

$\Xi$ is the length scale of the static correlations in the gel, which can be attributed to the “frozen-in” crosslinks. $\xi$ is the dynamic correlation length, which can be attributed to the fluctuating polymer chains between crosslinks. $I_G(0)$ and $I_L(0)$ are the scaling factors for each of these structures. Think carefully about how these map to your particular system!

**Note:** The peaked structure at higher $q$ values (Figure 2 from the reference) is not reproduced by the model. Peaks can be introduced into the model by summing this model with the *gaussian_peak* model.

For 2D data the scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$
q = \sqrt{q_x^2 + q_y^2}
$$

Fig. 1.100: 1D plot corresponding to the default parameters of the model.

**References**


*gaussian_peak*

Gaussian shaped peak
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
<td>0.001</td>
</tr>
<tr>
<td>peak_pos</td>
<td>Peak position</td>
<td>Å(^{-1})</td>
<td>0.05</td>
</tr>
<tr>
<td>sigma</td>
<td>Peak width (standard deviation)</td>
<td>Å(^{-1})</td>
<td>0.005</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

**Definition**

This model describes a Gaussian shaped peak on a flat background

\[
I(q) = (\text{scale}) \exp \left[ -\frac{1}{2} \left( q - q_0 \right)^2 / \sigma^2 \right] + \text{background}
\]

with the peak having height of \( \text{scale} \) centered at \( q_0 \) and having a standard deviation of \( \sigma \). The FWHM (full-width half-maximum) is \( 2.354\sigma \).

For 2D data, scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

![1D plot corresponding to the default parameters of the model.](image)

Fig. 1.101: 1D plot corresponding to the default parameters of the model.

**References**

None.

**gel_fit**

Fitting using fine-scale polymer distribution in a gel.
The returned value is scaled to units of \( \text{cm}^{-1} \text{ sr}^{-1} \), absolute scale.

This model was implemented by an interested user!

Unlike a concentrated polymer solution, the fine-scale polymer distribution in a gel involves at least two characteristic length scales, a shorter correlation length \( a_1 \) to describe the rapid fluctuations in the position of the polymer chains that ensure thermodynamic equilibrium, and a longer distance (denoted here as \( a_2 \)) needed to account for the static accumulations of polymer pinned down by junction points or clusters of such points. The latter is derived from a simple Guinier function. Compare also the gauss_lorentz_gel model.

**Definition**

The scattered intensity \( I(q) \) is calculated as

\[
I(Q) = I(0) L \left( \frac{1}{1 + \left[ (D + 1/3)Q^2 a_1^2 \right]^{D/2}} \right) + I(0) \exp \left( -Q^2 a_2^2 \right) + B
\]

where

\[
a_2^2 \approx \frac{R_g^2}{3}
\]

Note that the first term reduces to the Ornstein-Zernicke equation when \( D = 2 \); i.e., when the Flory exponent is 0.5 (theta conditions). In gels with significant hydrogen bonding \( D \) has been reported to be ~2.6 to 2.8.

Fig. 1.102: 1D plot corresponding to the default parameters of the model.

**References**

Mitsuhiro Shibayama, Toyoichi Tanaka, Charles C Han, *J. Chem. Phys.* 1992, 97 (9), 6829-6841

The returned value is scaled to units of \( \text{cm}^{-1} \text{sr}^{-1} \), absolute scale.

**Definition**

This model fits the Guinier function

\[
I(q) = \text{scale} \cdot \exp \left( \frac{-Q^2 R_g^2}{3} \right) + \text{background}
\]

to the data directly without any need for linearisation (cf. the usual plot of \( \ln I(q) \) vs \( q^2 \)). Note that you may have to restrict the data range to include small \( q \) only, where the Guinier approximation actually applies. See also the guinier_porod model.

For 2D data the scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

In scattering, the radius of gyration \( R_g \) quantifies the object’s distribution of SLD (not mass density, as in mechanics) from the object’s SLD centre of mass. It is defined by

\[
R_g^2 = \frac{\sum_i \rho_i (r_i - r_0)^2}{\sum_i \rho_i}
\]

where \( r_0 \) denotes the object’s SLD centre of mass and \( \rho_i \) is the SLD at a point \( i \).

Notice that \( R_g^2 \) may be negative (since SLD can be negative), which happens when a form factor \( P(Q) \) is increasing with \( Q \) rather than decreasing. This can occur for core/shell particles, hollow particles, or for composite particles with domains of different SLDs in a solvent with an SLD close to the average match point. (Alternatively, this might be regarded as there being an internal inter-domain “structure factor” within a single particle which gives rise to a peak in the scattering).

To specify a negative value of \( R_g^2 \) in SasView, simply give \( R_g \) a negative value (\( R_g^2 \) will be evaluated as \( R_g^2 | R_g | \)). Note that the physical radius of gyration, of the exterior of the particle, will still be large and positive. It is only the apparent size from the small \( Q \) data that will give a small or negative value of \( R_g^2 \).

**References**


---

**guinier**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
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<tbody>
<tr>
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<td>Source intensity</td>
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<tr>
<td>background</td>
<td>Source background</td>
<td>( \text{cm}^{-1} )</td>
<td>0.001</td>
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<td>rg</td>
<td>Radius of Gyration</td>
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**guinier_porod**

Guinier-Porod function

<table>
<thead>
<tr>
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<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
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<td>rg</td>
<td>Radius of gyration</td>
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</tr>
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<td>s</td>
<td>Dimension variable</td>
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<td>porod_exp</td>
<td>Porod exponent</td>
<td>None</td>
<td>3</td>
</tr>
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</table>

The returned value is scaled to units of \( \text{cm}^{-1} \text{sr}^{-1} \), absolute scale.

Calculates the scattering for a generalized Guinier/power law object. This is an empirical model that can be used to determine the size and dimensionality of scattering objects, including asymmetric objects such as rods or...
platelets, and shapes intermediate between spheres and rods or between rods and platelets, and overcomes some of the deficiencies of the (Beaucage) Unified_Power_Rg model (see Hammouda, 2010).

Definition
The following functional form is used

\[
I(q) = \begin{cases} 
\frac{G}{Q} \exp \left[ \frac{-Q^2 R_g^2}{4 - s} \right] & Q \leq Q_1 \\
D/Q^m & Q > Q_1 
\end{cases}
\]

This is based on the generalized Guinier law for such elongated objects (see the Glatter reference below). For 3D globular objects (such as spheres), \(s = 0\) and one recovers the standard Guinier formula. For 2D symmetry (such as for rods) \(s = 1\), and for 1D symmetry (such as for lamellae or platelets) \(s = 2\). A dimensionality parameter \((3 - s)\) is thus defined, and is 3 for spherical objects, 2 for rods, and 1 for plates.

Enforcing the continuity of the Guinier and Porod functions and their derivatives yields

\[
Q_1 = \frac{1}{R_g} \sqrt{(m - s)(3 - s)/2}
\]

and

\[
D = G \exp \left[ \frac{-Q_1^2 R_g^2}{3 - s} \right] Q_1^{m - s}
\]

\[
= \frac{G}{R_g^{m - s}} \exp \left[ -\frac{m - s}{2} \right] \left( \frac{(m - s)(3 - s)}{2} \right)^{\frac{m - s}{2}}
\]

Note that the radius of gyration for a sphere of radius \(R\) is given by \(R_g = R \sqrt{3/5}\). For a cylinder of radius \(R\) and length \(L\), \(R_g^2 = \frac{L^2}{12} + \frac{R^2}{4}\) from which the cross-sectional radius of gyration for a randomly oriented thin cylinder is \(R_g = R / \sqrt{2}\) and the cross-sectional radius of gyration of a randomly oriented lamella of thickness \(T\) is given by \(R_g = T / \sqrt{12}\).

For 2D data: The 2D scattering intensity is calculated in the same way as 1D, where the \(q\) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]
Fig. 1.104: 1D plot corresponding to the default parameters of the model.

Reference


**line**

Line model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
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<td>background</td>
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<td>intercept</td>
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<td>slope</td>
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</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This model calculates intensity using simple linear function

**Definition**

The scattering intensity \(I(q)\) is calculated as

\[ I(q) = \text{scale}(A + B \cdot q) + \text{background} \]

**Note:** For 2D plots intensity has different definition than other shape independent models

\[ I(q) = \text{scale}(I(qx) \cdot I(qy)) + \text{background} \]
Fig. 1.105: 1D plot corresponding to the default parameters of the model.

References
None.

lorentz
Ornstein-Zernicke correlation length model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
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<tbody>
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<td>Screening length</td>
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</table>

The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

Lorentz (Ornstein-Zernicke Model)

Definition
The Ornstein-Zernicke model is defined by

$$I(q) = \frac{\text{scale}}{1 + (qL)^2} + \text{background}$$

The parameter $L$ is the screening length $\text{cor\_length}$.

For 2D data the scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

References
L.S. Ornstein and F. Zernike, Proc. Acad. Sci. Amsterdam 17, 793 (1914), and Z. Phys. 19, 134 (1918), and 27, 761 (1926); referred to as QZ.

1.1. Model Functions
mass_fractal

Mass Fractal model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
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<td>background</td>
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<td>radius</td>
<td>Particle radius</td>
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The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

Calculates the scattering from fractal-like aggregates based on the Mildner reference.

Definition

The scattering intensity \( I(q) \) is calculated as

\[
I(q) = \text{scale} \times P(q)S(q) + \text{background}
\]

\[
P(q) = F(qR)^2
\]

\[
F(x) = \frac{3\left[\sin(x) - x\cos(x)\right]}{x^3}
\]

\[
S(q) = \frac{\Gamma(D_m - 1)\zeta^{D_m - 1} \sin \left[ (D_m - 1)\tan^{-1}(q\zeta) \right]}{(1 + (q\zeta)^2)^{(D_m - 1)/2}}
\]

\[
\text{scale} = \text{scale\_factor} \times NV^2(\rho_{\text{particle}} - \rho_{\text{solvent}})^2
\]

\[
V = \frac{4}{3}\pi R^3
\]

where \( R \) is the radius of the building block, \( D_m \) is the mass fractal dimension, \( \zeta \) is the cut-off length, \( \rho_{\text{solvent}} \) is the scattering length density of the solvent, and \( \rho_{\text{particle}} \) is the scattering length density of particles.
Note: The mass fractal dimension \( D_m \) is only valid if \( 1 < mass\_dim < 6 \). It is also only valid over a limited \( q \) range (see the reference for details).

Fig. 1.107: 1D plot corresponding to the default parameters of the model.

References


**mass_surface_fractal**

Mass Surface Fractal model

<table>
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<th>Parameter</th>
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<td>4000</td>
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<tr>
<td>rg_primary</td>
<td>Primary particle radius of gyration</td>
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<td>86.7</td>
</tr>
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</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

A number of natural and commercial processes form high-surface area materials as a result of the vapour-phase aggregation of primary particles. Examples of such materials include soots, aerosols, and fume or pyrogenic silicas. These are all characterised by cluster mass distributions (sometimes also cluster size distributions) and internal surfaces that are fractal in nature. The scattering from such materials displays two distinct breaks in log-log representation, corresponding to the radius-of-gyration of the primary particles, \( rg \), and the radius-of-gyration of the clusters (aggregates), \( R_g \). Between these boundaries the scattering follows a power law related to the mass fractal dimension, \( D_m \), whilst above the high-Q boundary the scattering follows a power law related to the surface fractal dimension of the primary particles, \( D_s \).

Definition
The scattered intensity $I(q)$ is calculated using a modified Ornstein-Zernicke equation

$$I(q) = \text{scale} \times P(q) + \text{background}$$

$$P(q) = \left\{\left[1 + (q^2a)\right]^{D_m/2} \times \left[1 + (q^2b)\right]^{(6-D_s-D_m)/2}\right\}^{-1}$$

$$a = R_g^2/(3D_m/2)$$

$$b = r_g^2/[-3(D_s + D_m - 6)/2]$$

$$\text{scale} = \text{scale\_factor} \times NV^2(\rho_{\text{particle}} - \rho_{\text{solvent}})^2$$

where $R_g$ is the size of the cluster, $r_g$ is the size of the primary particle, $D_s$ is the surface fractal dimension, $D_m$ is the mass fractal dimension, $\rho_{\text{solvent}}$ is the scattering length density of the solvent, and $\rho_{\text{particle}}$ is the scattering length density of particles.

**Note:** The surface ($D_s$) and mass ($D_m$) fractal dimensions are only valid if $0 < surface\_dim < 6$, $0 < mass\_dim < 6$, and $(surface\_dim + mass\_dim) < 6$. Older versions of sasview may have the default primary particle radius larger than the cluster radius, this was an error, also present in the Schmidt review paper below. The primary particle should be the smaller as described in the original Hurd et.al. who also point out that polydispersity in the primary particle sizes may affect their apparent surface fractal dimension.

![Graph](image)

Fig. 1.108: 1D plot corresponding to the default parameters of the model.

**References**

**Authorship and Verification**

- Converted to sasmodels by: Piotr Rozyczko Date: Jan 20, 2016
- Last Reviewed by: Richard Heenan Date: May 30, 2018

**mono_gauss_coil**

Scattering from monodisperse polymer coils
The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

This Debye Gaussian coil model strictly describes the scattering from *monodisperse* polymer chains in theta solvents or polymer melts, conditions under which the distances between segments follow a Gaussian distribution. Provided the number of segments is large (i.e., high molecular weight polymers) the single-chain form factor $P(Q)$ is that described by Debye (1947).

To describe the scattering from *polydisperse* polymer chains see the *poly_gauss_coil* model.

**Definition**

$$I(q) = \text{scale} \cdot I_0 \cdot P(q) + \text{background}$$

where

$$I_0 = \phi_{\text{poly}} \cdot V \cdot (\rho_{\text{poly}} - \rho_{\text{solv}})^2$$

$$P(q) = \frac{2[\exp(-Z) + Z - 1]}{Z^2}$$

$$Z = (qR_g)^2$$

$$V = \frac{M}{(N_A\delta)}$$

Here, $\phi_{\text{poly}}$ is the volume fraction of polymer, $V$ is the volume of a polymer coil, $M$ is the molecular weight of the polymer, $N_A$ is Avogadro’s Number, $\delta$ is the bulk density of the polymer, $\rho_{\text{poly}}$ is the sld of the polymer, $\rho_{\text{solv}}$ is the sld of the solvent, and $R_g$ is the radius of gyration of the polymer coil.

The 2D scattering intensity is calculated in the same way as the 1D, but where the $q$ vector is redefined as

$$q = \sqrt{q_x^2 + q_y^2}$$

![Fig. 1.109: 1D plot corresponding to the default parameters of the model.](image-url)
References

peak_lorentz
A Lorentzian peak on a flat background

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
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<td>Source intensity</td>
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<tr>
<td>background</td>
<td>Source background</td>
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<tr>
<td>peak_pos</td>
<td>Peak position in q</td>
<td>Å^{-1}</td>
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<tr>
<td>peak_hwhm</td>
<td>HWHM of peak</td>
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<td>0.005</td>
</tr>
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</table>

The returned value is scaled to units of cm^{-1} sr^{-1}, absolute scale.

This model describes a Lorentzian shaped peak on a flat background.

Definition
The scattering intensity \( I(q) \) is calculated as

\[
I(q) = \frac{scale}{(1 + \left(\frac{q - q_0}{B}\right)^2)} + background
\]

with the peak having height of \( I_0 \) centered at \( q_0 \) and having a HWHM (half-width half-maximum) of \( B \).

For 2D data the scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

![Fig. 1.110: 1D plot corresponding to the default parameters of the model.](image)
**References**

None.

**poly_gauss Coil**

Scattering from polydisperse polymer coils

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
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<td>background</td>
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<td>i_zero</td>
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<td>rg</td>
<td>Radius of gyration</td>
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<tr>
<td>polydispersity</td>
<td>Polymer Mw/Mn</td>
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The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

This empirical model describes the scattering from *polydisperse* polymer chains in theta solvents or polymer melts, assuming a Schulz-Zimm type molecular weight distribution.

To describe the scattering from *monodisperse* polymer chains, see the *mono_gauss_coil* model.

**Definition**

\[
I(q) = \text{scale} \cdot I_0 \cdot P(q) + \text{background}
\]

where

\[
I_0 = \phi_{\text{poly}} \cdot V \cdot (\rho_{\text{poly}} - \rho_{\text{solv}})^2
\]

\[
P(q) = 2[(1 + UZ)^{-1/U} + Z - 1]/[(1 + U)Z^2]
\]

\[
Z = (qR_g)^2/(1 + 2U)
\]

\[
U = (M_w/M_n) - 1 = \text{polydispersity ratio} - 1
\]

\[
V = M/(N_A \delta)
\]

Here, \(\phi_{\text{poly}}\) is the volume fraction of polymer, \(V\) is the volume of a polymer coil, \(M\) is the molecular weight of the polymer, \(N_A\) is Avogadro's Number, \(\delta\) is the bulk density of the polymer, \(\rho_{\text{poly}}\) is the sld of the polymer, \(\rho_{\text{solv}}\) is the sld of the solvent, and \(R_g\) is the radius of gyration of the polymer coil.

The 2D scattering intensity is calculated in the same way as the 1D, but where the \(q\) vector is redefined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

**References**


**polymer_excl_volume**

Polymer Excluded Volume model
The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

This model describes the scattering from polymer chains subject to excluded volume effects and has been used as a template for describing mass fractals.

**Definition**

The form factor was originally presented in the following integral form (Benoit, 1957)

\[
P(Q) = 2 \int_{0}^{1} dx (1 - x) \exp \left[ -\frac{Q^2 a^2 n^2 \nu^2 x^2}{6} \right]
\]

where $\nu$ is the excluded volume parameter (which is related to the Porod exponent $m$ as $\nu = 1/m$), $a$ is the statistical segment length of the polymer chain, and $n$ is the degree of polymerization.

This integral was put into an almost analytical form as follows (Hammouda, 1993)

\[
P(Q) = \frac{1}{\nu U^{1/2\nu}} \left\{ \gamma \left( \frac{1}{2\nu}, U \right) - \frac{1}{U^{1/2\nu}} \gamma \left( \frac{1}{\nu}, U \right) \right\}
\]

and later recast as (for example, Hore, 2013; Hammouda & Kim, 2017)

\[
P(Q) = \frac{1}{\nu U^{1/2\nu}} \gamma \left( \frac{1}{2\nu}, U \right) - \frac{1}{\nu U^{1/\nu}} \gamma \left( \frac{1}{\nu}, U \right)
\]

where $\gamma(x, U)$ is the incomplete gamma function

\[
\gamma(x, U) = \int_{0}^{U} dt \, \exp(-t)t^{x-1}
\]

and the variable $U$ is given in terms of the scattering vector $Q$ as

\[
U = \frac{Q^2 a^2 n^2 \nu^2}{6} = \frac{Q^2 R_g^2(2\nu + 1)(2\nu + 2)}{6}
\]
The two analytic forms are equivalent. In the 1993 paper
\[ \frac{1}{\nu U^{1/2}} \]
has been factored out.

**SasView implements the 1993 expression.**

The square of the radius-of-gyration is defined as
\[ R_g^2 = \frac{a^2 \pi^{2\nu}}{(2\nu + 1)(2\nu + 2)} \]

**Note:** This model applies only in the mass fractal range (ie, \( 5/3 < m <= 3 \)) and does not apply to surface fractals (\( 3 < m <= 4 \)). It also does not reproduce the rigid rod limit (\( m=1 \)) because it assumes chain flexibility from the outset. It may cover a portion of the semi-flexible chain range (\( 1 < m < 5/3 \)).

A low-Q expansion yields the Guinier form and a high-Q expansion yields the Porod form which is given by
\[ P(Q \to \infty) = \frac{1}{\nu U^{1/2}} \Gamma \left( \frac{1}{2\nu} \right) - \frac{1}{\nu U^{1/2}} \Gamma \left( \frac{1}{\nu} \right) \]

Here \( \Gamma(x) = \gamma(x, \infty) \) is the gamma function.

The asymptotic limit is dominated by the first term
\[ P(Q \to \infty) \sim \frac{1}{\nu U^{1/2}} \Gamma \left( \frac{1}{2\nu} \right) = \frac{m}{(QR_g)^m} \left[ \frac{6}{(2\nu + 1)(2\nu + 2)} \right]^{m/2} \Gamma(m/2) \]

The special case when \( \nu = 0.5 \) (or \( m = 1/\nu = 2 \)) corresponds to Gaussian chains for which the form factor is given by the familiar Debye function.
\[ P(Q) = \frac{2}{Q^4 R_g^4} \left[ \exp(-Q^2 R_g^2) - 1 + Q^2 R_g^2 \right] \]

For 2D data: The 2D scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as
\[ q = \sqrt{q_x^2 + q_y^2} \]

**References**

H Benoit, *Comptes Rendus*, 245 (1957) 2244-2247


**porod**

Porod function

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
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</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm^{-1}</td>
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</tr>
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</table>
The returned value is scaled to units of \( \text{cm}^{-1} \text{ sr}^{-1} \), absolute scale.

This model fits the Porod function

\[ I(q) = \frac{C}{q^4} \]

to the data directly without any need for linearisation (cf. \( \log I(q) \) vs \( \log q \)).

Here \( C = 2\pi (\Delta \rho)^2 S_v \) is the scale factor where \( S_v \) is the specific surface area (ie, surface area / volume) of the sample, and \( \Delta \rho \) is the contrast factor.

For 2D data: The 2D scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[ q = \sqrt{q_x^2 + q_y^2} \]

References


**power Law**

Simple power law with a flat background

<table>
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<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
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The returned value is scaled to units of \( \text{cm}^{-1} \text{ sr}^{-1} \), absolute scale.

This model calculates a simple power law with a flat background.
Definition

\[ I(q) = \text{scale} \cdot q^{-\text{power}} + \text{background} \]

Note the minus sign in front of the exponent. The exponent \text{power} should therefore be entered as a \textbf{positive} number for fitting.

Also note that unlike many other models, \text{scale} in this model is NOT explicitly related to a volume fraction. Be careful if combining this model with other models.

References

None.

\textbf{rpa}

Random Phase Approximation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm(^{-1})</td>
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</tr>
<tr>
<td>case_num</td>
<td>Component organization</td>
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<td>1</td>
</tr>
<tr>
<td>N[4]</td>
<td>Degree of polymerization</td>
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<td>1000</td>
</tr>
<tr>
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<td>volume fraction</td>
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<tr>
<td>v[4]</td>
<td>molar volume</td>
<td>mL/mol</td>
<td>100</td>
</tr>
<tr>
<td>L[4]</td>
<td>scattering length</td>
<td>fm</td>
<td>10</td>
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<tr>
<td>b[4]</td>
<td>segment length</td>
<td>Å</td>
<td>5</td>
</tr>
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<td>K12</td>
<td>A:B interaction parameter</td>
<td>None</td>
<td>-0.0004</td>
</tr>
<tr>
<td>K13</td>
<td>A:C interaction parameter</td>
<td>None</td>
<td>-0.0004</td>
</tr>
<tr>
<td>K14</td>
<td>A:D interaction parameter</td>
<td>None</td>
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<tr>
<td>K23</td>
<td>B:C interaction parameter</td>
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<td>C:D interaction parameter</td>
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</table>

The returned value is scaled to units of cm\(^{-1}\) sr\(^{-1}\), absolute scale.

1.1. Model Functions
Definition

Calculates the macroscopic scattering intensity for a multi-component homogeneous mixture of polymers using the Random Phase Approximation. This general formalism contains 10 specific cases:

- Case 0: C/D binary mixture of homopolymers
- Case 1: C-D diblock copolymer
- Case 2: B/C/D ternary mixture of homopolymers
- Case 3: C/C-D mixture of a homopolymer B and a diblock copolymer C-D
- Case 4: B-C-D triblock copolymer
- Case 5: A/B/C/D quaternary mixture of homopolymers
- Case 6: A/B/C-D mixture of two homopolymers A/B and a diblock C-D
- Case 7: A/B-C-D mixture of a homopolymer A and a triblock B-C-D
- Case 8: A-B/C-D mixture of two diblock copolymers A-B and C-D
- Case 9: A-B-C-D tetra-block copolymer

Note: These case numbers are different from those in the NIST SANS package!

Usage notes:

The models are based on the papers by Akcasu et al. and by Hammouda assuming the polymer follows Gaussian statistics such that \( R_g^2 = nb^2/6 \) where \( b \) is the statistical segment length and \( n \) is the number of statistical segment lengths. A nice tutorial on how these are constructed and implemented can be found in chapters 28 and 39 of Boualem Hammouda’s ‘SANS Toolbox’.

In brief the macroscopic cross sections are derived from the general forms for homopolymer scattering and the multiblock cross-terms while the inter polymer cross terms are described in the usual way by the \( \chi \) parameter.

Usage Notes:

- Only one case can be used at any one time.
- The RPA (mean field) formalism only applies only when the multicomponent polymer mixture is in the homogeneous mixed-phase region.
• Component D is assumed to be the “background” component (i.e., all contrasts are calculated with respect to component D). So the scattering contrast for a C/D blend $= \left[ \text{SLD(component C)} - \text{SLD(component D)} \right]^2$.

• Depending on which case is being used, the number of fitting parameters can vary.

**Note:**

- In general the degrees of polymerization, the volume fractions, the molar volumes, and the neutron scattering lengths for each component are obtained from other methods and held fixed while the scale parameter should be held equal to unity.
- The variables are normally the segment lengths ($b_a, b_b, \text{etc.}$) and $\chi$ parameters ($K_{ab}, K_{ac}, \text{etc.}$).

Fig. 1.115: 1D plot corresponding to the default parameters of the model.

**References**


**Authorship and Verification**

- **Author:** Boualem Hammouda - NIST IGOR/DANSE **Date:** pre 2010
- **Converted to sasmodels by:** Paul Kienzle **Date:** July 18, 2016
- **Last Modified by:** Paul Butler **Date:** March 12, 2017
- **Last Reviewed by:** Paul Butler **Date:** March 12, 2017

**spinodal**

Spinodal decomposition model
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
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<tbody>
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<td>scale</td>
<td>Source intensity</td>
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</tr>
<tr>
<td>background</td>
<td>Source background</td>
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<td>gamma</td>
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<td>None</td>
<td>3</td>
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<tr>
<td>q_0</td>
<td>Correlation peak position</td>
<td>Å⁻¹</td>
<td>0.1</td>
</tr>
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</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

This model calculates the SAS signal of a phase separating system undergoing spinodal decomposition. The scattering intensity \( I(q) \) is calculated as

\[
I(q) = I_{\text{max}} \frac{(1 + \gamma/2)x^2}{\gamma/2 + x^{2+\gamma}} + B
\]

where \( x = q/q_0, q_0 \) is the peak position, \( I_{\text{max}} \) is the intensity at \( q_0 \) (parameterised as the \textit{scale} parameter), and \( B \) is a flat background. The spinodal wavelength, \( \Lambda \), is given by \( 2\pi/q_0 \).

The definition of \( I_{\text{max}} \) in the literature varies. Hashimoto \textit{et al} (1991) define it as

\[
I_{\text{max}} = \Lambda^3 \Delta \rho^2
\]

whereas Meier \& Strobl (1987) give

\[
I_{\text{max}} = V_z \Delta \rho^2
\]

where \( V_z \) is the volume per monomer unit.

The exponent \( \gamma \) is equal to \( d + 1 \) for off-critical concentration mixtures (smooth interfaces) and \( 2d \) for critical concentration mixtures (entangled interfaces), where \( d \) is the dimensionality (ie, 1, 2, 3) of the system. Thus \( 2 <\gamma < 6 \). A transition from \( \gamma = d + 1 \) to \( \gamma = 2d \) is expected near the percolation threshold.

As this function tends to zero as \( q \) tends to zero, in practice it may be necessary to combine it with another function describing the low-angle scattering, or to simply omit the low-angle scattering from the fit.

![Graph](image.png)

**Fig. 1.116**: 1D plot corresponding to the default parameters of the model.

**References**


Revision History

- **Author:** Dirk Honecker  **Date:** Oct 7, 2016
- **Revised:** Steve King  **Date:** Oct 25, 2018

**star_polymer**

Star polymer model with Gaussian statistics

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
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<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
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</tr>
<tr>
<td>rg_squared</td>
<td>Ensemble radius of gyration SQUARED of the full polymer</td>
<td>Å²</td>
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<tr>
<td>arms</td>
<td>Number of arms in the model</td>
<td>None</td>
<td>3</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

Calculates the scattering from a simple star polymer with f equal Gaussian coil arms. A star being defined as a branched polymer with all the branches emanating from a common central (in the case of this model) point. It is derived as a special case of on the Benoit model for general branched polymers¹ as also used by Richter et al.²

For a star with f arms the scattering intensity \( I(q) \) is calculated as

\[
I(q) = \frac{2}{f v^2} \left[ v - 1 + \exp(-v) + \frac{f - 1}{2} \left[ 1 - \exp(-v) \right]^2 \right]
\]

where

\[
v = \frac{uf}{(3f - 2)}
\]

and

\[
u = \langle R_g^2 \rangle q^2
\]

contains the square of the ensemble average radius-of-gyration of the full polymer while \( v \) contains the radius of gyration of a single arm \( R_{arm} \). The two are related as:

\[
R_{arm}^2 = \frac{f}{3f - 2} R_g^2
\]

Note that when there is only one arm, \( f = 1 \), the Debye Gaussian coil equation is recovered.

**Note:** Star polymers in solutions tend to have strong interparticle and osmotic effects. Thus the Benoit equation may not work well for many real cases. A newer model for star polymer incorporating excluded volume has been developed by Li et al in arXiv:1404.6269 [physics.chem-ph]. Also, at small \( q \) the scattering, i.e. the Guinier term, is not sensitive to the number of arms, and hence ‘scale’ here is simply \( I(q = 0) \) as described for the mono_gauss_coil model, using volume fraction \( \phi \) and volume \( V \) for the whole star polymer.

¹ H Benoit J. Polymer Science, 11, 507-510 (1953)
Fig. 1.117: 1D plot corresponding to the default parameters of the model.

References

Authorship and Verification

- **Author:** Kieran Campbell **Date:** July 24, 2012
- **Last Modified by:** Paul Butler **Date:** Auguts 26, 2017
- **Last Reviewed by:** Ziang Li and Richard Heenan **Date:** May 17, 2017

**surface_fractal**

Fractal-like aggregates based on the Mildner reference

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
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<td>Source intensity</td>
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<tr>
<td>background</td>
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</tr>
<tr>
<td>radius</td>
<td>Particle radius</td>
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<td>fractal_dim_surf</td>
<td>Surface fractal dimension</td>
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<tr>
<td>cutoff_length</td>
<td>Cut-off Length</td>
<td>Å</td>
<td>500</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

This model calculates the scattering from fractal-like aggregates based on the Mildner reference.

**Definition**
The scattering intensity $I(q)$ is calculated as

$$I(q) = \text{scale} \times P(q)S(q) + \text{background}$$

$$P(q) = F(qR)^2$$

$$F(x) = \frac{3}{x^3} [\sin(x) - x \cos(x)]$$

$$S(q) = \Gamma(5 - D_S)\xi^{5-D_S} \left[1 + (q\xi)^2\right]^{-\frac{5-D_S}{2}} \sin \left[-(5 - D_S) \tan^{-1}(q\xi)\right] q^{-1}$$

where $R$ is the radius of the building block, $D_S$ is the surface fractal dimension, $\xi$ is the cut-off length, $\rho_{\text{solvent}}$ is the scattering length density of the solvent and $\rho_{\text{particle}}$ is the scattering length density of particles.

**Note:** The surface fractal dimension is only valid if $1 < D_S < 3$. The result is only valid over a limited $q$ range, $\frac{5}{3-D_S} \xi^{-1} < q < R^{-1}$. See the reference for details.

![Fig. 1.118: 1D plot corresponding to the default parameters of the model.](image)

**References**


teubner_strey

Teubner-Strey model of microemulsions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm$^{-1}$</td>
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<td>0.5</td>
</tr>
<tr>
<td>sld_a</td>
<td>SLD of phase a</td>
<td>$10^6$Å$^{-2}$</td>
<td>0.3</td>
</tr>
<tr>
<td>sld_b</td>
<td>SLD of phase b</td>
<td>$10^6$Å$^{-2}$</td>
<td>6.3</td>
</tr>
<tr>
<td>d</td>
<td>Domain size (periodicity)</td>
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<td>100</td>
</tr>
<tr>
<td>xi</td>
<td>Correlation length</td>
<td>Å</td>
<td>30</td>
</tr>
</tbody>
</table>

1.1. Model Functions
The returned value is scaled to units of cm$^{-1}$ sr$^{-1}$, absolute scale.

**Definition**

This model calculates the scattered intensity of a two-component system using the Teubner-Strey model. Unlike `dab` this function generates a peak. A two-phase material can be characterised by two length scales - a correlation length and a domain size (periodicity).

The original paper by Teubner and Strey defined the function as:

$$I(q) \propto \frac{1}{a_2 + c_1 q^2 + c_2 q^4} + \text{background}$$

where the parameters $a_2$, $c_1$ and $c_2$ are defined in terms of the periodicity, $d$, and correlation length $\xi$ as:

$$a_2 = \left[1 + \left(\frac{2\pi \xi}{d}\right)^2\right]^2$$

$$c_1 = -2\xi^2 \left(\frac{2\pi \xi}{d}\right)^2 + 2\xi^2$$

$$c_2 = \xi^4$$

and thus, the periodicity, $d$ is given by

$$d = 2\pi \left[\frac{1}{2} \left(\frac{a_2}{c_2}\right)^{1/2} - \frac{1}{4} \frac{c_1}{c_2}\right]^{-1/2}$$

and the correlation length, $\xi$, is given by

$$\xi = \left[\frac{1}{2} \left(\frac{a_2}{c_2}\right)^{1/2} + \frac{1}{4} \frac{c_1}{c_2}\right]^{-1/2}$$

Here the model is parameterised in terms of $d$ and $\xi$ and with an explicit volume fraction for one phase, $\phi_a$, and contrast, $\delta \rho^2 = (\rho_a - \rho_b)^2$:

$$I(q) = \frac{8\pi \phi_a (1 - \phi_a)(\Delta \rho)^2 c_2 / \xi}{a_2 + c_1 q^2 + c_2 q^4}$$

where $8\pi \phi_a (1 - \phi_a)(\Delta \rho)^2 c_2 / \xi$ is the constant of proportionality from the first equation above.

In the case of a microemulsion, $a_2 > 0$, $c_1 < 0$, and $c_2 > 0$.

For 2D data, scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

**References**


**two_lorentzian**

This model calculates an empirical functional form for SAS data characterized by two Lorentzian-type functions.
Fig. 1.119: 1D plot corresponding to the default parameters of the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
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<tbody>
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</tr>
<tr>
<td>background</td>
<td>Source background</td>
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</tr>
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</tr>
<tr>
<td>lorentz_length_1</td>
<td>First Lorentzian screening length</td>
<td>Å</td>
<td>100</td>
</tr>
<tr>
<td>lorentz_exp_1</td>
<td>First exponent of power law</td>
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<td>3</td>
</tr>
<tr>
<td>lorentz_scale_2</td>
<td>Second scale factor for broad Lorentzian peak</td>
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<td>1</td>
</tr>
<tr>
<td>lorentz_length_2</td>
<td>Second Lorentzian screening length</td>
<td>Å</td>
<td>10</td>
</tr>
<tr>
<td>lorentz_exp_2</td>
<td>Second exponent of power law</td>
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<td>2</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

The scattering intensity $I(q)$ is calculated as

$$I(q) = \frac{A}{1 + (Q\xi_1)^n} + \frac{C}{1 + (Q\xi_2)^m} + B$$

where $A = $ Lorentzian scale factor #1, $C = $ Lorentzian scale #2, $\xi_1$ and $\xi_2$ are the corresponding correlation lengths, and $n$ and $m$ are the respective power law exponents (set $n = m = 2$ for Ornstein-Zernicke behaviour).

For 2D data the scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

**References**

None.

- **Author:** NIST IGOR/DANSE Date: pre 2010
- **Last Modified by:** Piotr rozyczko Date: January 29, 2016
- **Last Reviewed by:** Paul Butler Date: March 21, 2016
two_power_law

This model calculates an empirical functional form for SAS data characterized by two power laws.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
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</tr>
<tr>
<td>coefficent_1</td>
<td>coefficient A in low Q region</td>
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<td>1</td>
</tr>
<tr>
<td>crossover</td>
<td>crossover location</td>
<td>Å⁻¹</td>
<td>0.04</td>
</tr>
<tr>
<td>power_1</td>
<td>power law exponent at low Q</td>
<td>None</td>
<td>1</td>
</tr>
<tr>
<td>power_2</td>
<td>power law exponent at high Q</td>
<td>None</td>
<td>4</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

**Definition**

The scattering intensity $I(q)$ is calculated as

$$I(q) = \begin{cases} 
  Aq^{-m_1} + \text{background} & q \leq q_c \\
  Cq^{-m_2} + \text{background} & q > q_c 
\end{cases}$$

where $q_c$ is the location of the crossover from one slope to the other, $A$ is the scaling coefficient that sets the overall intensity of the lower Q power law region, $m_1$ is power law exponent at low Q, and $m_2$ is power law exponent at high Q. The scaling of the second power law region (coefficient $C$) is then automatically scaled to match the first by following formula:

$$C = \frac{Aq_c^{-m_2}}{q_c^{-m_1}}$$

**Note:** Be sure to enter the power law exponents as positive values!

For 2D data the scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$
unified_power_Rg

Unified Power Rg

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>scale</td>
<td>Source intensity</td>
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<td>1</td>
</tr>
<tr>
<td>background</td>
<td>Source background</td>
<td>cm⁻¹</td>
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</tr>
<tr>
<td>level</td>
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</tr>
<tr>
<td>rg[level]</td>
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<td>Power</td>
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<tr>
<td>B[level]</td>
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<td>4.5e-06</td>
</tr>
<tr>
<td>G[level]</td>
<td>cm⁻¹</td>
<td></td>
<td>400</td>
</tr>
</tbody>
</table>

The returned value is scaled to units of cm⁻¹ sr⁻¹, absolute scale.

Definition

This model employs the empirical multiple level unified Exponential/Power-law fit method developed by Beaucage. Four functions are included so that 1, 2, 3, or 4 levels can be used. In addition a 0 level has been added which simply calculates

\[ I(q) = \frac{\text{scale}}{q} + \text{background} \]

The Beaucage method is able to reasonably approximate the scattering from many different types of particles, including fractal clusters, random coils (Debye equation), ellipsoidal particles, etc.
The model works best for mass fractal systems characterized by Porod exponents between $5/3$ and $3$. It should not be used for surface fractal systems. Hammouda (2010) has pointed out a deficiency in the way this model handles the transitioning between the Guinier and Porod regimes and which can create artefacts that appear as kinks in the fitted model function.

Also see the Guinier_Porod model.

The empirical fit function is:

$$ I(q) = \text{background} + \sum_{i=1}^{N} \left[ G_i \exp \left( -\frac{q^2 R_{gi}^2}{3} \right) + B_i \exp \left( -\frac{q^2 R_{gi(i+1)}^2}{3} \right) \left( \frac{1}{q^2} \right)^{P_i} \right] $$

where

$$ q_i^* = q \left[ \text{erf} \left( \frac{q R_{gi}}{\sqrt{6}} \right) \right]^{-3} $$

For each level, the four parameters $G_i$, $R_{gi}$, $B_i$ and $P_i$ must be chosen. Beaucage has an additional factor $k$ in the definition of $q_i^*$ which is ignored here.

For example, to approximate the scattering from random coils (Debye equation), set $R_{gi}$ as the Guinier radius, $P_i = 2$, and $B_i = 2G_i / R_{gi}$.

See the references for further information on choosing the parameters.

For 2D data: The 2D scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$ q = \sqrt{q_x^2 + q_y^2} $$

![Fig. 1.122: 1D plot corresponding to the default parameters of the model.](image)

**References**


1.1.8 Structure Factors

**hardsphere**

Hard sphere structure factor, with Percus-Yevick closure

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>radius_effective</td>
<td>effective radius of hard sphere</td>
<td>Å</td>
<td>50</td>
</tr>
<tr>
<td>volfraction</td>
<td>volume fraction of hard spheres</td>
<td>None</td>
<td>0.2</td>
</tr>
</tbody>
</table>

The returned value is a dimensionless structure factor, $S(q)$.

Calculate the interparticle structure factor for monodisperse spherical particles interacting through hard sphere (excluded volume) interactions. May be a reasonable approximation for other shapes of particles that freely rotate, and for moderately polydisperse systems. Though strictly the maths needs to be modified (no Beta(Q) correction yet in sasview).

radius_effective is the effective hard sphere radius. volfraction is the volume fraction occupied by the spheres.

In sasview the effective radius may be calculated from the parameters used in the form factor $P(q)$ that this $S(q)$ is combined with.

For numerical stability the computation uses a Taylor series expansion at very small $qR$, there may be a very minor glitch at the transition point in some circumstances.

The $S(Q)$ uses the Percus-Yevick closure where the interparticle potential is

$$ U(r) = \begin{cases} 
\infty & r < 2R \\
0 & r \geq 2R 
\end{cases} $$

where $r$ is the distance from the center of the sphere of a radius $R$.

For a 2D plot, the wave transfer is defined as

$$ q = \sqrt{q_x^2 + q_y^2} $$

![Graph](image.png)

Fig. 1.123: 1D plot corresponding to the default parameters of the model.
References


**hayter_msa**

Hayter-Penfold rescaled MSA, charged sphere, interparticle S(Q) structure factor

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>radius_effective</td>
<td>effective radius of charged sphere</td>
<td>Å</td>
<td>20.75</td>
</tr>
<tr>
<td>volfraction</td>
<td>volume fraction of spheres</td>
<td>None</td>
<td>0.0192</td>
</tr>
<tr>
<td>charge</td>
<td>charge on sphere (in electrons)</td>
<td>e</td>
<td>19</td>
</tr>
<tr>
<td>temperature</td>
<td>temperature, in Kelvin, for Debye length calculation</td>
<td>K</td>
<td>318.16</td>
</tr>
<tr>
<td>concentration_salt</td>
<td>conc of salt, moles/litre, 1:1 electrolyte, for Debye length</td>
<td>M</td>
<td>0</td>
</tr>
<tr>
<td>dielectconst</td>
<td>dielectric constant (relative permittivity) of solvent, default water, for Debye length</td>
<td>None</td>
<td>71.08</td>
</tr>
</tbody>
</table>

The returned value is a dimensionless structure factor, \( S(q) \).

This calculates the structure factor (the Fourier transform of the pair correlation function \( g(r) \)) for a system of charged, spheroidal objects in a dielectric medium. When combined with an appropriate form factor (such as sphere, core+shell, ellipsoid, etc), this allows for inclusion of the interparticle interference effects due to screened coulomb repulsion between charged particles.

**This routine only works for charged particles.** If the charge is set to zero the routine may self-destruct! For non-charged particles use a hard sphere potential.

The salt concentration is used to compute the ionic strength of the solution which in turn is used to compute the Debye screening length. At present there is no provision for entering the ionic strength directly nor for use of any multivalent salts, though it should be possible to simulate the effect of this by increasing the salt concentration. The counterions are also assumed to be monovalent.

In sasview the effective radius may be calculated from the parameters used in the form factor \( P(q) \) that this \( S(q) \) is combined with.

The computation uses a Taylor series expansion at very small rescaled \( qR \), to avoid some serious rounding error issues, this may result in a minor artefact in the transition region under some circumstances.

For 2D data, the scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

**References**


**squarewell**

Square well structure factor, with MSA closure

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>radius_effective</td>
<td>effective radius of hard sphere</td>
<td>Å</td>
<td>50</td>
</tr>
<tr>
<td>volfraction</td>
<td>volume fraction of spheres</td>
<td>None</td>
<td>0.04</td>
</tr>
<tr>
<td>welldepth</td>
<td>depth of well, epsilon</td>
<td>kT</td>
<td>1.5</td>
</tr>
<tr>
<td>wellwidth</td>
<td>width of well in diameters (=2R) units, must be &gt; 1</td>
<td>diameters</td>
<td>1.2</td>
</tr>
</tbody>
</table>
The returned value is a dimensionless structure factor, $S(q)$.

This calculates the interparticle structure factor for a square well fluid spherical particles. The mean spherical approximation (MSA) closure was used for this calculation, and is not the most appropriate closure for an attractive interparticle potential. This solution has been compared to Monte Carlo simulations for a square well fluid, showing this calculation to be limited in applicability to well depths $\epsilon < 1.5 \, kT$ and volume fractions $\phi < 0.08$.

Positive well depths correspond to an attractive potential well. Negative well depths correspond to a potential “shoulder”, which may or may not be physically reasonable. The stickyhard sphere model may be a better choice in some circumstances. Computed values may behave badly at extremely small $qR$.

The well width ($\lambda$) is defined as multiples of the particle diameter ($2R$).

The interaction potential is:

$$U(r) = \begin{cases} 
\infty & r < 2R \\
-\epsilon & 2R \leq r \leq 2R\lambda \\
0 & r \geq 2R
\end{cases}$$

where $r$ is the distance from the center of the sphere of a radius $R$.

In sasview the effective radius may be calculated from the parameters used in the form factor $P(q)$ that this $S(q)$ is combined with.

For 2D data: The 2D scattering intensity is calculated in the same way as 1D, where the $q$ vector is defined as

$$q = \sqrt{q_x^2 + q_y^2}$$

References

Fig. 1.125: 1D plot corresponding to the default parameters of the model.

**stickyhardsphere**

Sticky hard sphere structure factor, with Percus-Yevick closure

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Units</th>
<th>Default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>radius_effective</td>
<td>effective radius of hard sphere</td>
<td>Å</td>
<td>50</td>
</tr>
<tr>
<td>volfrac</td>
<td>volume fraction of hard spheres</td>
<td>None</td>
<td>0.2</td>
</tr>
<tr>
<td>perturb</td>
<td>perturbation parameter, epsilon</td>
<td>None</td>
<td>0.05</td>
</tr>
<tr>
<td>stickiness</td>
<td>stickiness, tau</td>
<td>None</td>
<td>0.2</td>
</tr>
</tbody>
</table>

The returned value is a dimensionless structure factor, $S(Q)$.

This calculates the interparticle structure factor for a hard sphere fluid with a narrow attractive well. A perturbative solution of the Percus-Yevick closure is used. The strength of the attractive well is described in terms of “stickiness” as defined below.

The perturb (perturbation parameter), $\epsilon$, should be held between 0.01 and 0.1. It is best to hold the perturbation parameter fixed and let the “stickiness” vary to adjust the interaction strength. The stickiness, $\tau$, is defined in the equation below and is a function of both the perturbation parameter and the interaction strength. $\tau$ and $\epsilon$ are defined in terms of the hard sphere diameter ($\sigma = 2R$), the width of the square well, $\Delta$ (same units as $R$), and the depth of the well, $U_o$, in units of $kT$. From the definition, it is clear that smaller $\tau$ means stronger attraction.

$$
\tau = \frac{1}{12\epsilon} \exp\left(\frac{U_o}{kT}\right)
$$

$$
\epsilon = \frac{\Delta}{(\sigma + \Delta)}
$$

where the interaction potential is

$$
U(r) = \begin{cases} 
\infty & r < \sigma \\
-U_o & \sigma \leq r \leq \sigma + \Delta \\
0 & r > \sigma + \Delta
\end{cases}
$$

The Percus-Yevick (PY) closure was used for this calculation, and is an adequate closure for an attractive interparticle potential. This solution has been compared to Monte Carlo simulations for a square well fluid, with good agreement.
The true particle volume fraction, \( \phi \), is not equal to \( h \), which appears in most of the reference. The two are related in equation (24) of the reference. The reference also describes the relationship between this perturbation solution and the original sticky hard sphere (or adhesive sphere) model by Baxter.

**NB**: The calculation can go haywire for certain combinations of the input parameters, producing unphysical solutions - in this case errors are reported to the command window and the \( S(q) \) is set to -1 (so it will disappear on a log-log plot). Use tight bounds to keep the parameters to values that you know are physical (test them) and keep nudging them until the optimization does not hit the constraints.

In sasview the effective radius may be calculated from the parameters used in the form factor \( P(q) \) that this \( S(q) \) is combined with.

For 2D data the scattering intensity is calculated in the same way as 1D, where the \( q \) vector is defined as

\[
q = \sqrt{q_x^2 + q_y^2}
\]

Fig. 1.126: 1D plot corresponding to the default parameters of the model.

**References**


### 1.2 Menu Bar

The menu bar at the top of the *SasView* window gives you access to additional features of the program:

#### 1.2.1 File

The File option allows you load data into *SasView* for analysis, or to save the work you have been doing. Data can be loaded one file at a time, or by selecting multiple files, or by loading an entire folder of files (in which case *SasView* will attempt to make an intelligent guess as to what to load based on the file formats it recognises in the folder!).

A *SasView* session can also be saved and reloaded as an ‘Analysis’ (an individual model fit or invariant calculation, etc), or as a ‘Project’ (everything you have done since starting your *SasView* session).
1.2.2 Edit

The Edit option allows you to:

- undo/redo your recent changes;
- copy and paste parameters between SasView analysis windows;
- copy parameters from a SasView analysis window to the Clipboard as either tab-delimited text (compatible with Microsoft Excel) or LaTeX-wrapped text;
- generate a summary ‘Report’ of the most recent analysis performed;
- reset parameter values in the P(r) Inversion analysis page.

1.2.3 View

The View option allows you to:

- show the Batch Fitting Results Panel if it has been closed;
- show/hide the Data Explorer Panel;
- show/hide the Toolbar of icons below the Menu Bar;
- select the default location that SasView looks in for data to analyse (the SasView installation directory, the initial default, or a custom folder). NB: any change only takes effect when SasView is restarted;
- change the default assignment of categories (Shapes, Shape-independent, Structure Factor) for fitting model functions.

1.2.4 Tools

The Tools option provides access to a comprehensive range of tools and utilities. See Tools & Utilities for more information.

1.2.5 Window

The Window option allows you to select which SasView windows are visible.

1.2.6 Analysis

The Analysis option provides access to the key functionality of SasView:

- Model Fitting;
- P(r) Inversion;
- Invariant Analysis;
- Correlation Function Analysis (SasView 4.1 and later)

See Fitting & Other Analyses for more information.

1.2.7 Fitting

The Fitting option allows you to:

- create a new FitPage;
- change optimiser (under Fit Options);
- view fit parameter correlations, distributions, and convergence traces (under Fit Results);
• create/edit a Plugin Model.

Additional functionality is available under this menu option during particular types of model fitting, including:

• setting up a Constrained or Simultaneous Fit;
• combining a Batch Fit (an obscure capability);
• setting up Chain Fitting.

1.2.8 Help

The Help option provides access to:

• this help documentation;
• a Tutorials on using SasView (in pdf format);
• information on how to acknowledge SasView in publications;
• information about the version of SasView you are using;
• the Model Marketplace;
• a check to see if there is a more recent version of SasView.

Note: This help document was last changed by Steve King, 10Oct2016

1.3 Fitting & Other Analyses

Note: In Windows use [Alt]-[Cursor left] to return to the previous page

1.3.1 Fitting Documentation

Note: In Windows use [Alt]-[Cursor left] to return to the previous page

Fitting

Note: If some code blocks are not readable, expand the documentation window

Preparing to fit data

To fit some data you must first load some data, activate one or more data sets, send those data sets to fitting, and select a model to fit to each data set.

Instructions on how to load and activate data are in the section Loading Data.

SasView can fit data in one of three ways:

• in Single fit mode - individual data sets are fitted independently one-by-one
in *Simultaneous* fit mode - multiple data sets are fitted simultaneously to the *same* model with/without constrained parameters (this might be useful, for example, if you have measured the same sample at different contrasts)

- in *Batch* fit mode - multiple data sets are fitted sequentially to the *same* model (this might be useful, for example, if you have performed a kinetic or time-resolved experiment and have *lots* of data sets!)

### Selecting a model

The models in SasView are grouped into categories. By default these consist of:

- **Cylinder** - cylindrical shapes (disc, right cylinder, cylinder with endcaps etc)
- **Ellipsoid** - ellipsoidal shapes (oblate, prolate, core shell, etc)
- **Parellelepiped** - as the name implies
- **Sphere** - sheredial shapes (sphere, core multishell, vesicle, etc)
- **Lamellae** - lamellar shapes (lamellar, core shell lamellar, stacked lamellar, etc)
- **Shape-Independent** - models describing structure in terms of density correlation functions, fractals, peaks, power laws, etc
- **Paracrystal** - semi ordered structures (bcc, fcc, etc)
- **Structure Factor** - S(Q) models
- **Plugin Models** - User-created (custom/non-library) Python models

Use the *Category* drop-down menu to chose a category of model, then select a model from the drop-down menu beneath. A graph of the chosen model, calculated using default parameter values, will appear. The graph will update dynamically as the parameter values are changed.

You can decide your own model categorizations using the *Category Manager*.

Once you have selected a model you can read its help documentation by clicking on the *Description* button to the right.

### Show 1D/2D

Models are normally fitted to 1D (ie, I(Q) vs Q) data sets, but some models in SasView can also be fitted to 2D (ie, I(Qx,Qy) vs Qx vs Qy) data sets.

*NB: Magnetic scattering can only be fitted in SasView in 2D.*

To activate 2D fitting mode, click the *Show 2D* button on the *Fit Page*. To return to 1D fitting model, click the same button (which will now say *Show 1D*).

### Category Manager

To change the model categorizations, either choose *Category Manager* from the *View* option on the menubar, or click on the *Modify* button on the *Fit Page*.
The categorization of all models except the user supplied Plugin Models can be reassigned, added to, and removed using Category Manager. Models can also be hidden from view in the drop-down menus.

Changing category

To change category, highlight a model in the list by left-clicking on its entry and then click the Modify button. Use the Change Category panel that appears to make the required changes.
To create a category for the selected model, click the Add button. In order to delete a category, select the category name and click the Remove Selected button. Then click Done.

**Showing/hiding models**

Use the Enable All / Disable All buttons and the check boxes beside each model to select the models to show/hide. To apply the selection, click Ok. Otherwise click Cancel.

NB: It may be necessary to change to a different category and then back again before any changes take effect.

**Model Functions**

For a complete list of all the library models available in SasView, see the Model Documentation.

It is also possible to add your own models.

**Adding your own Models**

There are essentially three ways to generate new fitting models for SasView:

- Using the SasView New Plugin Model helper dialog (best for beginners and/or relatively simple models)
• By copying/editing an existing model (this can include models generated by the New Plugin Model* dialog) in the Python Shell-Editor Tool or Advanced Plugin Editor (suitable for all use cases)

• By writing a model from scratch outside of SasView (only recommended for code monkeys!)

Please read the guidance on Writing a Plugin Model before proceeding.

To be found by SasView your model must reside in the ~/.sasview/plugin_models* folder.

Plugin Model Operations

From the Fitting option in the menu bar, select Plugin Model Operations

1.3. Fitting & Other Analyses
When using this feature, be aware that even if your code has errors, including syntax errors, a model file is still generated. When you then correct the errors and click ‘Apply’ again to re-compile you will get an error informing you that the model already exists if the ‘Overwrite’ box is not checked. In this case you will need to supply a new model function name. By default the ‘Overwrite’ box is checked.

A model file generated by this option can be viewed and further modified using the Advanced Plugin Editor.

Note that the New Plugin Model Feature currently does not allow for parameters to be polydisperse. However they can be edited in the Advanced Editor.

**SasView version 4.2** made it possible to specify whether a plugin created with the New Plugin Model dialog is actually a form factor $P(Q)$ or a structure factor $S(Q)$. To do this, simply add one or other of the following lines under the `import` statements.

For a form factor:

```python
form_factor = True
```

or for a structure factor:

```python
structure_factor = True
```

If the plugin is a structure factor it is also necessary to add two variables to the parameter list:

```python
parameters = [
    ['radius_effective', '', 1, [0.0, numpy.inf], 'volume', ''],
    ...]
```

(continues on next page)
and to the declarations of the functions Iq and Iqxy:

```python
def Iq(x, radius_effective, volfraction, ...):
def Iqxy(x, y, radius_effective, volfraction, ...):
```

Such a plugin should then be available in the S(Q) drop-down box on a FitPage (once a P(Q) model has been selected).

**Sum|Multi(p1,p2)**

![Easy Sum/Multi Editor](image)

This option creates a custom Plugin Model of the form:

```plaintext
Plugin Model = scale_factor \times \{(scale_1 \times model_1) \pm (scale_2 \times model_2)\} + background
```

or:

```plaintext
Plugin Model = scale_factor \times (model1 \times model2) + background
```

In the *Easy Sum/Multi Editor* give the new model a function name and brief description (to appear under the *Details* button on the *FitPage*). Then select two existing models, as p1 and p2, and the required operator, ‘+’ or ‘*’ between them. Finally, click the *Apply* button to generate and test the model and then click *Close*.

Any changes to a plugin model generated in this way only become effective after it is re-selected from the plugin models drop-down menu on the FitPage. If the model is not listed you can force a recompilation of the plugins by selecting *Fitting > Plugin Model Operations > Load Plugin Models*. 

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SasView version 4.2 introduced a much simplified and more extensible structure for plugin models generated through the Easy Sum/Multi Editor. For example, the code for a combination of a sphere model with a power law model now looks like this:

```python
from sasmodels.core import load_model_info
from sasmodels.sasview_model import make_model_from_info

model_info = load_model_info('sphere+power_law')
model_info.name = 'MyPluginModel'
model_info.description = 'sphere + power_law'
Model = make_model_from_info(model_info)
```

To change the models or operators contributing to this plugin it is only necessary to edit the string in the brackets after `load_model_info`, though it would also be a good idea to update the model name and description too!!!

The model specification string can handle multiple models and combinations of operators (+ or ) which are processed according to normal conventions. Thus ‘model1+model2*model3’ would be valid and would multiply model2 by model3 before adding model1. In this example, parameters in the *FitPage would be prefixed A (for model2), B (for model3) and C (for model1). Whilst this might appear a little confusing, unless you were creating a plugin model from multiple instances of the same model the parameter assignments ought to be obvious when you load the plugin.

If you need to include another plugin model in the model specification string, just prefix the name of that model with custom. For instance:

```
sphere+custom.MyPluginModel
```

To create a P(Q)*S(Q) model use the @ symbol instead of * like this:

```
sphere@hardsphere
```

This streamlined approach to building complex plugin models from existing library models, or models available on the Model Marketplace, also permits the creation of P(Q)*S(Q) plugin models, something that was not possible in earlier versions of SasView.

Advanced Plugin Editor

Selecting this option shows all the plugin models in the plugin model folder, on Windows this is

```
C:\Users\{username}.sasview\plugin_models
```

You can edit, modify, and save the Python code in any of these models using the Advanced Plugin Model Editor. Note that this is actually the same tool as the Python Shell-Editor Tool.

For details of the SasView plugin model format see Writing a Plugin Model.

**Note:** Model files generated with the Sum/Multi option are still using the SasView 3.x model format. Unless you are confident about what you are doing, it is recommended that you only modify lines denoted with the ## <— comments!

When editing is complete, select Run > Check Model from the Advanced Plugin Model Editor menu bar. An Info box will appear with the results of the compilation and model unit tests. The model will only be usable if the tests ‘pass’.
To use the model, go to the relevant Fit Page, select the Plugin Models category and then select the model from the drop-down menu.

Any changes to a plugin model generated in this way only become effective after it is re-selected from the model drop-down menu on the FitPage.

Delete Plugin Models

Simply highlight the plugin model to be removed. The operation is final!!!

NB: Models shipped with SasView cannot be removed in this way.

Load Plugin Models

This option loads (or re-loads) all models present in the ~/.sasview/plugin_models folder.

Fitting Options

It is possible to specify which optimiser SasView should use to fit the data, and to modify some of the configura-
tional parameters for each optimiser.

From Fitting in the menu bar select Fit Options, then select one of the following optimisers:
The DREAM optimiser is the most sophisticated, but may not necessarily be the best option for fitting simple models. If uncertain, try the Levenberg-Marquardt optimiser initially.

These optimisers form the Bumps package written by P Kienzle. For more information on each optimiser, see the Fitting Documentation.

Fitting Limits

By default, SasView will attempt to model fit the full range of the data; ie, across all $Q$ values. If necessary, however, it is possible to specify only a sub-region of the data for fitting.

In a FitPage or BatchPage change the $Q$ values in the Min and/or Max text boxes. Vertical coloured bars will appear on the graph with the data and ‘theory’ indicating the current $Q$ limits (red = $Q_{min}$, purple = $Q_{max}$).

To return to including all data in the fit, click the Reset button.

Shortcuts

Copy/Paste Parameters

It is possible to copy the parameters from one Fit Page and to paste them into another Fit Page using the same model.

To copy parameters, either:

- Select Edit -> Copy Params from the menu bar, or
- Use Ctrl(Cmd on Mac) + Left Mouse Click on the Fit Page.

To paste parameters, either:

- Select Edit -> Paste Params from the menu bar, or
- Use Ctrl(Cmd on Mac) + Shift + Left-click on the Fit Page.

If either operation is successful a message will appear in the info line at the bottom of the SasView window.

Bookmark

To Bookmark a Fit Page either:

- Select a Fit Page and then click on Bookmark in the tool bar, or
- Right-click and select the Bookmark in the popup menu.

Status Bar & Console

The status bar is located at the bottom of the SasView window and displays messages, hints, warnings and errors.

At the right-hand side of the status bar is a button marked Console. The Console displays available message history and some run-time traceback information.

During a long task the Console can also be used to monitor the progress.
**Single Fit Mode**

*NB: Before proceeding, ensure that the Single Mode radio button at the bottom of the Data Explorer is checked (see the section Loading Data).*

This mode fits one data set.

When data is sent to the fitting it is plotted in a graph window as markers.

If a graph does not appear, or a graph window appears but is empty, then the data has not loaded correctly. Check to see if there is a message in the Status Bar & Console or in the Console window.

Assuming the data has loaded correctly, when a model is selected a green model calculation (or what SasView calls a ‘Theory’) line will appear in the earlier graph window, and a second graph window will appear displaying the residuals (the difference between the experimental data and the theory) at the same X-data values. See Assessing Fit Quality.

The objective of model-fitting is to find a physically-plausible model, and set of model parameters, that generate a theory that reproduces the experimental data and minimizes the values of the residuals.

Change the default values of the model parameters by hand until the theory line starts to represent the experimental data. Then check the tick boxes alongside the ‘background’ and ‘scale’ parameters. Click the Fit button. SasView will optimise the values of the ‘background’ and ‘scale’ and also display the corresponding uncertainties on the optimised values.

**Note:** If the uncertainty on a fitted parameter is unrealistically large, or if it displays as NaN, the model is most likely a poor representation of the data, the parameter in question is highly correlated with one or more of the other fitted parameters, or the model is relatively insensitive to the value of that particular parameter.

In the bottom left corner of the Fit Page is a box displaying a normalised value of the statistical $\chi^2$ parameter (the reduced $\chi^2$, See Assessing Fit Quality) returned by the optimiser.

Now check the box for another model parameter and click Fit again. Repeat this process until all relevant parameters are checked and have been optimised. As the fit of the theory to the experimental data improves, the value of ‘Reduced Chi2’ will decrease. A good model fit should produce values of Reduced Chi2 close to one, and certainly << 100. See Assessing Fit Quality.

SasView has a number of different optimisers (see the section Fitting Options). The DREAM optimiser is the most sophisticated, but may not necessarily be the best option for fitting simple models. If uncertain, try the Levenberg-Marquardt optimiser initially.

**Simultaneous Fit Mode**

*NB: Before proceeding, ensure that the Single Mode radio button at the bottom of the Data Explorer is checked (see the section Loading Data).*

This mode is an extension of the Single Fit Mode that allows for some relatively extensive constraints between fitted parameters in a single FitPage or between several FitPage’s (eg, to constrain all fitted parameters to be the same in a contrast series of FitPages except for the solvent sld parameter, constrain the length to be twice that of the radius in a single FitPage, fix the radius of the sphere in one FitPage to be the same as the radius of the cylinder in a second FitPage, etc).

If the data to be fit are in multiple files, load each file, then select each file in the Data Explorer, and Send To Fitting. If multiple data sets are in one file, load that file. Unselect All Data, select just those data sets to be fitted, and Send To Fitting. Either way, the result should be that for $n$ data sets you have $2n$ graphs ($n$ of the data and model fit, and $n$ of the resulting residuals). But it may be helpful to minimise the residuals plots for clarity. Also see Assessing Fit Quality.

**NB: If you need to use a custom Plugin Model, you must ensure that model is available first (see Adding your own Models).**
Method

Now go to each FitPage in turn and:

Select the required category and model;

Unselect all the model parameters;

Enter some starting guesses for the parameters;

Enter any parameter limits (recommended);

Select which parameters will refine (selecting all is generally a bad idea…):

When done, select Constrained or Simultaneous Fit under Fitting in the menu bar.

In the Const & Simul Fit page that appears, select which data sets are to be simultaneously fitted (this will probably be all of them or you would not have loaded them in the first place!).

To tie parameters between the data sets with constraints, check the ‘yes’ radio button next to Add Constraint? in the Fit Constraints box.

To constrain all identically named parameters to fit simultaneously to the same value across all the Fitpages use the Easy Setup drop-down buttons in the Const & Simul Fit page.

NB: You can only constrain parameters that are set to refine.

Constraints will generally be of the form

Mi Parameter1 = Mj.Parameter1

however the text box after the ‘=’ sign can be used to adjust this relationship; for example

Mi Parameter1 = scalar * Mj.Parameter1

A ‘free-form’ constraint box is also provided.

Many constraints can be entered for a single fit.

When ready, click the Fit button on the Const & Simul Fit page, NOT the Fit button on the individual FitPage’s.

The results of the model-fitting will be returned to each of the individual FitPage’s.

Note that the Reduced Chi2 value returned is the SUM of the Reduced Chi2 of each fit. To see the Reduced Chi2 value for a specific FitPage, click the Compute button at the bottom of that FitPage to recalculate. Note that in doing so the degrees of freedom will be set to Npts. See Assessing Fit Quality. Moreover in the case of constraints the degrees of freedom are less than one might think due to those constraints.

Batch Fit Mode

NB: Before proceeding, ensure that the Single Mode radio button at the bottom of the Data Explorer is checked (see the section Loading Data). The Batch Mode button will be used later on!

This mode sequentially fits two or more data sets to the same model. Unlike in simultaneous fitting, in batch fitting it is not possible to constrain fit parameters between data sets.

If the data to be fit are in multiple files, load each file in the Data Explorer. If multiple data sets are in one file, load just that file. Unselect All Data, then select a single initial data set to be fitted. Fit that selected data set as described above under Single Fit Mode.

NB: If you need to use a custom Plugin Model, you must ensure that model is available first (see Adding your own Models).
Method

Now Select All Data in the Data Explorer, check the Batch Mode radio button at the bottom of that panel and Send To Fitting. A BatchPage will be created.

NB: The Batch Page can also be created by checking the Batch Mode radio button and selecting New Fit Page under Fitting in the menu bar.

Using the drop-down menus in the BatchPage, now set up the same data set with the same model that you just fitted in single fit mode. A quick way to set the model parameter values is to just copy them from the earlier Single Fit. To do this, go back to the Single Fit FitPage, select Copy Params under Edit in the menu bar, then go back to the BatchPage and Paste Params.

When ready, use the Fit button on the BatchPage to perform the fitting, NOT the Fit button on the individual FitPage's.

Unlike in single fit mode, the results of batch fits are not returned to the BatchPage. Instead, a spreadsheet-like Grid Window will appear.
If you want to visually check a graph of a particular fit, click on the name of a Data set in the Grid Window and then click the View Fits button. The data and the model fit will be displayed. If you select multiple data sets they will all appear on one graph.

NB: In theory, returning to the BatchPage and changing the name of the I(Q) data source should also work, but at the moment whilst this does change the data set displayed it always superimposes the ‘theory’ corresponding to the starting parameters.

If you select a ‘Chi2’ value and click the View Fits button a graph of the residuals for that data set is displayed. Again, if you select multiple ‘Chi2’ values then all the residuals data will appear on one graph. Also see Assessing Fit Quality.

Chain Fitting

By default, the same parameter values copied from the initial single fit into the BatchPage will be used as the starting parameters for all batch fits. It is, however, possible to get SasView to use the results of a fit to a preceding data set as the starting parameters for the next fit in the sequence. This variation of batch fitting is called Chain Fitting, and will considerably speed up model-fitting if you have lots of very similar data sets where a few parameters are gradually changing. Do not use chain fitting on disparate data sets.

To use chain fitting, select Chain Fitting under Fitting in the menu bar. It toggles on/off, so selecting it again will switch back to normal batch fitting.

Grid Window

The Grid Window provides an easy way to view the results from batch fitting. It will be displayed automatically when a batch fit completes, but may be opened at any time by selecting Show Grid Window under View in the menu bar.
Once a batch fit is completed, all model parameters are displayed but *not* their uncertainties. To view the uncertainties, click on a given column then go to *Edit* in the menu bar, select *Insert Column Before* and choose the required data from the list. An empty column can be inserted in the same way.

To remove a column from the grid, click on the column header and choose *Remove Column* under *Edit* in the menu bar. The same functionality also allows you to re-order columns.

*NB: You cannot insert/remove/re-order the rows in the Grid Window.*

All of the above functions are also available by right-clicking on a column label.

*NB: If there is an existing Grid Window and another batch fit is performed, an additional ‘Table’ tab will be added to the Grid Window.*

The parameter values in the *currently selected* table of the *Grid Window* can be output to a CSV file by choosing *Save As* under *File* in the (*Grid Window*) menu bar. The default filename includes the date and time that the batch fit was performed.

Saved CSV files can be reloaded by choosing *Open* under *File* in the *Grid Window* menu bar. The loaded parameters will appear in a new table tab.
NB: Saving the Grid Window does not save any experimental data, residuals or actual model fits. Consequently if you reload a saved CSV file the ability to View Fits will be lost.

Parameter Plots

Any column of numeric parameter values can be plotted against another using the Grid Window. Simply select one column at the time and click the Add button next to the required XY-axis Selection Range text box. When both the X and Y axis boxes have been completed, click the Plot button.

When the Add button is clicked, SasView also automatically completes the XY-axis Label text box with the heading from Row 1 of the selected table, but different labels and units can be entered manually.

The XY-axis Selection Range can be edited manually. The text control box recognises the operators +, -, *, /, or ‘pow’, and allows the following types of expression:

1. if an axis label range is a function of 1 or more columns, write this type of expression
   
   constant1 * column_name1 [minimum row index : maximum row index] operator constant2 * column_name2 [minimum row index : maximum row index]
Example: \( \text{radius} [2 : 5] \cdot 3 \cdot \text{scale} [2 : 5] \)

2. if only some values of a given column are needed but the range between the first row and the last row used is not continuous, write this type of expression

\[ \text{column}_1 \left[ \text{minimum row index}_1 : \text{maximum row index}_1 \right], \text{column}_2 \left[ \text{minimum row index}_2 : \text{maximum row index}_2 \right] \]

Example: \( \text{radius} [2 : 5], \text{radius} [10 : 25] \)

**Combined Batch Fit Mode**

The purpose of the Combined Batch Fit is to allow running two or more batch fits in sequence without overwriting the output table of results. This may be of interest for example if one is fitting a series of data sets where there is a shape change occurring in the series that requires changing the model part way through the series; for example a sphere to rod transition. Indeed the regular batch mode does not allow for multiple models and requires all the files in the series to be fit with single model and set of parameters. While it is of course possible to just run part of the series as a batch fit using model one followed by running another batch fit on the rest of the series with model two (and/or model three etc), doing so will overwrite the table of outputs from the previous batch fit(s). This may not be desirable if one is interested in comparing the parameters: for example the sphere radius of set one and the cylinder radius of set two.

**Method**

In order to use the Combined Batch Fit, first load all the data needed as described in **Loading Data**. Next start up two or more BatchPage fits following the instructions in **Batch Fit Mode** but DO NOT PRESS FIT. At this point the Combine Batch Fit menu item under the Fitting menu should be active (if there is one or no BatchPage the menu item will be greyed out and inactive). Clicking on Combine Batch Fit will bring up a new panel, similar to the Const & Simult Fit panel. In this case there will be a checkbox for each BatchPage instead of each FitPage that should be included in the fit. Once all are selected, click the Fit button on the BatchPage to run each batch fit in sequence.

The batch table will then pop up at the end as for the case of the simple Batch Fitting with the following caveats:

**Note:** The order matters. The parameters in the table will be taken from the model used in the first BatchPage of the list. Any parameters from the second and later BatchPage s that have the same name as a parameter in the first...
will show up allowing for plotting of that parameter across the models. The other parameters will not be available in the grid.

**Note:** a corralary of the above is that currently models created as a sum|multiply model will not work as desired because the generated model parameters have a p#_ appended to the beginning and thus radius and p1_radius will not be recognized as the same parameter.

In the example shown above the data is a time series with a shifting peak. The first part of the series was fitted using the `broad_peak` model, while the rest of the data were fit using the `gaussian_peak` model. Unfortunately the time is not listed in the file but the file name contains the information. As described in *Grid Window*, a column can be added manually, in this case called time, and the peak position plotted against time.
Note the discontinuity in the peak position. This reflects the fact that the Gaussian fit is a rather poor model for the data and is not actually finding the peak.

**Assessing Fit Quality**

When performing model-fits to some experimental data it is helpful to be able to gauge how good an individual fit is, how it compares to a fit of the same model to another set of data, or how it compares to a fit of a different model to the same data.

One way is obviously to just inspect the graph of the experimental data and to see how closely (or not!) the ‘theory’ calculation matches it. But SasView also provides two other measures of the quality of a fit:

- $\chi^2$ (or ‘Chi2’; pronounced ‘chi-squared’)
- Residuals
Chi2

$\chi^2$ is a statistical parameter that quantifies the differences between an observed data set and an expected dataset (or ‘theory’) calculated as

$$\chi^2 = \sum [(Y_i - \text{theory}_i)^2 / \text{error}_i^2]$$

Fitting typically minimizes the value of $\chi^2$. For assessing the quality of the model and its “fit” however, SasView displays the traditional reduced $\chi^2_R$ which normalizes this parameter by dividing it by the number of degrees of freedom (or DOF). The DOF is the number of data points being considered, $N_{\text{pts}}$, reduced by the number of free (i.e. fitted) parameters, $N_{\text{par}}$. Note that model parameters that are kept fixed do not contribute to the DOF (they are not “free”). This reduced value is then given as

$$\chi^2_R = \sum [(Y_i - \text{theory}_i)^2 / \text{error}_i^2] / [N_{\text{pts}} - N_{\text{par}}]$$

Note that this means the displayed value will vary depending on the number of parameters used in the fit. In particular, when doing a calculation without a fit (e.g. manually changing a parameter) the DOF will now equal $N_{\text{pts}}$ and the $\chi^2_R$ will be the smallest possible for that combination of model, data set, and set of parameter values. When $N_{\text{pts}} \gg N_{\text{par}}$ as it should for proper fitting, the value of the reduced $\chi^2_R$ will not change very much.

For a good fit, $\chi^2_R$ tends to 1. $\chi^2_R$ is sometimes referred to as the ‘goodness-of-fit’ parameter.

Residuals

A residual is the difference between an observed value and an estimate of that value, such as a ‘theory’ calculation (whereas the difference between an observed value and its true value is its error).

SasView calculates ‘normalized residuals’, $R_i$, for each data point in the fit:

$$R_i = (Y_i - \text{theory}_i) / \text{error}_i$$

Think of each normalized residual as the number of standard deviations between the measured value and the theory. For a good fit, 68% of $R_i$ will be within one standard deviation, which will show up in the Residuals plot as $R_i$ values between $-1$ and $+1$. Almost all the values should be between $-3$ and $+3$.

Residuals values larger than $\pm 3$ indicate that the model is not fit correctly, the wrong model was chosen (e.g., because there is more than one phase in your system), or there are problems in the data reduction. Since the goodness of fit is calculated from the sum-squared residuals, these extreme values will drive the choice of fit parameters. Any uncertainties calculated for the fitting parameters will be meaningless.

Document History

2015-06-08 Steve King
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Polydispersity & Orientational Distributions

For some models we can calculate the average intensity for a population of particles that possess size and/or orientational (i.e., angular) distributions. In SasView we call the former polydispersity but use the parameter $PD$ to parameterise both. In other words, the meaning of $PD$ in a model depends on the actual parameter it is being applied too.

The resultant intensity is then normalized by the average particle volume such that

$$P(q) = \text{scale}(F^*F)/V + \text{background}$$
where $F$ is the scattering amplitude and $\langle \cdot \rangle$ denotes an average over the distribution $f(x; \bar{x}, \sigma)$, giving

$$P(q) = \frac{\text{scale}}{V} \int_{\mathbb{R}} f(x; \bar{x}, \sigma) F^2(q, x) \, dx + \text{background}$$

Each distribution is characterized by a center value $\bar{x}$ or $x_{\text{med}}$, a width parameter $\sigma$ (note this is not necessarily the standard deviation, so read the description of the distribution carefully), the number of sigmas $N_\sigma$ to include from the tails of the distribution, and the number of points used to compute the average. The center of the distribution is set by the value of the model parameter.

The distribution width applied to volume (ie, shape-describing) parameters is relative to the center value such that $\sigma = \text{PD} \cdot \bar{x}$. However, the distribution width applied to orientation parameters is just $\sigma = \text{PD}$.

$N_\sigma$ determines how far into the tails to evaluate the distribution, with larger values of $N_\sigma$ required for heavier tailed distributions. The scattering in general falls rapidly with $q \sigma$ so the usual assumption that $f(r - 3\sigma_r) / f(r - 3\sigma_r)$ will not contribute much to the average may not hold when particles are large. This, too, will require increasing $N_\sigma$.

Users should note that the averaging computation is very intensive. Applying polydispersion and/or orientational distributions to multiple parameters at the same time, or increasing the number of points in the distribution, will require patience! However, the calculations are generally more robust with more data points or more angles.

The following distribution functions are provided:

- **Uniform Distribution**
- **Rectangular Distribution**
- **Gaussian Distribution**
- **Boltzmann Distribution**
- **Lognormal Distribution**
- **Schulz Distribution**
- **Array Distribution**

These are all implemented as number-average distributions.

Additional distributions are under consideration.

**Beware:** when the Polydispersity & Orientational Distribution panel in SasView is first opened, the default distribution for all parameters is the Gaussian Distribution. This may not be suitable. See Suggested Applications below.

**Note:** In 2009 IUPAC decided to introduce the new term ‘dispersity’ to replace the term ‘polydispersity’ (see Pure Appl. Chem., (2009), 81(2), 351-353 in order to make the terminology describing distributions of chemical properties unambiguous. However, these terms are unrelated to the proportional size distributions and orientational distributions used in SasView models.

**Suggested Applications**

If applying polydispersion to parameters describing particle sizes, consider using the Lognormal or Schulz distributions.

If applying polydispersion to parameters describing interfacial thicknesses or angular orientations, consider using the Gaussian or Boltzmann distributions.

If applying polydispersion to parameters describing angles, use the Uniform distribution. Beware of using distributions that are always positive (eg, the Lognormal) because angles can be negative!

The array distribution allows a user-defined distribution to be applied.
Uniform Distribution

The Uniform Distribution is defined as

\[ f(x) = \frac{1}{\text{Norm}} \begin{cases} 1 & \text{for } |x - \bar{x}| \leq \sigma \\ 0 & \text{for } |x - \bar{x}| > \sigma \end{cases} \]

where \( \bar{x} \) (\( x_{\text{mean}} \) in the figure) is the mean of the distribution, \( \sigma \) is the half-width, and \( \text{Norm} \) is a normalization factor which is determined during the numerical calculation.

The polydispersity in sasmodels is given by

\[ \text{PD} = \sigma / \bar{x} \]

Note that the standard deviation and the half width \( w \) are different!

\[ \sigma = \frac{w}{\sqrt{3}} \]

Rectangular Distribution

The Rectangular Distribution is defined as

\[ f(x) = \frac{1}{\text{Norm}} \begin{cases} 1 & \text{for } |x - \bar{x}| \leq w \\ 0 & \text{for } |x - \bar{x}| > w \end{cases} \]

where \( \bar{x} \) (\( x_{\text{mean}} \) in the figure) is the mean of the distribution, \( w \) is the half-width, and \( \text{Norm} \) is a normalization factor which is determined during the numerical calculation.

Note that the standard deviation and the half width \( w \) are different!

The standard deviation is

\[ \sigma = \frac{w}{\sqrt{3}} \]

whilst the polydispersity in sasmodels is given by

\[ \text{PD} = \sigma / \bar{x} \]

Note: The Rectangular Distribution is deprecated in favour of the Uniform Distribution above and is described here for backwards compatibility with earlier versions of SasView only.
The Gaussian Distribution is defined as

\[ f(x) = \frac{1}{\text{Norm}} \exp \left( -\frac{(x - \bar{x})^2}{2\sigma^2} \right) \]

where \( \bar{x} \) (\( x_{\text{mean}} \) in the figure) is the mean of the distribution and \( \text{Norm} \) is a normalization factor which is determined during the numerical calculation.

The polydispersity in sasmodels is given by

\[ \text{PD} = \frac{\sigma}{\bar{x}} \]
Boltzmann Distribution

The Boltzmann Distribution is defined as

\[ f(x) = \frac{1}{\text{Norm}} \exp \left( -\frac{|x - \bar{x}|}{\sigma} \right) \]

where \( \bar{x} \) (\( x_{\text{mean}} \) in the figure) is the mean of the distribution and \( \text{Norm} \) is a normalization factor which is determined during the numerical calculation.

The width is defined as

\[ \sigma = \frac{kT}{E} \]

which is the inverse Boltzmann factor, where \( k \) is the Boltzmann constant, \( T \) the temperature in Kelvin and \( E \) a characteristic energy per particle.

Lognormal Distribution

The Lognormal Distribution describes a function of \( x \) where \( \ln(x) \) has a normal distribution. The result is a distribution that is skewed towards larger values of \( x \).

The Lognormal Distribution is defined as

\[ f(x) = \frac{1}{\text{Norm}} \frac{1}{x\sigma} \exp \left( -\frac{1}{2} \left( \frac{\ln(x) - \mu}{\sigma} \right)^2 \right) \]

where \( \text{Norm} \) is a normalization factor which will be determined during the numerical calculation, \( \mu = \ln(x_{\text{med}}) \) and \( x_{\text{med}} \) is the median value of the lognormal distribution, but \( \sigma \) is a parameter describing the width of the underlying normal distribution.

\( x_{\text{med}} \) will be the value given for the respective size parameter in sasmodels, for example, \( \text{radius}=60 \).

The polydispersity in sasmodels is given by

\[ \text{PD} = \frac{\sigma}{x_{\text{med}}} \]

The mean value of the distribution is given by \( \bar{x} = \exp(\mu + \sigma^2/2) \) and the peak value by \( \max x = \exp(\mu - \sigma^2) \).

The variance (the square of the standard deviation) of the lognormal distribution is given by

\[ \nu = [\exp(\sigma^2) - 1] \exp(2\mu + \sigma^2) \]

Note that larger values of PD might need a larger number of points and \( N_\sigma \).

Schulz Distribution

The Schulz (sometimes written Schultz) distribution is similar to the Lognormal distribution, in that it is also skewed towards larger values of \( x \), but which has computational advantages over the Lognormal distribution.

The Schulz distribution is defined as

\[
f(x) = \frac{1}{\text{Norm}} \left( z + 1 \right)^{z+1} \left( \frac{x}{\bar{x}} \right)^z \exp \left[ - \left( z + 1 \right) \frac{x}{\bar{x}} \right] \frac{\Gamma(z+1)}{\bar{x}}
\]

where \( \bar{x} \) (\( x_{\text{mean}} \) in the figure) is the mean of the distribution, \( \text{Norm} \) is a normalization factor which is determined during the numerical calculation, and \( z \) is a measure of the width of the distribution such that

\[
z = \frac{1 - p^2}{p^2}
\]

where \( p \) is the polydispersity in sasmodels given by

\[
PD = p = \sigma / \bar{x}
\]

and \( \sigma \) is the RMS deviation from \( \bar{x} \).

Note that larger values of PD might need a larger number of points and \( N_\sigma \). For example, for PD=0.7 with radius=60 Å, at least \( N_{\text{pts}} \geq 160 \) and \( N_{\text{sigmas}} \geq 15 \) are required.

Array Distribution

This user-definable distribution should be given as a simple ASCII text file where the array is defined by two columns of numbers: \( x \) and \( f(x) \). The \( f(x) \) will be normalized to 1 during the computation.

Example of what an array distribution file should look like:

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0.1</td>
</tr>
<tr>
<td>32</td>
<td>0.3</td>
</tr>
<tr>
<td>35</td>
<td>0.4</td>
</tr>
<tr>
<td>36</td>
<td>0.5</td>
</tr>
<tr>
<td>37</td>
<td>0.6</td>
</tr>
<tr>
<td>39</td>
<td>0.7</td>
</tr>
<tr>
<td>41</td>
<td>0.9</td>
</tr>
</tbody>
</table>

Only these array values are used computation, therefore the parameter value given for the model will have no affect, and will be ignored when computing the average. This means that any parameter with an array distribution will not be fitable.

Note about DLS polydispersity

Several measures of polydispersity abound in Dynamic Light Scattering (DLS) and it should not be assumed that any of the following can be simply equated with the polydispersity \( PD \) parameter used in SasView.

The dimensionless Polydispersity Index (PI) is a measure of the width of the distribution of autocorrelation function decay rates (not the distribution of particle sizes itself, though the two are inversely related) and is defined by ISO 22412:2017 as

\[
PI = \frac{\mu_2}{\bar{\Gamma}^2}
\]

where \( \mu_2 \) is the second cumulant, and \( \bar{\Gamma}^2 \) is the intensity-weighted average value, of the distribution of decay rates. If the distribution of decay rates is Gaussian then

\[
PI = \frac{\sigma^2}{2\bar{\Gamma}^2}
\]

where \( \sigma \) is the standard deviation, allowing a Relative Polydispersity (RP) to be defined as

\[
RP = \frac{\sigma}{\bar{\Gamma}} = \sqrt{2 \cdot PI}
\]

PI values smaller than 0.05 indicate a highly monodisperse system. Values greater than 0.7 indicate significant polydispersity.

The size polydispersity P-parameter is defined as the relative standard deviation coefficient of variation

\[
P = \frac{\sqrt{\nu}}{\bar{R}}
\]

where \( \nu \) is the variance of the distribution and \( \bar{R} \) is the mean value of \( R \). Here, the product \( P\bar{R} \) is equal to the standard deviation of the Lognormal distribution.

P values smaller than 0.13 indicate a monodisperse system.

For more information see:

Polydispersity: What does it mean for DLS and Chromatography.
Resolution Functions

Sometimes the instrumental geometry used to acquire the experimental data has an impact on the clarity of features in the reduced scattering curve. For example, peaks or fringes might be slightly broadened. This is known as $Q$ resolution smearing. To compensate for this effect one can either try and remove the resolution contribution - a process called desmearing - or add the resolution contribution into a model calculation/simulation (which by definition will be exact) to make it more representative of what has been measured experimentally - a process called smearing. Sasmodels does the latter.

Both smearing and desmearing rely on functions to describe the resolution effect. Sasmodels provides three smearing algorithms:

- Slit Smearing
- Pinhole Smearing
- 2D Smearing

The $Q$ resolution values should be determined by the data reduction software for the instrument and stored with the data file. If not, they will need to be set manually before fitting.

Slit Smearing

This type of smearing is normally only encountered with data from X-ray Kratky cameras or X-ray/neutron Bonse-Hart USAXS/USANS instruments.

The slit-smeared scattering intensity is defined by

$$I_s = \frac{1}{\text{Norm}} \int_{-\infty}^{\infty} dv \, W_v(v) \int_{-\infty}^{\infty} du \, W_u(u) \, I \left( \sqrt{(q + v)^2 + [u]^2} \right)$$

where $\text{Norm}$ is given by

$$\int_{-\infty}^{\infty} dv \, W_v(v) \int_{-\infty}^{\infty} du \, W_u(u)$$

[Equation 1]

The functions $W_v(v)$ and $W_u(u)$ refer to the slit width weighting function and the slit height weighting determined at the given $q$ point, respectively. It is assumed that the weighting function is described by a rectangular function, such that

$$W_v(v) = \delta(|v| \leq \Delta q_v)$$

[Equation 2]

and

$$W_u(u) = \delta(|u| \leq \Delta q_u)$$

[Equation 3]

so that $\Delta q_v = \int_{0}^{\infty} d\alpha \, W_v(\alpha)$ for $\alpha$ as $v$ and $u$.

Here $\Delta q_u$ and $\Delta q_v$ stand for the the slit height (FWHM/2) and the slit width (FWHM/2) in $q$ space.
This simplifies the integral in Equation 1 to

$$I_s(q) = \frac{2}{\text{Norm}} \int_{-\Delta q_u}^{\Delta q_u} dv \int_{0}^{\Delta q_v} du I \left( \sqrt{(q + v)^2 + u^2} \right)$$

[Equation 4]

which may be solved numerically, depending on the nature of $\Delta q_u$ and $\Delta q_v$.

Solution 1

For $\Delta q_v = 0$ and $\Delta q_u = \text{constant}$

$$I_s(q) \approx \int_{0}^{\Delta q_u} du I \left( \sqrt{q^2 + u^2} \right) = \int_{0}^{\Delta q_u} d \left( \sqrt{q'^2 - q^2} \right) I(q')$$

For discrete $q$ values, at the $q$ values of the data points and at the $q$ values extended up to $q_N = q_i + \Delta q_u$ the smeared intensity can be approximately calculated as

$$I_s(q_i) \approx \sum_{j=1}^{N-1} \left[ \sqrt{q_{j+1}^2 + q_i^2} - \sqrt{q_j^2 + q_i^2} \right] I(q_j) \sum_{j=1}^{N-1} W_{ij} I(q_j)$$

[Equation 5]

where $W_{ij} = 0$ for $I_s$ when $j < i$ or $j > N - 1$.

Solution 2

For $\Delta q_v = \text{constant}$ and $\Delta q_u = 0$

Similar to Case 1

$$I_s(q_i) \approx \sum_{j=p}^{N-1} [q_{j+1} - q_i] I(q_j) \approx \sum_{j=p}^{N-1} W_{ij} I(q_j)$$

for $q_p = q_i - \Delta q_v$ and $q_N = q_i + \Delta q_v$

[Equation 6]

where $W_{ij} = 0$ for $I_s$ when $j < p$ or $j > N - 1$.

Solution 3

For $\Delta q_v = \text{constant}$ and $\Delta q_u = \text{constant}$

In this case, the best way is to perform the integration of Equation 1 numerically for both slit height and slit width. However, the numerical integration is imperfect unless a large number of iterations, say, at least 10000 by 10000 for each element of the matrix $W$, is performed. This is usually too slow for routine use.

An alternative approach is used in sasmodels which assumes slit width $<<$ slit height. This method combines Solution 1 with the numerical integration for the slit width. Then

$$I_s(q_i) \approx \sum_{j=p}^{N-1} \sum_{k=-L}^{L} \left[ \sqrt{q_{j+1}^2 - (q_i + (k\Delta q_v/L))^2} - \sqrt{q_j^2 - (q_i + (k\Delta q_v/L))^2} \right] (\Delta q_v/L) I(q_j)$$

$$\approx \sum_{j=p}^{N-1} W_{ij} I(q_j)$$

[Equation 7]

for $q_p = q_i - \Delta q_v$ and $q_N = q_i + \Delta q_v$

where $W_{ij} = 0$ for $I_s$ when $j < p$ or $j > N - 1$. 
Pinhole Smearing

This is the type of smearing normally encountered with data from synchrotron SAXS cameras and SANS instruments.

The pinhole smearing computation is performed in a similar fashion to the slit-smeared case above except that the weight function used is a Gaussian. Thus Equation 6 becomes

\[ I_s(q_i) \approx \sum_{j=0}^{N-1} \left[ \text{erf}(q_{j+1}) - \text{erf}(q_j) \right] I(q_j) \]

\[ \approx \sum_{j=0}^{N-1} W_{ij} I(q_j) \]

[Equation 8]

2D Smearing

The 2D smearing computation is performed in a similar fashion to the 1D pinhole smearing above except that the weight function used is a 2D elliptical Gaussian. Thus

\[ I_s(x_0, y_0) = A \int_{x_0} \int_{y_0} \exp \left[ -\frac{(x' - x_0)^2}{2\sigma_x^2} + \frac{(y' - y_0)^2}{2\sigma_y^2} \right] I(x', y') \]

\[ = A\sigma_x\sigma_y \int dX dY \exp \left[ -\frac{(X^2 + Y^2)}{2} \right] I(x_0 X + y_0 Y + x'_0, y'_0) \]

\[ = A\sigma_x\sigma_y \int dR d\Theta R \exp \left( -\frac{R^2}{2} \right) I(x_0 R \cos \Theta + x'_0, y_0 R \sin \Theta + y'_0) \]

[Equation 9]

In Equation 9, \( x_0 = q \cos(\theta) \), \( y_0 = q \sin(\theta) \), and the primed axes are all in the coordinate rotated by an angle \( \theta \) about the \( z \)-axis (see the figure below) so that \( x'_0 = x_0 \cos(\theta) + y_0 \sin(\theta) \) and \( y'_0 = -x_0 \sin(\theta) + y_0 \cos(\theta) \). Note that the rotation angle is zero for a \( x-y \) symmetric elliptical Gaussian distribution. The \( A \) is a normalization factor.

Now we consider a numerical integration where each of the bins in \( \theta \) and \( R \) are evenly (this is to simplify the equation below) distributed by \( \Delta \theta \) and \( \Delta R \) respectively, and it is further assumed that \( I(x', y') \) is constant within the bins. Then

\[ I_s(x_0, y_0) \approx A\sigma_x\sigma_y \sum_1^N \Delta \Theta \left[ \exp \left( \frac{(R_i - \Delta R/2)^2}{2} \right) - \exp \left( \frac{(R_i + \Delta R/2)^2}{2} \right) \right] I(x_0 R_i \cos \Theta_i + x'_0, y_0 R_i \sin \Theta_i + y'_0) \]

\[ \approx \sum_1^n W_i I(x_0 R_i \cos \Theta_i + x'_0, y_0 R_i \sin \Theta_i + y'_0) \]

[Equation 10]

Since the weighting factor on each of the bins is known, it is convenient to transform \( x'-y' \) back to \( x-y \) coordinates (by rotating it by \( -\theta \) around the \( z \)-axis).

Then, for a polar symmetric smear

\[ I_s(x_0, y_0) \approx \sum_1^n W_i I(x' \cos \theta - y' \sin \theta, x' \sin \theta + y' \cos \theta) \]

[Equation 11]

where

\[ x' = \sigma_x R_i \cos \Theta_i + x'_0 \]
\[ y' = \sigma_y R_i \sin \Theta_i + y'_0 \]
\[ x'_0 = q = \sqrt{x_0^2 + y_0^2} \]
\[ y'_0 = 0 \]
Fig. 1.133: Coordinate axis rotation for 2D resolution calculation.
while for a $x$–$y$ symmetric smear

$$I_s(x_0, y_0) \approx \sum_i^n W_i I(x', y')$$  

[Equation 12]

where

$$x' = \sigma x'_0 R_i \cos \Theta_i + x'_0$$

$$y' = \sigma y'_0 R_i \sin \Theta_i + y'_0$$

$$x'_0 = x_0 = q_x$$

$$y'_0 = y_0 = q_y$$

The current version of sasmodels uses Equation 11 for 2D smearing, assuming that all the Gaussian weighting functions are aligned in the polar coordinate.

**Weighting & Normalization**

In all the cases above, the weighting matrix $W$ is calculated on the first call to a smearing function, and includes ~60 $q$ values (finely and evenly binned) below ($>0$) and above the $q$ range of data in order to smear all data points for a given model and slit/pinhole size. The $Norm$ factor is found numerically with the weighting matrix and applied on the computation of $I_s$.

**Document History**

2015-05-01 Steve King
2017-05-08 Paul Kienzle

**Polarisation/Magnetic Scattering**

Models which define a scattering length density parameter can be evaluated as magnetic models. In general, the scattering length density (SLD = $\beta$) in each region where the SLD is uniform, is a combination of the nuclear and magnetic SLDs and, for polarised neutrons, also depends on the spin states of the neutrons.

For magnetic scattering, only the magnetization component $M_\perp$ perpendicular to the scattering vector $Q$ contributes to the magnetic scattering length.

The magnetic scattering length density is then

$$\beta_M = \frac{\gamma r_0}{2\mu_B} \sigma \cdot M_\perp = D_M \sigma \cdot M_\perp$$

where $\gamma = -1.913$ is the gyromagnetic ratio, $\mu_B$ is the Bohr magneton, $r_0$ is the classical radius of electron, and $\sigma$ is the Pauli spin.

Assuming that incident neutrons are polarized parallel (+) and anti-parallel (−) to the $x'$ axis, the possible spin states after the sample are then:

- Non spin-flip (++) and (−−)
- Spin-flip (+−) and (−+)  

Each measurement is an incoherent mixture of these spin states based on the fraction of $+$ neutrons before ($u_i$) and after ($u_f$) the sample, with weighting:

$$-\ = (1 - u_i)(1 - u_f)$$

$$-+ = (1 - u_i)(u_f)$$

$$+- = (u_i)(1 - u_f)$$

$$++ = (u_i)(u_f)$$
Ideally the experiment would measure the pure spin states independently and perform a simultaneous analysis of the four states, tying all the model parameters together except $u_i$ and $u_f$.

If the angles of the $Q$ vector and the spin-axis $x'$ to the $x$-axis are $\phi$ and $\theta_{up}$, respectively, then, depending on the spin state of the neutrons, the scattering length densities, including the nuclear scattering length density ($\beta_N$) are

$$\beta_{\pm \pm} = \beta_N \mp D_M M_{\perp x'}$$ for non-spin-flip states

and

$$\beta_{\pm \mp} = -D_M (M_{\perp y'} \pm i M_{\perp z'})$$ for spin-flip states

where

$$M_{\perp x'} = M_{0x} \cos(\theta_{up}) + M_{0y} \sin(\theta_{up})$$
$$M_{\perp y'} = M_{0y} \cos(\theta_{up}) - M_{0x} \sin(\theta_{up})$$
$$M_{\perp z'} = M_{0z}$$
$$M_{0x} = (M_{0x} \cos \phi - M_{0y} \sin \phi) \cos \phi$$
$$M_{0y} = (M_{0y} \sin \phi - M_{0x} \cos \phi) \sin \phi$$
Here, \( M_{0x}, M_{0y}, M_{0z} \) are the x, y and z components of the magnetization vector given in the laboratory \( xyz \) frame given by

\[
\begin{align*}
M_{0x} &= M_0 \cos \theta_M \cos \phi_M \\
M_{0y} &= M_0 \sin \theta_M \\
M_{0z} &= -M_0 \cos \theta_M \sin \phi_M
\end{align*}
\]

and the magnetization angles \( \theta_M \) and \( \phi_M \) are defined in the figure above.

The user input parameters are:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>sld_M0</td>
<td>( D M_0 )</td>
</tr>
<tr>
<td>sld_mtheta</td>
<td>( \theta_M )</td>
</tr>
<tr>
<td>sld_mphi</td>
<td>( \phi_M )</td>
</tr>
<tr>
<td>up_frac_i</td>
<td>( u_i = (\text{spin up})/(\text{spin up} + \text{spin down}) ) before the sample</td>
</tr>
<tr>
<td>up_frac_f</td>
<td>( u_f = (\text{spin up})/(\text{spin up} + \text{spin down}) ) after the sample</td>
</tr>
<tr>
<td>up_angle</td>
<td>( \theta_{up} )</td>
</tr>
</tbody>
</table>

**Note:** The values of the ‘up_frac_i’ and ‘up_frac_f’ must be in the range 0 to 1.

**Document History**

2015-05-02 Steve King
2017-11-15 Paul Kienzle
2018-06-02 Adam Washington

**Oriented particles**

With two dimensional small angle diffraction data sasmodels will calculate scattering from oriented particles, applicable for example to shear flow or orientation in a magnetic field.

In general we first need to define the reference orientation of the particle’s \( a-b-c \) axes with respect to the incoming neutron or X-ray beam. This is done using three angles: \( \theta \) and \( \phi \) define the orientation of the \( c \)-axis of the particle, and angle \( \Psi \) is defined as the orientation of the major axis of the particle cross section with respect to its starting position along the beam direction (or equivalently, as rotation about the \( c \) axis). There is an unavoidable ambiguity when \( c \) is aligned with \( z \) in that \( \phi \) and \( \Psi \) both serve to rotate the particle about \( c \), but this symmetry is destroyed when \( \theta \) is not a multiple of 180.

The figures below are for an elliptical cross section cylinder, but may be applied analogously to other shapes of particle.

**Note:** It is very important to note that these angles, in particular \( \theta \) and \( \phi \), are NOT in general the same as the \( \theta \) and \( \phi \) appearing in equations for the scattering form factor which gives the scattered intensity or indeed in the equation for scattering vector \( Q \). The \( \theta \) rotation must be applied before the \( \phi \) rotation, else there is an ambiguity.

Having established the mean direction of the particle (the view) we can then apply angular orientation distributions (jitter). This is done by a numerical integration over a range of angles in a similar way to particle size dispersity. The orientation dispersity is defined with respect to the \( a-b-c \) axes of the particle, with roll angle \( \Psi \) about the \( c \)-axis, yaw angle \( \theta \) about the \( b \)-axis and pitch angle \( \phi \) about the \( a \)-axis.

You can explore the view and jitter angles interactively using `sasmodels.jitter.run()`. Enter the following into the python interpreter:

```python
from sasmodels import jitter
jitter.run()
```
Fig. 1.134: Definition of angles for oriented elliptical cylinder, where axis_ratio b/a is shown >1. Note that rotation θ, initially in the x-z plane, is carried out first, then rotation φ about the z-axis, finally rotation Ψ is around the axis of the cylinder. The neutron or X-ray beam is along the −z axis.
Fig. 1.135: Some examples of the orientation angles for an elliptical cylinder, with $\Psi = 0$. 

- $\theta = 90$, $\phi = 0$
- $\theta = 45$, $\phi = 90$
More formally, starting with axes $a$-$b$-$c$ of the particle aligned with axes $x$-$y$-$z$ of the laboratory frame, the orientation dispersity is applied first, using the Tait-Bryan $x$-$y$-$z''$ convention with angles $\Delta \phi$-$\Delta \theta$-$\Delta \Psi$. The reference orientation then follows, using the Euler angles $z$-$y'$-$z''$ with angles $\phi$-$\theta$-$\Psi$. This is implemented using rotation matrices as

$$R = R_z(\phi) R_y(\theta) R_z(\Psi) R_x(\Delta \phi) R_y(\Delta \theta) R_z(\Delta \Psi)$$

To transform detector $(q_x, q_y)$ values into $(q_a, q_b, q_c)$ for the shape in its canonical orientation, use

$$(q_a, q_b, q_c)^T = R^{-1} [q_x, q_y, 0]^T$$

The inverse rotation is easily calculated by rotating the opposite directions in the reverse order, so

$$R^{-1} = R_z(-\Delta \Psi) R_y(-\Delta \theta) R_x(-\Delta \phi) R_z(-\Psi) R_y(-\theta) R_z(-\phi)$$

The $\theta$ and $\phi$ orientation parameters for the cylinder only appear when fitting 2d data. On introducing “Orientational Distribution” in the angles, “distribution of theta” and “distribution of phi” parameters will appear. These are actually rotations about the axes $\delta_1$ and $\delta_2$ of the cylinder, which correspond to the $b$ and $a$ axes of the cylinder cross section. (When $\theta = \phi = 0$ these are parallel to the $Y$ and $X$ axes of the instrument.) The third orientation distribution, in $\Psi$, is about the $c$ axis of the particle. Some experimentation may be required to understand the 2d patterns fully. A number of different shapes of distribution are available, as described for size dispersity, see Polydispersity & Orientational Distributions.

Given that the angular dispersion distribution is defined in cartesian space, over a cube defined by

$$[-\Delta \theta, \Delta \theta] \times [-\Delta \phi, \Delta \phi] \times [-\Delta \Psi, \Delta \Psi]$$

but the orientation is defined over a sphere, we are left with a map projection problem, with different tradeoffs depending on how values in $\Delta \theta$ and $\Delta \phi$ are translated into latitude/longitude on the sphere.

Sasmodels is using the equirectangular projection. In this projection, square patches in angular dispersity become wedge-shaped patches on the sphere. To correct for the changing point density, there is a scale factor of $\sin(\Delta \theta)$ that applies to each point in the integral. This is not enough, though. Consider a shape which is tumbling freely around the $b$ axis, with $\Delta \theta$ uniform in $[-180, 180]$. At $\pm 90$, all points in $\Delta \phi$ map to the pole, so the jitter will have a distinct angular preference. If the spin axis is along the beam (which will be the case for $\theta = 90$ and $\Psi = 90$) the scattering pattern should be circularly symmetric, but it will go to zero at $q_x = 0$ due to the $\sin(\Delta \theta)$ correction. This problem does not appear for a shape that is tumbling freely around the $a$ axis, with $\Delta \phi$ uniform in $[-180, 180]$, so swap the $a$ and $b$ axes so $\Delta \theta < \Delta \phi$ and adjust $\Psi$ by 90. This works with the current sasmodels shapes due to symmetry.

Alternative projections were considered. The sinusoidal projection works by scaling $\Delta \phi$ as $\Delta \theta$ increases, and dropping those points outside $[-180, 180]$. The distortions are a little less for middle ranges of $\Delta \theta$, but they are still severe for large $\Delta \theta$ and the model is much harder to explain. The azimuthal equidistance projection also improves on the equirectangular projection by extending the range of reasonable values for the $\Delta \theta$ range, with $\Delta \phi$ forming a wedge that cuts to the opposite side of the sphere rather than cutting to the pole. This projection has the nice property that distance from the center are preserved, and that $\Delta \theta$ and $\Delta \phi$ act the same. The azimuthal equal area projection is like the azimuthal equidistance projection, but it preserves area instead of distance. It also has the same behaviour for $\Delta \theta$ and $\Delta \phi$. The Guyou projection has an excellent balance with reasonable distortion in both $\Delta \theta$ and $\Delta \phi$, as well as preserving small patches. However, it requires considerably more computational overhead, and we have not yet derived the formula for the distortion correction, measuring the degree of stretch at the point $(\Delta \theta, \Delta \phi)$ on the map.

**Note:** Note that the form factors for oriented particles are performing numerical integrations over one or more variables, so care should be taken, especially with very large particles or more extreme aspect ratios. In such cases results may not be accurate, particularly at very high $Q$, unless the model has been specifically coded to use limiting forms of the scattering equations.

For best numerical results keep the $\theta$ distribution narrower than the $\phi$ distribution. Thus for asymmetric particles, such as elliptical cylinder, you may need to reorder the sizes of the three axes to achieve the desired result. This is due to the issues of mapping a rectangular distribution onto the surface of a sphere.
Users can experiment with the values of Npts and Nsigs, the number of steps used in the integration and the range spanned in number of standard deviations. The standard deviation is entered in units of degrees. For a “rectangular” distribution the full width should be \( \pm \sqrt{3} \sim 1.73 \) standard deviations. The new “uniform” distribution avoids this by letting you directly specify the half width.

The angular distributions may be truncated outside of the range -180 to +180 degrees, so beware of using a broad Gaussian distribution with large value of Nsigs, as the array of Npts may be truncated to many fewer points than would give a good integration, as well as becoming rather meaningless. (At some point in the future the actual dispersion arrays may be made available to the user for inspection.)

Some more detailed technical notes are provided in the developer section of this manual Orientation and Numerical Integration.

This definition of orientation is new to SasView 4.2. In earlier versions, the orientation distribution appeared as a distribution of view angles. This led to strange effects when \( c \) was aligned with \( z \), where changes to the \( \phi \) angle served only to rotate the shape about \( c \), rather than having a consistent interpretation as the pitch of the shape relative to the flow field defining the reference orientation. Prior to SasView 4.1, the reference orientation was defined using a Tait-Bryan convention, making it difficult to control. Now, rotation in \( \theta \) modifies the spacings in the refraction pattern, and rotation in \( \phi \) rotates it in the detector plane.

Document History

2017-11-06 Richard Heenan
2017-12-20 Paul Kienzle

Optimizer Selection

Bumps has a number of different optimizers available, each with its own control parameters:

- Levenberg-Marquardt
- Nelder-Mead Simplex
- DREAM
- Differential Evolution
- Quasi-Newton BFGS
- Random Lines [experimental]
- Particle Swarm [experimental]
- Parallel Tempering [experimental]

In general there is a trade-off between convergence rate and robustness, with the fastest algorithms most likely to find a local minimum rather than a global minimum. The gradient descent algorithms (Levenberg-Marquardt, Quasi-Newton BFGS) tend to be fast but they will find local minima only, while the population algorithms (DREAM, Differential Evolution) are more robust and likely slower. Nelder-Mead Simplex is somewhere between, with a small population keeping the search local but more robust than the gradient descent algorithms.

Each algorithm has its own set of control parameters for adjusting the search process and the stopping conditions. The same option may mean slightly different things to different optimizers. The bumps package provides a dialog box for selecting the optimizer and its options when running the fit wx application. This only includes the common options for the most useful optimizers. For full control, the fit will need to be run from the command line interface or through a python script.

For parameter uncertainty, most algorithms use the covariance matrix at the optimum to estimate an uncertainty ellipse. This is okay for a preliminary analysis, but only works reliably for weakly correlated parameters. For full uncertainty analysis, DREAM uses a random walk to explore the parameter space near the minimum, showing pairwise correlations amongst the parameter values. In order for DREAM to return the correct uncertainty, the function to be optimized should be a conditional probability density, with nllf as the negative log likelihood function of seeing point \( x \) in the parameter space. Other functions can be fitted, but uncertainty estimates will be meaningless.
Most algorithms have been adapted to run in parallel at least to some degree. The implementation is not heavily tuned, either in terms of minimizing the overhead per function evaluation or for distributing the problem across multiple processors. If the theory function is implemented in parallel, then the optimizer should be run in serial. Mixed mode is also possible when running on a cluster with a multi-threaded theory function. In this case, only one theory function will be evaluated on each cluster node, but the optimizer will distribute the parameters values to the cluster nodes in parallel. Do not run serial algorithms (Levenberg-Marquardt, Quasi-Newton BFGS) on a cluster.

We have included a number of optimizers in Bumps that did not perform particularly well on our problem sets. However, they may be perfect for your problem, so we have left them in the package for you to explore. They are not available in the GUI selection.

**Levenberg-Marquardt**

![Levenberg-Marquardt](image)

The Levenberg-Marquardt algorithm has been the standard method for non-linear data fitting. As a gradient descent trust region method, it starts at the initial value of the function and steps in the direction of the derivative until it reaches the minimum. Set up as an explicit minimization of the sum of square differences between theory
and model, it uses a numerical approximation of the Jacobian matrix to set the step direction and an adaptive algorithm to set the size of the trust region.

**When to use**

Use this method when you have a reasonable fit near the minimum, and you want to get the best possible value. This can then be used as the starting point for uncertainty analysis using DREAM. This method requires that the problem definition includes a residuals method, but this should always be true when fitting data.

When modeling the results of an experiment, the best fit value is an accident of the measurement. Redo the same measurement, and the slightly different values you measure will lead to a different best fit. The important quantity to report is the credible interval covering 68% (1-\(\sigma\)) or 95% (2-\(\sigma\)) of the range of parameter values that are somewhat consistent with the data.

This method uses lmfit from scipy, and does not run in parallel.

**Options**

*Steps* is the number of gradient steps to take. Each step requires a calculation of the Jacobian matrix to determine the direction. This needs \(2mn\) function evaluations, where \(n\) is the number of parameters and each function is evaluated and \(m\) data points (assuming center point formula for finite difference estimate of the derivative). The resulting linear equation is then solved, but for small \(n\) and expensive function evaluation this overhead can be ignored. Use `--steps=n` from the command line.

\(f(x)\) tolerance and \(x\) tolerance are used to determine when the fit has reached the point where no significant improvement is expected. If the function value does not improve significantly within the step, or the step is too short, then the fit will terminate. Use `--ftol=v` and `--xtol=v` from the command line.

From the command line, `--starts=n` will automatically restart the algorithm after it has converged so that a slightly better value can be found. If `--keep_best` is included then restart will use a value near the minimum, otherwise it will restart the fit from a random point in the parameter space.

Use `--fit=lm` to select the Levenberg-Marquardt fitter from the command line.
The Nelder-Mead downhill simplex algorithm is a robust optimizer which does not require the function to be continuous or differentiable. It uses the relative values of the function at the corners of a simplex (an n-dimensional triangle) to decide which points of the simplex to update. It will take the worst value and try moving it inward or outward, or reflect it through the centroid of the remaining values stopping if it finds a better value. If none of these values are better, then it will shrink the simplex and start again. The name amoeba comes from the book *Numerical Recipes* [Press1992] wherein they describe the search as acting like an amoeba, squeezing through narrow valleys as it makes its way down to the minimum.

**When to use**

Use this method as a first fit to your model. If your fitting function is well behaved with few local minima this will give a quick estimate of the model, and help you decide if the model needs to be refined. If your function is
poorly behaved, you will need to select a good initial value before fitting, or use a more robust method such as \textit{Differential Evolution} or \textit{DREAM}.

The uncertainty reported comes from a numerical derivative estimate at the minimum.

This method requires a series of function updates, and does not benefit much from running in parallel.

\textbf{Options}

\textit{Steps} is the simplex update iterations to perform. Most updates require one or two function evaluations, but shrinking the simplex evaluates every value in the simplex. Use \texttt{--steps=n} from the command line.

\textit{Starts} tells the optimizer to restart a given number of times. Each time it restarts it uses a random starting point. Use \texttt{--starts=n} from the command line.

\textit{Simplex radius} is the initial size of the simplex, as a portion of the bounds defining the parameter space. If a parameter is unbounded, then the radius will be treated as a portion of the parameter value. Use \texttt{--radius=n} from the command line.

\textit{x tolerance} and \textit{f(x) tolerance} are used to determine when the fit has reached the point where no significant improvement is expected. If the simplex is tiny (that is, the corners are close to each other) and flat (that is, the values at the corners are close to each other), then the fit will terminate. Use \texttt{--xtol=v} and \texttt{--ftol=v} from the command line.

From the command line, use \texttt{--keep_best} so that restarts are centered on a value near the minimum rather than restarting from a random point within the parameter bounds.

Use \texttt{--fit=amoeba} to select the Nelder-Mead simplex fitter from the command line.
Quasi-Newton BFGS

Broyden-Fletcher-Goldfarb-Shanno is a gradient descent method which uses the gradient to determine the step direction and an approximation of the Hessian matrix to estimate the curvature and guess a step size. The step is further refined with a one-dimensional search in the direction of the gradient.

**When to use**

Like Levenberg-Marquardt, this method converges quickly to the minimum. It does not assume that the problem is in the form of a sum of squares and does not require a residuals method.

The $n$ partial derivatives are computed in parallel.
Options

*Steps* is the number of gradient steps to take. Each step requires a calculation of the Jacobian matrix to determine the direction. This needs \(2mn\) function evaluations, where \(n\) is the number of parameters and each function is evaluated and \(m\) data points (assuming center point formula for finite difference estimate of the derivative). The resulting linear equation is then solved, but for small \(n\) and expensive function evaluation this overhead can be ignored. Use \(--\text{steps}=n\) from the command line.

*Starts* tells the optimizer to restart a given number of times. Each time it restarts it uses a random starting point. Use \(--\text{starts}=n\) from the command line.

*f(x) tolerance* and *x tolerance* are used to determine when the fit has reached the point where no significant improvement is expected. If the function is small or the step is too short then the fit will terminate. Use \(--\text{ftol}=v\) and \(--\text{xtol}=v\) from the command line.

From the command line, \(--\text{keep_best}\) uses a value near the previous minimum when restarting instead of using a random value within the parameter bounds.

Use \(--\text{fit= newton}\) to select BFGS from the command line.
Differential evolution is a population based algorithm which uses differences between points as a guide to selecting new points. For each member of the population a pair of points is chosen at random, and a difference vector is computed. This vector is scaled, and a random subset of its components are added to the current point based on crossover ratio. This new point is evaluated, and if its value is lower than the current point, it replaces it in the population. There are many variations available within DE that have not been exposed in Bumps. Interested users can modify `bumps.fitters.DEFit` and experiment with different crossover and mutation algorithms, and perhaps add them as command line options.

Differential evolution is a robust directed search strategy. Early in the search, when the population is disperse, the difference vectors are large and the search remains broad. As the search progresses, more of the population goes into the valleys and eventually all the points end up in local minima. Now the differences between random pairs will often be small and the search will become more localized.

The population is initialized according to the prior probability distribution for each each parameter. That is, if the
parameter is bounded, it will use a uniform random number generate within the bounds. If it is unbounded, it will use a uniform value in $[0,1]$. If the parameter corresponds to the result of a previous measurement with mean $\mu$ and standard deviation $\sigma$, then the initial values will be pulled from a gaussian random number generator.

**When to use**

Convergence with differential evolution will be slower, but more robust.

Each update will evaluate $k$ points in parallel, where $k$ is the size of the population.

**Options**

*Steps* is the number of iterations. Each step updates each member of the population. The population size scales with the number of fitted parameters. Use `--steps=n` from the command line.

*Population* determines the size of the population. The number of individuals, $k$, is equal to the number of fitted parameters times the population scale factor. Use `--pop=k` from the command line.

*Crossover ratio* determines what proportion of the dimensions to update at each step. Smaller values will likely lead to slower convergence, but more robust results. Values must be between 0 and 1. Use `--CR=v` from the command line.

*Scale* determines how much to scale each difference vector before adding it to the candidate point. The selected mutation algorithm chooses a scale factor uniformly in $[0, F]$. Use `--F=v` from the command line.

*f(x) tolerance* and *x tolerance* are used to determine when the fit has reached the point where no significant improvement is expected. If the population is flat (that is, the minimum and maximum values are within tolerance) and tiny (that is, all the points are close to each other) then the fit will terminate. Use `ftol=v` and `xtol=v` from the command line.

Use `--fit=de` to select differential evolution from the commandline.
DREAM is a population based algorithm like differential evolution, but instead of only keeping individuals which improve each generation, it will sometimes keep individuals which get worse. Although it is not fast and does not give the very best value for the function, we have found it to be a robust fitting engine which will give a good value given enough time.

The progress of each individual in the population from generation to generation can considered a Markov chain, whose transition probability is equal to the probability of taking the step times the probability that it keeps the step based on the difference in value between the points. By including a purely random stepper with some probability, the detailed balance condition is preserved, and the Markov chain converges onto the underlying equilibrium distribution. If the theory function represents the conditional probability of selecting each point in the parameter space, then the resulting chain is a random draw from the posterior distribution.

This means that the DREAM algorithm can be used to determine the parameter uncertainties. Unlike the hessian estimate at the minimum that is used to report uncertainties from the other fitters, the resulting uncertainty need not
gaussian. Indeed, the resulting distribution can even be multi-modal. Fits to measured data using theory functions that have symmetric solutions have shown all equivalent solutions with approximately equal probability.

When to use

Use DREAM when you need a robust fitting algorithm. It takes longer but it does an excellent job of exploring different minima and getting close to the global optimum.

Use DREAM when you want a detailed analysis of the parameter uncertainty.

Like differential evolution, DREAM will evaluate \( k \) points in parallel, where \( k \) is the size of the population.

Options

*Samples* is the number of points to be drawn from the Markov chain. To estimate the 68% interval to two digits of precision, at least 1e5 (or 100,000) samples are needed. For the 95% interval, 1e6 (or 1,000,000) samples are needed. The default 1e4 samples gives a rough approximation of the uncertainty relatively quickly. Use `--samples=n` from the command line.

*Burn-in Steps* is the number of iterations to required for the Markov chain to converge to the equilibrium distribution. If the fit ends early, the tail of the burn will be saved to the start of the steps. Use `--burn=n` from the command line.

*Population* determines the size of the population. The number of individuals, \( k \), is equal to the number of fitted parameters times the population scale factor. Use `--pop=k` from the command line.

*Initializer* determines how the population will be initialized. The options are as follows:

- *eps* (epsilon ball), in which the entire initial population is chosen at random from within a tiny hypersphere centered about the initial point
- *lhs* (latin hypersquare), which chops the bounds within each dimension in \( k \) equal sized chunks where \( k \) is the size of the population and makes sure that each parameter has at least one value within each chunk across the population.
- *cov* (covariance matrix), in which the uncertainty is estimated using the covariance matrix at the initial point, and points are selected at random from the corresponding gaussian ellipsoid
- *random* (uniform random), in which the points are selected at random within the bounds of the parameters

Use `--init=type` from the command line.

*Thinning* is the amount of thinning to use when collecting the population. If the fit is somewhat stuck, with most steps not improving the fit, then you will need to thin the population to get proper statistics. Use `--thin=k` from the command line.

*Calculate entropy*, if true, computes the entropy for the fit. This is an estimate of the amount of information in the data. Use `--entropy` from the command line.

*Steps*, if not zero, determines the number of iterations to use for drawing samples after burn in. Each iteration updates the full population, which is \( (\text{population} \times \text{number of fitted parameters}) \) points. This option is available for compatibility; it is more useful to set the number of samples directly. Use `--steps=n` from the command line.

Use `--fit=dream` to select DREAM from the commandline.

Output

DREAM produces a number of different outputs, and there are a number of things to check before using its reported uncertainty values. The main goal of selecting `--burn=n` is to wait long enough to reach the equilibrium distribution.
Fig. 1.136: This DREAM fit is incomplete, as can be seen on all four plots. The Convergence plot is still decreasing, Parameter Trace plot does not show random mixing of Markov chain values, the Correlations plots are fuzzy and mostly empty, the Uncertainty plot shows black histograms (indicating that there are a few stray values far away from the best) and green maximum likelihood spikes not matching the histogram (indicating that the region around the best value has not been adequately explored).
Fig. 1.137: This DREAM fit completed successfully. The Convergence plot is flat, the Parameter Trace plot is flat and messy, the Correlations plots show nice blobs (and a bit of correlation between the $M1.radius$ parameter and the $M1.radius.width$ parameter), and the uncertainty plots show a narrow range of $-\log(P)$ values in the mostly brown histograms and a good match to the green constrained maximum likelihood line.
For each parameter in the fit, DREAM finds the mean, median and best value, as well as the 68% and 95% credible intervals. The mean value is defined as \( \int x P(x)dx \), which is just the expected value of the probability distribution for the parameter. The median value is the 50% point in the probability distribution, and the best value is the maximum likelihood value seen in the random walk. The credible intervals are the central intervals which capture 68% and 95% of the parameter values respectively. You need approximately 100,000 samples to get two digits of precision on the 68% interval, and 1,000,000 samples for the 95% interval.

Table 1.1: Example fit output

<table>
<thead>
<tr>
<th>#</th>
<th>Parameter</th>
<th>mean</th>
<th>median</th>
<th>best</th>
<th>[ 68% interval]</th>
<th>[ 95% interval]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>M1.background</td>
<td>0.059925(41)</td>
<td>0.059924</td>
<td>0.059922</td>
<td>[0.05988 0.05997]</td>
<td>[0.05985 0.06000]</td>
</tr>
<tr>
<td>2</td>
<td>M1.radius</td>
<td>2345.3(15)</td>
<td>2345.234</td>
<td>2345.174</td>
<td>[2343.83 2346.74]</td>
<td>[2342.36 2348.29]</td>
</tr>
<tr>
<td>3</td>
<td>M1.radius.width</td>
<td>0.00775(41)</td>
<td>0.00774</td>
<td>0.00777</td>
<td>[0.0074 0.0081]</td>
<td>[0.0070 0.0086]</td>
</tr>
<tr>
<td>4</td>
<td>M1.scale</td>
<td>0.21722(20)</td>
<td>0.217218</td>
<td>0.217244</td>
<td>[0.21702 0.21743]</td>
<td>[0.21681 0.21761]</td>
</tr>
</tbody>
</table>

The Convergence plot shows the range of \( \chi^2 \) values in the population for each iteration. The band shows the 68% of values around the median, and the solid line shows the minimum value. If the distribution has reached equilibrium, then convergence graph should be roughly flat, with little change in the minimum value throughout the graph. If there is no convergence, then the remaining plots don’t mean much.

The Correlations plot shows cross correlation between each pair of parameters. If the parameters are completely uncorrelated then the boxes should contain circles. Diagonals indicate strong correlation. Square blocks indicate that the fit is not sensitive to one of the parameters. The range plotted on the correlation plot is determined by the 95% interval of the data. The individual correlation plots are too small to show the range of values for the parameters. These can instead be read from the Uncertainty plot for each parameter, which covers the same range of values and indicates 68% and 95% intervals. If there are some chains that are wandering around away from the minimum, then the plot will look fuzzy, and not have a nice blob in the center. If a correlation plot has multiple blobs, then there are multiple minima in your problem space, usually because there are symmetries in the problem definition. For example, a model fitting \( x + a^2 \) will have identical solutions for \( \pm a \).

The Uncertainty plot shows histograms for each fitted parameter generated from the values for that parameter across all chains. Within each histogram bar the values are sorted and displayed as a gradient from black to copper, with black values having the lowest \( \chi^2 \) and copper values having the highest. The resulting histogram should be dark brown, with a black hump in the center and light brown tips. If there are large lumps of light brown, or excessive black then its likely that the optimizer did not converge. The green line over the histogram shows the best value seen within each histogram bin (the maximum likelihood given \( p_k = x \)). With enough samples and proper convergence, it should roughly follow the outline of the histogram. The yellow band in the center of the plot represents the 68% interval for the data. The histogram cuts off at 95%. These values along with the median are shown as labels along the x axis. The green asterisk represents the best value, the green \( \mu \) the mean value and the vertical green line the median value. If the fit is not sensitive to a parameter, or if two parameters are strongly correlated, the parameter histogram will show a box rather than a hump. Spiky shapes (either in the histogram or the maximum likelihood line) indicate lack of convergence or maybe not enough steps. A chopped histograms indicates that the range for that parameter is too small.

The Parameter Trace plot is diagnostic for models which have poor mixing. In this cases no matter how the parameter values are changing, they are landing on much worse values for the \( \chi^2 \). This can happen if the problem is highly constrained with many tight and twisty values.

The Data and Theory plot should show theory and data lining up pretty well, with the theory overlaying about 2/3 of the error bars on the data (1-\( \sigma = 68\% \)). The Residuals plot shows the difference between theory and data divided by uncertainty. The residuals should be 2/3 within [-1, 1]. They should not show any structure, such as humps where the theory misses the data for long stretches. This indicates some feature missing from the model, or a lack of convergence to the best model.

If entropy is requested, then bumps will show the total number of bits of information in the fit. This derives from the entropy term:

Using entropy and simulation we hope to be able to make experiment planning decisions in a way that maximizes information, by estimating whether it is better to measure more precisely or to measure different but related values and fit them with shared parameters.
Particle Swarm

Inspired by bird flocking behaviour, the particle swarm algorithm is a population-based method which updates an individual according to its momentum and a force toward the current best fit parameter values. We did not explore variations of this algorithm in any detail.

When to use

Particle swarm performed well enough in our low dimensional test problems, but made little progress when more fit parameters were added.

The population updates can run in parallel, but the tiny population size limits the amount of parallelism.

Options

--steps=n is the number of iterations. Each step updates each member of the population. The population size scales with the number of fitted parameters.

--pop=k determines the size of the population. The number of individuals, $k$, is equal to the number of fitted parameters times the population scale factor. The default scale factor is 1.

Use --fit=ps to select particle swarm from the commandline.

Add a few more lines

Random Lines

Most of the population based algorithms ignore the value of the function when choosing the points in the next iteration. Random lines is a new style of algorithm which fits a quadratic model to a selection from the population, and uses that model to propose a new point in the next generation of the population. The hope is that the method will inherit the robustness of the population based algorithms as well as the rapid convergence of the newton descent algorithms.

When to use

Random lines works very well for some of our test problems, showing rapid convergence to the optimum, but on other problems it makes very little progress.

The population updates can run in parallel.

Options

--steps=n is the number of iterations. Each step updates each member of the population. The population size scales with the number of fitted parameters.

--pop=k determines the size of the population. The number of individuals, $k$, is equal to the number of fitted parameters times the population scale factor. The default scale factor is 0.5.

--CR=v is the crossover ratio, determining what proportion of the dimensions to update at each step. Values must be between 0 and 1.
--starts=n tells the optimizer to restart a given number of times. Each time it restarts it uses a random starting point.

--keep_best uses a value near the previous minimum when restarting instead of using a random value within the parameter bounds. This option is not available in the options dialog.

Use --fit=rl to select random lines from the commandline.

References

Parallel Tempering

Parallel tempering is an MCMC algorithm for uncertainty analysis. This version runs at multiple temperatures simultaneously, with chains at high temperature able to more easily jump between minima and chains at low temperature to fully explore the minima. Like DREAM it has a differential evolution stepper, but this version uses the chain history as the population rather than maintaining a population at each temperature.

This is an experimental algorithm which does not yet perform well.

When to use

When complete, parallel tempering should be used for problems with widely spaced local minima which dream cannot fit.

Options

--steps=n is the number of iterations to include in the Markov chain. Each iteration updates the full population. The population size scales with the number of fitted parameters.

--burn=n is the number of iterations to required for the Markov chain to converge to the equilibrium distribution. If the fit ends early, the tail of the burn will be saved to the start of the steps.

--CR=v is the differential evolution crossover ratio to use when computing step size and direction. Use a small value to step through the dimensions one at a time, or a large value to step through all at once.

--nT=k, --Tmin=v and --Tmax=v specify a log-spaced initial distribution of temperatures. The default is 25 points between 0.1 and 10. DREAM runs at a fixed temperature of 1.0.

Use --fit=pt to select parallel tempering from the commandline.

References

SANS to SESANS conversion

The conversion from SANS into SESANS in absolute units is a simple Hankel transformation when all the small-angle scattered neutrons are detected. First we calculate the Hankel transform including the absolute intensities by

\[ G(\delta) = 2\pi \int_0^{\infty} J_0(Q\delta) \frac{d\Sigma}{d\Omega}(Q) Q dQ, \]

in which \( J_0 \) is the zeroth order Bessel function, \( \delta \) the spin-echo length, \( Q \) the wave vector transfer and \( \frac{d\Sigma}{d\Omega}(Q) \) the scattering cross section in absolute units.

Out of necessity, a 1-dimensional numerical integral approximates the exact Hankel transform. The upper bound of the numerical integral is \( Q_{\text{max}} \), which is calculated from the wavelength and the instrument’s maximum acceptance angle, both of which are included in the file. While the true Hankel transform has a lower bound of zero, most scattering models are undefined at \( Q=0 \), so the integral requires an effective lower bound. The
lower bound of the integral is \( Q_{\text{min}} = 0.1 \times 2\pi / R_{\text{max}} \), in which \( R_{\text{max}} \) is the maximum length scale probed by the instrument multiplied by the number of data points. This lower bound is the minimum expected \( Q \) value for the given length scale multiplied by a constant. The constant, 0.1, was chosen empirically by integrating multiple curves and finding where the value at which the integral was stable. A constant value of 0.3 gave numerical stability to the integral, so a factor of three safety margin was included to give the final value of 0.1.

From the equation above we can calculate the polarisation that we measure in a SESANS experiment:

\[
P(\delta) = e^{t(\frac{2\pi}{\lambda})^2 (G(\delta) - G(0))}
\]

in which \( t \) is the thickness of the sample and \( \lambda \) is the wavelength of the neutrons.

**Fitting SESANS Data**

*Note: A proper installation of the developers setup of SasView (http://trac.sasview.org/wiki/AnacondaSetup) is a prerequisite for using these instructions.*

It is possible to fit SESANS measurements from the command line in Python.

**Simple Fits**

In the folder sasmodels/example the file sesans_sphere_2micron.py gives an example of how to fit a shape to a measurement.

The command:

```
>python fit_sesans.py sesans_sphere_2micron.py
```

then results in a GUI from which you can control the fit.
All the parameters and names in sesans_sphere_2micron.py (shown below) can be adjusted to fit your own problem:

```python
# This is a data file used to load in sesans data and fit it using the bumps engine
#
# from bumps.names import *
# import sesansfit
#
# Enter the model name to use
model_name = "sphere"
#
# DO NOT MODIFY THIS LINE
model = sesansfit.get_bumps_model(model_name)
#
# Enter any custom parameters
# name = Parameter(initial_value, name='name')
phi = Parameter(0.0855, name='phi')
#
# Add the parameters to this list that should be displayed in the fitting window
custom_params = {"phi" : phi}
#
# SESANS data file name
sesans_file = "spheres2micron.ses"
#
# Initial parameter values (if other than defaults)
```

(continues on next page)
Incorporating a Structure Factor

An example of how to also include a structure factor can be seen in the following example taken from Washington et al., *Soft Matter*, (2014), 10, 3016 (dx.doi.org/10.1039/C3SM53027B). These are time-of-flight measurements, which is the reason that not the polarisation is plotted, but the $\log_\lambda \left( \frac{P}{P_0} \right)$. The sample is a dispersion of core-shell colloids at a high volume fraction with hard sphere interactions.

The fit can be started by:

```bash
>python fit_sesans.py sesans_parameters_css-hs.py
```

This yields after the fitting:
The code `sesans_parameters_css-hs.py` can then be used as a template for a fitting problem with a structure factor:

```python
###
This is a data file used to load in sesans data and fit it using the bumps engine
###
from bumps.names import *

import sesansfit

# Enter the model name to use
model_name = "core_shell_sphere+hardsphere"

# DO NOT MODIFY THIS LINE
model = sesansfit.get_bumps_model(model_name)

# Enter any custom parameters
phi = Parameter(0.45, name='phi')
pen = Parameter(0.95, name='solvent penetration')
custom_params = {"phi" : phi, "pen" : pen}

# SESANS data file
sesans_file = "core_shell.ses"

# Initial parameter values (if other than defaults)
initial_vals = {
    "sld_core" : 1.05,
    "sld_shell" : 2.88*pen-0.05*(1-pen),
    "sld_solvent" : 2.88,
    "radius" : 730,
    "thickness" : 20,
    "volfraction" : phi,
}
```

(continues on next page)
"scale" : (1-\phi)
}

# Ranges for parameters if other than default
param_range = {
    "phi" : [0.2, 0.5],
    "pen" : [0,1],
    "radius" : [500, 3000],
    "thickness" : [0,200]
}

# Constraints
# model.param_name = f(other params)
# EXAMPLE: model.scale = model.radius*model.radius*(1 - phi) - where radius
# and scale are model functions and phi is a custom parameter
model.scale = phi*(1-phi)
model.volfraction = phi
model.shell_sld = pen*2.88

# Send to the fitting engine
problem = sesansfit.sesans_fit(sesans_file, model_name, initial_vals, custom_params, param_range)

Writing a Plugin Model

Overview

In addition to the models provided with the sasmodels package, you are free to create your own models.

Models can be of three types:

- A pure python model: Example - broadpeak.py
- A python model with embedded C: Example - sphere.py
- A python wrapper with separate C code: Example - cylinder.py, cylinder.c

When using SasView, plugin models should be saved to the SasView plugin_models folder C:\Users\{username}.sasview\plugin_models (on Windows) or /Users/{username}/.sasview/plugin_models (on Mac). The next time SasView is started it will compile the plugin and add it to the list of Plugin Models in a FitPage. Scripts can load the models from anywhere.

The built-in modules are available in the models subdirectory of the sasmodels package. For SasView on Windows, these will be found in C:\Program Files (x86)\SasView\sasmodels-data\models. On Mac OSX, these will be within the application bundle as /Applications/SasView 4.0.app/Contents/Resources/sasmodels-data/models.

Other models are available for download from the Model Marketplace. You can contribute your own models to the Marketplace as well.

Create New Model Files

Copy the appropriate files to your plugin models directory (we recommend using the examples above as templates) as mymodel.py (and mymodel.c, etc) as required, where “mymodel” is the name for the model you are creating.

Please follow these naming rules:

- No capitalization and thus no CamelCase
- If necessary use underscore to separate words (i.e. barbell not BarBell or broad_peak not BroadPeak)
- Do not include “model” in the name (i.e. barbell not BarBellModel)
Edit New Model Files

Model Contents

The model interface definition is in the .py file. This file contains:

• a model name:
  – this is the name string in the .py file
  – titles should be:
    – all in lower case
    – without spaces (use underscores to separate words instead)
    – without any capitalization or CamelCase
    – without incorporating the word “model”
    – examples: barbell not BarBell; broad_peak not BroadPeak; barbell not BarBellModel

• a model title:
  – this is the title string in the .py file
  – this is a one or two line description of the model, which will appear at the start of the model documentation and as a tooltip in the SasView GUI

• a short description:
  – this is the description string in the .py file
  – this is a medium length description which appears when you click Description on the model FitPage

• a parameter table:
  – this will be auto-generated from the parameters in the .py file

• a long description:
  – this is ReStructuredText enclosed between the r”””” and “””” delimiters at the top of the .py file
  – what you write here is abstracted into the SasView help documentation
  – this is what other users will refer to when they want to know what your model does; so please be helpful!

• a definition of the model:
  – as part of the long description

• a formula defining the function the model calculates:
  – as part of the long description

• an explanation of the parameters:
  – as part of the long description
  – explaining how the symbols in the formula map to the model parameters

• a plot of the function, with a figure caption:
  – this is automatically generated from your default parameters

• at least one reference:
  – as part of the long description
  – specifying where the reader can obtain more information about the model

• the name of the author
as part of the **long description**

- the *.py* file should also contain a comment identifying who converted/created the model file

Models that do not conform to these requirements will **never** be incorporated into the built-in library.

---

**Model Documentation**

The *.py* file starts with an `r` (for raw) and three sets of quotes to start the doc string and ends with a second set of three quotes. For example:

```python
r""
Definition
-------------
The 1D scattering intensity of the sphere is calculated in the following way (Guinier, 1955)
.. math::
   \[ I(q) = \frac{\text{scale}}{V} \cdot \left[ 3V(\Delta\rho) \cdot \frac{\sin(qr) - qr\cos(qr))}{(qr)^3} \right]^2 + \text{background} \]
where \texttt{scale} is a volume fraction, \texttt{V} is the volume of the scatterer, \texttt{r} is the radius of the sphere and \texttt{background} is the background level. \texttt{sld} and \texttt{sld_solvent} are the scattering length densities (SLDs) of the scatterer and the solvent respectively, whose difference is \texttt{\Delta\rho}.

You can included figures in your documentation, as in the following figure for the cylinder model.
.. figure:: img/cylinder_angle_definition.jpg
   Definition of the angles for oriented cylinders.

References
---------
""
```

This is where the FULL documentation for the model goes (to be picked up by the automatic documentation system). Although it feels odd, you should start the documentation immediately with the **definition**—the model name, a brief description and the parameter table are automatically inserted above the definition, and the a plot of the model is automatically inserted before the **reference**.

Figures can be included using the `figure` command, with the name of the *.png* file containing the figure and a caption to appear below the figure. Figure numbers will be added automatically.

See this *Sphinx cheat sheet* for a quick guide to the documentation layout commands, or the *Sphinx Documentation* for complete details.

The model should include a **formula** written using LaTeX markup. The example above uses the `math` command to make a displayed equation. You can also use `$formula$` for an inline formula. This is handy for defining the relationship between the model parameters and formula variables, such as the phrase “\texttt{r} is the radius” used above. The live demo MathJax page [http://www.mathjax.org/](http://www.mathjax.org/) is handy for checking that the equations will look like you intend.

Math layout uses the `amsmath` package for aligning equations (see amsldoc.pdf on that page for complete documentation). You will automatically be in an aligned environment, with blank lines separating the lines of the equation. Place an ampersand before the operator on which to align. For example:
.. math::

\begin{align*}
  x + y &= 1 \\
  y &= x - 1
\end{align*}

produces

\begin{align*}
  x + y &= 1 \\
  y &= x - 1
\end{align*}

If you need more control, use:

.. math::

    :nowrap:

Model Definition

Following the documentation string, there are a series of definitions:

```py
name = "sphere"  # optional: defaults to the filename without .py

# Model

title = "Spheres with uniform scattering length density"

description = ""

\[
    P(q) = (scale/V) \times \left[ 3V(sld-sld\_solvent) \times (\sin(qr)-qr \cos(qr)) \right] \\
        / (qr)^3 \right]^2 + background
\]

- **r**: radius of sphere
- **V**: The volume of the scatter
- **sld**: the SLD of the sphere
- **sld\_solvent**: the SLD of the solvent

```""

category = "shape:sphere"

# optional: defaults to True

single = True

# optional: defaults to True

opencl = False

# optional: defaults to False

structure_factor = False

```

name = “mymodel” defines the name of the model that is shown to the user. If it is not provided it will use the name of the model file. The name must be a valid variable name, starting with a letter and contains only letters, numbers or underscore. Spaces, dashes, and other symbols are not permitted.

title = “short description” is short description of the model which is included after the model name in the automatically generated documentation. The title can also be used for a tooltip.

description = “doc string” is a longer description of the model. It shows up when you press the “Description” button of the SasView FitPage. It should give a brief description of the equation and the parameters without the need to read the entire model documentation. The triple quotes allow you to write the description over multiple lines. Keep the lines short since the GUI will wrap each one separately if they are too long. Make sure the parameter names in the description match the model definition!

category = “shape:sphere” defines where the model will appear in the model documentation. In this example, the model will appear alphabetically in the list of spheroid models in the Shape category.

single = True indicates that the model can be run using single precision floating point values. Set it to False if the numerical calculation for the model is unstable, which is the case for about 20 of the built in models. It is worthwhile modifying the calculation to support single precision, allowing models to run up to 10 times faster. The section Test_Your_New_Model describes how to compare model values for single vs. double precision so you can decide if you need to set single to False.
opencl = False indicates that the model should not be run using OpenCL. This may be because the model definition includes code that cannot be compiled for the GPU (for example, goto statements). It can also be used for large models which can’t run on most GPUs. This flag has not been used on any of the built-in models; models which were failing were streamlined so this flag was not necessary.

structure_factor = True indicates that the model can be used as a structure factor to account for interactions between particles. See Form_Factors for more details.

model_info = ... lets you define a model directly, for example, by loading and modifying existing models. This is done implicitly by sasmodels.core.load_model_info(), which can create a mixture model from a pair of existing models. For example:

```python
from sasmodels.core import load_model_info
model_info = load_model_info('sphere+cylinder')
```

See sasmodels.modelinfo.ModelInfo for details about the model attributes that are defined.

**Model Parameters**

Next comes the parameter table. For example:

```python
# pylint: disable=bad-whitespace, line-too-long
# ["name", "units", default, [min, max], "type", "description"],
parameters = [
    ["sld", "1e-6/Ang^2", 1, [-inf, inf], "sld", "Layer scattering - length density"],
    ["sld_solvent", "1e-6/Ang^2", 6, [-inf, inf], "sld", "Solvent scattering - length density"],
    ["radius", "Ang", 50, [0, inf], "volume", "Sphere radius"],
]
# pylint: enable=bad-whitespace, line-too-long
parameters = [[‘name’, ‘units’, default, [min,max], ‘type’, ‘tooltip’],... ] defines the parameters that form the model.

Note: The order of the parameters in the definition will be the order of the parameters in the user interface and the order of the parameters in Iq(), Iqac(), Iqabc() and form_volume(). And scale and background parameters are implicit to all models, so they do not need to be included in the parameter table.

- “name” is the name of the parameter shown on the FitPage.
  - the name must be a valid variable name, starting with a letter and containing only letters, numbers and underscore.
  - parameter names should follow the mathematical convention; e.g., radius_core not core_radius, or sld_solvent not solvent_sld.
  - model parameter names should be consistent between different models, so sld_solvent, for example, should have exactly the same name in every model.
  - to see all the parameter names currently in use, type the following in the python shell/editor under the Tools menu:

```python
import sasmodels.list_pars
sasmodels.list_pars.list_pars()
```

- use “name[n]” for multiplicity parameters, where n is the name of the parameter defining the number of shells/layers/segments, etc.

- “units” are displayed along with the parameter name
  - every parameter should have units; use “None” if there are no units.
- sld’s should be given in units of 1e-6/Ang^2, and not simply 1/Ang^2 to be consistent with the built-in models. Adjust your formulas appropriately.

- fancy units markup is available for some units, including:

| Ang, 1/Ang, 1/Ang^2, 1e-6/Ang^2, degrees, 1/cm, Ang/cm, g/cm^3, mg/m^2 |

- the list of units is defined in the variable RST_UNITS within sasmodels/generate.py
  * new units can be added using the macros defined in doc/rst_prolog in the sasmodels source.
  * units should be properly formatted using sub-/super-scripts and using negative exponents instead of the / operator, though the unit name should use the / operator for consistency.
  * please post a message to the SasView developers mailing list with your changes.

- **default** is the initial value for the parameter.
  - the parameter default values are used to auto-generate a plot of the model function in the documentation.

- **[min, max]** are the lower and upper limits on the parameter.
  - lower and upper limits can be any number, or -inf or inf.
  - the limits will show up as the default limits for the fit making it easy, for example, to force the radius to always be greater than zero.
  - these are hard limits defining the valid range of parameter values; polydispersity distributions will be truncated at the limits.

- **“type”** can be one of: “”, “sld”, “volume”, or “orientation”.
  - “sld” parameters can have magnetic moments when fitting magnetic models; depending on the spin polarization of the beam and the q value being examined, the effective sld for that material will be used to compute the scattered intensity.
  - “volume” parameters are passed to Iq(), Iqac(), Iqabc() and form_volume(), and have polydispersity loops generated automatically.
  - “orientation” parameters are not passed, but instead are combined with orientation dispersity to translate qx and qy to qa, qb and qc. These parameters should appear at the end of the table with the specific names theta, phi and for asymmetric shapes psi, in that order.

Some models will have integer parameters, such as number of pearls in the pearl necklace model, or number of shells in the multi-layer vesicle model. The optimizers in BUMPS treat all parameters as floating point numbers which can take arbitrary values, even for integer parameters, so your model should round the incoming parameter value to the nearest integer inside your model you should round to the nearest integer. In C code, you can do this using:

```c
static double
Iq(double q, ..., double fp_n, ...)
{
    int n = (int)(fp_n + 0.5);
    ...
}
```

In python:

```python
def Iq(q, ..., n, ...):
    n = int(n+0.5)
    ...
```

Derivative based optimizers such as Levenberg-Marquardt will not work for integer parameters since the partial derivative is always zero, but the remaining optimizers (DREAM, differential evolution, Nelder-Mead simplex) will still function.
Model Computation

Models can be defined as pure python models, or they can be a mixture of python and C models. C models are run on the GPU if it is available, otherwise they are compiled and run on the CPU.

Models are defined by the scattering kernel, which takes a set of parameter values defining the shape, orientation and material, and returns the expected scattering. Polydispersity and angular dispersion are defined by the computational infrastructure. Any parameters defined as “volume” parameters are polydisperse, with polydispersity defined in proportion to their value. “orientation” parameters use angular dispersion defined in degrees, and are not relative to the current angle.

Based on a weighting function \( G(x) \) and a number of points \( n \), the computed value is

\[
\hat{I}(q) = \frac{\int G(x)I(q, x) \, dx}{\int G(x)V(x) \, dx} \approx \frac{\sum_{i=1}^{n} G(x_i)I(q, x_i)}{\sum_{i=1}^{n} G(x_i)V(x_i)}
\]

That is, the individual models do not need to include polydispersity calculations, but instead rely on numerical integration to compute the appropriately smeared pattern.

Each .py file also contains a function:

```python
def random():
    ...
```

This function provides a model-specific random parameter set which shows model features in the USANS to SANS range. For example, core-shell sphere sets the outer radius of the sphere logarithmically in [20, 20,000], which sets the Q value for the transition from flat to falling. It then uses a beta distribution to set the percentage of the shape which is shell, giving a preference for very thin or very thick shells (but never 0% or 100%). Using -sets=10 in sascomp should show a reasonable variety of curves over the default sascomp q range. The parameter set is returned as a dictionary of \{parameter: value, ...\}. Any model parameters not included in the dictionary will default according to the code in the _randomize_one() function from sasmodels/compare.py.

Python Models

For pure python models, define the \( Iq \) function:

```python
import numpy as np
from numpy import cos, sin, ...

def Iq(q, par1, par2, ...):
    return I(q, par1, par2, ...)
Iq.vectorized = True
```

The parameters \( par1, par2, \ldots \) are the list of non-orientation parameters to the model in the order that they appear in the parameter table. Note that the auto-generated model file uses \( x \) rather than \( q \).

The .py file should import trigonometric and exponential functions from numpy rather than from math. This lets us evaluate the model for the whole range of \( q \) values at once rather than looping over each \( q \) separately in python. With \( q \) as a vector, you cannot use if statements, but must instead do tricks like

\[
a = x\cdot q (q>0) + y\cdot q (q\leq0)
\]

or

```python
a = np.empty_like(q)
index = q>0
a[index] = x*q[index]
a[~index] = y*q[~index]
```

which sets \( a \) to \( q \cdot x \) if \( q \) is positive or \( q \cdot y \) if \( q \) is zero or negative. If you have not converted your function to use \( q \) vectors, you can set the following and it will only receive one \( q \) value at a time:

---

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Iq.vectorized = False

Return np.NaN if the parameters are not valid (e.g., cap_radius < radius in barbell). If I(q; pars) is NaN for any q, then those parameters will be ignored, and not included in the calculation of the weighted polydispersity.

Models should define form_volume(par1, par2, ...) where the parameter list includes the volume parameters in order. This is used for a weighted volume normalization so that scattering is on an absolute scale. If form_volume is not defined, then the default form_volume = 1.0 will be used.

Embedded C Models

Like pure python models, inline C models need to define an Iq function:

```c
Iq = ***
*** return I(q, par1, par2, ...);
```

This expands into the equivalent C code:

```c
#include <math.h>
double Iq(double q, double par1, double par2, ...);
double Iq(double q, double par1, double par2, ...)
{
    return I(q, par1, par2, ...);
}
```

form_volume defines the volume of the shape. As in python models, it includes only the volume parameters.

source=['fn.c', ...] includes the listed C source files in the program before Iq and form_volume are defined. This allows you to extend the library of C functions available to your model.

c_code includes arbitrary C code into your kernel, which can be handy for defining helper functions for Iq and form_volume. Note that you can put the full function definition for Iq and form_volume (include function declaration) into c_code as well, or put them into an external C file and add that file to the list of sources.

Models are defined using double precision declarations for the parameters and return values. When a model is run using single precision or long double precision, each variable is converted to the target type, depending on the precision requested.

Floating point constants must include the decimal point. This allows us to convert values such as 1.0 (double precision) to 1.0f (single precision) so that expressions that use these values are not promoted to double precision expressions. Some graphics card drivers are confused when functions that expect floating point values are passed integers, such as 4*atan(1); it is safest to not use integers in floating point expressions. Even better, use the builtin constant M_PI rather than 4*atan(1); it is faster and smaller!

The C model operates on a single q value at a time. The code will be run in parallel across different q values, either on the graphics card or the processor.

Rather than returning NAN from Iq, you must define the INVALID(v). The v parameter lets you access all the parameters in the model using v.par1, v.par2, etc. For example:

```c
#define INVALID(v) (v.bell_radius < v.radius)
```

The INVALID define can go into Iq, or c_code, or an external C file listed in source.

Oriented Shapes

If the scattering is dependent on the orientation of the shape, then you will need to include orientation parameters theta, phi and psi at the end of the parameter table. As described in the section Oriented particles, the individual (q_x, q_y) points on the detector will be rotated into (q_a, q_b, q_c) points relative to the sample in its canonical orientation with a-b-c aligned with x-y-z in the laboratory frame and beam travelling along -z.
The oriented C model is called using $I_{qabc}(qa, qb, qc, par1, par2, \ldots)$ where $par1,$ etc. are the parameters to the model. If the shape is rotationally symmetric about $c$ then $psi$ is not needed, and the model is called as $I_{qac}(qab, qc, par1, par2, \ldots).$ In either case, the orientation parameters are not included in the function call.

For 1D oriented shapes, an integral over all angles is usually needed for the $I_q$ function. Given symmetry and the substitution $u = \cos(\alpha), du = -\sin(\alpha) d\alpha$ this becomes

$$I(q) = \frac{1}{4\pi} \int_{-\pi/2}^{\pi/2} F(q_a, q_b, q_c)^2 \sin(\alpha) d\beta d\alpha$$

$$= \frac{8}{4\pi} \int_{0}^{\pi/2} \int_{0}^{\pi/2} F^2(\sin(\alpha)) d\beta d\alpha$$

$$= \frac{8}{4\pi} \int_{0}^{1} \int_{0}^{\pi/2} -F^2 d\beta du$$

$$= \frac{8}{4\pi} \int_{0}^{1} \int_{0}^{\pi/2} F^2 d\beta du$$

for

$$q_a = q \sin(\alpha) \sin(\beta) = q \sqrt{1 - u^2 \sin^2(\beta)}$$

$$q_b = q \sin(\alpha) \cos(\beta) = q \sqrt{1 - u^2 \cos^2(\beta)}$$

$$q_c = q \cos(\alpha) = qu$$

Using the $z, w$ values for Gauss-Legendre integration in "lib/gauss76.c", the numerical integration is then:

```c
double outer_sum = 0.0;
for (int i = 0; i < GAUSS_N; i++) {
    const double cos_alpha = 0.5*GAUSS_Z[i] + 0.5;
    const double sin_alpha = sqrt(1.0 - cos_alpha*cos_alpha);
    const double qc = cos_alpha * q;
    double inner_sum = 0.0;
    for (int j = 0; j < GAUSS_N; j++) {
        const double beta = M_PI_4 * GAUSS_Z[j] + M_PI_4;
        double sin_beta, cos_beta;
        SINCOS(beta, sin_beta, cos_beta);
        const double qa = sin_alpha * sin_beta * q;
        const double qb = sin_alpha * cos_beta * q;
        const double form = Fq(qa, qb, qc, ...);
        inner_sum += GAUSS_W[j] * form * form;
    }
    outer_sum += GAUSS_W[i] * inner_sum;
}
outer_sum *= 0.25; // = 8/(4 pi) * outer_sum * (pi/2) / 4
```

The $z$ values for the Gauss-Legendre integration extends from -1 to 1, so the double sum of $w[i]w[j]$ explains the factor of 4. Correcting for the average $dz[i]dz[j]$ gives $(1 - 0) \cdot (\pi/2 - 0) = \pi/2.$ The $8/(4\pi)$ factor comes from the integral over the quadrant. With less symmetry (eg., in the bcc and fcc paracrystal models), then an integral over the entire sphere may be necessary.

For simpler models which are rotationally symmetric a single integral suffices:

$$I(q) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} F(q_{ab}, q_c)^2 \sin(\alpha) d\alpha/\pi$$

$$= \frac{2}{\pi} \int_{0}^{1} F^2 du$$

for

$$q_{ab} = q \sin(\alpha) = q \sqrt{1 - u^2}$$

$$q_c = q \cos(\alpha) = qu$$

with integration loop:

```c
for (int i = 0; i < GAUSS_N; i++) {
    double cos_alpha = GAUSS_Z[i];
    double sin_alpha = sqrt(1.0 - cos_alpha*cos_alpha);
    double qc = cos_alpha * q;
    for (int j = 0; j < GAUSS_N; j++) {
        double beta = M_PI_4 * GAUSS_Z[j] + M_PI_4;
        double sin_beta, cos_beta;
        SINCOS(beta, sin_beta, cos_beta);
        double qa = sin_alpha * sin_beta * q;
        double qb = sin_alpha * cos_beta * q;
        double form = Fq(qa, qb, qc);
        inner_sum += GAUSS_W[j] * form;
    }
    outer_sum += GAUSS_W[i] * inner_sum;
}
outer_sum *= 0.25; // = 2/(\pi) * outer_sum * (pi/2) / 4
```
double sum = 0.0;
for (int i = 0; i < GAUSS_N; i++) {
    const double cos_alpha = 0.5*GAUSS_Z[i] + 0.5;
    const double sin_alpha = sqrt(1.0 - cos_alpha*cos_alpha);
    const double qab = sin_alpha * q;
    const double qc = cos_alpha * q;
    const double form = Fq(qab, qc, ...);
    sum += GAUSS_W[j] * form * form;
}
sum *= 0.5; // = 2/pi * sum * (pi/2) / 2

Magnetism

Magnetism is supported automatically for all shapes by modifying the effective SLD of particle according to the Halpern-Johnson vector describing the interaction between neutron spin and magnetic field. All parameters marked as type sld in the parameter table are treated as possibly magnetic particles with magnitude $M_0$ and direction $m\theta$ and $m\phi$. Polarization parameters are also provided automatically for magnetic models to set the spin state of the measurement.

For more complicated systems where magnetism is not uniform throughout the individual particles, you will need to write your own models. You should not mark the nuclear sld as type sld, but instead leave them unmarked and provide your own magnetism and polarization parameters. For 2D measurements you will need $(q_x, q_y)$ values for the measurement to compute the proper magnetism and orientation, which you can implement using $I_{qxy}(q_x, q_y, \text{par1}, \text{par2}, \ldots)$.

Special Functions

The C code follows the C99 standard, with the usual math functions, as defined in OpenCL. This includes the following:

\begin{itemize}
    \item $M_{\text{PI}}, M_{\text{PI2}}, M_{\text{PI4}}, M_{\text{SQRT1_2}}, M_{\text{E}}$: $\pi, \pi/2, \pi/4, 1/\sqrt{2}$ and Euler’s constant $e$
    \item $\exp, \log, \text{pow}(x,y), \expm1, \log1p, \text{sqrt}, \text{cbrt}$: Power functions $e^x$, $\ln x$, $x^y$, $e^x - 1$, $\ln 1 + x$, $\sqrt{x}$. The functions $\expm1(x)$ and $\log1p(x)$ are accurate across all $x$, including $x$ very close to zero.
    \item $\sin, \cos, \tan, \text{asin}, \text{acos}, \text{atan}$: Trigonometry functions and inverses, operating on radians.
    \item $\sinh, \cosh, \text{tanh}, \text{asinh}, \text{acosh}, \text{atanh}$: Hyperbolic trigonometry functions.
    \item $\text{atan2}(y,x)$: Angle from the $x$-axis to the point $(x, y)$, which is equal to $\tan^{-1}(y/x)$ corrected for quadrant. That is, if $x$ and $y$ are both negative, then $\text{atan2}(y,x)$ returns a value in quadrant III where $\text{atan}(y/x)$ would return a value in quadrant I. Similarly for quadrants II and IV when $x$ and $y$ have opposite sign.
    \item $\text{fabs}(x), \text{fmin}(x,y), \text{fmax}(x,y), \text{trunc}, \text{rint}$: Floating point functions. $\text{rint}(x)$ returns the nearest integer.
    \item $\text{NAN}$: NaN, Not a Number, 0/0. Use $\text{isnan}(x)$ to test for NaN. Note that you cannot use $x == \text{NAN}$ to test for NaN values since that will always return false. $\text{NAN}$ does not equal $\text{NAN}$! The alternative, $x != x$ may fail if the compiler optimizes the test away.
    \item $\text{INFINITY}$: $\infty, 1/0$. Use $\text{isinf}(x)$ to test for infinity, or $\text{isfinite}(x)$ to test for finite and not NaN.
    \item $\text{erf, erfc, tgamma, lgamma}$: do not use Special functions that should be part of the standard, but are missing or inaccurate on some platforms. Use $\text{sas}_{-}\text{erf, sas}_{-}\text{erfc, sas}_{-}\text{gamma} and\text{ sas}_{-}\text{lgamma}$ instead (see below).
\end{itemize}

Some non-standard constants and functions are also provided:

\begin{itemize}
    \item $M_{\text{PI180}}, M_{\text{4PI3}}$: $\frac{\pi}{180}, \frac{4\pi}{3}$
\end{itemize}
SINCSOS(x, s, c): Macro which sets \( s=\sin(x) \) and \( c=\cos(x) \). The variables \( c \) and \( s \) must be declared first.

\( \text{square}(x): x^2 \)

\( \text{cube}(x): x^3 \)

\( \text{sas\_sin}_x(x): \sin(x)/x \), with limit \( \sin(0)/0 = 1 \).

\( \text{powr}(x, y): x^y \) for \( x \geq 0 \); this is faster than general \( x^y \) on some GPUs.

\( \text{pown}(x, n): x^n \) for \( n \) integer; this is faster than general \( x^n \) on some GPUs.

FLOAT_SIZE: The number of bytes in a floating point value. Even though all variables are declared double, they may be converted to single precision float before running. If your algorithm depends on precision (which is not uncommon for numerical algorithms), use the following:

```c
#if FLOAT_SIZE>4
... code for double precision ...
#else
... code for single precision ...
#endif
```

SAS_DOUBLE: A replacement for double so that the declared variable will stay double precision; this should generally not be used since some graphics cards do not support double precision. There is no provision for forcing a constant to stay double precision.

The following special functions and scattering calculations are defined in `sasmodels/models/lib`. These functions have been tuned to be fast and numerically stable down to \( q = 0 \) even in single precision. In some cases they work around bugs which appear on some platforms but not others, so use them where needed. Add the files listed in `source = \[ "lib/file.c", ... \]` to your `model.py` file in the order given, otherwise these functions will not be available.

\( \text{polevl}(x, c, n): \) Polynomial evaluation \( p(x) = \sum_{i=0}^{n} c_i x^i \) using Horner’s method so it is faster and more accurate.

\( c = \{c_0, c_{n-1}, \ldots, c_0\} \) is the table of coefficients, sorted from highest to lowest.

source = \[ "lib/polevl.c", ... \] (link to code)

\( \text{p1evl}(x, c, n): \) Evaluation of normalized polynomial \( p(x) = x^n + \sum_{i=0}^{n-1} c_i x^i \) using Horner’s method so it is faster and more accurate.

\( c = \{c_{n-1}, c_{n-2}, \ldots, c_0\} \) is the table of coefficients, sorted from highest to lowest.

source = \[ "lib/polevl.c", ... \] (polevl.c)

\( \text{sas\_gamma}(x): \) Gamma function \( \text{sas\_gamma}(x) = \Gamma(x) \).

The standard math function, \( \text{tgamma}(x) \), is unstable for \( x < 1 \) on some platforms.

source = \[ "lib/sas\_gamma.c", ... \] (sas\_gamma.c)

\( \text{sas\_gammaln}(x): \) log gamma function \( \text{sas\_gammaln}(x) = \log \Gamma(|x|) \).

The standard math function, \( \text{lgamma}(x) \), is incorrect for single precision on some platforms.

source = \[ "lib/sas\_gammaln.c", ... \] (sas\_gammaln.c)

\( \text{sas\_gammainc}(a, x), \text{sas\_gammaincc}(a, x): \) Incomplete gamma function \( \text{sas\_gammainc}(a, x) = \int_x^\infty t^{a-1} e^{-t} dt/\Gamma(a) \) and complementary incomplete gamma function \( \text{sas\_gammaincc}(a, x) = \int_0^x t^{a-1} e^{-t} dt/\Gamma(a) \).

source = \[ "lib/sas\_gammainc.c", ... \] (sas\_gammainc.c)

\( \text{sas\_erf}(x), \text{sas\_erfc}(x): \) Error function \( \text{sas\_erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \) and complementary error function \( \text{sas\_erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt \).

The standard math functions \( \text{erf}(x) \) and \( \text{erfc}(x) \) are slower and broken on some platforms.
sas_J0(x): Bessel function of the first kind \( sas_J0(x) = J_0(x) \) where \( J_0(x) = \frac{1}{\pi} \int_0^\pi \cos(x \sin(\tau)) d\tau. \)

The standard math function \( j0(x) \) is not available on all platforms.

sas_J1(x): Bessel function of the first kind \( sas_J1(x) = J_1(x) \) where \( J_1(x) = \frac{1}{\pi} \int_0^\pi \cos(\tau - x \sin(\tau)) d\tau. \)

The standard math function \( j1(x) \) is not available on all platforms.

sas_JN(n, x): Bessel function of the first kind and integer order \( n \), \( sas_JN(n, x) = J_n(x) \) where \( J_n(x) = \frac{1}{\pi} \int_0^\pi \cos(n\tau - x \sin(\tau)) d\tau. \) If \( n = 0 \) or 1, it uses \( sas_J0(x) \) or \( sas_J1(x) \), respectively.

Warning: \( JN(n, x) \) can be very inaccurate (0.1%) for \( x \) not in \([0.1, 100]\).

The standard math function \( jn(n, x) \) is not available on all platforms.

sas_Si(x): Sine integral \( Si(x) = \int_0^x \frac{\sin(t)}{t} dt. \)

Warning: \( Si(x) \) can be very inaccurate (0.1%) for \( x \) in \([0.1, 100]\).

This function uses Taylor series for small and large arguments:

For large arguments use the following Taylor series,

\[
\begin{align*}
Si(x) & \sim \frac{\pi}{2} - \frac{\cos(x)}{x} \left( 1 - \frac{2!}{x^2} + \frac{4!}{x^4} - \frac{6!}{x^6} \right) - \frac{\sin(x)}{x} \left( \frac{1}{x} - \frac{3!}{x^3} + \frac{5!}{x^5} - \frac{7!}{x^7} \right) \\
& \approx \frac{x^3}{3 \times 3!} + \frac{x^5}{5 \times 5!} - \frac{x^7}{7 \times 7!} + \frac{x^9}{9 \times 9!} - \frac{x^{11}}{11 \times 11!}
\end{align*}
\]

For small arguments,

\[
Si(x) \sim x - \frac{x^3}{3 \times 3!} + \frac{x^5}{5 \times 5!} - \frac{x^7}{7 \times 7!} + \frac{x^9}{9 \times 9!} - \frac{x^{11}}{11 \times 11!}
\]

sas_3j1x_x(x): Spherical Bessel form \( sph_j1c(x) = 3j1(x)/x = 3(sin(x) - x \cos(x))/x^3 \), with a limiting value of 1 at \( x = 0 \), where \( j1(x) \) is the spherical Bessel function of the first kind and first order.

This function uses a Taylor series for small \( x \) for numerical accuracy.

sas_2J1x_x(x): Bessel form \( sas_J1c(x) = 2J1(x)/x \), with a limiting value of 1 at \( x = 0 \), where \( J1(x) \) is the Bessel function of first kind and first order.

Gauss76Z[i], Gauss76Wt[i]: Points \( z_i \) and weights \( w_i \) for 76-point Gaussian quadrature, respectively, computing \( \int_{-1}^1 f(z) dz \approx \sum_{i=1}^{76} w_i f(z_i). \)

Similar arrays are available in gauss20.c for 20-point quadrature and in gauss150.c for 150-point quadrature. The macros GAUSS_N, GAUSS_Z and GAUSS_W are defined so that you can change the order of the integration by selecting an different source without touching the C code.
Problems with C models

The graphics processor (GPU) in your computer is a specialized computer tuned for certain kinds of problems. This leads to strange restrictions that you need to be aware of. Your code may work fine on some platforms or for some models, but then return bad values on other platforms. Some examples of particular problems:

1. **Code is too complex, or uses too much memory.** GPU devices only have a limited amount of memory available for each processor. If you run programs which take too much memory, then rather than running multiple values in parallel as it usually does, the GPU may only run a single version of the code at a time, making it slower than running on the CPU. It may fail to run on some platforms, or worse, cause the screen to go blank or the system to reboot.

2. **Code takes too long.** Because GPU devices are used for the computer display, the OpenCL drivers are very careful about the amount of time they will allow any code to run. For example, on OS X, the model will stop running after 5 seconds regardless of whether the computation is complete. You may end up with only some of your 2D array defined, with the rest containing random data. Or it may cause the screen to go blank or the system to reboot.

3. **Memory is not aligned.** The GPU hardware is specialized to operate on multiple values simultaneously. To keep the GPU simple the values in memory must be aligned with the different GPU compute engines. Not following these rules can lead to unexpected values being loaded into memory, and wrong answers computed. The conclusion from a very long and strange debugging session was that any arrays that you declare in your model should be a multiple of four. For example:

```c
double Iq(q, p1, p2, ...)
{
    double vector[8]; // Only going to use seven slots, but declare 8
    ...
}
```

The first step when your model is behaving strangely is to set `single=False`. This automatically restricts the model to only run on the CPU, or on high-end GPU cards. There can still be problems even on high-end cards, so you can force the model off the GPU by setting `opencl=False`. This runs the model as a normal C program without any GPU restrictions so you know that strange results are probably from your code rather than the environment. Once the code is debugged, you can compare your output to the output on the GPU.

Although it can be difficult to get your model to work on the GPU, the reward can be a model that runs 1000x faster on a good card. Even your laptop may show a 50x improvement or more over the equivalent pure python model.

Form Factors

Away from the dilute limit you can estimate scattering including particle-particle interactions using \( I(q) = P(q) * S(q) \) where \( P(q) \) is the form factor and \( S(q) \) is the structure factor. The simplest structure factor is the *hardsphere* interaction, which uses the effective radius of the form factor as an input to the structure factor model. The effective radius is the average radius of the form averaged over all the polydispersity values.

```python
def ER(radius, thickness):
    """Effective radius of a core-shell sphere."""
    return radius + thickness
```

Now consider the *core_shell_sphere*, which has a simple effective radius equal to the radius of the core plus the thickness of the shell, as shown above. Given polydispersity over \((r_1, r_2, \ldots, r_m)\) in radius and \((t_1, t_2, \ldots, t_n)\) in thickness, \(ER\) is called with a mesh grid covering all possible combinations of radius and thickness. That is, \(radius\) is \((r_1, r_2, \ldots, r_m, r_1, r_2, \ldots, r_m, \ldots)\) and \(thickness\) is \((t_1, t_1, t_1, t_2, t_2, t_2, \ldots, t_2, \ldots)\). The \(ER\) function returns one effective radius for each combination. The effective radius calculator weights each of these according to the polydispersity distributions and calls the structure factor with the average \(ER\).
def VR(radius, thickness):
    """Sphere and shell volumes for a core-shell sphere."""
    whole = 4.0/3.0 * pi * (radius + thickness)**3
    core = 4.0/3.0 * pi * radius**3
    return whole, whole - core

Core-shell type models have an additional volume ratio which scales the structure factor. The VR function returns the volume of the whole sphere and the volume of the shell. Like ER, there is one return value for each point in the mesh grid.

NOTE: we may be removing or modifying this feature soon. As of the time of writing, core-shell sphere returns (1., 1.) for VR, giving a volume ratio of 1.0.

Unit Tests

THESE ARE VERY IMPORTANT. Include at least one test for each model and PLEASE make sure that the answer value is correct (i.e. not a random number).

tests = [[{}], 0.2, 0.726362],
        ["scale": 1., "background": 0., "sld": 6., "sld_solvent": 1.,
         "radius": 120., "radius_pd": 0.2, "radius_pd_n":45},
         0.2, 0.228843],
        ["radius": 120., "radius_pd": 0.2, "radius_pd_n":45}, "ER", 120.],
        ["radius": 120., "radius_pd": 0.2, "radius_pd_n":45}, "VR", 1.],

```
tests=[[\{parameters\}, q, result], ...] is a list of lists. Each list is one test and contains, in order:

* a dictionary of parameter values. This can be {} using the default parameters, or filled with some parameters that will be different from the default, such as {"radius":10.0, "sld":4}. Unlisted parameters will be given the default values.

* the input $q$ value or tuple of $(q_x, q_y)$ values.

* the output $I(q)$ or $I(q_x, q_y)$ expected of the model for the parameters and input value given.

* input and output values can themselves be lists if you have several $q$ values to test for the same model parameters.

* for testing ER and VR, give the inputs as “ER” and “VR” respectively; the output for VR should be the sphere/shell ratio, not the individual sphere and shell values.

Test Your New Model

Minimal Testing

From SasView either open the Python shell (Tools > Python Shell/Editor) or the plugin editor (Fitting > Plugin Model Operations > Advanced Plugin Editor), load your model, and then select Run > Check Model from the menu bar. An Info box will appear with the results of the compilation and a check that the model runs.

If you are not using sasmodels from SasView, skip this step.

Recommended Testing

If the model compiles and runs, you can next run the unit tests that you have added using the test = values.

From SasView, switch to the Shell tab and type the following:
from sasmodels.model_test import run_one
run_one("~/.sasview/plugin_models/model.py")

This should print:
test_model_python (sasmodels.model_test.ModelTestCase) ... ok

To check whether single precision is good enough, type the following:

from sasmodels.compare import main as compare
compare("~/.sasview/plugin_models/model.py")

This will pop up a plot showing the difference between single precision and double precision on a range of $q$ values.

demo = dict(scale=1, background=0,
            sld=6, sld_solvent=1,
            radius=120,
            radius_pd=.2, radius_pd_n=45)

demo={'par': value, ...} in the model file sets the default values for the comparison. You can include polydispersity parameters such as radius_pd=0.2, radius_pd_n=45 which would otherwise be zero.

These commands can also be run directly in the python interpreter:

$ python -m sasmodels.model_test -v ~/.sasview/plugin_models/model.py $ python -m sasmodels.compare ~/.sasview/plugin_models/model.py

The options to compare are quite extensive; type the following for help:

compare()

Options will need to be passed as separate strings. For example to run your model with a random set of parameters:

compare("-random", "-pars", "~/.sasview/plugin_models/model.py")

For the random models,

- $sld$ will be in the range (-0.5,10.5),
- angles ($theta$, $phi$, $psi$) will be in the range (-180,180),
- angular dispersion will be in the range (0,45),
- polydispersity will be in the range (0,1)
- other values will be in the range (0, 2$v$), where $v$ is the value of the parameter in demo.

Dispersion parameters $n$, $sigma$ and $type$ will be unchanged from demo so that run times are more predictable (polydispersity calculated across multiple parameters can be very slow).

If your model has 2D orientation calculation, then you should also test with:

compare("-2d", "~/.sasview/plugin_models/model.py")

Check The Docs

You can get a rough idea of how the documentation will look using the following:

compare("-help", "~/.sasview/plugin_models/model.py")

This does not use the same styling as the rest of the docs, but it will allow you to check that your ReStructuredText and LaTeX formatting. Here are some tools to help with the inevitable syntax errors:
There is also a neat online WYSIWYG ReStructuredText editor at http://rst.ninjs.org.

Clean Lint - (Developer Version Only)

NB: For now we are not providing pylint with the installer version of SasView; so unless you have a SasView build environment available, you can ignore this section!

Run the lint check with:

```python
python -m pylint --rcfile=extra/pylint.rc ~/.sasview/plugin_models/model.py
```

We are not aiming for zero lint just yet, only keeping it to a minimum. For now, don’t worry too much about invalid-name. If you really want a variable name $R_g$ for example because $R_g$ is the right name for the model parameter then ignore the lint errors. Also, ignore missing-docstring for standard model functions $I_q$, $I_{qac}$, etc.

We will have delinting sessions at the SasView Code Camps, where we can decide on standards for model files, parameter names, etc.

For now, you can tell pylint to ignore things. For example, to align your parameters in blocks:

```python
# pylint: disable=bad-whitespace,line-too-long
# "["name", "units", default, [lower, upper], "type", "description"],
parameters = [
  ["contrast_factor", "barns", 10.0, [\inf, \inf], ", "Contrast factor of the polymer"],
  ["bjerrum_length", "\text{Ang}", 7.1, [0, \inf], ", "Bjerrum length"],
  ["virial_param", "1/\text{Ang}^2", 12.0, [\inf, \inf], ", "Virial parameter"],
  ["monomer_length", "\text{Ang}", 10.0, [0, \inf], ", "Monomer length"],
  ["salt_concentration", "\text{mol/L}", 0.0, [\inf, \inf], ", "Concentration of monovalent salt"],
  ["ionization_degree", ", \text{0.05, [0, \inf], ", "Degree of ionization"],
  ["polymer_concentration", "\text{mol/L}", 0.7, [0, \inf], ", "Polymer molar concentration"],
]
# pylint: enable=bad-whitespace,line-too-long
```

Don’t put in too many pylint statements, though, since they make the code ugly.

Share Your Model!

Once compare and the unit test(s) pass properly and everything is done, consider adding your model to the Model Marketplace so that others may use it!

Document History

2016-10-25 Steve King
2017-05-07 Paul Kienzle - Moved from sasview to sasmodels docs
GPU Setup

SAS model evaluations can run on your graphics card (GPU) or they can run on the processor (CPU). In general, calculations performed on the GPU will run faster.

OpenCL Installation

Warning! GPU devices do not in general offer the same level of memory protection as CPU devices. If your code attempts to write outside allocated memory buffers unpredictable behaviour may result (eg, your video display may freeze, or your system may crash, etc). Do not install OpenCL drivers without first checking for known issues (eg, some computer manufacturers install modified graphics drivers so replacing these may not be a good idea!). If in doubt, seek advice from an IT professional before proceeding further.

Check if you have OpenCL already installed

Windows

The following instructions are based on http://web.engr.oregonstate.edu/~mjb/cs475/DoIHaveOpenCL.pdf

- Go to: Start -> Control Panel -> System & Security -> Administrative Tools
- Double Click on Computer Management
- Click on Device Manager
- Click open Display Adapters
- Right-click on available adapter and select Properties
- Click on Driver
- Go to Driver Details
- Scroll down and see if OpenCL is installed (look for OpenCL*.dll files)

Mac OSX

For OS X operating systems higher than 10.6 OpenCL is shipped along with the system.

However, OpenCL has had a rocky history on Macs. Apple provide a useful compatibility table at https://support.apple.com/en-us/HT202823

Installation

Windows

Depending on the graphic card in your system, drivers can be obtained from different sources:

- NVIDIA: https://developer.nvidia.com/opencl

Mac OSX

N/A

You cannot download OpenCL driver updates for your Mac. They are packaged with the normal quarterly OS X updates from Apple.

Note: Intel provides OpenCL drivers for Intel processors at https://software.intel.com/en-us/articles/opencl-drivers These can sometimes make use of special vector instructions across multiple processors, so it is worth installing if the GPU does not support double precision. You can install this driver alongside the GPU driver for NVIDIA or AMD.
GPU Selection

The logic for choosing the compute platform is a little bit complicated. If the model has the line `single=False` then it requires double precision. If the GPU is single precision only, then it will try running via OpenCL on the CPU. If the OpenCL driver is not available for the CPU then it will run as a normal program on the CPU.

For models with a large number of parameters or with a lot of code, the GPU may be too small to run the program effectively. In this case, you should try simplifying the model, maybe breaking it into several different models so that you don't need IF statements in your code. If it is still too big, you can set `opencl=False` in the model file and the model will only run as a normal program on the CPU. This will not usually be necessary.

Device Selection

If you have multiple GPU devices you can tell the program which device to use. By default, the program looks for one GPU and one CPU device from available OpenCL platforms. It prefers AMD or NVIDIA drivers for GPU, and prefers Intel or Apple drivers for CPU. Both GPU and CPU are included on the assumption that CPU is always available and supports double precision.

The device order is important: GPU is checked before CPU on the assumption that it will be faster. By examining `~sasview.log` you can see which device was used to run the model.

**If you don’t want to use OpenCL, you can set `SAS_OPENCL=None` in your environment settings, and it will only use normal programs.**

If you want to use one of the other devices, you can run the following from the python console:

```python
import pyopencl as cl
cl.create_some_context()
```

This will provide a menu of different OpenCL drivers available. When one is selected, it will say “set PYOPENCL_CTX=...” Use that value as the value of `SAS_OPENCL`.

Device Testing

Unfortunately, not all vendors provide working OpenCL implementations for their GPU devices. For example, the HD 6000 Intel GPUs with double precision support fail for some of the double precision models.

The SasView user interface provides a Fitting OpenCL Options dialog for selecting amongst and testing the available devices. After a few minutes of seeming to freeze, the application will return a list of model tests which have passed. The same tests can be run directly from the python console using:

```python
from sasmodels.model_tests import main as model_tests
model_tests("-v", "opencl", "all")
```

Compiler Selection

For models run as normal programs, you may need to specify a compiler. This is done using the `SAS_COMPILER` environment variable, and the `SAS_OPENMP` environment variable if OpenMP support is available for the compiler.

On Windows, set `SAS_COMPILER=tinycc` for the tinycc compiler, `SAS_COMPILER=msvc` for the Microsoft Visual C compiler, or `SAS_COMPILER=mingw` for the MinGW compiler. If TinyCC is available on the python path (it is provided with SasView), that will be the default. If you want one of the other compilers, be sure to have it available in your `PATH` so we can find it!

On Mac OS/X and Linux, set `SAS_COMPILER=unix` for the compiler. This will use the unix cc command to compile the model, with gcc style command line options. For OS/X you will need to install the Xcode package to make the compiler available.
Scripting Interface

Need some basic details here of how to load models and data via script, evaluate them at given parameter values and run bumps fits.

The key functions are `sasmodels.core.load_model()` for loading the model definition and compiling the kernel and `sasmodels.data.load_data()` for calling sasview to load the data.

Preparing data

Usually you will load data via the sasview loader, with the `sasmodels.data.load_data()` function. For example:

```python
from sasmodels.data import load_data
data = load_data("sasmodels/example/093191_201.dat")
```

You may want to apply a data mask, such a beam stop, and trim high \(q\):

```python
from sasmodels.data import set_beam_stop
set_beam_stop(data, qmin, qmax)
```

The `sasmodels.data.set_beam_stop()` method simply sets the `mask` attribute for the data.

The data defines the resolution function and the \(q\) values to evaluate, so even if you simulating experiments prior to making measurements, you still need a data object for reference. Use `sasmodels.data.empty_data1D()` or `sasmodels.data.empty_data2D()` to create a container with a given \(q\) and \(\Delta q/q\). For example:

```python
import numpy as np
from sasmodels.data import empty_data1D
# 120 points logarithmically spaced from 0.005 to 0.2, with \(dq/q = 5\%\)
q = np.logspace(np.log10(5e-3), np.log10(2e-1), 120)
data = empty_data1D(q, resolution=0.05)
```

To use a more realistic model of resolution, or to load data from a file format not understood by SasView, you can use `sasmodels.data.Data1D` or `sasmodels.data.Data2D` directly. The 1D data uses \(x, y, dx, dy\) for \(x = q\) and \(y = I(q)\), and 2D data uses \(x, y, z, dx, dy, dz\) for \(x, y = qr, qy\) and \(z = I(qr, qy)\). [Note: internally, the Data2D object uses SasView conventions, \(qx, qy, data, dqx, dqy, err\).]

For USANS data, use 1D data, but set \(dxl\) and \(dxw\) attributes to indicate slit resolution:

```python
data.dxl = 0.117
```

See `sasmodels.resolution.slit_resolution()` for details.

SESANS data is more complicated; if your SESANS format is not supported by SasView you need to define a number of attributes beyond \(x, y\). For example:

```python
SElength = np.linspace(0, 2400, 61) # [A]
data = np.ones_like(SElength)
err_data = np.ones_like(SElength)*0.03
class Source:
    wavelength = 6 # [A]
    wavelength_unit = "A"
```

(continues on next page)
The `data` module defines various data plotters as well.

**Using sasmodels directly**

Once you have a computational kernel and a data object, you can evaluate the model for various parameters using `sasmodels.direct_model.DirectModel`. The resulting object will be callable as `f(par=value, ...)`, returning the $I(q)$ for the $q$ values in the data. For example:

```python
import numpy as np
from sasmodels.data import empty_data1D
from sasmodels.core import load_model
from sasmodels.direct_model import DirectModel

q = np.logspace(np.log10(5e-3), np.log10(2e-1), 120)
data = empty_data1D(q, resolution=0.05)
kern = load_model("ellipsoid")
f = DirectModel(data, kern)
Iq = f(radius_polar=100)
```

Polydispersity information is set with special parameter names:

- `par_pd` for polydispersity width, $\Delta p/p$,
- `par_pd_n` for the number of points in the distribution,
- `par_pd_type` for the distribution type (as a string), and
- `par_pd_nsigmas` for the limits of the distribution.

**Using sasmodels through the bumps optimizer**

Like `DirectModel`, you can wrap data and a kernel in a `bumps` model with class:`sasmodels.bumps_model.Model` and create an class:`sasmodels.bumps_model.Experiment` that you can fit with the `bumps` interface. Here is an example from the `example` directory such as `example/model.py`:

```python
import sys
from bumps.names import *
from sasmodels.core import load_model
from sasmodels.bumps_model import Model, Experiment
from sasmodels.data import load_data, set_beam_stop, set_top

""" IMPORT THE DATA USED """
```
radial_data = load_data('DEC07267.DAT')
set_beam_stop(radial_data, 0.00669, outer=0.025)
set_top(radial_data, -.0185)
kernel = load_model("ellipsoid")
model = Model(kernel,
  scale=0.08,
  radius_polar=15, radius_equatorial=800,
  sld=.291, sld_solvent=7.105,
  background=0,
  theta=90, phi=0,
  theta_pd=15, theta_pd_n=40, theta_pd_nsigma=3,
  radius_polar_pd=0.222296, radius_polar_pd_n=1, radius_polar_pd_nsigma=0,
  radius_equatorial_pd=.000128, radius_equatorial_pd_n=1, radius_equatorial_pd_nsigma=0,
  phi_pd=0, phi_pd_n=20, phi_pd_nsigma=3,
)

# SET THE FITTING PARAMETERS
model.radius_polar.range(15, 1000)
model.radius_equatorial.range(15, 1000)
model.theta_pd.range(0, 360)
model.background.range(0,1000)
model.scale.range(0, 10)

cutoff = 1e-3

cutoff = 1e-3  # low precision cutoff
M = Experiment(data=radial_data, model=model, cutoff=cutoff)
problem = FitProblem(M)

Assume that bumps has been installed and the bumps command is available. Maybe need to set the path to sasmodels/sasview using PYTHONPATH=path/to/sasmodels:path/to/sasview/src. To run the model use the bumps program:

$ bumps example/model.py --preview

Note that bumps and sasmodels are included as part of the SasView distribution. On windows, bumps can be called from the cmd prompt as follows:

SasViewCom bumps.cli example/model.py --preview

Calling the computation kernel

Getting a simple function that you can call on a set of q values and return a result is not so simple. Since the time critical use case (fitting) involves calling the function over and over with identical q values, we chose to optimize the call by only transferring the q values to the GPU once at the start of the fit. We do this by creating a sasmodels.kernel.Kernel object from the sasmodels.kernel.KernelModel returned from sasmodels.core.load_model() using the sasmodels.kernel.KernelModel.make_kernel() method. What it actual does depends on whether it is running as a DLL, as OpenCL or as a pure python kernel. Once the kernel is in hand, we can then marshal a set of parameters into a sasmodels.details.CallDetails object and ship it to the kernel using the sasmodels.direct_model.call_kernel() function. An example should help, example/cylinder_eval.py:

from numpy import logspace
from matplotlib import pyplot as plt
from sasmodels.core import load_model

(continues on next page)
```python
from sasmodels.direct_model import call_kernel

model = load_model('cylinder')
q = logspace(-3, -1, 200)
kernel = model.make_kernel([q])
Iq = call_kernel(kernel, dict(radius=200.))
plt.loglog(q, Iq)
plt.show()
```

On windows, this can be called from the cmd prompt using sasview as:

```
SasViewCom example/cylinder_eval.py
```

## References


S J Henderson *Biophys. J.* 70, (1996), 1618-1627


Also see the references at the end of the each model function descriptions.

### 1.3.2 P(r) Calculation

#### Description

This tool calculates a real-space distance distribution function, $P(r)$, using the inversion approach (Moore, 1980). $P(r)$ is set to be equal to an expansion of base functions of the type

$$\Phi_n(r) = 2rsin\left(\frac{\pi nr}{D_{max}}\right)$$

The coefficient of each base function in the expansion is found by performing a least square fit with the following fit function

$$\chi^2 = \sum_i (\frac{I_{meas}(Q_i) - I_{th}(Q_i)}{error_i})^2 + Reg\_term$$

where $I_{meas}(Q_i)$ is the measured scattering intensity and $I_{th}(Q_i)$ is the prediction from the Fourier transform of the $P(r)$ expansion.

The $Reg\_term$ term is a regularization term set to the second derivative $d^2P(r)/d^2r$ integrated over $r$. It is used to produce a smooth $P(r)$ output.
Using P(r) inversion

The user must enter

- **Number of terms**: the number of base functions in the P(r) expansion.
- **Regularization constant**: a multiplicative constant to set the size of the regularization term.
- **Maximum distance**: the maximum distance between any two points in the system.

P(r) inversion requires that the background be perfectly subtracted. This is often difficult to do well and thus many data sets will include a background. For those cases, the user should check the “Estimate background level” option and the module will do its best to estimate it. If you know the background value for your data, select the “Input manual background level” option. Note that this value will be treated as having 0 error.

The P(r) module is constantly computing in the background what the optimum number of terms should be as well as the optimum regularization constant. These are constantly updated in the buttons next to the entry boxes on the GUI. These are almost always close and unless the user has a good reason to choose differently they should just click on the buttons to accept both. \( D_{\text{max}} \) must still be set by the user. However, besides looking at the output, the user can click the explore button which will bring up a graph of chi^2 vs Dmax over a range around the current Dmax. The user can change the range and the number of points to explore in that range. They can also choose to plot several other parameters as a function of Dmax including: I0, Rg, Oscillation parameter, background, positive fraction, and 1-sigma positive fraction.

Reference


Note: This help document was last modified by Paul Butler, 05 September, 2016
Low-$Q$ region ($\leq Q_{\text{min}}$ in data)

- The Guinier function $I_0 \exp(-R_g^2Q^2/3)$ where $I_0$ and $R_g$ are obtained by fitting as for the high-$Q$ region above. Alternatively a power law can be used.

Using invariant analysis

1. Select Invariant from the Analysis menu on the SasView toolbar.
2. Load some data with the Data Explorer.
3. Select a dataset and use the Send To button on the Data Explorer to load the dataset into the Invariant panel.
4. Use the Customised Input boxes on the Invariant panel to subtract any background, specify the contrast (i.e. difference in SLDs - this must be specified for the eventual value of $Q^*$ to be on an absolute scale), or to rescale the data.
5. Adjust the extrapolation range as necessary. In most cases the default values will suffice.
6. Click the Compute button.
7. To include a lower and/or higher $Q$ range, check the relevant Enable Extrapolate check boxes.
   
   If power law extrapolations are chosen, the exponent can be either held fixed or fitted. The number of points, Npts, to be used for the basis of the extrapolation can also be specified.
8. If the value of $Q^*$ calculated with the extrapolated regions is invalid, a red warning will appear at the top of the Invariant panel.
   
   The details of the calculation are available by clicking the Details button in the middle of the panel.
Parameters

Volume Fraction

The volume fraction $\phi$ is related to $Q^*$ by

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

where $\Delta\rho$ is the SLD contrast.

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

Specific Surface Area

The specific surface area $S_v$ is related to $Q^*$ by

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

where $C_p$ is the Porod constant.

Reference


Note: This help document was last changed by Steve King, 01May2015

1.3.4 Correlation Function Analysis

Description

This currently performs correlation function analysis on SAXS/SANS data, but in the the future is also planned to generate model-independent volume fraction profiles from the SANS from adsorbed polymer/surfactant layers. The two types of analyses differ in the mathematical transform that is applied to the data (Fourier vs Hilbert). However, both functions are returned in real space.

A correlation function may be interpreted in terms of an imaginary rod moving through the structure of the material. $\Gamma(x)$ is the probability that a rod of length $x$ has equal electron/neutron scattering length density at either end. Hence a frequently occurring spacing within a structure will manifest itself as a peak in $\Gamma(x)$. SasView will return both the one-dimensional ($\Gamma_1(x)$) and three-dimensional ($\Gamma_3(x)$) correlation functions, the difference being that the former is only averaged in the plane of the scattering vector.

A volume fraction profile $\Phi(z)$ describes how the density of polymer segments/surfactant molecules varies with distance, $z$, normal to an (assumed locally flat) interface. The form of $\Phi(z)$ can provide information about the arrangement of polymer/surfactant molecules at the interface. The width of the profile provides measures of the layer thickness, and the area under the profile is related to the amount of material that is adsorbed.

Both analyses are performed in 3 stages:

- Extrapolation of the scattering curve to $q = 0$ and toward $q = \infty$
- Smoothed merging of the two extrapolations into the original data
• Fourier / Hilbert Transform of the smoothed data to give the correlation function or volume fraction profile, respectively
• (Optional) Interpretation of $\Gamma_1(x)$ assuming the sample conforms to an ideal lamellar morphology

**Extrapolation**

**To $q = 0$**

The data are extrapolated to $q = 0$ by fitting a Guinier function to the data points in the low-$q$ range.

The equation used is:

$$I(q) = Ae^{Bq^2}$$

Where the parameter $B$ is related to the effective radius-of-gyration of a spherical object having the same small-angle scattering in this region.

Note that as $q$ tends to zero this function tends to a limiting value and is therefore less appropriate for use in systems where the form factor does not do likewise. However, because of the transform, the correlation functions are most affected by the Guinier back-extrapolation at large values of $x$ where the impact on any extrapolated parameters will be least significant.

**To $q = \infty$**

The data are extrapolated towards $q = \infty$ by fitting a Porod model to the data points in the high-$q$ range and then computing the extrapolation to 100 times the maximum $q$ value in the experimental dataset. This should be more than sufficient to ensure that on transformation any truncation artefacts introduced are at such small values of $x$ that they can be safely ignored.

The equation used is:

$$I(q) = Kq^{-4}e^{-q^2\sigma^2} + Bg$$

Where $Bg$ is the background, $K$ is the Porod constant, and $\sigma$ (which must be $> 0$) describes the width of the electron/neutron scattering length density profile at the interface between the crystalline and amorphous regions as shown below.

**Smoothing**

The extrapolated data set consists of the Guinier back-extrapolation from $q \sim 0$ up to the lowest $q$ value in the original data, then the original scattering data, and then the Porod tail-fit beyond this. The joins between the original data and the Guinier/Porod extrapolations are smoothed using the algorithm below to try and avoid the formation of truncation ripples in the transformed data:

Functions $f(x_i)$ and $g(x_i)$ where $x_i \in \{x_1, x_2, ..., x_n\}$, are smoothed over the range $[a, b]$ to produce $y(x_i)$, by the following equations:

$$y(x_i) = h_i g(x_i) + (1 - h_i) f(x_i)$$

where:

$$h_i = \frac{1}{1 + \frac{(x_i-b)^2}{(x_i-a)^2}}$$
If “Fourier” is selected for the transform type, SasView will perform a discrete cosine transform on the extrapolated data in order to calculate the 1D correlation function as:

$$\Gamma(x) = \frac{1}{Q^*} \int_0^{\infty} I(q)q^2\cos(qx) dq$$

where $Q^*$ is the Scattering (also called Porod) Invariant.

The following algorithm is applied:

$$\Gamma(x_k) = 2 \sum_{n=0}^{N-1} x_n \cos \left[ \frac{\pi}{N} \left( n + \frac{1}{2} \right) k \right] \quad \text{for } k = 0, 1, \ldots, N - 1, N$$

The 3D correlation function is calculated as:

$$\Gamma_3(x) = \frac{1}{Q^*} \int_0^{\infty} I(q)q^2 \frac{\sin(qx)}{qx} dq$$

**Note:** It is always advisable to inspect $\Gamma_1(x)$ and $\Gamma_3(x)$ for artefacts arising from the extrapolation and transformation processes:

- do they tend to zero as $x$ tends to $\infty$?
- do they smoothly curve onto the ordinate at $x = 0$? (if not check the value of $\sigma$ is sensible)
- are there ripples at $x$ values corresponding to $(2 \pi)$ over the two $q$ values at which the extrapolated and experimental data are merged?
- are there any artefacts at $x$ values corresponding to $2 \pi / q_{\text{max}}$ in the experimental data?
- and lastly, do the significant features/peaks in the correlation functions actually correspond to anticipated spacings in the sample?!!!
Finally, the program calculates the interface distribution function (IDF) \( g_1(x) \) as the discrete cosine transform of:

\[-q^4 I(q)\]

The IDF is proportional to the second derivative of \( \Gamma_1(x) \) and represents a superposition of thickness distributions from all the contributing lamellae.

**Hilbert**

If “Hilbert” is selected for the transform type, the analysis will perform a Hilbert transform on the extrapolated data in order to calculate the Volume Fraction Profile.

**Note:** The Hilbert transform functionality is not yet implemented in SasView.

**Interpretation**

**Correlation Function**

Once the correlation functions have been calculated SasView can be asked to try and interpret \( \Gamma_1(x) \) in terms of an ideal lamellar morphology as shown below.

The structural parameters extracted are:

- Long Period = \( L_p \)
- Average Hard Block Thickness = \( L_c \)
- Average Core Thickness = \( D_0 \)
- Average Interface Thickness = \( D_{tr} \)
- Polydispersity = \( \Gamma_{\text{min}}/\Gamma_{\text{max}} \)
- Local Crystallinity = \( L_c/L_p \)

**Warning:** If the sample does not possess lamellar morphology then “Compute Parameters” will return garbage!

**Volume Fraction Profile**

SasView does not provide any automatic interpretation of volume fraction profiles in the same way that it does for correlation functions. However, a number of structural parameters are obtainable by other means:

- Surface Coverage = \( \theta \)
- Anchor Separation = \( D \)
- Bound Fraction = \( <p> \)
- Second Moment = \( \sigma \)
- Maximum Extent = \( \delta_h \)
- Adsorbed Amount = \( \Gamma \)

The reader is directed to the references for information on these parameters.
Extraction of ideal lamellar parameters from the one dimensional correlation function.

\[ \Gamma_1(R) \]

\[ \Gamma^* \]

\( R = D_{tr} \) at start of linear section

\( R = D_0 \) at end of linear section

\( \Gamma_{\text{max}} \)

\( \Gamma_{\text{min}} \)

\( L_0 \)

\( L_p^*/2 \)

\( L_p \) (Real space coord)
References

Correlation Function


Volume Fraction Profile


Usage

Upon sending data for correlation function analysis, it will be plotted (minus the background value), along with a red bar indicating the upper end of the low-Q range (used for Guinier back-extrapolation), and 2 purple bars indicating the range to be used for Porod forward-extrapolation. These bars may be moved by grabbing and dragging, or by entering appropriate values in the Q range input boxes.

Once the Q ranges have been set, click the “Calculate Bg” button to determine the background level. Alternatively, enter your own value into the box. If the box turns yellow this indicates that background subtraction has created some negative intensities. This may still be fine provided the peak intensity is very much greater than the background level. The important point is that the extrapolated dataset must approach zero at high-q.

Now click the “Extrapolate” button to extrapolate the data. The graph window will update to show the extrapolated data, and the values of the parameters used for the Guinier and Porod extrapolations will appear in the “Extrapolation Parameters” section of the SasView GUI.

Now select which type of transform you would like to perform, using the radio buttons:
- **Fourier**: to perform a Fourier Transform to calculate the correlation functions
- **Hilbert**: to perform a Hilbert Transform to calculate the volume fraction profile

and click the “Transform” button to perform the selected transform and plot the results.

If a Fourier Transform was performed, the “Compute Parameters” button can now be clicked to interpret the correlation function as described earlier. The parameters will appear in the “Output Parameters” section of the SasView GUI.

1.3. Fitting & Other Analyses
1.3. Fitting & Other Analyses
1.4 Tools & Utilities

Note: In Windows use [Alt]-[Cursor left] to return to the previous page

1.4.1 Data Operations Tool

Description

This tool permits arithmetic operations between two data sets. Alternatively, the last data set can be a number.

NOTE! When Data1 and Data2 are both data, their Q (or Qx and Qy for 2D) value(s) must match with each other UNLESS using the 'append' operator.

Using the tool

1. Ensure you have loaded data into the Data Explorer (see Loading Data).
2. Select Data Operation from the Tool menu on the SasView toolbar.
3. Select a dataset/theory in the drop-down menu Data1. A mini-plot of the data will appear underneath.
4. Select a dataset/theory in the drop-down menu Data2 or select Number and enter a number in the box that appears alongside.
5. Select an arithmetic operator symbol from the Operator drop-down. The available operators are:
   • + (for addition)
   • - (for subtraction)
   • * (for multiplication)
   • / (for division)
   • | (for combination of two data sets)
   If two data sets do not match, the operation will fail and the background color of the combo box items will turn to red (WIN only).
6. If the operation is successful, hit the Apply button to make the new dataset. The new dataset will appear in the Data Explorer.

NOTE! Any errors and warnings will be displayed at the bottom of the SasView window.
1.4.2 SLD Calculator Tool

Description

The neutron scattering length density (SLD, $\beta_N$) is defined as

$$\beta_N = \frac{b_{c1} + b_{c2} + \ldots + b_{cn}}{V_m}$$

where $b_{ci}$ is the bound coherent scattering length of ith of n atoms in a molecule with the molecular volume $V_m$.

Specifying the Compound Name

To calculate scattering length densities enter the empirical formula of a compound and its mass density and click “Calculate”. Entering a wavelength value is optional (a default value of 6.0 Å will be used).

TIPS!

- Formula strings consist of atoms and the number of them, such as “CaCO3+6H2O”.
- Groups can be separated by ‘+’ or space, so “CaCO3 6H2O” works as well.
- Groups can be defined using parentheses, such as “CaCO3(H2O)6”.
- Parentheses can be nested, such as “(CaCO3(H2O)6)1”.
- Isotopes are represented by their atomic number in square brackets, such as “CaCO[18]3+6H2O”, H[1], or H[2].
- Numbers of atoms can be integer or decimal, such as “CaCO3+(3HO0.5)2”.
- The SLD of mixtures can be calculated as well. For example, for a 70-30 mixture of H2O/D2O write “H14O7+D6O3” or more simply “H7D3O5” (i.e. this says 7 hydrogens, 3 deuteriums, and 5 oxygens) and enter a mass density calculated on the percentages of H2O and D2O.
1.4.3 Density/Volume Calculator Tool

Description

This tool calculates the mass density from the molar volume or vice versa. To calculate the mass density, the chemical formula and molar volume should be provided.

Using the tool

1. Select Density/Volume Calculator from the Tool menu on the SasView toolbar.
2. Enter the empirical formula of a molecule. For mixtures, the ratio of each of the molecules should be used, for example, (H2O)0.5(D2O)0.5.
3. Use the input combo box to choose between molar volume or mass density and then type in an input value.
4. Click the ‘Calculate’ button to perform the calculation.

Note: This help document was last changed by Steve King, 01May2015

1.4.4 Slit Size Calculator Tool

Description

This tool enables X-ray users to calculate the slit size (FWHM/2) for resolution smearing purposes based on their half beam profile data (as Q vs Intensity; any other data fields are ignored).
Method

The tool works by sequentially summing 10 or more intensity values until a maximum value is attained. It then locates the Q values for the points just before, and just after, half of this maximum value and interpolates between them to get an accurate value for the Q value for the half maximum.

NOTE! Whilst it may have some more generic applicability, the calculator has only been tested with beam profile data from Anton-Paar SAXSess™ software. The beam profile file does not carry any information about the units of the Q data. It is probably nm⁻¹ but the resolution calculations assume the slit height/width has units of Å⁻¹. If the beam profile data is not in these units then it, or the result, must be manually converted.

Using the tool

1. Select Slit Size Calculator from the Tool menu on the SasView toolbar.
2. Load a beam profile file in the Data field using the Browse button.
   NOTE! To see an example of the beam profile file format, visit the file beam profile.DAT in your {installation_directory}/SasView/test_1d folder.
3. Once a data is loaded, the slit size is automatically computed and displayed in the tool window.

Note: This help document was last changed by Steve King, 09Sep2018

1.4.5 Kiessig Thickness Calculator Tool

Description

This tool estimates real space dimensions from the position or spacing of features in reciprocal space. In particular a particle of size \( d \) will give rise to Bragg peaks with spacing \( \Delta q \) according to the relation

\[
d = \frac{2\pi}{\Delta q}
\]

Similarly, the spacing between the peaks in Kiessig fringes in reflectometry data arise from layers of thickness \( d \).

Using the tool

To get a rough thickness or particle size, simply type the fringe or peak position (in units of 1/Å) and click on the Compute button.

Note: This help document was last changed by Paul Kienzle, 05Apr2017

1.4.6 Q Resolution Estimator Tool

Description

This tool is approximately estimates the resolution of \( Q \) from SAS instrumental parameter values assuming that the detector is flat and normal to the incident beam.
Using the tool

1. Select SAS Resolution Estimator from the Tool menu on the SasView toolbar.

2. Select the source (Neutron or Photon) and source type (Monochromatic or TOF).

   **NOTE!** The computational difference between the sources is only the gravitational contribution due to the mass of the particles.

3. Change the default values of the instrumental parameters as required. Be careful to note that distances are specified in cm!

4. Enter values for the source wavelength(s), \( \lambda \), and its spread (\( = \text{FWHM}/\lambda \)).

   For monochromatic sources, the inputs are just one value. For TOF sources, the minimum and maximum values should be separated by a ‘-’ to specify a range.

   Optionally, the wavelength (BUT NOT of the wavelength spread) can be extended by adding ‘; nn’ where the ‘nn’ specifies the number of the bins for the numerical integration. The default value is \( nn = 10 \). The same number of bins will be used for the corresponding wavelength spread.

5. For TOF, the default wavelength spectrum is flat. A custom spectral distribution file (2-column text: wavelength (Å) vs Intensity) can also be loaded by selecting Add new in the combo box.

6. When ready, click the Compute button. Depending on the computation the calculation time will vary.

7. 1D and 2D \( dQ \) values will be displayed at the bottom of the panel, and a 2D resolution weight distribution (a 2D elliptical Gaussian function) will also be displayed in the plot panel even if the \( Q \) inputs are outside of the detector limit (the red lines indicate the limits of the detector).

   TOF only: green lines indicate the limits of the maximum \( Q \) range accessible for the longest wavelength due to the size of the detector.

   Note that the effect from the beam block/stop is ignored, so in the small \( Q \) region near the beam block/stop

   \( \{ i.e., \ Q < (2\pi \cdot w)/(d_s \cdot \lambda_{\text{min}}), \text{ where } w \text{ is the beam block diameter, } d_s \text{ is the sample-to-detector distance, and } \lambda_{\text{min}} \text{ is the minimum wavelength.} \} \)

   the variance is slightly under estimated.

8. A summary of the calculation is written to the SasView Console at the bottom of the main SasView window.
Theory

The scattering wave transfer vector is by definition

\[ \mathbf{q} = \mathbf{k}_2 - \mathbf{k}_1 \]

\[ |q| = 4\pi/\lambda \sin(\theta/2) \]

Variance of \( q \),

\[ \sigma_q^2 \approx q^2 \left( \frac{(\Delta x)^2}{\Delta^2} + \frac{(\Delta y)^2}{\theta^2} \right) \]

\[ = \sigma_{k_1}^2 + \sigma_{k_2}^2 + \sigma_{\text{sample}}^2 + \sigma_{\text{spect}}^2 \]

where

\[ \sigma_{k_1}^2 = \sigma_{k_2}^2 + \sigma_{\text{sample}}^2 + \sigma_{\text{spect}}^2 \]

\[ = \langle \mathbf{q}^2 \rangle - \langle \mathbf{q} \rangle^2 \]

\[ = k^2 \left[ \langle T_0 \rangle + \langle T_1(r) \rangle + \langle T_2(r) \rangle + \ldots \right] \]

setting \( q = 2\pi/\lambda [T_0 + T_1(r) + T_2(r) + \ldots] \)

In the small-angle limit, the variance of \( Q \) is to a first-order approximation
The geometric and gravitational contributions can then be summarised as

<table>
<thead>
<tr>
<th>Geometric Contribution Case I:</th>
<th>Geometric Contribution Case II:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rectangular shape w/ ( x ) by ( y ) :</td>
<td>Circular shape w/ ( R ) = radius of an aperture,</td>
</tr>
<tr>
<td>( \langle r^2 \rangle_x = x^2 / 12 ), ( \langle r^2 \rangle_y = y^2 / 12 )</td>
<td>( \langle r^2 \rangle_x = R^2 / 4 ), ( \langle r^2 \rangle_y = R^2 / 4 )</td>
</tr>
<tr>
<td>1D: ( \langle r^2 \rangle_{1D} = \langle r^2 \rangle_x + \langle r^2 \rangle_y )/2</td>
<td>1D: ( \langle r^2 \rangle_{1D} = \langle r^2 \rangle_x + \langle r^2 \rangle_y )/2</td>
</tr>
</tbody>
</table>

**The wavelength contribution is always in \( R \) direction (including the gravitational effect)**

- Triangular pulse: \( b = 2 \)
- Rectangular pulse: \( b = 1 \)

\[
\sigma_{\lambda,1D}^2 = \frac{k^2}{12} \left[ \frac{b(2A \lambda^2 R^2 - R^2)^2}{L^2} \left( \frac{\Delta \lambda}{\lambda} \right)^2 \right]
\]

1D: \( \langle \sigma_{\lambda,1D}^2 \rangle = \sigma_{\lambda,1D}^2 \)

**The gravitational contribution is always in \( y \) (vertical) direction and cannot be separated from the wavelength contribution.**

See above.

The terms with \( A \) are due to the gravitation.

Finally, a Gaussian function is used to describe the 2D weighting distribution of the uncertainty in \( Q \).

**References**

1.4.7 Generic SANS Calculator Tool

Description

This tool attempts to simulate the SANS expected from a specified shape/structure or scattering length density profile. The tool can handle both nuclear and magnetic contributions to the scattering.

Theory

In general, a particle with a volume $V$ can be described by an ensemble containing $N$ 3-dimensional rectangular pixels where each pixel is much smaller than $V$.

Assuming that all the pixel sizes are the same, the elastic scattering intensity from the particle is

$$ I(\vec{Q}) = \frac{1}{V} \left| \sum_{j}^{N} v_j \beta_j \exp(i\vec{Q} \cdot \vec{r}_j) \right|^2 $$

Equation 1.

where $\beta_j$ and $r_j$ are the scattering length density and the position of the $j^{th}$ pixel respectively.

The total volume $V$

$$ V = \sum_{j}^{N} v_j $$

for $\beta_j \neq 0$ where $v_j$ is the volume of the $j^{th}$ pixel (or the $j^{th}$ natural atomic volume (= atomic mass / (natural molar density * Avogadro number) for the atomic structures).

$V$ can be corrected by users. This correction is useful especially for an atomic structure (such as taken from a PDB file) to get the right normalization.

*NOTE!* $\beta_j$ displayed in the GUI may be incorrect but this will not affect the scattering computation if the correction of the total volume $V$ is made.

The scattering length density (SLD) of each pixel, where the SLD is uniform, is a combination of the nuclear and magnetic SLDs and depends on the spin states of the neutrons as follows.

Magnetic Scattering

For magnetic scattering, only the magnetization component, $M_\perp$, perpendicular to the scattering vector $\vec{Q}$ contributes to the magnetic scattering length.
The magnetic scattering length density is then
\[
\beta_M = \frac{\gamma r_0^2 \mu_B \sigma \cdot M_{\perp}}{D_M \sigma \cdot M_{\perp}}
\]
where the gyromagnetic ratio is \( \gamma = -1.913 \), \( \mu_B \) is the Bohr magneton, \( r_0 \) is the classical radius of electron, and \( \sigma \) is the Pauli spin.

For a polarized neutron, the magnetic scattering is depending on the spin states.

Let us consider that the incident neutrons are polarised both parallel (+) and anti-parallel (-) to the \( x' \) axis (see below). The possible states after scattering from the sample are then

- Non-spin flips: (+ +) and (- -)
- Spin flips: (+ -) and (- +)

Now let us assume that the angles of the \( \vec{Q} \) vector and the spin-axis \( (x') \) to the \( x \)-axis are \( \phi \) and \( \theta_{up} \) respectively (see above). Then, depending upon the polarization (spin) state of neutrons, the scattering length densities, including the nuclear scattering length density \( \beta_N \) are given as

- for non-spin-flips
\[ \beta_{\pm \pm} = \beta_N \mp DM_{\perp x'} \]

- for spin-flips

\[ \beta_{\pm \mp} = -DM(M_{\perp y'} \pm iM_{\perp z'}) \]

where

\[
M_{\perp x'} = M_{0x} \cos \theta_{up} + M_{0y} \sin \theta_{up} \\
M_{\perp y'} = M_{0x} \cos \theta_{up} - M_{0y} \sin \theta_{up} \\
M_{\perp z'} = M_{0z} \\
M_{0x} = (M_{0x} \cos \phi - M_{0y} \sin \phi) \cos \phi \\
M_{0y} = (M_{0y} \sin \phi - M_{0y} \cos \phi) \sin \phi
\]

Here the \( M_{0x}, M_{0y} \) and \( M_{0z} \) are the \( x, y \) and \( z \) components of the magnetisation vector in the laboratory \( x-y-z \) frame.

### Using the tool

After computation the result will appear in the Theory box in the SasView Data Explorer panel.

\( Up\_frac\_in \) and \( Up\_frac\_out \) are the ratio

\[
\frac{\text{spin up}}{\text{spin up} + \text{spin down}}
\]
of neutrons before the sample and at the analyzer, respectively.

**NOTE 1.** The values of $Up_{frac\_in}$ and $Up_{frac\_out}$ must be in the range 0.0 to 1.0. Both values are 0.5 for unpolarized neutrons.

**NOTE 2.** This computation is totally based on the pixel (or atomic) data fixed in xyz coordinates. No angular orientational averaging is considered.

**NOTE 3.** For the nuclear scattering length density, only the real component is taken account.

### Using PDB/OMF or SLD files

The SANS Calculator tool can read some PDB, OMF or SLD files but ignores polarized/magnetic scattering when doing so, thus related parameters such as $Up_{frac\_in}$, etc, will be ignored.

The calculation for fixed orientation uses Equation 1 above resulting in a 2D output, whereas the scattering calculation averaged over all the orientations uses the Debye equation below providing a 1D output

$$I(|\vec{Q}|) = \frac{1}{V} \sum_{j}^{N} v_{j} \beta_{j} \sum_{k}^{N} v_{k} \beta_{k} \frac{\sin(|\vec{Q}||r_{j} - r_{k}|)}{|\vec{Q}||r_{j} - r_{k}|}$$

where $v_{j} \beta_{j} \equiv b_{j}$ is the scattering length of the $j^{th}$ atom. The calculation output is passed to the Data Explorer for further use.

---

**Note:** This help document was last changed by Steve King, 01May2015
1.4.8 Python Shell-Editor Tool

Description

This is a Python shell/editor provided with WxPython.

For the help about Python, visit the website http://docs.python.org/tutorial/

Note: This shell/editor has its own help, but the Help() and Credits() calls do not work on Macs.

The NumPy, SciPy, and Matplotlib, etc, libraries are shipped with SasView and so functions from these can be imported into the shell/editor, however, some functionality may not work.

When a Python file, for example a fitting model, is created or loaded with the New or Open options from the menu, a new tab opens with an editing notebook.
If a Python (.py) model has a linked C (.c) subroutine in the same folder then the shell/editor will open both! However input focus is usually transferred to the tab with the .c file.

To compile a model, select Run > Check Model from the shell/editor menu. If the model contains a unit test (which it should!!!) then this will also run and a popup window will report the success/failure of the test.

**Note:** This help document was last changed by Steve King, 10Oct2015

### 1.4.9 Image Viewer Tool

**Description**

This tool loads image files and displays them as 2D (x-y coordinate against counts per pixel). The plot can then can be saved, printed, and copied. The plot can also be resized by dragging the corner of the panel.

The supported input image formats are:

- BMP (bitmap format)
- GIF (graphical interchange format)
- JPG (joint photographic experts group format)
- PNG (portable network graphics format)
- TIF (tagged image format)

Using the tool

1. Select Image Viewer from the Tool menu on the SasView toolbar.
2. Select a file and then click Open. If the loading is successful the image will be displayed.
3. To save, print, or copy the image, or to apply a grid overlay, right-click anywhere in the plot.
4. If the image is taken from a 2D detector, SasView can attempt to convert the colour/grey scale into pseudo-intensity 2D data using

\[ z = (0.299 \times R) + (0.587 \times G) + (0.114 \times B) \]

unless the image is formatted as 8-bit grey-scale TIF.

5. In the Convert to Data dialog, set the parameters relevant to the data and then click the OK.

**Note:** This help document was last changed by Steve King, 01May2015
1.4.10 File Converter Tool

Description

This tool converts file formats with the Q data and Intensity data stored in separate files, into a single CanSAS (XML) or NXcanSAS (HDF5) file.

It can also convert 2D BSL/OTOKO files into a NXcanSAS file.

Supported input file formats (examples may be found in the /test/convertible_files folder):

- Single-column ASCII data, with lines that end without any delimiter, or with a comma or semi-colon delimiter
- 2D ISIS ASCII formatted data
- 1D BSL/OTOKO format data
- 2D BSL/OTOKO format data

Supported output file formats:

- CanSAS
- NXcanSAS

Using the Tool

1. Select the files containing your Q-axis and Intensity-axis data
2. Choose whether the files are in ASCII 1D, ASCII 2D, 1D BSL/OTOKO or 2D BSL/OTOKO format
3. Choose where you would like to save the converted file
4. Optionally, input some metadata such as sample size, detector name, etc
5. Click Convert to save the converted file

Files With Multiple Frames

If a BSL/OTOKO file with multiple frames is selected for the Intensity-axis file, a dialog will appear asking which frames you would like converted. You may enter a start frame, end frame & increment, and all frames in that subset will be converted. For example, entering 0, 50 and 10 will convert frames 0, 10, 20, 30, 40 & 50.

To convert a single frame, enter the same value for first frame & last frame, and 1 as the increment.

CanSAS XML files can become quite large when exporting multiple frames to a single file, so there is an option in the Select Frame dialog to output each frame to its own file. The single file option will produce one file with multiple <SASdata> elements. The multiple file option will output a separate file with one <SASdata> element for each frame. The frame number will also be appended to the file name.

The multiple file option is not available when exporting to NXcanSAS because the HDF5 format is more efficient at handling large amounts of data.

Note: This help document was last changed by Steve King, 08Oct2016

1.5 Working with SasView

Note: In Windows use [Alt]-[Cursor left] to return to the previous page
1.5.1 Data Formats

SasView reads several different 1D SAS ($I(Q)$ vs $Q$), 2D SAS($I(Q_x,Q_y)$ vs $(Q_x,Q_y)$) and 1D SESANS ($P(z)$ vs $z$) data files. From SasView 4.1 onwards, a File Converter Tool allows some legacy formats to be converted into modern formats that SasView will read.

1D SAS Formats

SasView will read ASCII (‘text’) files with 2 to 4 columns of numbers in the following order:

$Q, I(Q), (dI(Q), dQ(Q))$

where $dQ(Q)$ is the instrumental resolution in $Q$ and assumed to have originated from pinhole geometry.

Numbers can be separated by spaces or commas.

SasView recognises the following file extensions which are not case-sensitive:

- .TXT
- .DAT
- .XML (in canSAS format v1.0 and 1.1)
- .H5 (as NeXus NXcanSAS only)
- .NXS (as NeXus NXcanSAS only)

Note: From SasView version 4.2 onwards files written in the NIST .ASC format are no longer read. This is because that format normally represents raw and not reduced data.

If using CSV output from, for example, a spreadsheet, ensure that it is not using commas as delimiters for thousands.

The SasView File Converter Tool available in SasView 4.1 onwards can be used to convert data sets with separated $I(Q)$ and $Q$ files (for example, BSL/OTOKO, and some output from FIT2D and other SAXS-oriented software) into either the canSAS SASXML (XML) format or the NeXus NXcanSAS (HDF5) format.

For a description of the CanSAS/SASXML format see: http://www.cansas.org/formats/canSAS1d/1.1/doc/

For a description of the ISIS 1D format see: https://www.isis.stfc.ac.uk/Pages/colette-ascii-file-format-descriptions.pdf

For a description of the NXcanSAS format see: http://cansas-org.github.io/NXcanSAS/classes/contributed_definitions/NXcanSAS.html

All the above formats are written by the Mantid Framework.

For a description of the NIST 1D format see: http://danse.chem.utk.edu/trac/wiki/NCNROutput1D_IQ

For a description of the BSL/OTOKO format see: http://www.diamond.ac.uk/Beamlines/Soft-Condensed-Matter/small-angle/SAXS-Software/CCP13/BSL.html

2D SAS Formats

SasView will read ASCII (‘text’) files in the NIST 2D format (with the extension .DAT) or files in the NeXus NXcanSAS (HDF5) format (with the extension .H5 or .NXS). File extensions are not case-sensitive. Both of these formats are written by the Mantid Framework.

Most of the header lines in the NIST 2D format can actually be removed except the last line, and only the first three columns ($Q_x$, $Q_y$, and $I(Q_x,Q_y)$) are actually required.
Note: From SasView version 4.2 onwards files written in the NIST .ASC format are no longer read. This is because that format normally represents raw and not reduced data.

Note: SasView does not read the standard NeXus format, only the NXcanSAS subset.

The SasView File Converter Tool available in SasView 4.1 onwards can be used to convert data sets in the 2D BSL/OTOKO format into the NeXus NXcanSAS (HDF5) format.

For a description of the NIST 2D format see: http://danse.chem.utk.edu/trac/wiki/NCNROutput1D_2DQxQy

For a description of the NXcanSAS format see: http://cansas-org.github.io/NXcanSAS/classes/contributed_definitions/NXcanSAS.html

For a description of the BSL/OTOKO format see: http://www.diamond.ac.uk/Beamlines/Soft-Condensed-Matter/small-angle/SAXS-Software/CCP13/BSL.html

1D SESANS Format

SasView version 4.1 onwards will read ASCII (‘text’) files in a prototype SESANS standard format (with the extensions .SES or .SESANS). The file extensions are not case-sensitive.

The file format has a list of name-value pairs at the top of the file which detail the general experimental parameters necessary for fitting and analyzing data. This list should contain all the information necessary for the file to be ‘portable’ between users.

Following the header is a 8 (only the first 4 are really needed) column list of instrument experimental variables:

- Spin echo length (z, in Angstroms)
- depolarization ($\log(P/P_0)/(\lambda^2 \times \text{thickness})$, in Angstrom$^{-1}$ cm$^{-1}$)
- depolarization error in the same unit (measurement error)
- Spin echo length error ($\Delta z$, in Angstroms) (experimental resolution)
- Neutron wavelength ($\lambda$, in Angstroms)
- Neutron wavelength error ($\Delta \lambda$, in Angstroms)
- Normalized polarization ($P/P_0$, unitless)
- Normalized polarization error ($\Delta (P/P_0)$, unitless) (measurement error)

Note: This help document was last changed by Wim Bouwman, 05Apr2017

1.5.2 Loading Data

The data explorer

Data Explorer is a panel that allows the user more interactions with data. Some functionalities provided by the Data Explorer are also available through the context menu of plot panels or other menus within the application.

Under View in the menu bar, Data Explorer can be toggled between Show and Hide by clicking Show/Hide Data Explorer.

NOTE! When Data Explorer is hidden, all data loaded will be sent directly to the current active analysis, if possible. When Data Explorer is shown, data go first to the Data Explorer.
Loading data

To load data, do one of the following:
- Select File -> Load Data File(s), and navigate to your data;
- Select File -> Load Data Folder, which will attempt to load all the data in the specified folder;
- Or, in the Data Explorer click the button Load Data, then select one or more (by holding down the Ctrl key) files to load into SasView.

The name of each loaded file will be listed in the Data Explorer. Clicking the + symbol alongside will display any available metadata read from the file.

The handy menu

Right-clicking on a loaded dataset (or model calculation, what SasView calls a ‘theory’) brings up a Handy Menu from which it is possible to access Data Info, Save the data/theory, or Plot the data/theory.

Activating data

To interact with data it must be activated. This is accomplished by checking the box next to the file name in the Data Explorer. A green tick will appear.

Unchecking/unticking a box deactivates that data set.

There is also a combo box labeled Selection Options from which you can activate or deactivate multiple data sets in one go.

Removing data

WARNING! Remove Data will stop any data operations currently using the selected data sets.

Remove Data removes all references to selected data from SasView.
Creating a new plot

Click on the New Plot button to create a new plot panel where the currently selected data will be plotted.

Appending plots to a graph

This operation can currently only be performed on 1D data and plot panels containing 1D data.

Click on the button Append Plot To to add selected data to a plot panel. Next to the button is a combo box containing the names of available plot panels. Selecting a name from this combo box will move that plot into focus.

If a plot panel is not available, the combo box and button will be disabled.

2D Data cannot be appended to any plot panels.

Freezing the theory

The Freeze Theory button generates data from the selected theory.

NOTE! This operation can only be performed when theory labels are selected in the Data panel.

Sending data to applications

Click on the Send To button to send the currently selected data to one of the available types of analysis (Fitting, P(r) Inversion, or Invariant calculation).

The Single/Batch mode radio buttons only apply to Fitting.

Batch mode provides serial (batch) fitting with one model function, that is, fitting one data set followed by another. If several data sets need to be fitted at the same time, use Simultaneous fitting under the Fitting option on the menu bar.

1.5.3 Plotting Data/Models

SasView generates three different types of graph window: one that displays 1D data (i.e., $I(Q)$ vs $Q$), one that displays 1D residuals (i.e., the difference between the experimental data and the theory at the same $Q$ values), and 2D color maps.

Graph window options

Invoking the graph menu

To invoke the Graph Menu simply right-click on a data/theory plot, or click the Graph Menu (bullet list) icon in the toolbar at the bottom of the plot. Then select a menu item.

How to Hide-Show-Delete a graph

To expand a plot window, click the Maximise (square) icon in the top-right corner.

To shrink a plot window, click the Restore down (square-on-square) icon in the top-right corner.

To hide a plot, click the Minimise (-) icon in the top-right corner of the plot window.
To show a hidden plot, select the *Restore up* (square-on-square) icon on the minimised window.

To delete a plot, click the *Close* (x) icon in the top-right corner of the plot window.

**Note:** If a residuals graph (when fitting data) is hidden, it will not show up after computation.

**Dragging a plot**

Select the *Pan* (crossed arrows) icon in the toolbar at the bottom of the plot to activate this option. Move the mouse pointer to the plot. It will change to a hand. Then left-click and drag the plot around. The axis values will adjust accordingly.

To disable dragging mode, unselect the *crossed arrows* icon on the toolbar.

**Zooming In-Out on a plot**

Select the *Zoom* (magnifying glass) button in the toolbar at the bottom of the plot to activate this option. Move the mouse pointer to the plot. It will change to a cross-hair. Then left-click and drag the pointer around to generate a region of interest. Release the mouse button to generate the new view.

To disable zoom mode, unselect the *Zoom* button on the toolbar.

After zooming in on a a region, the *left arrow* or *right arrow* buttons on the toolbar will switch between recent views.

The axis range can also be specified manually. To do so go to the *Graph Menu* (see *Invoking the graph menu* for further details), choose the *Set Graph Range* option and enter the limits in the pop box.

**NOTE! If a wheel mouse is available scrolling the wheel will zoom in/out on the current plot (changing both axes). Alternatively, point at the numbers on one axis and scroll the wheel to zoom in/out on just that axis.**

To return to the original view of the data, click the the *Reset* (home) icon in the toolbar at the bottom of the plot (see *Resetting the graph* for further details).

**Saving a plot image**

To save the current plot as an image file, right click on the plot to bring up the *Graph Menu* (see *Invoking the graph menu*) and select *Save Image*. Alternatively, click on the *Save* (floppy disk) icon in the toolbar at the bottom of the plot.

A dialog window will open. Select a folder, enter a filename, choose an output image type, and click *Save*.

The currently supported image types are:

- EPS (encapsulated postscript)
- EMF (enhanced metafile)
- JPG/JPEG (joint photographics experts group)
- PDF (portable document format)
- PNG (portable network graphics)
- PS (postscript)
- RAW/RGHA (bitmap, stored as 935x635 pixels of depth 8)
- SVG/SVGA (scalable vector graphics)
- TIF/TIFF (tagged image file)
Printing a plot

To send the current plot to a printer, click on the Print (printer) icon in the toolbar at the bottom of the plot.

Resetting the graph

To reset the axis range of a graph to its initial values select Reset Graph Range on the Graph Menu (see Invoking_the_graph_menu). Alternatively, use the Reset (home) icon in the toolbar at the bottom of the plot.

Modifying the graph

It is possible to make custom modifications to plots including:
- changing the plot window title
- changing the default legend location and toggling it on/off
- changing the axis label text
- changing the axis label units
- changing the axis label font & font colour
- adding/removing a text string
- adding a grid overlay

The legend and text strings can be drag and dropped around the plot.

These options are accessed through the Graph Menu (see Invoking_the_graph_menu) and selecting Modify Graph Appearance (for axis labels, grid overlay and legend position) or Add Text to add textual annotations, selecting font, color, style and size. Remove Text will remove the last annotation added. To change the legend, Window Title allows a custom title to be entered instead of Graph x.

Changing scales

This menu option is only available with 1D data.

From the Graph Menu (see Invoking_the_graph_menu) select Change Scale. A dialog window will appear in which it is possible to choose different transformations of the x (usually Q) or y (usually I(Q)) axes, including:
- x, x^2, x^4, ln(x), log10(x), log10(x^4)
- y, 1/y, ln(y), y^2, y.(x^4), 1/sqrt(y), log10(y), ln(y.x), ln(y.x^2), ln(y.x^4), log10(y.x^4)

A View option includes short-cuts to common SAS transformations, such as:
- linear
- Guinier
- X-sectional Guinier
- Porod
- Kratky

For properly corrected and scaled data, these SAS transformations can be used to estimate, for example, Rg, rod diameter, or SANS incoherent background levels, via a linear fit (see Making_a_linear_fit).
Toggling scales

This menu option is only available with 2D data.

From the Graph Menu (see Invoking the graph menu) select Toggle Linear/Log Scale to switch between a linear to log intensity scale. The type of scale selected is written alongside the colour scale.

2D color maps

This menu option is only available with 2D data.

From the Graph Menu (see Invoking the graph menu) select 2D Color Map to choose a different color scale for the image and/or change the maximum or minimum limits of the scale.

Getting data coordinates

Clicking anywhere in the plot window will cause the current coordinates to be displayed in the status bar at the very bottom-left of the SasView window.

Dataset menu options

Invoking the dataset menu

From the Graph Menu (see Invoking the graph menu) highlight a plotted dataset.

Getting data info

In the Dataset Menu (see Invoking the dataset menu), highlight a data set and select DataInfo to bring up a data information dialog panel for that data set.

Saving data

In the Dataset Menu (see Invoking the dataset menu), select Save Points as a File (if 1D data) or Save as a file(DAT) (if 2D data). A save dialog will appear.

1D data can be saved in either ASCII text (.TXT) or CanSAS/SASXML (.XML) formats (see Data Formats).

2D data can only be saved in the NIST 2D format (.DAT) (see Data Formats).

Making a linear fit

Linear fit performs a simple \( y(x) = ax + b \) linear fit within the plot window.

In the Dataset Menu (see Invoking the dataset menu), select Linear Fit. A fitting dialog will appear. Set some initial parameters and data limits and click Fit. The fitted parameter values are displayed and the resulting line calculated from them is added to the plot.

This option is most useful for performing simple Guinier, XS Guinier, and Porod type analyses, for example, to estimate \( R_g \), a rod diameter, or incoherent background level, respectively.

The following figure shows an example of a Guinier analysis using this option.
Removing data from the plot

In the Dataset Menu (see Invoking_the_dataset_menu), select Remove. The selected data will be removed from the plot.

**Note:** The Remove data set action cannot be undone.

Show-Hide error bars

In the Dataset Menu (see Invoking_the_dataset_menu), select Show Error Bar or Hide Error Bar to switch between showing/hiding the errors associated with the chosen dataset.

Modify plot properties

In the Dataset Menu (see Invoking_the_dataset_menu), select Modify Plot Property to change the size, color, or shape of the displayed marker for the chosen dataset, or to change the dataset label that appears in the plot legend box.

2D data averaging

**Purpose**

This feature is only available with 2D data.

2D data averaging allows you to perform different types of averages on your data. The region to be averaged is displayed in the plot window and its limits can be modified by dragging the boundaries around.
How to average

In the Dataset Menu (see Invoking_the_dataset_menu), select one of the following averages

- Perform Circular Average
- Sector [Q view]
- Annulus [Phi view]
- Box sum
- Box averaging in Qx
- Box averaging on Qy

A ‘slicer’ will appear (except for Perform Circular Average) in the plot that you can drag by clicking on a slicer’s handle. When the handle is highlighted in red, it means that the slicer can move/change size.

**NOTE! The slicer size will reset if you try to select a region greater than the size of the data.**

Alternatively, once a ‘slicer’ is active you can also select the region to average by bringing back the Dataset Menu and selecting Edit Slicer Parameters and Batch Fitting. A dialog window will appear in which you can enter values to define a region, select the number of points to plot (nbins), or apply the slicer to any or all other 2D data plots.

A separate plot window will also have appeared, displaying the requested average.

**Note:** The displayed average only updates when input focus is moved back to that window; ie, when the mouse pointer is moved onto that plot.

Selecting Box Sum automatically brings up the ‘Slicer Parameters’ dialog in order to display the average numerically, rather than graphically.

To remove a ‘slicer’, bring back the Dataset menu and select Clear Slicer.

**Batch Slicing**

A slicer can be applied to any or all existing 2D data plots using the ‘Slicer Parameters’ window. To open the window, select Edit Slicer Parameters and Batch Fitting in the Dataset Menu (see Invoking_the_dataset_menu). Batch slicing options are available at the bottom of the window.

Select the 2D plots you want to apply the slicer to. All 2D plots are selected by default. The resulting 1D data for all slicers can be saved as a text file and then sent to fitting by selecting the Auto save generated 1D check box. Sending data to the fitting perspective requires the data be saved.

Once the auto save check box is selected, you can select where the files are saved. The file name for the saved data is the slicer name plus the file name of the original data set, plus what is in the Append to file name field. The default value in the append to field includes the names and values for all of the slicer parameters.

The batch of slices can be sent to fitting if desired, with three options available. The first is to not fit the data, the second is to send the slices to individual fit pages, and the third is to send all sliced data to a single batch fit window.

Clicking Apply Slicer to Selected Plots will create a slicer for each selected plot with the parameters entered in the ‘Slicer Parameters’ window. Depending on the options selected the data may then be saved, loaded as separate data sets in the data manager panel, and finally sent to fitting.

**Unmasked circular average**

This operation will perform an average in constant $Q$ rings around the (x,y) pixel location of the beam center.
**Masked circular average**

This operation is the same as ‘Unmasked Circular Average’ except that any masked region is excluded.

**Sector average [Q View]**

This operation averages in constant $Q$ arcs.

The width of the sector is specified in degrees ($\pm \delta |\phi|$) each side of the central angle $\phi$.

**Annular average [$\phi$]**

This operation performs an average between two $Q$ values centered on (0,0), and averaged over a specified number of pixels.

The data is returned as a function of angle $\phi$ in degrees with zero degrees at the 3 O’clock position.

**Box sum**

This operation performs a sum of counts in a 2D region of interest.

When editing the slicer parameters, the user can enter the length and the width the rectangular slicer and the coordinates of the center of the rectangle.

**Box Averaging in Qx**

This operation computes an average $I(Q_x)$ for the region of interest.

When editing the slicer parameters, the user can control the length and the width the rectangular slicer. The averaged output is calculated from constant bins with rectangular shape. The resultant $Q$ values are nominal values, that is, the central value of each bin on the x-axis.

**Box Averaging in Qy**

This operation computes an average $I(Q_y)$ for the region of interest.

When editing the slicer parameters, the user can control the length and the width the rectangular slicer. The averaged output is calculated from constant bins with rectangular shape. The resultant $Q$ values are nominal values, that is, the central value of each bin on the x-axis.

---

**Note:** This help document was last modified by Paul Butler, 05 September, 2016

### 1.5.4 Test Data

Test data sets are included as a convenience to our users. Look in the test sub-folder in your SasView installation folder.

The test data sets are organized based on their data structure:

- 1D data
- convertible 1D data files
- 2D data
1D Data

1D data sets EITHER have:

• at least two columns of data with I(Q) (assumed to be in absolute units) on the y-axis and Q on the x-axis. And additional columns of data may carry uncertainty data, resolution data, or other metadata.

OR:

• the I(Q) and Q data in separate files with no other information.

Data in the latter format need to be converted to a single file format with the File Converter Tool before they can be analysed in SasView. Test files are located in the /convertible_files folder.

1D Test Data

33837rear_1D_1.75_16.5
• Data from a magnetically-oriented surfactant liquid crystal output by the Mantid framework. The data was collected on the SANS2D instrument at ISIS.

10wtAOT_Reline_120_reduced / Anton-Paar / sascess_example
• Data from Anton-Paar SAXSess instruments saved in Otto Glatter’s PDH format.

AOT_Microemulsion
• Aerosol-OT surfactant stabilised oil-in-water microemulsion data at three contrasts: core (oil core), drop (oil core + surfactant layer), and shell (surfactant layer).
• Suitable for testing simultaneous fitting.

APS_DND-CAT
• ASCII data from the DND-CAT beamline at the APS.

hSDS_D2O
• h25-sodium dodecyl sulphate solutions at two concentrations: 0.5wt% (just above the cmc), 2wt% (well above the cmc), and 2wt% but with 0.2mM NaCl electrolyte.
• Suitable for testing charged S(Q) models.

ISIS_83404 / ISIS_98929
• Polyamide-6 fibres hydrated in D2O exhibiting a broad lamellar peak from the semi-crystalline nanostructure.
• This is the same data as that in the BSL/OTOKO Z8300* / Z9800* files but in an amalgamated ASCII format!
• Suitable for testing Correlation Function Analysis.

ISIS_Polymer_Blend_TK49
• Monodisperse (Mw/Mn~1.02) 49wt% d8-polystyrene : 51wt% h8-polystyrene polymer blend.
• Suitable for testing Poly_GaussCoil and RPA10 models.

P123_D2O
• Lyotropic liquid crystalline solutions of non-ionic ABA block copolymer Pluronic P123 in water at three concentrations: 10wt%, 30wt%, and 40wt%.
• Suitable for testing paracrystal models.

Convertible 1D Data

APS_X / APS_Y
• ASCII data output by a reduction software package at the APS.
• Suitable for testing the File Converter Tool.

FIT2D_I / FIT2D_Q
• ASCII data output by the FIT2D software package at the ESRF.
• Suitable for testing the File Converter Tool.

Z8300*.I1D / Z8300*.QAX / Z9800*.I1D / Z9800*.QAX
• BSL/OTOKO data from polyamide-6 fibres hydrated in D2O exhibiting a broad lamellar peak from the semi-crystalline nanostructure.
• This is the same data as that in ISIS_83404 / ISIS_98929 but in an older separated format!
• Suitable for testing the File Converter Tool.
• Suitable for testing Correlation Function Analysis.

2D Data

2D data sets are data sets that give the reduced intensity for each Qx-Qy bin. Depending on the file format, uncertainty data and metadata may also be available.

2D Test Data

33837rear_2D_1.75_16.5
• Data from a magnetically-oriented surfactant liquid crystal output by the Mantid framework. The data was collected on the SANS2D instrument at ISIS.

P123_D2O
• Lyotropic liquid crystalline solutions of non-ionic ABA block copolymer Pluronic P123 in water at three concentrations: 10wt%, 30wt%, and 40wt%.
• Suitable for testing paracrystal models.

Coordinate Data

Coordinate data sets, such as PDB or OMF files, and which describe a specific structure, are designed to be read and viewed in the Generic SANS Calculator Tool.

Coordinate Test Data

A_Raw_Example-1
• OMF format data file from a simulation of magnetic spheres.

diamond
• PDB format data file for diamond.
dna

- PDB format data file for DNA.

sld_file

- Example SLD format data file.

**Image Data**

Image data sets are designed to be read by the *Image Viewer Tool*. They can be converted into synthetic 2D data.

**Image Test Data**

**ISIS_98940**

- Polyamide-6 fibres hydrated in D2O exhibiting a broad lamellar peak from the semi-crystalline nanostructure.
- Data is presented in Windows Bitmap (BMP), GIF, JPEG (JPG), PNG, and TIFF (TIF) formats.

**SESANS Data**

SESANS (Spin-Echo SANS) data sets primarily contain the neutron polarisation as a function of the spin-echo length. Also see *SANS to SESANS conversion*.

**SESANS Test Data**

**spheres2micron**

- SESANS data from 2 micron polystyrene spheres in 53% H2O / 47% D2O.

**Save States**

Saved states are projects and analyses saved by the SasView program. A single analysis file contains the data and parameters for a single fit (.fit), p(r) inversion (.prv), or invariant calculation (.inv). A project file (.svs) contains the results for every active analysis in a SasView session.

**Saved State Test Data**

**fitstate.fitv**

- a saved fitting analysis.

**test.inv**

- a saved invariant analysis.

**test002.inv**

- a saved invariant analysis.

**prstate.prv**

- a saved P(r) analysis.

**newone.svs**

- a saved SasView project.
Upcoming Formats

Data in this folder are in formats that are not yet implemented in SasView but which might be in future versions of the program.

Other Test Data

phi_weights.txt
radius_dist.txt
THETA_weights.txt

Note: This help document was last changed by Steve King, 06Oct2016

1.5.5 Tutorials

Note: In Windows use [Alt]-[Cursor left] to return to the previous page

The following tutorial was written for Version 2.x but is still a useful overview of much of the analysis capability in SasView (but disregard Appendix XIII if using Version 4.2 or later)

Old Tutorial
The following tutorials have been written for Version 4.x
Getting Started with Sasview
Basic 1D Fitting in Sasview
Simultaneous 1D Fitting in Sasview
Correlation Function Analysis in SasView

1.5.6 Environment Variables

SasView creates and uses a number of environment variables:

- **SAS_MODELPATH=path**
  - sets the directory containing custom models
- **SAS_DLL_PATH=path**
  - sets the path to the compiled modules
- **SAS_WEIGHTS_PATH=~/.sasview/weights**
  - sets the path to custom distribution files (see Polydispersity & Orientational Distributions)
- **XDG_CACHE_HOME=~/.cache**
  - sets the pyopencl cache root (linux only)
- **SAS_COMPILER=tinycc|msvc|mingw|unix**
  - sets the DLL compiler
- **SAS_OPENCL=vendor:device|none**
  - sets the target OpenCL device for GPU computations
- use none to disable

- SAS_OPENMP=1|0
  - turns on/off OpenMP multi-processing of the DLLs

Document History

2018-07-20 Steve King

1.5.7 Model Marketplace

The Model Marketplace allows members of the SAS Community to contribute plug-in fitting models for SasView for all to use.

**Note:** These plug-in models require SasView version 4.0 or later. However, not all models may work with every version of SasView because of changes to our API.

Contributed models should be written in Python (only version 2.7.x is currently supported) or, if computational speed is an issue, in a combination of Python and C. You only need to upload the .py/.c source code files to the Marketplace!

Please put a comment in your code to indicate which version of SasView you wrote the model for.

For guidance on how to write a plugin model see *Writing a Plugin Model*. It may also be helpful to examine the library models in the /sasmodels-data/models sub-folder of your SasView installation directory.

The Marketplace also provides the option to upload a SasView text file of the scattering function data computed by your model. If you do this a graph of the scattering function will appear under the Marketplace entry for your model.

**Note:** The SasView Development Team regret to say that they do not have the resources to fix the bugs or polish the code in every model contributed to the Marketplace!
2.1 Contents

2.1.1 SasView

sas package

Subpackages

sas.sascalc package

Subpackages

sas.sascalc.calculator package

Submodules

sas.sascalc.calculator.BaseComponent module

Provide base functionality for all model components

```python
class sas.sascalc.calculator.BaseComponent.BaseComponent
    Basic model component

    Since version 0.5.0, basic operations are no longer supported.

calculate_ER()
    Calculate effective radius

calculate_VR()
    Calculate volume fraction ratio

close()
    Returns a new object identical to the current object

evalDistribution(qdist)
    Evaluate a distribution of q-values.
    * For 1D, a numpy array is expected as input:
```
where \( q \) is a numpy array.

- For 2D, a list of numpy arrays are expected: \([q_{x\prime}, q_{y\prime}]\), where 1D arrays,

\[
q_{x\prime} = [ qx[0], qx[1], qx[2], ... ]
\]

and

\[
q_{y\prime} = [ qy[0], qy[1], qy[2], ... ]
\]

Then get

\[
q = np.sqrt(q_{x\prime}^2 + q_{y\prime}^2)
\]

that is a qr in 1D array;

\[
q = [q[0], q[1], q[2], ...]
\]

**Note:** Due to 2D speed issue, no anisotropic scattering is supported for python models, thus C-models should have their own evalDistribution methods.

The method is then called the following way:

\[
evalDistribution(q)
\]

where \( q \) is a numpy array.

**Parameters**

- \( qdist \) – ndarray of scalar q-values or list \([qx, qy]\) where \(qx, qy\) are 1D ndarrays

getDispParamList()  
Return a list of all available parameters for the model

getParam(name)  
Set the value of a model parameter :param name: name of the parameter

getParamList()  
Return a list of all available parameters for the model

getParamListWithToken(token, member)  
get Param List With Token

getParamWithToken(name, token, member)  
get Param With Token

getProfile()  
Get SLD profile  
: return: \((z, beta)\) where \(z\) is a list of depth of the transition points \(beta\) is a list of the corresponding SLD values

is_fittable(par_name)  
Check if a given parameter is fittable or not

Parameters \(par\_name\) – the parameter name to check

run(x)  
run 1d

runXY(x)  
run 2d

setParam(name, value)  
Set the value of a model parameter

Parameters
• name – name of the parameter
• value – value of the parameter

```
setParamWithToken (name, value, token, member)
set Param With Token
set Dispersion (parameter, dispersion)
model dispersions
```

**sas.sascalc.calculator.instrument module**

This module is a small tool to allow user to control instrumental parameters.

**class** sas.sascalc.calculator.instrument.Aperture

Bases: object

An object class that defines the aperture variables

```
set_sample_distance (distance=[])
Set the sample aperture distance
set_sample_size (size=[])
Set the sample aperture size
set_source_size (size=[])
Set the source aperture size
```

**class** sas.sascalc.calculator.instrument.Detector

Bases: object

An object class that defines the detector variables

```
set_distance (distance=[])
Set the detector distance
set_pix_size (size=[])
Set the detector pix_size
set_size (size=[])
Set the detector size
```

**class** sas.sascalc.calculator.instrument.Neutron

Bases: object

An object that defines the wavelength variables

```
get_band ()
To get the wavelength band
get_default_spectrum ()
get default spectrum
get_intensity ()
To get the value of intensity
get_mass ()
To get the neutron mass
get_random_value ()
To get the value of wave length
get_spectrum ()
To get the wavelength spectrum
get_wavelength ()
To get the value of wavelength
```
get_wavelength_spread()
To get the value of wavelength spread

plot_spectrum()
To plot the wavelength spectrum: requirement: matplotlib.pyplot

set_band(band=[1])
To set the wavelength band

    Parameters band – array of [min, max]

set_full_band()
set band to default value

set_intensity(intensity=368428)
Sets the intensity in counts/sec

set_mass(mass=1.67492729e-24)
Sets the wavelength

set_spectrum(spectrum)
Set spectrum

    Parameters spectrum – numpy array

set_wavelength(wavelength=6.0)
Sets the wavelength

set_wavelength_spread(spread=0.125)
Sets the wavelength spread

setup_spectrum()
To set the wavelength spectrum, and intensity, assumes wavelength is already within the spectrum

class sas.sascalc.calculator.instrument.Sample
Bases: object
An object class that defines the sample variables

set_distance(distance=[])
Set the sample distance

set_size(size=[])
Set the sample size

set_thickness(thickness=0.0)
Set the sample thickness

class sas.sascalc.calculator.instrument.TOF
Bases: sas.sascalc.calculator.instrument.Neutron
TOF: make list of wavelength and wave length spreads

get_intensity_list()
get list of the intensity wrt wavelength_list

get_wave_list()
Get wavelength and wavelength_spread list

set_wave_list(wavelength=[])
Set wavelength list

    Parameters wavelength – list of wavelengths

set_wave_spread_list(wavelength_spread=[])
Set wavelength_spread list

    Parameters wavelength_spread – list of wavelength spreads

sas.sascalc.calculator.instrument.validate(value=None)
Check if the value is float > 0.0
**sas.sascalc.calculator.kiessig_calculator module**

This module is a small tool to allow user to quickly determine the size value in real space from the fringe width in q space.

```python
class sas.sascalc.calculator.kiessig_calculator.KiessigThicknessCalculator
    Bases: object
    compute thickness from the fringe width of data
    compute_thickness()
        Calculate thickness.
        Returns the thickness.
    get_deltaq()
        return deltaQ value in 1/A unit
    get_thickness_unit()
        Returns the thickness unit.
    set_deltaq(dq=None)
        Receive deltaQ value
        Parameters dq – q fringe width in 1/A unit
```

**sas.sascalc.calculator.resolution_calculator module**

This object is a small tool to allow user to quickly determine the variance in q from the instrumental parameters.

```python
class sas.sascalc.calculator.resolution_calculator.ResolutionCalculator
    Bases: object
    compute resolution in 2D
    compute(wavelength, wavelength_spread, qx_value, qy_value, coord='cartesian', tof=False)
        Compute the Q resoltuion in ll and + direction of 2D : qx_value: x component of q : qy_value: y component of q
    compute_and_plot(qx_value, qy_value, qx_min, qx_max, qy_min, qy_max, coord='cartesian')
        Compute the resolution : qx_value: x component of q : qy_value: y component of q
    get_all_instrument_params()
        Get all instrumental parameters
    get_default_spectrum()
        Get default_spectrum
    get_detector_pix_size()
        Get detector pixel size
    get_detector_qrange()
        get max detector q ranges
        : return: qx_min, qx_max, qy_min, qy_max tuple
    get_detector_size()
        Get detector size
    get_image(qx_value, qy_value, sigma_1, sigma_2, sigma_r, qx_min, qx_max, qy_min, qy_max, coord='cartesian', full_cal=True)
        Get the resolution in polar coordinate ready to plot : qx_value: qx_value value : qy_value: qy_value
```
value : sigma_1: variance in r direction : sigma_2: variance in phi direction : coord: coordinate system of image, ‘polar’ or ‘cartesian’

**get_intensity** ()
Get intensity

**get_intensity_list** ()
Set wavelength spread

**get_neutron_mass** ()
Get Neutron mass

**get_sample2detector_distance** ()
Get detector sample2detector_distance

**get_sample2sample_distance** ()
Get detector sampleslitsample_distance

**get_sample_aperture_size** ()
Get sample aperture size

**get_source2sample_distance** ()
Get detector source2sample_distance

**get_source_aperture_size** ()
Get source aperture size

**get_spectrum** ()
Get _spectrum

**get_variance** (size=[], distance=0, phi=0, comp='radial')
Get the variance when the slit/pinhole size is given : size: list that can be one(diameter for circular) or two components(lengths for rectangular) : distance: [z, x] where z along the incident beam, x // qx_value : comp: direction of the sigma; can be ‘phi’, ‘y’, ‘x’, and ‘radial’
: return variance: sigma^2

**get_variance_gravity** (s_distance, d_distance, wavelength, spread, phi, comp='radial',
switch='on')
Get the variance from gravity when the wavelength spread is given
: return variance: sigma^2

**get_variance_wave** (A_value, radius, distance, spread, phi, comp='radial', switch='on')
Get the variance when the wavelength spread is given
: radius: the radial distance from the beam center to the pix of q : distance: sample to detector distance : spread: wavelength spread (ratio) : comp: direction of the sigma; can be ‘phi’, ‘y’, ‘x’, and ‘radial’
: return variance: sigma^2 for 2d, sigma^2 for 1d [tuple]

**get_wave_list** ()
Set wavelength spread

**get_wavelength** ()
Get wavelength

**get_wavelength_spread** ()
Get wavelength spread

**plot_image** (image)
Plot image using pyplot : image: 2d resolution image
: return plt: pylab object
reset_image()  
Reset image to default (=[])  

set_detector_pix_size(size)  
Set detector pixel size  

set_detector_size(size)  
Set detector size in number of pixels : param size: [pixel_nums] or [x_pix_num, yx_pix_num]  

set_intensity(intensity)  
Set intensity  

set_neutron_mass(mass)  
Set Neutron mass  

set_sample2detector_distance(distance)  
Set detector sample2detector_distance  
: param distance: [distance, x_offset]  

set_sample2sample_distance(distance)  
Set detector sample_slit2sample_distance  
: param distance: [distance, x_offset]  

set_sample_aperture_size(size)  
Set sample aperture size  
: param size: [dia_value] or [xheight_value, yheight_value]  

set_source2sample_distance(distance)  
Set detector source2sample_distance  
: param distance: [distance, x_offset]  

set_source_aperture_size(size)  
Set source aperture size  
: param size: [dia_value] or [x_value, y_value]  

set_spectrum(spectrum)  
Set spectrum  

set_wave(wavelength)  
Set wavelength list or wavelength  

set_wave_list(wavelength_list, wavelengthspread_list)  
Set wavelength and its spread list  

set_wave_spread(wavelength_spread)  
Set wavelength spread or wavelength spread  

set_wavelength(wavelength)  
Set wavelength  

set_wavelength_spread(wavelength_spread)  
Set wavelength spread  

setup_tof(wavelength, wavelength_spread)  
Setup all parameters in instrument  
: param ind: index of lambda, etc  

sas.sascalc calculator.sas_gen module  
SAS generic computation and sld file readers
class sas.sascalc.calculator.sas_gen.GenSAS
    Bases: sas.sascalc.calculator.BaseComponent.BaseComponent

Generic SAS computation Model based on sld (n & m) arrays

evalDistribution(qdist)
    Evaluate a distribution of q-values.
        Parameters qdist – ndarray of scalar q-values (for 1D) or list [qx,qy] where qx,qy are 1D ndarrays (for 2D).

getProfile()
    Get SLD profile : return: sld_data

run(x=0.0)
    Evaluate the model :param x: simple value :return: (I value)

runXY(x=0.0)
    Evaluate the model :param x: simple value :return: I value :Use this runXY() for the computation

set_is_avg(is_avg=False)
    Sets is_avg: [bool]

set_pixel_volumes(volume)
    Set the volume of a pixel in (A^3) unit :Param volume: pixel volume [float]

set_sld_data(sld_data=None)
    Sets sld_data

class sas.sascalc.calculator.sas_gen.MagSLD(pos_x, pos_y, pos_z, sld_n=None, sld_mx=None, sld_my=None, sld_mz=None, vol_pix=None)

    Bases: object

    Magnetic SLD.

    get_sldn()
        Returns nuclear sld

    pos_x = None

    pos_y = None

    pos_z = None

    set_conect_lines(line_x, line_y, line_z)
        Set bonding line data if taken from pdb

    set_nodes()
        Set xnodes, ynodes, and znodes

    set_pix_type(pix_type)
        Set pixel type :Param pix_type: string, ‘pixel’ or ‘atom’

    set_pixel_symbols(symbol='pixel')
        Set pixel :Params pixel: str; pixel or atomic symbol, or array of strings

    set_pixel_volumes(vol)
        Set pixel volumes :Params pixel: str; pixel or atomic symbol, or array of strings

    set_sldms(sld_mx, sld_my, sld_mz)
        Sets mx, my, mz and abs(m).

    set_sldn(sld_n)
        Sets neutron SLD

    set_stepsize()
        Set xstepsize, ystepsize, and zstepsize

    sld_mx = None
sld_my = None
sld_mz = None
sld_n = None

class sas.sascalc.calculator.sas_gen.OMF2SLD
Bases: object
Convert OMFData to MAgData

    get_magsld()
    return MagSLD

    get_omfdata()
    Return all data

    get_output()
    Return output

    remove_null_points(remov=False, recenter=False)
    Removes any mx, my, and mz = 0 points

    set_data(omfdata, shape='rectangular')
    Set all data

class sas.sascalc.calculator.sas_gen.OMFData
Bases: object
OMF Data.

    set_m(mx, my, mz)
    Set the Mx, My, Mz values

class sas.sascalc.calculator.sas_gen.OMFReader
Bases: object
Class to load omf/ascii files (3 columns w/header).

    ext = ['*.omf', '*.OMF']

    read(path)
    Load data file :param path: file path :return: x, y, z, sld_n, sld_mx, sld_my, sld_mz

    type = ['OMF files (*.OMF, *.omf)|*.omf']

    type_name = 'OMF ASCII'

class sas.sascalc.calculator.sas_gen.PDBReader
Bases: object
PDB reader class: limited for reading the lines starting with ‘ATOM’

    ext = ['*.pdb', '*.PDB']

    read(path)
    Load data file

        Parameters path – file path

        Returns MagSLD

        Raises RuntimeError – when the file can’t be opened

    type = ['pdb files (*.PDB, *.pdb)|*.pdb']

    type_name = 'PDB'

    write(path, data)
    Write
class sas.sascalc.calculator.sas_gen.SLDReader
    Bases: object
    Class to load ascii files (7 columns).
    ext = ['.sld', '.SLD', '.txt', '.TXT', '.*']

    read(path)
        Load data file :param path: file path :return MagSLD: x, y, z, sld_n, sld_mx, sld_my, sld_mz
        :raise RuntimeError: when the file can’t be opened :raise ValueError: when the length of the data vectors are inconsistent

    type = ['sld files (*.SLD, *.sld)|*.sld', 'txt files (*.TXT, *.txt)|*.txt', 'all files (*.*)|*.*'
    type_name = 'SLD ASCII'

write(path, data)
    Write sld file :Param path: file path :Param data: MagSLD data object

sas.sascalc.calculator.sas_gen.decode(s)

sas.sascalc.calculator.sas_gen.mag2sld(mag, v_unit=None)
    Convert magnetization to magnetic SLD sldm = Dm * mag where Dm = gamma * classical elec. radius/(2*Bohr magneton) Dm ~ 2.853E-12 [A^(-2)]
    Shouldn’t be 2.90636E-12 [A^(-2)]???

sas.sascalc.calculator.sas_gen.test()
    Test code

sas.sascalc.calculator.sas_gen.test_load()
    Test code

sas.sascalc.calculator.sas_gen.test_save()

sas.sascalc.calculator.sas_gen.transform_center(pos_x, pos_y, pos_z)
    re-center :return: posx, posy, posz [arrays]

sas.sascalc.calculator.slit_length_calculator module

This module is a small tool to allow user to quickly determine the slit length value of data.

class sas.sascalc.calculator.slit_length_calculator.SlitlengthCalculator
    Bases: object
    compute slit length from SAXSess beam profile (1st col. Q, 2nd col. I, and 3rd col. dI.: don’t need the 3rd)

    calculate_slit_length()
        Calculate slit length.

        Returns the slit length calculated value.

    get_slit_length_unit()
        Returns the slit length unit.

    set_data(x=None, y=None)
        Receive two vector x, y and prepare the slit calculator for computation.

        Parameters
        * x – array
        * y – array
Module contents

`sas.sascalc.corfunc` package

Submodules

`sas.sascalc.corfunc.corfunc_calculator` module

This module implements `corfunc_calculator`.

```python
class sas.sascalc.corfunc.corfunc_calculator.CorfuncCalculator(data=None, lowerq=None, upperq=None, scale=1):

    Bases: object

    def compute_background(self, upperq=None):
        Compute the background level from the Porod region of the data

    def compute_extrapolation(self):
        Extrapolate and interpolate scattering data
        Returns The extrapolated data

    def compute_transform(self, extrapolation, trans_type, background=None, completefn=None, updatefn=None):
        Transform an extrapolated scattering curve into a correlation function.
        Parameters
            • extrapolation – The extrapolated data
            • background – The background value (if not provided, previously calculated value will be used)
            • extrap_fn – A callable function representing the extrapolated data
            • completefn – The function to call when the transform calculation is complete
            • updatefn – The function to call to update the GUI with the status of the transform calculation
        Returns The transformed data

    def extract_parameters(self, transformed_data):
        Extract the interesting measurements from a correlation function

    def set_data(self, data, scale=1):
        Prepares the data for analysis
        Returns new_data = data * scale - background

    def stop_transform(self):

    def transform_isrunning(self):
```

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sas.sascalc.corfunc.transform_thread module

```python
class sas.sascalc.corfunc.transform_thread.FourierThread(raw_data, extrapolated_data, bg, updatefn=None, completefn=None)

Bases: sas.sascalc.data_util.calcthread.CalcThread

check_if_cancelled()
compute()
```

```python
class sas.sascalc.corfunc.transform_thread.HilbertThread(raw_data, extrapolated_data, bg, updatefn=None, completefn=None)

Bases: sas.sascalc.data_util.calcthread.CalcThread

compute()
```

Module contents

sas.sascalc.data_util package

Submodules

sas.sascalc.data_util.calcthread module

```python
class sas.sascalc.data_util.calcthread.CalcCommandline(n=20000)

Test method

complete(total=0.0)
update(i=0)
```

```python
class sas.sascalc.data_util.calcthread.CalcDemo(completefn=None, updatefn=None, yieldtime=0.01, worktime=0.01, exception_handler=None)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Example of a calculation thread.

compute(n)
```

```python
class sas.sascalc.data_util.calcthread.CalcThread(completefn=None, updatefn=None, yieldtime=0.01, worktime=0.01, exception_handler=None)

Threaded calculation class. Inherit from here and specialize the compute() method to perform the appropriate operations for the class.

If you specialize the __init__ method be sure to call CalcThread.__init__, passing it the keyword arguments for yieldtime, worktime, update and complete.

When defining the compute() method you need to include code which allows the GUI to run. They are as follows:

```python
self.isquit()  # call frequently to check for interrupts
self.update(kw=...)  # call when the GUI could be updated
self.complete(kw=...)  # call before exiting compute()
```
The update() and complete() calls accept field=value keyword arguments which are passed to the called function. complete() should be called before exiting the GUI function. A KeyboardInterrupt event is triggered if the GUI signals that the computation should be halted.

The following documentation should be included in the description of the derived class.

The user of this class will call the following:

```python
thread = Work(...,kw=...)  # prepare the work thread.
thread.queue(...,kw=...)    # queue a work unit.
thread.requeue(...,kw=...)  # replace work unit on the end of queue.
thread.reset(...,kw=...)    # reset the queue to the given work unit.
thread.stop()               # clear the queue and halt.
thread.interrupt()          # halt the current work unit but continue.
thread.ready(delay=0.)      # request an update signal after delay.
thread.isrunning()          # returns true if compute() is running.
```

Use queue() when all work must be done. Use requeue() when intermediate work items don’t need to be done (e.g., in response to a mouse move event). Use reset() when the current item doesn’t need to be completed before the new event (e.g., in response to a mouse release event). Use stop() to halt the current and pending computations (e.g., in response to a stop button).

The methods queue(), requeue() and reset() are proxies for the compute() method in the subclass. Look there for a description of the arguments. The compute() method can be called directly to run the computation in the main thread, but it should not be called if isrunning() returns true.

The constructor accepts additional keywords yieldtime=0.01 and worktime=0.01 which determine the cooperative multitasking behaviour. Yield time is the duration of the sleep period required to give other processes a chance to run. Work time is the duration between sleep periods.

Notifying the GUI thread of work in progress and work complete is done with updatefn=updatefn and completefn=completefn arguments to the constructor. Details of the parameters to the functions depend on the particular calculation class, but they will all be passed as keyword arguments. Details of how the functions should be implemented vary from framework to framework.

For wx, something like the following is needed:

```python
import wx, wx.lib.newevent
(CalcCompleteEvent, EVT_CALC_COMPLETE) = wx.lib.newevent.NewEvent()

# methods in the main window class of your application
def __init__(self):
    ...
    # Prepare the calculation in the GUI thread.
    self.work = Work(completefn=self.CalcComplete)
    self.Bind(EVT_CALC_COMPLETE, self.OnCalcComplete)
    ...
    # Bind work queue to a menu event.
    self.Bind(wx.EVT_MENU, self.OnCalcStart, id=idCALCSTART)
    ...

def OnCalcStart(self, event):
    # Start the work thread from the GUI thread.
    self.work.queue(...work unit parameters...)

def CalcComplete(self,**kwargs):
    # Generate CalcComplete event in the calculation thread.
    # kwargs contains field1, field2, etc. as defined by
    # the Work thread class.
    event = CalcCompleteEvent(**kwargs)
    wx.PostEvent(self, event)

def OnCalcComplete(self, event):
    # Process CalcComplete event in GUI thread.
```

(continues on next page)
# Use values from event.field1, event.field2 etc. as defined by the Work thread class to show the results.

...  

complete(**kwargs)
Update the GUI with the completed results from a work unit.

compute(*args, **kwargs)
Perform a work unit. The subclass will provide details of the arguments.

exception()
An exception occurred during computation, so call the exception handler if there is one. If not, then log the exception and continue.

interrupt()
Stop the current work item. To clear the work queue as well call the stop() method.

isquit()
Check for interrupts. Should be called frequently to provide user responsiveness. Also yields to other running threads, which is required for good performance on OS X.

isrunning()

queue(*args, **kwargs)
Add a work unit to the end of the queue. See the compute() method for details of the arguments to the work unit.

ready(delay=0.0)
Ready for another update after delay=t seconds. Call this for threads which can show intermediate results from long calculations.

requeue(*args, **kwargs)
Replace the work unit on the end of the queue. See the compute() method for details of the arguments to the work unit.

reset(*args, **kwargs)
Clear the queue and start a new work unit. See the compute() method for details of the arguments to the work unit.

stop()
Clear the queue and stop the thread. New items may be queued after stop. To stop just the current work item, and continue the rest of the queue call the interrupt method.

update(**kwargs)
Update GUI with the latest results from the current work unit.

sas.sascalc.data_util.err1d module

Error propagation algorithms for simple arithmetic

Warning: like the underlying numpy library, the inplace operations may return values of the wrong type if some of the arguments are integers, so be sure to create them with floating point inputs.

sas.sascalc.data_util.err1d.add(X, varX, Y, varY)
Addition with error propagation

sas.sascalc.data_util.err1d.add_inplace(X, varX, Y, varY)
In-place addition with error propagation

sas.sascalc.data_util.err1d.div(X, varX, Y, varY)
Division with error propagation

sas.sascalc.data_util.err1d.div_inplace(X, varX, Y, varY)
In-place division with error propagation
sas.sascalc.data_util.err1d.exp(X, varX)
    Exponentiation with error propagation
sas.sascalc.data_util.err1d.log(X, varX)
    Logarithm with error propagation
sas.sascalc.data_util.err1d.mul(X, varX, Y, varY)
    Multiplication with error propagation
sas.sascalc.data_util.err1d.mul_inplace(X, varX, Y, varY)
    In-place multiplication with error propagation
sas.sascalc.data_util.err1d.pow(X, varX, n)
    X**n with error propagation
sas.sascalc.data_util.err1d.pow_inplace(X, varX, n)
    In-place X**n with error propagation
sas.sascalc.data_util.err1d.sub(X, varX, Y, varY)
    Subtraction with error propagation
sas.sascalc.data_util.err1d.sub_inplace(X, varX, Y, varY)
    In-place subtraction with error propagation

sas.sascalc.data_util.formatnum module

Format values and uncertainties nicely for printing.

format_uncertainty_pm() produces the expanded format v +/- dv.
format_uncertainty_compact() produces the compact format v(##), where the number in parenthesis is
the uncertainty in the last two digits of v.

format_uncertainty() uses the compact format by default, but this can be changed to use the expanded +/-
format by setting format_uncertainty.compact to False.

The formatted string uses only the number of digits warranted by the uncertainty in the measurement.

If the uncertainty is 0 or not otherwise provided, the simple %g floating point format option is used.

Infinite and indefinite numbers are represented as inf and NaN.

Example:

```python
>>> v, dv = 757.2356, 0.01032
>>> print format_uncertainty_pm(v, dv)
757.236 +/- 0.010
>>> print format_uncertainty_compact(v, dv)
757.236(10)
>>> print format_uncertainty(v, dv)
757.236(10)
>>> format_uncertainty.compact = False
>>> print format_uncertainty(v, dv)
757.236 +/- 0.010
```

UncertaintyFormatter() returns a private formatter with its own formatter.compact flag.

sas.sascalc.data_util.formatnum.format_uncertainty_pm(value, uncertainty)
    Given value v and uncertainty dv, return a string v +/- dv.

sas.sascalc.data_util.formatnum.format_uncertainty_compact(value, uncertainty)
    Given value v and uncertainty dv, return the compact representation v(##), where ## are the first two digits of the uncertainty.
sas.sascalc.data_util.nxsunit module

Define unit conversion support for NeXus style units.

The unit format is somewhat complicated. There are variant spellings and incorrect capitalization to worry about, as well as forms such as "mili*metre" and "1e-7 seconds".

This is a minimal implementation of units including only what I happen to need now. It does not support the complete dimensional analysis provided by the package udunits on which NeXus is based, or even the units used in the NeXus definition files.

Unlike other units packages, this package does not carry the units along with the value but merely provides a conversion function for transforming values.

Usage example:

```
import nxsunit
u = nxsunit.Converter('mili*metre')  # Units stored in mm
v = u(3000,'m')  # Convert the value 3000 mm into meters
```

NeXus example:

```
# Load sample orientation in radians regardless of how it is stored.
# 1. Open the path
file.openpath('/entry1/sample/sample_orientation')
# 2. scan the attributes, retrieving 'units'
units = [for attr,value in file.attrs() if attr == 'units']
# 3. set up the converter (assumes that units actually exists)
u = nxsunit.Converter(units[0])
# 4. read the data and convert to the correct units
v = u(file.read(),'radians')
```

This is a standalone module, not relying on either DANSE or NeXus, and can be used for other unit conversion tasks.

Note: minutes are used for angle and seconds are used for time. We cannot tell what the correct interpretation is without knowing something about the fields themselves. If this becomes an issue, we will need to allow the application to set the dimension for the unit rather than inferring the dimension from an example unit.

```
class sas.sascalc.data_util.nxsunit.Converter (name)
    Bases: object

    Unit converter for NeXus style units.

    dims = [{'kilometre': 1000.0, 'centi*Metre': 0.01, 'mili*meter': 0.001, 'gigameter': 1000000000.0, 'meter': 1, 'milli*meter': 0.001, '1/cm': 1e-08, 'nm^-1': 0.1, 'nm-1': 0.1, '1/A': 1, 'cm^{-1}': 1e-08, '10^-3 Angstrom^-1': 0.001, 'invAngstroms': 1, '1/cm^2': 1, '1/m^2': 1, '1/A*rad': 1e-10, '1/m*A': 1e-10, '1/m*deg': 1e-10, '1/m*A*deg': 1e-10, '1/m^2*A*deg': 1e-10, '1/m^2*A*rad': 1e-10, '1/m^3': 1, '1/m^3/A': 1e-10, '1/m^3/A*deg': 1e-10, '1/m^3/A*rad': 1e-10, '1/m^3*deg': 1e-10, '1/m^3*rad': 1e-10, '1/m^4/A^2': 1e-10, '1/m^4/A^2*deg': 1e-10, '1/m^4/A^2*rad': 1e-10, '1/m^4/A*deg': 1e-10, '1/m^4*A^2': 1e-10, '1/m^4*A^2*deg': 1e-10, '1/m^4*A^2*rad': 1e-10, '1/m^4/A*deg': 1e-10, '1/m^4*A*rad': 1e-10, '1/m^4*deg': 1e-10, '1/m^4*rad': 1e-10, '1/m^5/A': 1e-10, '1/m^5/A*deg': 1e-10, '1/m^5/A*rad': 1e-10, '1/m^5*deg': 1e-10, '1/m^5*rad': 1e-10, '1/m^6/A': 1e-10, '1/m^6/A*deg': 1e-10, '1/m^6/A*rad': 1e-10, '1/m^6*deg': 1e-10, '1/m^6*rad': 1e-10, '1/m^7/A': 1e-10, '1/m^7/A*deg': 1e-10, '1/m^7/A*rad': 1e-10, '1/m^7*deg': 1e-10, '1/m^7*rad': 1e-10, '1/m^8/A': 1e-10, '1/m^8/A*deg': 1e-10, '1/m^8/A*rad': 1e-10, '1/m^8*deg': 1e-10, '1/m^8*rad': 1e-10, '1/m^9/A': 1e-10, '1/m^9/A*deg': 1e-10, '1/m^9/A*rad': 1e-10, '1/m^9*deg': 1e-10, '1/m^9*rad': 1e-10, '1/m^10/A': 1e-10, '1/m^10/A*deg': 1e-10, '1/m^10/A*rad': 1e-10, '1/m^10*deg': 1e-10, '1/m^10*rad': 1e-10}
```

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All normal dictionary methods are available. Update and comparison is restricted to other OrderedDict
objects.
Various sequence methods are available, including the ability to explicitly mutate the key ordering.
__contains__ tests:
>>> d = OrderedDict(((1, 3),))
>>> 1 in d
1
>>> 4 in d
0

__getitem__ tests:
>>> OrderedDict(((1, 3), (3, 2), (2, 1)))[2]
1
>>> OrderedDict(((1, 3), (3, 2), (2, 1)))[4]
Traceback (most recent call last):
KeyError: 4

__len__ tests:
>>> len(OrderedDict())
0
>>> len(OrderedDict(((1, 3), (3, 2), (2, 1))))
3

get tests:
>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.get(1)
3
>>> d.get(4) is None
1
>>> d.get(4, 5)
5
>>> d
OrderedDict([(1, 3), (3, 2), (2, 1)])

has_key tests:
>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.has_key(1)
1
>>> d.has_key(4)
0

clear()
>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.clear()
>>> d
OrderedDict([])

copy()
>>> OrderedDict(((1, 3), (3, 2), (2, 1))).copy()
OrderedDict([(1, 3), (3, 2), (2, 1)])

index(key)
Return the position of the specified key in the OrderedDict.
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```python
>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.index(3)
1
>>> d.index(4)
Traceback (most recent call last):
  ValueError: list.index(x): x not in list
```

**insert** (*index*, *key*, *value*)

Takes *index*, *key*, and *value* as arguments.

Sets *key* to *value*, so that *key* is at position *index* in the OrderedDict.

```python
>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.insert(0, 4, 0)
>>> d
OrderedDict([(4, 0), (1, 3), (3, 2), (2, 1)])
>>> d.insert(0, 2, 1)
>>> d
OrderedDict([(2, 1), (4, 0), (1, 3), (3, 2)])
>>> d.insert(8, 8, 1)
>>> d
OrderedDict([(2, 1), (4, 0), (1, 3), (3, 2), (8, 1)])
```

**items()**

`items()` returns a list of tuples representing all the (*key*, *value*) pairs in the dictionary.

```python
>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.items()
[(1, 3), (3, 2), (2, 1)]
>>> d.clear()
>>> d.items()
[]
```

**iteritems()**

```python
>>> ii = OrderedDict(((1, 3), (3, 2), (2, 1))).iteritems()
>>> ii.next()
(1, 3)
>>> ii.next()
(3, 2)
>>> ii.next()
(2, 1)
>>> ii.next()
Traceback (most recent call last):
  StopIteration
```

**iterkeys()**

```python
>>> ii = OrderedDict(((1, 3), (3, 2), (2, 1))).iterkeys()
>>> ii.next()
1
>>> ii.next()
3
>>> ii.next()
2
>>> ii.next()
Traceback (most recent call last):
  StopIteration
```

**itervalues()**

```python
```
iv = OrderedDict(((1, 3), (3, 2), (2, 1))).itervalues()
>>> iv.next()
3
>>> iv.next()
2
>>> iv.next()
1
>>> iv.next()
Traceback (most recent call last):
StopIteration

keys()
Return a list of keys in the OrderedDict.

>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.keys()
[1, 3, 2]

pop(key, *args)
No dict.pop in Python 2.2, gotta reimplement it

>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.pop(3)
2
>>> d.pop(4)
Traceback (most recent call last):
KeyError: 4
>>> d.pop(4, 0)
0
>>> d.pop(4, 0, 1)
Traceback (most recent call last):
TypeError: pop expected at most 2 arguments, got 3

popitem(i=-1)
Delete and return an item specified by index, not a random one as in dict. The index is -1 by default (the last item).

>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.popitem()
(2, 1)
>>> d.popitem(0)
(3, 2)
>>> d.popitem(0)
Traceback (most recent call last):
Traceback (most recent call last):
KeyError: 'popitem(): dictionary is empty'
>>> d.popitem(2)
Traceback (most recent call last):
IndexError: popitem(): index 2 not valid

rename(old_key, new_key)
Rename the key for a given value, without modifying sequence order.

For the case where new_key already exists this raise an exception, since if new_key exists, it is ambiguous as to what happens to the associated values, and the position of new_key in the sequence.

>>> od = OrderedDict()
>>> od['a'] = 1
>>> od['b'] = 2
(continues on next page)
>> od.items()
[('a', 1), ('b', 2)]
>> od.rename('b', 'c')
>> od.items()
[('a', 1), ('c', 2)]
>> od.rename('c', 'a')
Traceback (most recent call last):
  ValueError: New key already exists: 'a'
>> od.rename('d', 'b')
Traceback (most recent call last):
  KeyError: 'd'

reverse()
Reverse the order of the OrderedDict.

>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.reverse()
>>> d
OrderedDict([(2, 1), (3, 2), (1, 3)])

setdefault (key, defval=\text{None})

>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.setdefault(1)
3
>>> d.setdefault(4) \text{ is None}
True
>>> d
OrderedDict([(1, 3), (3, 2), (2, 1), (4, None)])
>>> d.setdefault(5, 0)
0
>>> d
OrderedDict([(1, 3), (3, 2), (2, 1), (4, None), (5, 0)])

setitems (items)
This method allows you to set the items in the dict.
It takes a list of tuples - of the same sort returned by the \text{items} method.

>>> d = OrderedDict()
>>> d.setitems(((3, 1), (2, 3), (1, 2)))
>>> d
OrderedDict([(3, 1), (2, 3), (1, 2)])

setkeys (keys)
setkeys all ows you to pass in a new list of keys which will replace the current set. This must contain the same set of keys, but need not be in the same order.
If you pass in new keys that don’t match, a KeyError will be raised.

>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.keys()
[1, 3, 2]
>>> d.setkeys((1, 2, 3))
>>> d
OrderedDict([(1, 3), (2, 1), (3, 2)])
>>> d.setkeys(['a', 'b', 'c'])
  Traceback (most recent call last):
  KeyError: 'Keylist is not the same as current keylist.'

setvalues (values)
You can pass in a list of values, which will replace the current list. The value list must be the same length as the OrderedDict.

(Or a ValueError is raised.)

```python
>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.setvalues((1, 2, 3))
>>> d
OrderedDict([(1, 1), (3, 2), (2, 3)])
>>> d.setvalues([6])
Traceback (most recent call last):
ValueError: Value list is not the same length as the OrderedDict.
```

**sort** (*args, **kwargs*)

Sort the key order in the OrderedDict.

This method takes the same arguments as the list.sort method on your version of Python.

```python
>>> d = OrderedDict(((4, 1), (2, 2), (3, 3), (1, 4)))
>>> d.sort()
>>> d
OrderedDict([(1, 4), (2, 2), (3, 3), (4, 1)])
```

**update** (*from_od*)

Update from another OrderedDict or sequence of (key, value) pairs

```python
>>> d = OrderedDict(((1, 0), (0, 1)))
>>> d.update(OrderedDict(((1, 3), (3, 2), (2, 1))))
>>> d
OrderedDict([(1, 3), (0, 1), (3, 2), (2, 1)])
>>> d.update({4: 4})
Traceback (most recent call last):
TypeError: undefined order, cannot get items from dict
>>> d.update((4, 4))
Traceback (most recent call last):
TypeError: cannot convert dictionary update sequence element "4" to a 2-item sequence
```

**values** (*values=None*)

Return a list of all the values in the OrderedDict.

Optionally you can pass in a list of values, which will replace the current list. The value list must be the same length as the OrderedDict.

```python
>>> d = OrderedDict(((1, 3), (3, 2), (2, 1)))
>>> d.values()
[3, 2, 1]
```

**Experimental version of OrderedDict that has a custom object for keys, values, and items.**

These are callable sequence objects that work as methods, or can be manipulated directly as sequences.

```python
class sas.sascalc.data_util.odict.SequenceOrderedDict (init_val=(), strict=True)
Bases: sas.sascalc.data_util.odict.OrderedDict

Test for keys, items and values.

```python
>>> d = SequenceOrderedDict(((1, 2), (2, 3), (3, 4)))
>>> d
SequenceOrderedDict([(1, 2), (2, 3), (3, 4)])
>>> d.keys
[1, 2, 3]
>>> d.keys()
[1, 2, 3]
```
>>> d.setkeys((3, 2, 1))
>>> d
SequenceOrderedDict([(3, 4), (2, 3), (1, 2)])
>>> d.setkeys((1, 2, 3))
>>> d.keys[0]
1
>>> d.keys[:]
[1, 2, 3]
>>> d.keys[-1]
3
>>> d.keys[-2]
2
>>> d.keys[0:2] = [2, 1]
>>> d
SequenceOrderedDict([(2, 3), (1, 2), (3, 4)])
>>> d.keys.reverse()
>>> d.keys
[3, 1, 2]
>>> d.keys = [1, 2, 3]
>>> d
SequenceOrderedDict([(1, 2), (2, 3), (3, 4)])
>>> d.keys = [3, 1, 2]
>>> d
SequenceOrderedDict([(3, 4), (1, 2), (2, 3)])
>>> a = SequenceOrderedDict()
>>> b = SequenceOrderedDict()
>>> a.keys == b.keys
1
>>> a['a'] = 3
>>> a.keys == b.keys
0
>>> b['a'] = 3
>>> a.keys == b.keys
1
>>> b['b'] = 3
>>> a.keys == b.keys
0
>>> a.keys > b.keys
0
>>> a.keys < b.keys
1
>>> 'a' in a.keys
1
>>> len(b.keys)
2
>>> 'c' in d.keys
0
>>> 1 in d.keys
1
>>> [v for v in d.keys]
[3, 1, 2]
>>> d.keys.sort()
>>> d.keys
[1, 2, 3]
>>> d = SequenceOrderedDict(((1, 2), (2, 3), (3, 4)), strict=True)
>>> d.keys[::-1] = [1, 2, 3]
>>> d
SequenceOrderedDict([(1, 2), (2, 3), (3, 4)])
>>> d.keys[:2]
[1, 2]
>>> d.keys[:2] = [1, 3]
Traceback (most recent call last):
  KeyError: 'Keylist is not the same as current keylist.'

>>> d = SequenceOrderedDict(((1, 2), (2, 3), (3, 4)))
>>> d
SequenceOrderedDict([(1, 2), (2, 3), (3, 4)])
>>> d.values
[2, 3, 4]
>>> d.values()
[2, 3, 4]
>>> d.setvalues((4, 3, 2))
>>> d
SequenceOrderedDict([(1, 4), (2, 3), (3, 2)])
>>> d.values[:=-1]
[2, 3, 4]
>>> d.values[0]
4
>>> d.values[-2]
3
>>> del d.values[0]
Traceback (most recent call last):
  TypeError: Can't delete items from values
>>> d.values[:2] = [2, 4]
>>> d
SequenceOrderedDict([(1, 2), (2, 3), (3, 4)])
>>> 7 in d.values
0
>>> len(d.values)
3
>>> [val for val in d.values]
[2, 3, 4]
>>> d.values[-1] = 2
>>> d.values.count(2)
2
>>> d.values.index(2)
0
>>> d.values[-1] = 7
>>> d.values
[2, 3, 7]
>>> d.values.reverse()
>>> d.values
[7, 3, 2]
>>> d.values.sort()
>>> d.values
[2, 3, 7]
>>> d.values.append('anything')
Traceback (most recent call last):
  TypeError: Can't append items to values
>>> d.values = (1, 2, 3)
>>> d
SequenceOrderedDict([(1, 1), (2, 2), (3, 3)])

>>> d = SequenceOrderedDict(((1, 2), (2, 3), (3, 4)))
>>> d
SequenceOrderedDict([(1, 2), (2, 3), (3, 4)])
>>> d.items()
[(1, 2), (2, 3), (3, 4)]
>>> d.setitems([(3, 4), (2, 3), (1, 2)])
>>> d
SequenceOrderedDict([(3, 4), (2, 3), (1, 2)])

(continues on next page)
sas.sascalc.data_util.ordereddict module

Backport from python2.7 to python <= 2.6.

class sas.sascalc.data_util.ordereddict.OrderedDict (*args, **kwargs)
Bases: dict

clear() → None. Remove all items from D.

copy() → a shallow copy of D

classmethod fromkeys(S, v) → New dict with keys from S and values equal to v.
   v defaults to None.

items() → list of D’s (key, value) pairs, as 2-tuples

keys() → list of D’s keys

pop(k[, d]) → v, remove specified key and return the corresponding value.
   If key is not found, d is returned if given, otherwise KeyError is raised

popitem() → (k, v), remove and return some (key, value) pair as a
   2-tuple; but raise KeyError if D is empty.

setdefault(k[, d]) → D.get(k,d), also set D[k]=d if k not in D

update([E, **F]) → None. Update D from dict/iterable E and F.
   If E present and has a .keys() method, does: for k in E: D[k] = E[k] If E present and lacks .keys()
   method, does: for (k, v) in E: D[k] = v In either case, this is followed by: for k in F: D[k] = F[k]

values() → list of D’s values

sas.sascalc.data_util.ordereddicttest module

class sas.sascalc.data_util.ordereddicttest.TestOrderedDict (methodName='runTest')
   Bases: unittest.case.TestCase

   test_clear()
   test_copying()
   test_delitem()
   test_equality()
   test_init()
   test_iterators()
   test_pop()
   test_popitem()
   test_reinsert()
   test_repr()
   test_setdefault()
   test_setitem()
   test_update()

sas.sascalc.data_util.pathutils module

Utilities for path manipulation. Not to be confused with the pathutils module from the pythonutils package (http://groups.google.com/group/pythonutils).

sas.sascalc.data_util.pathutils.relpath(p1, p2)
   Compute the relative path of p1 with respect to p2.
**sas.sascalc.data_util.registry module**

File extension registry.

This provides routines for opening files based on extension, and registers the built-in file extensions.

```python
class sas.sascalc.data_util.registry.ExtensionRegistry(**kw)
    Bases: object

    Associate a file loader with an extension.
    
    Note that there may be multiple loaders for the same extension.
    
    Example:
    ```
    registry = ExtensionRegistry()
    # Add an association by setting an element
    registry['.zip'] = unzip
    # Multiple extensions for one loader
    registry['.tgz'] = untar
    registry['.tar.gz'] = untar
    # Generic extensions to use after trying more specific extensions;
    # these will be checked after the more specific extensions fail.
    registry['.gz'] = gunzip
    # Multiple loaders for one extension
    registry['.cx'] = cx1
    registry['.cx'] = cx2
    registry['.cx'] = cx3
    # Show registered extensions
    print registry.extensions()
    # Can also register a format name for explicit control from caller
    registry['cx3'] = cx3
    print registry.formats()
    # Retrieve loaders for a file name
    registry.lookup('hello.cx') -> [cx3,cx2,cx1]
    # Run loader on a filename
    registry.load('hello.cx') ->
        try:
            return cx3('hello.cx')
        except:
            try:
                return cx2('hello.cx')
            except:
                return cx1('hello.cx')
    # Load in a specific format ignoring extension
    registry.load('hello.cx', format='cx3') ->
        return cx3('hello.cx')
```

- `extensions()` Return a sorted list of registered extensions.
- `formats()` Return a sorted list of the registered formats.
- `load(path, format=None)` Call the loader for the file type of path.
Raises

- `ValueError` – if no loader is available.
- `KeyError` – if format is not available.

May raise a loader-defined exception if loader fails.

`lookup(path)`

Return the loader associated with the file type of path.

Parameters

path – Data file path

Raises `ValueError` – When no loaders are found for the file.

Returns List of available readers for the file extension

`sas.sascalc.data_util.uncertainty module`

Uncertainty propagation class for arithmetic, log and exp.

Based on scalars or numpy vectors, this class allows you to store and manipulate values+uncertainties, with propagation of gaussian error for addition, subtraction, multiplication, division, power, exp and log.

Storage properties are determined by the numbers used to set the value and uncertainty. Be sure to use floating point uncertainty vectors for inplace operations since numpy does not do automatic type conversion. Normal operations can use mixed integer and floating point. In place operations such as $a *= b$ create at most one extra copy for each operation. By contrast, $c = a*b$ uses four intermediate vectors, so shouldn’t be used for huge arrays.

```python
class sas.sascalc.data_util.uncertainty.Uncertainty(x, variance=None)
Bases: object
    dx
    standard deviation
    exp()
    log()
```

Module contents

`sas.sascalc.dataloader package`

Subpackages

`sas.sascalc.dataloader.readers package`

Submodules

`sas.sascalc.dataloader.readers.abs_reader module`

IGOR 1D data reader

```python
class sas.sascalc.dataloader.readers.abs_reader.Reader
    Bases: sas.sascalc.dataloader.file_reader_base_class.FileReader

    Class to load IGOR reduced .ABS files
    ext = ['abs', 'cor']

    get_file_contents()
        Get the contents of the file
```

2.1. Contents
 Raises

  • RuntimeError – when the file can’t be opened
  • ValueError – when the length of the data vectors are inconsistent

```python
type = ['IGOR 1D files (*.abs)|*.abs', 'IGOR 1D USANS files (*.cor)|*.cor']
type_name = 'IGOR 1D'
```

*sas.sascalc.dataloader.readers.anton_paar_saxs_reader module*

CanSAS 2D data reader for reading HDF5 formatted CanSAS files.

```python
class sas.sascalc.dataloader.readers.anton_paar_saxs_reader.Reader(xml=None, schema=None):
    Bases: sas.sascalc.dataloader.readers.xml_reader.XMLreader
    A class for reading in Anton Paar .pdh files
    allow_all = False
    errors = None
    ext = ['.pdh', '.PDH']
    get_file_contents()
    This is the general read method that all SasView data_loaders must have.
    Parameters
    filename – A path for an XML formatted Anton Paar SAXSess data file.
    Returns
    List of Data1D objects or a list of errors.
    logging = None
    parent_list = None
    raw_data = None
    read_data()
    reset_state()
    Resets the class state to a base case when loading a new data file so previous data files do not appear a second time
    type = ['Anton Paar SAXSess Files (*.pdh)|*.pdh']
type_name = 'Anton Paar SAXSess'
```

*sas.sascalc.dataloader.readers.ascii_reader module*

Generic multi-column ASCII data reader

```python
class sas.sascalc.dataloader.readers.ascii_reader.Reader:
    Bases: sas.sascalc.dataloader.file_reader_base_class.FileReader
    Class to load ascii files (2, 3 or 4 columns).
    allow_all = True
    ext = ['.txt', '.dat', '.abs', '.csv']
    get_file_contents()
    Get the contents of the file
    min_data_pts = 5
    type = ['ASCII files (*.txt)|*.txt', 'ASCII files (*.dat)|*.dat', 'ASCII files (*.abs)|*.abs']
type_name = 'ASCII'
```
sas.sascalc.dataloader.readers.associations module

Module to associate default readers to file extensions. The module reads an xml file to get the readers for each file extension. The readers are tried in order they appear when reading a file.

```python
sas.sascalc.dataloader.readers.associations.readAssociations(loader, settings={'.abs': 'abs_reader', '.cor': 'abs_reader', '.dat': 'red2d_reader', '.h5': 'cansas_reader_HDF5', '.nxs': 'cansas_reader_HDF5', '.pdh': 'anton_paar_saxs_reader', '.sans': 'danse_reader', '.ses': 'sesans_reader', '.txt': 'ascii_reader', '.xml': 'cansas_reader'})
```

Read the specified settings file to associate default readers to file extension.

**Parameters**

- `loader` – Loader object
- `settings` – path to the json settings file [string]

sas.sascalc.dataloader.readers.cansas_constants module

Information relating to the CanSAS data format. These constants are used in the cansas_reader.py file to read in any version of the canساس format.

```python
class sas.sascalc.dataloader.readers.cansas_constants.CansasConstants
```

The base class to define where all of the data is to be saved by cansas_reader.py.

```python
ANY = {'storeas': 'content'}
CANSAS_FORMAT = {'SASentry': {'attributes': {'name': {}}, 'units_optional': True}, ...
CANSAS_NS = {'1.0': {'ns': 'cansas1d/1.0', 'schema': 'cansas1d_v1_0.xsd'}, '1.1': ...
RUN = {'attributes': {'name': {}}}
SASDATA = {'attributes': {'name': {}}, 'children': {'zacceptance': {'storeas': ...
SASDATA_IDATA = {'attributes': {'timestamp': {'storeas': 'timestamp'}, 'name': {}}
SASDATA_IDATA_DQL = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': ...
SASDATA_IDATA_DQW = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': ...
SASDATA_IDATA_I = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': ...
SASDATA_IDATA_IDEV = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': ...
SASDATA_IDATA_Q = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': ...
```

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SASDATA_IDATA_QDEV = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'x_unit'}
SASDATA_IDATA_QMEAN = {'attributes': {'unit': '{}}, 'unit': 'x_unit'}
SASDATA_IDATA_SHADOWFACTOR = {}
SASINSTR_SRC_WL = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'wavelength_unit'}
SASINSTR_SRC_WL_MAX = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'wavelength_max_unit'}
SASINSTR_SRC_WL_MIN = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'wavelength_min_unit'}
SASINSTR_SRC_WL_SPR = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'wavelength_spread_unit'}
SASNOTE = {}
SASPROCESS = {'children': {'term': {'attributes': {'name': {}, 'unit': {}}}, '<any>': {'storeas': 'content'}, 'description': {}, 'SASprocessnote': {'children': {'<any>': {'storeas': 'content'}}}, 'date': {}, 'name': {}}}
SASPROCESS_SASPROCESSNOTE = {'children': {'<any>': {'storeas': 'content'}}}
SASPROCESS_TERM = {'attributes': {'name': {}, 'unit': {}}}
SASSAMPLE = {'attributes': {'name': {}}, 'children': {'<any>': {'storeas': 'content'}, 'orientation': {'children': {'yaw': {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'orientation_unit'}, ... 'details': {}, 'ID': {}, 'thickness': {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'thickness_unit'}}}}
SASSAMPLE_ORIENT = {'children': {'yaw': {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'orientation_unit'}, ... 'unit': 'orientation_unit'}, 'pitch': {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'orientation_unit'}}
SASSAMPLE_ORIENT_ATTR = {'unit': {}}
SASSAMPLE_ORIENT_PITCH = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'orientation_unit'}
SASSAMPLE_ORIENT_ROLL = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'orientation_unit'}
SASSAMPLE_ORIENT_YAW = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'orientation_unit'}
SASSAMPLE_POS = {'children': {'y': {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'position_unit'}, 'x': ... 'float', 'unit': 'position_unit'}, 'z': {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'position_unit'}}
SASSAMPLE_POS_ATTR = {'unit': {}}
SASSAMPLE_POS_X = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'position_unit'}
SASSAMPLE_POS_Y = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'position_unit'}
SASSAMPLE_POS_Z = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'position_unit'}
SASSAMPLE_TEMP = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'temperature_unit'}
SASSAMPLE_THICK = {'attributes': {'unit': {}}, 'storeas': 'float', 'unit': 'thickness_unit'}
SASTRANSSPEC = {'attributes': {'timestamp': {}, 'name': {}}, 'children': {'Tdata': {'children': {'Tdev': {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'wavelength_unit'}}}, '<any>': {'storeas': 'content'}}}
SASTRANSSPEC_TDATA = {'children': {'Tdev': {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': ... 'Lambda': {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'wavelength_unit'}}}
SASTRANSSPEC_TDATA_LAMDBA = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'wavelength_unit'}
SASTRANSSPEC_TDATA_T = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'transmission_unit'}
SASTRANSSPEC_TDATA_TDEV = {'attributes': {'unit': {'storeas': 'content'}}, 'storeas': 'float', 'unit': 'transmission_deviation_unit'}
TITLE = {}
format = ''
get_namespace_map()
Helper method to get the names namespace list
iterate_namespace (namespace)
Method to iterate through a canساس constants tree based on a list of names
Parameters namespace – A list of names that match the tree structure of canساس constants
names = ''
class sas.sascalc.dataloader.readers.cansas_constants.CurrentLevel
    Bases: object
    A helper class to hold information on where you are in the constants tree
    current_level = ''
get_current_level()  
Helper method to get the current_level map

get_data_type()  
Helper method to get the ns_datatype label

get_variable()  
Helper method to get the ns_variable label

ns_datatype = ''
ns_optional = True

sas.sascalc.dataloader.readers.cansas_reader module

class sas.sascalc.dataloader.readers.cansas_reader.Reader(xml=None, schema=None):
    Bases: sas.sascalc.dataloader.readers.xml_reader.XMLreader

    allow_all = True
    base_ns = '{cansas1d/1.0}'
    cansas_defaults = None
    cansas_version = '1.0'
    current_data1d = None
    data = None
    errors = set([])
    ext = ['.xml', '.XML', '.svs', '.SVS']
    frm = ''

    get_file_contents(xml_file=None, schema_path='', invalid=True)
        Reader specific class to access the contents of the file All reader classes that inherit from FileReader must implement

        invalid = True

        is_cansas(ext='xml')
            Checks to see if the XML file is a CanSAS file

            Parameters ext -- The file extension of the data file

            Raises FileContentsException -- Raised if XML file isn’t valid CanSAS

    load_file_and_schema(xml_file, schema_path='')

    logging = None
    names = None
    ns_list = None

    read(xml_file, schema_path='', invalid=True)
        Basic file reader

            Parameters filepath -- The full or relative path to a file to be loaded

    reset_state()
        Resets the class state to a base case when loading a new data file so previous data files do not appear a second time

    type = ['XML files (*.xml)|*.xml', 'SasView Save Files (*.svs)|*.svs']
    type_name = 'canSAS'
write(filename, datainfo)

Write the content of a Data1D as a CanSAS XML file

Parameters

• filename – name of the file to write
• datainfo – Data1D object

write_node(parent, name, value, attr=None)

Parameters

• doc – document DOM
• parent – parent node
• name – tag of the element
• value – value of the child text node
• attr – attribute dictionary

Returns True if something was appended, otherwise False

sas.sascalc.dataloader.readers.cansas_reader.get_content(location, node)

Get the first instance of the content of a xpath location.

Parameters

• location – xpath location
• node – node to start at

Returns Element, or None

sas.sascalc.dataloader.readers.cansas_reader.getattrchain(obj, chain, default=None)

Like getattr, but the attr may contain multiple parts separated by ‘.’

sas.sascalc.dataloader.readers.cansas_reader.setattrchain(obj, chain, value)

Like setattr, but the attr may contain multiple parts separated by ‘.’

sas.sascalc.dataloader.readers.cansas_reader.write_node(doc, parent, name, value, attr=None)

Parameters

• doc – document DOM
• parent – parent node
• name – tag of the element
• value – value of the child text node
• attr – attribute dictionary

Returns True if something was appended, otherwise False

sas.sascalc.dataloader.readers.cansas_reader_HDF5 module

NXcanSAS data reader for reading HDF5 formatted CanSAS files.

class sas.sascalc.dataloader.readers.cansas_reader_HDF5.Reader

Bases: sas.sascalc.dataloader.file_reader_base_class.FileReader

A class for reading in NXcanSAS data files. The current implementation has been tested to load data generated by multiple facilities, all of which are known to produce NXcanSAS standards compliant data. Any number of data sets may be present within the file and any dimensionality of data may be used. Currently 1D and 2D SAS data sets are supported, but should be immediately extensible to SESANS data.
Any number of SASdata groups may be present in a SASentry and the data within each SASdata group can be a single 1D I(Q), multi-framed 1D I(Q), 2D I(Qx, Qy) or multi-framed 2D I(Qx, Qy).

Dependencies The NXcanSAS HDF5 reader requires h5py => v2.5.0 or later.

```
add_data_set(key="")
```

Adds the current dataset to the list of outputs after preforming final processing on the data and then calls a private method to generate a new data set.

**Parameters**
- `key` – NeXus group name for current tree level

```
add_intermediate()
```

This method stores any intermediate objects within the final data set after fully reading the set.

**Parameters**
- `parent` – The NXclass name for the h5py Group object that just finished being processed

```
allow_all = True
```

```
static as_list_or_array(iterable)
```

Return value as a list if not already a list or array.

```
cansas_version = 2.0
```

```
ext = ['\.h5', '\.H5']
```

```
final_data_cleanup()
```

Does some final cleanup and formatting on self.current_datainfo and all data1D and data2D objects and then combines the data and info into Data1D and Data2D objects

```
get_file_contents()
```

This is the general read method that all SasView data_loaders must have.

**Parameters**
- `filename` – A path for an HDF5 formatted CanSAS 2D data file.

**Returns** List of Data1D/2D objects and/or a list of errors.

```
process_1d_data_object(data_set, key, unit)
```

SASdata processor method for 1d data items

```
process_2d_data_object(data_set, key, unit)
```

```
process_aperture(data_point, key)
```

SASaperture processor

```
process_collimation(data_point, key, unit)
```

SAScollimation processor

```
process_detector(data_point, key, unit)
```

SASdetector processor

```
process_process(data_point, key)
```

SASprocess processor

```
process_sample(data_point, key)
```

SASsample processor

```
process_source(data_point, key, unit)
```

SASsource processor
process_trans_spectrum\((\text{data\_set}, \text{key})\)

SAS transmission spectrum processor:
- \text{param data\_set: data from HDF5 file}
- \text{param key: canSAS\_class attribute}

read_children\((\text{data, parent\_list})\)

A recursive method for stepping through the hierarchical data file.

Parameters

- \text{data} – h5py Group object of any kind
- \text{parent} – h5py Group parent name

reset_state()

Create the reader object and define initial states for class variables

type = ['NXcanSAS HDF5 Files (*.h5)|*.h5|']

type\_name = 'NXcanSAS'

\text{sas.sascalc.dataloader.readers.cansas_reader\_HDF5.h5attr(node, key, default=None)}

sas.sascalc.dataloader.readers.danse_reader module

DANSE/SANS file reader

\text{class sas.sascalc.dataloader.readers.danse_reader.Reader}

- \text{Bases: sas.sascalc.dataloader.file\_reader\_base\_class.FileReader}

Example data manipulation

\text{ext = ['.sans', '.SANS']}

\text{get\_file\_contents()}

Reader specific class to access the contents of the file All reader classes that inherit from FileReader must implement

type = ['DANSE files (*.sans)|*.sans']

type\_name = 'DANSE'

sas.sascalc.dataloader.readers.red2d_reader module

TXT/IGOR 2D Q Map file reader

\text{class sas.sascalc.dataloader.readers.red2d_reader.Reader}

- \text{Bases: sas.sascalc.dataloader.file\_reader\_base\_class.FileReader}

Simple data reader for Igor data files

\text{ext = ['.DAT', '.dat']}

\text{get\_file\_contents()}

Reader specific class to access the contents of the file All reader classes that inherit from.FileReader must implement

type = ['IGOR/DAT 2D file in Q\_map (*.dat)|*.DAT']

type\_name = 'IGOR/DAT 2D Q\_map'

write\((\text{filename, data})\)

Write to .dat

Parameters

- \text{filename} – file name to write
• data – data2D
sas.sascalc.dataloader.readers.red2d_reader.check_point(x_point)
  check point validity

sas.sascalc.dataloader.readers.sesans_reader module

SESANS reader (based on ASCII reader)
Reader for .ses or .sesans file format
Jurrian Bakker

class sas.sascalc.dataloader.readers.sesans_reader.Reader
  Bases: sas.sascalc.dataloader.file_reader_base_class.FileReader
  Class to load sesans files (6 columns).
  allow_all = True
  ext = ['.ses', '.SES', '.sesans', '.SESANS']
  get_file_contents()
    Reader specific class to access the contents of the file All reader classes that inherit from FileReader
    must implement
    type = ['SESANS files (*.ses)|*.ses', 'SESANS files (*.sesans)|*.sesans']
    type_name = 'SESANS'

sas.sascalc.dataloader.readers.tiff_reader module

Image reader. Untested.

class sas.sascalc.dataloader.readers.tiff_reader.Reader
  Example data manipulation
  ext = ['.tif', '.tiff']
  read(filename=None)
    Open and read the data in a file
      Parameters file – path of the file
      type = ['TIF files (*.tif)|*.tif', 'TIFF files (*.tiff)|*.tiff']
      type_name = 'TIF'

sas.sascalc.dataloader.readers.xml_reader module

Generic XML read and write utility
Usage: Either extend xml_reader or add as a class variable.

class sas.sascalc.dataloader.readers.xml_reader.XMLreader(xml=None,
  schema=None)
  Bases: sas.sascalc.dataloader.file_reader_base_class.FileReader
  Generic XML read and write class. Mostly helper functions. Makes reading/writing XML a bit easier than
calling lxml libraries directly.
    Dependencies This class requires lxml 2.3 or higher.
  append(element, tree)
    Append an etree Element to an ElementTree.
Parameters

• **element** – etree Element to append
• **tree** – ElementTree object to append to

`break_processing_instructions(string, dic)`
Method to break a processing instruction string apart and add to a dict

Parameters

• **string** – A processing instruction as a string
• **dic** – The dictionary to save the PIs to

`create_element(name, attrib=None, nsmap=None)`
Create an XML element for writing to file

Parameters

**name** – The name of the element to be created

`create_element_from_string(xml_string)`
Create an element from an XML string

Parameters

**xml_string** – A string of xml

`create_tree(root)`
Create an element tree for processing from an etree element

Parameters

**root** – etree Element(s)

`ebuilder(parent, elementname, text=None, attrib=None)`
Use lxml E builder class with arbitrary inputs.

Parameters

• **parent** – The parent element to append a child to
• **elementname** – The name of the child in string form
• **text** – The element text
• **attrib** – A dictionary of attribute names to attribute values

encoding = None

`find_invalid_xml()`
Finds the first offending element that should not be present in XML file

`parse_schema_and_doc()`
Creates a dictionary of the parsed schema and xml files.

`processing_instructions = None`

`reader()`
Read in an XML file into memory and return an lxml dictionary

`return_processing_instructions()`
Get all processing instructions saved when loading the document

Parameters

**tree** – etree.ElementTree object to write PIs to

`schema = None`

`schemadoc = None`

`set_encoding(attr_str)`
Find the encoding in the xml declaration and save it as a string

Parameters

**attr_str** – All attributes as a string e.g. “foo1=‘bar1’” foo2=‘bar2’ foo3=‘bar3’ ... foo_n=‘bar_n’”
**set_processing_instructions()**
Take out all processing instructions and create a dictionary from them If there is a default encoding, the value is also saved

**set_schema(schema)**
Set the schema file and parse

**set_xml_file(xml)**
Set the XML file and parse

**set_xml_string(tag_soup)**
Set an XML string as the working XML.

  **Parameters**
  - *tag_soup* – XML formatted string

**to_string(elem, pretty_print=False, encoding=None)**
Converts an etree element into a string

**validate_xml()**
Checks to see if the XML file meets the schema

**write_attribute(elem, attr_name, attr_value)**
Write attributes to an Element

  **Parameters**
  - *elem* – etree.Element object
  - *attr_name* – attribute name to write
  - *attr_value* – attribute value to set

**write_text(elem, text)**
Write text to an etree Element

  **Parameters**
  - *elem* – etree.Element object
  - *text* – text to write to the element

```python
xml = None
xmldoc = None
xmlroot = None
```

**Module contents**

**Submodules**

**sas.sascalc.dataloader.data_info module**

Module that contains classes to hold information read from reduced data files.
A good description of the data members can be found in the CanSAS 1D XML data format:
http://www.smallangles.net/wgwiki/index.php/cansas1d_documentation

```python
class sas.sascalc.dataloader.data_info.Aperture
    Bases: object
    distance = None
distance_unit = 'mm'
name = None
size = None
```
size_name = None
size_unit = 'mm'
type = None
class sas.sascalc.dataloader.data_info.Collimation
    Bases: object
    Class to hold collimation information
    aperture = None
    length = None
    length_unit = 'mm'
    name = None
class sas.sascalc.dataloader.data_info.Data1D(x=None, y=None, dx=None, dy=None, lam=None, dlam=None, isSesans=None)
    Bases: sas.sascalc.dataloader.data_info.plottable_1D, sas.sascalc.dataloader.data_info.DataInfo
    1D data class
    clone_without_data(length=0, clone=None)
    Clone the current object, without copying the data (which will be filled out by a subsequent operation).
    The data arrays will be initialized to zero.
    Parameters
    • length – length of the data array to be initialized
    • clone – if provided, the data will be copied to clone
    is_slit_smeared()
    Check whether the data has slit smearing information :return: True is slit smearing info is present,
    False otherwise
class sas.sascalc.dataloader.data_info.Data2D(data=None, err_data=None, qx_data=None, qy_data=None, q_data=None, mask=None, dqx_data=None, dqy_data=None)
    Bases: sas.sascalc.dataloader.data_info.plottable_2D, sas.sascalc.dataloader.data_info.DataInfo
    2D data class
    I_unit = '1/cm'
    Q_unit = '1/A'
    clone_without_data(length=0, clone=None)
    Clone the current object, without copying the data (which will be filled out by a subsequent operation).
    The data arrays will be initialized to zero.
    Parameters
    • length – length of the data array to be initialized
    • clone – if provided, the data will be copied to clone
    isSesans = False
    x_bins = None
    y_bins = None
class sas.sascalc.dataloader.data_info.DataInfo
    Bases: object
    
    Class to hold the data read from a file. It includes four blocks of data for the instrument description, the sample description, the data itself and any other meta data.

    add_notes(message="")
    Add notes to datainfo

    append_empty_process()

    collimation = None
    detector = None
    errors = None
    filename = ''
    instrument = ''
    isSesans = None
    meta_data = None
    notes = None
    process = None
    run = None
    run_name = None
    sample = None
    source = None
    title = ''
    trans_spectrum = None

class sas.sascalc.dataloader.data_info.Detector
    Bases: object
    
    Class to hold detector information

    beam_center = None
    beam_center_unit = 'mm'
    distance = None
    distance_unit = 'mm'
    name = None
    offset = None
    offset_unit = 'm'
    orientation = None
    orientation_unit = 'degree'
    pixel_size = None
    pixel_size_unit = 'mm'
    slit_length = None
    slit_length_unit = 'mm'

class sas.sascalc.dataloader.data_info.Process
    Bases: object
    
    Class that holds information about the processes performed on the data.
date = ''
description = ''

is_empty()
    Return True if the object is empty

name = ''

notes = None

single_line_desc()
    Return a single line string representing the process

term = None

class sas.sascalc.dataloader.data_info.Sample
    Bases: object
    
    Class to hold the sample description

    ID = ''
    details = None
    name = ''
    orientation = None
    orientation_unit = 'degree'
    position = None
    position_unit = 'mm'
    temperature = None
    temperature_unit = None
    thickness = None
    thickness_unit = 'mm'
    transmission = None
    yacceptance = (0, '')
    zacceptance = (0, '')

class sas.sascalc.dataloader.data_info.Source
    Bases: object
    
    Class to hold source information

    beam_shape = None
    beam_size = None
    beam_size_name = None
    beam_size_unit = 'mm'
    name = None
    radiation = None
    wavelength = None
    wavelength_max = None
    wavelength_max_unit = 'nm'
    wavelength_min = None
    wavelength_min_unit = 'nm'
wavelength_spread = None
wavelength_spread_unit = 'percent'
wavelength_unit = 'A'

class sas.sascalc.dataloader.data_info.TransmissionSpectrum
    Bases: object
    
    Class that holds information about transmission spectrum for white beams and spallation sources.
    
    name = ''
    timestamp = ''
    transmission = None
    transmission_deviation = None
    transmission_deviation_unit = ''
    transmission_unit = ''
    wavelength = None
    wavelength_unit = 'A'

class sas.sascalc.dataloader.data_info.Vector(x=None, y=None, z=None)
    Bases: object
    
    Vector class to hold multi-dimensional objects
    
    x = None
    y = None
    z = None

class sas.sascalc.dataloader.data_info.combine_data_info_with_plottable(data)

    A function that combines the DataInfo data in self.current_data into with a plottable_1D or 2D data object.

    Parameters
    data -- A plottable_1D or plottable_2D data object

    Returns
    A fully specified Data1D or Data2D object

class sas.sascalc.dataloader.data_info.plottable_1D(x, y, dx=None, dy=None, dxl=None, dxw=None, lam=None, dlam=None)

    Bases: object
    
    Data1D is a place holder for 1D plottables.
    
    dlam = None
    dx = None
    dxl = None
    dxw = None
    dy = None
    lam = None
    x = None
    xaxis(label, unit)
        set the x axis label and unit
    y = None
    yaxis(label, unit)
        set the y axis label and unit
class sas.sascalc.dataloader.data_info.plottable_2D (data=None, err_data=None, 
qx_data=None, 
qy_data=None, 
q_data=None, mask=None, 
dqx_data=None, 
dqy_data=None)

Bases: object

Data2D is a place holder for 2D plottables.

data = None
dqx_data = None
dqy_data = None
err_data = None
mask = None
q_data = None
qx_data = None
qy_data = None
xaxis (label, unit)
set the x axis label and unit

xmax = None
xmin = None

yaxis (label, unit)
set the y axis label and unit

ymax = None
ymin = None

zaxis (label, unit)
set the z axis label and unit

sas.sascalc.dataloader.file_reader_base_class module

This is the base file reader class most file readers should inherit from. All generic functionality required for a file loader/reader is built into this class

class sas.sascalc.dataloader.file_reader_base_class.FileReader

Bases: object

allow_all = False

convert_data_units (default_q_unit='1/A')
Converts all data to the sasview default of units of A^{-1} for Q and cm^{-1} for I. :param default_q_unit: The default Q unit used by Sasview

data_cleanup ()
Clean up the data sets and refresh everything :return: None

deprecated_extensions = ['asc']
ext = ['txt']

format_unit (unit=None)
Format units a common way :param unit: :return:
get_file_contents()
    Reader specific class to access the contents of the file. All reader classes that inherit from FileReader
    must implement

handle_error_message(msg)
    Generic error handler to add an error to the current datainfo to propagate the error up the error chain.
    :param msg: Error message

has_converter = True

nextline()
    Returns the next line in the file as a string.

nextlines()
    Returns the next line in the file as a string.

read(filepath)
    Basic file reader

        Parameters filepath -- The full or relative path to a file to be loaded

readall()
    Returns the entire file as a string.

remove_empty_q_values()
    Remove any point where Q == 0

reset_data_list(no_lines=0)
    Reset the plottable_1D object

reset_state()
    Resets the class state to a base case when loading a new data file so previous data files do not appear a
    second time

send_to_output()
    Helper that automatically combines the info and set and then appends it to output

set_all_to_none()
    Set all mutable values to None for error handling purposes

static set_default_1d_units(data)
    Set the x and y axes to the default 1D units
    :param data: 1D data set
    :return:

static set_default_2d_units(data)
    Set the x and y axes to the default 2D units
    :param data: 2D data set
    :return:

sort_data()
    Sort 1D data along the X axis for consistency

static splitline(line)
    Splits a line into pieces based on common delimiters
    :param line: A single line of text
    :return: list of values

type = ['Text files (*.txt|*.TXT)']
type_name = 'ASCII'

sas.sascalc.dataloader.file_reader_base_class.decode(s)

sas.sascalc.dataloader.loader module

File handler to support different file extensions. Uses reflectometer registry utility.

The default readers are found in the ‘readers’ sub-module and registered by default at initialization time.

To add a new default reader, one must register it in the register_readers method found in readers/__init__.py.
A utility method (find_plugins) is available to inspect a directory (for instance, a user plug-in directory) and look for new readers/writers.

```python
class sas.sascalc.dataloader.loader.Loader
    Bases: object

    Utility class to use the Registry as a singleton.

    associate_file_reader(ext, loader)
        Append a reader object to readers

        Parameters
        • ext – file extension [string]
        • module – reader object

    associate_file_type(ext, module)
        Look into a module to find whether it contains a Reader class. If so, append it to readers and (potentially) to the list of writers for the given extension

        Parameters
        • ext – file extension [string]
        • module – module object

    find_plugins(directory)
        Find plugins in a given directory

        Parameters dir – directory to look into to find new readers/writers

    get_wildcards()
        Return the list of wildcards

    load(file, format=None)
        Load a file

        Parameters
        • file – file name (path)
        • format – specified format to use (optional)

        Returns DataInfo object

    save(file, data, format)
        Save a DataInfo object to file

        Parameters file, data, format

    Bases: sas.sascalc.data_util.registry.ExtensionRegistry

    Registry class for file format extensions. Readers and writers are supported.

    associate_file_reader(ext, loader)
        Append a reader object to readers

        Parameters
        • ext – file extension [string]
        • module – reader object

    associate_file_type(ext, module)
        Look into a module to find whether it contains a Reader class. If so, append it to readers and (potentially) to the list of writers for the given extension

        Parameters
        • ext – file extension [string]
        • module – module object
```
**find_plugins(dir)**

Find readers in a given directory. This method can be used to inspect user plug-in directories to find new readers/writers.

**Parameters**

- dir – directory to search into

**Returns**

number of readers found

**load(path, format=None)**

Call the loader for the file type of path.

**Parameters**

- path – file path
- format – explicit extension, to force the use of a particular reader

Defaults to the ascii (multi-column), canas XML, and canas NeXuS readers if no reader was registered for the file’s extension.

**lookup_writers(path)**

Returns the loader associated with the file type of path.

Raises ValueError if file type is not known.

**save(path, data, format=None)**

Call the writer for the file type of path.

Raises ValueError if no writer is available. Raises KeyError if format is not available. May raise a writer-defined exception if writer fails.

### sas.sascalc.dataloader.loader_exceptions module

Exceptions specific to loading data.

**exception sas.sascalc.dataloader.loader_exceptions.DataReaderException(e=None)**

Bases: exceptions.Exception

Exception for files that were able to mostly load, but had minor issues along the way. Any exceptions of this type should be put into the datainfo.errors

**exception sas.sascalc.dataloader.loader_exceptions.DefaultReaderException(e=None)**

Bases: exceptions.Exception

Exception for files with no associated reader. This should be thrown by default readers only to tell Loader to try the next reader.

**exception sas.sascalc.dataloader.loader_exceptions.FileContentsException(e=None)**

Bases: exceptions.Exception

Exception for files with an associated reader, but with no loadable data. This is useful for catching loader or file format issues.

**exception sas.sascalc.dataloader.loader_exceptions.NoKnownLoaderException(e=None)**

Bases: exceptions.Exception

Exception for files with no associated reader based on the file extension of the loaded file. This exception should only be thrown by loader.py.

### sas.sascalc.dataloader.manipulations module

**class sas.sascalc.dataloader.manipulations.Binning(min_value, max_value, n_bins, base=None)**

Bases: object

This class just creates a binning object either linear or log
get_bin_index(value)
The general formula logarithm binning is: \( \text{bin} = \text{floor}(N \times (\log(x) - \log(\text{min})) / (\log(\text{max}) - \log(\text{min}))) \)

class sas.sascalc.dataloader.manipulations.Boxavg(x_min=0.0, x_max=0.0, y_min=0.0, y_max=0.0)
Bases: sas.sascalc.dataloader.manipulations.Boxsum
Perform the average of counts in a 2D region of interest.

class sas.sascalc.dataloader.manipulations.Boxcut(x_min=0.0, x_max=0.0, y_min=0.0, y_max=0.0)
Bases: object
Find a rectangular 2D region of interest.

class sas.sascalc.dataloader.manipulations.Boxsum(x_min=0.0, x_max=0.0, y_min=0.0, y_max=0.0)
Bases: object
Perform the sum of counts in a 2D region of interest.

class sas.sascalc.dataloader.manipulations.CircularAverage(r_min=0.0, r_max=0.0, bin_width=0.0005)
Bases: object
Perform circular averaging on 2D data
The data returned is the distribution of counts as a function of Q

class sas.sascalc.dataloader.manipulations.Ring(r_min=0, r_max=0, center_x=0, center_y=0, nbins=36)
Bases: object
Defines a ring on a 2D data set. The ring is defined by r_min, r_max, and the position of the center of the ring.
The data returned is the distribution of counts around the ring as a function of phi.
Phi_min and phi_max should be defined between 0 and 2*\pi in anti-clockwise starting from the x-axis on the left-hand side.

class sas.sascalc.dataloader.manipulations.Ringcut(r_min=0, r_max=0, center_x=0, center_y=0)
Bases: object
Defines a ring on a 2D data set. The ring is defined by r_min, r_max, and the position of the center of the ring.
The data returned is the region inside the ring
Phi_min and phi_max should be defined between 0 and 2*\pi in anti-clockwise starting from the x-axis on the left-hand side.

class sas.sascalc.dataloader.manipulations.SectorPhi(r_min, r_max, phi_min=0, phi_max=6.283185307179586, nbins=20, base=None)
Bases: sas.sascalc.dataloader.manipulations._Sector
Sector average as a function of phi. I(\phi) is return and the data is averaged over Q.
A sector is defined by r_min, r_max, phi_min, phi_max. The number of bin in phi also has to be defined.

class sas.sascalc.dataloader.manipulations.SectorQ(r_min, r_max, phi_min=0, phi_max=6.283185307179586, nbins=20, base=None)
Bases: sas.sascalc.dataloader.manipulations._Sector
Sector average as a function of Q for both symatric wings. I(Q) is return and the data is averaged over phi.
A sector is defined by \( r_{\text{min}}, r_{\text{max}}, \phi_{\text{min}}, \phi_{\text{max}} > 0 \). The number of bin in \( Q \) also has to be defined.

```python
class sas.sascalc.dataloader.manipulations.Sectorcut (phi_min=0, phi_max=3.141592653589793)

Bases: object

Defines a sector (major + minor) region on a 2D data set. The sector is defined by \( \phi_{\text{min}}, \phi_{\text{max}} \), where \( \phi_{\text{min}} \) and \( \phi_{\text{max}} \) are defined by the right and left lines wrt central line.

\( \phi_{\text{min}} \) and \( \phi_{\text{max}} \) are given in units of radian and (\( \phi_{\text{max}}-\phi_{\text{min}} \)) should not be larger than \( \pi \).
```

```python
class sas.sascalc.dataloader.manipulations.SlabX (x_min=0.0, x_max=0.0, y_min=0.0, y_max=0.0, bin_width=0.001)

Bases: sas.sascalc.dataloader.manipulations._Slab

Compute average \( I(Qx) \) for a region of interest
```

```python
class sas.sascalc.dataloader.manipulations.SlabY (x_min=0.0, x_max=0.0, y_min=0.0, y_max=0.0, bin_width=0.001)

Bases: sas.sascalc.dataloader.manipulations._Slab

Compute average \( I(Qy) \) for a region of interest
```

```python
class sas.sascalc.dataloader.manipulations.flip_phi (phi)

Correct phi to within the \( 0 \leq \phi \leq 2\pi \) range

Returns phi in \( >0 \) and \( \leq 2\pi \)
```

```python
class sas.sascalc.dataloader.manipulations.get_dq_data (data2D)

Get the \( dq \) for resolution averaging. The pinholes and det. pix contribution present in both direction of the 2D which must be subtracted when converting to 1D: \( dq \) overlap should calculated ideally at \( q = 0 \). Note This method works on only pinhole geometry. Extrapolate \( dqx(r) \) and \( dqy(\phi) \) at \( q = 0 \), and take an average.
```

```python
class sas.sascalc.dataloader.manipulations.get_intercept (q, q_0, q_1)

Returns the fraction of the side at which the \( q \)-value intercept the pixel, None otherwise. The values returned is the fraction ON THE SIDE OF THE LOWEST \( Q \).
```

```python
class sas.sascalc.dataloader.manipulations.get_pixel_fraction (qmax, q_00, q_01, q_10, q_11)

Returns the fraction of the pixel defined by the four corners \( (q_{00}, q_{01}, q_{10}, q_{11}) \) that has \( q < q_{\text{max}} \).
```

```python
class sas.sascalc.dataloader.manipulations.get_pixel_fraction_square (x, xmin, xmax)

Return the fraction of the length from \( xmin \) to \( x \).
```
### Parameters

- **x** – x-value
- **xmin** – minimum x for the length considered
- **xmax** – minimum x for the length considered

### Returns

\((x-xmin)/(xmax-xmin)\) when \(xmin < x < xmax\)

### SASCalc::Dataloader::Manipulations::GetQ(dx, dy, det_dist, wavelength)

#### Parameters

- **dx** – x-distance from beam center [mm]
- **dy** – y-distance from beam center [mm]

#### Returns

q-value at the given position

### SASCalc::Dataloader::Manipulations::GetQCompo(dx, dy, det_dist, wavelength, compo=None)

This reduces tiny error at very large q. Implementation of this function is not started yet.<–ToDo

### SASCalc::Dataloader::Reader2DConverter(data2d=None)

convert old 2d format opened by IHorReader or danse_reader to new Data2D format. This is mainly used by the Readers

#### Parameters

- **data2d** – 2d array of Data2D object

#### Returns

1d arrays of Data2D object

### Module contents

- **SASCalc::FileConverter package**

### Submodules

- **SASCalc::FileConverter::Ascii2DLoader module**

#### ASCII 2D Loader

##### Class

```python
class SASCalc::FileConverter::Ascii2DLoader::ASCII2DLoader(data_path)
    Bases: object

    load()
        Load the data from the file into a Data2D object

        Returns
            A Data2D instance containing data from the file

        Raises
            ValueError – Raises a ValueError if the file is incorrectly formatted
```

### SASCalc::FileConverter::BSLLoader module

##### Class

```python
class SASCalc::FileConverter::BSLLoader::BSLLoader(filename)
    Bases: CLoader

    Loads 2D SAS data from a BSL file. CLoader is a C extension (found in c_ext/bsl_loader.c)
```

```python
load_frames(frames)
```

```python
exception sas.sascalc.file_converter.bsl_loader.BSLParsingError
    Bases: exceptions.Exception
```

```python
sas.sascalc.file_converter.cansas_writer module
```

```python
class sas.sascalc.file_converter.cansas_writer.CansasWriter(xml=None, schema=None)
    Bases: sas.sascalc.dataloader.readers.cansas_reader.Reader
    write(filename, frame_data, sasentry_attrs=None)
        Write the content of a Data1D as a CanSAS XML file
        Parameters
            • filename -- name of the file to write
            • datainfo -- Data1D object
```

```python
sas.sascalc.file_converter.nxcansas_writer module
```

NXcanSAS 1/2D data reader for writing HDF5 formatted NXcanSAS files.

```python
class sas.sascalc.file_converter.nxcansas_writer.NXcanSASWriter
    Bases: sas.sascalc.dataloader.readers.cansas_reader_HDF5.Reader
    A class for writing in NXcanSAS data files. Any number of data sets may be written to the file. Currently 1D and 2D SAS data sets are supported
    NXcanSAS spec: http://download.nexusformat.org/sphinx/classes/contributed_definitions/NXcanSAS.html
    Dependencies The NXcanSAS writer requires h5py => v2.5.0 or later.
    write(dataset, filename)
        Write an array of Data1d or Data2D objects to an NXcanSAS file, as one SASEntry with multiple SASData elements. The metadata of the first element in the array will be written as the SASEntry metadata (detector, instrument, sample, etc).
        Parameters
            • dataset -- A list of Data1D or Data2D objects to write
            • filename -- Where to write the NXcanSAS file
```

```python
sas.sascalc.file_converter.otoko_loader module
```

Here we handle loading of “OTOKO” data (for more info about this format see the comment in load_otoko_data). Given the paths of header and data files, we aim to load the data into numpy arrays for use later.

```python
class sas.sascalc.file_converter.otoko_loader.CStyleStruct(**kwds)
    A nice and easy way to get “C-style struct” functionality.

class sas.sascalc.file_converter.otoko_loader.OTOKOData(q_axis, data_axis)

class sas.sascalc.file_converter.otoko_loader.OTOKOLoader(qaxis_path, data_path)
    Bases: object
```

---

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load_otoko_data()

Loads “OTOKO” data, which is a format that stores each axis separately. An axis is represented by a “header” file, which in turn will give details of one or more binary files where the actual data is stored.

Given the paths of two header files, this function will load each axis in turn. If loading is successful then an instance of the OTOKOData class will be returned, else an exception will be raised.

For more information on the OTOKO file format, please see: http://www.diamond.ac.uk/Home/Beamlines/small-angle/SAXS-Software/CCP13/XOTOKO.html

exception sas.sascalc.file_converter.otoko_loader.OTOKOParsingError
  Bases: exceptions.Exception

sas.sascalc.file_converter.red2d_writer module

class sas.sascalc.file_converter.red2d_writer.Red2DWriter
  Bases: sas.sascalc.dataloader.readers.red2d_reader.Reader

write (filename, data, thread)
  Write to .dat

  Parameters

  • filename – file name to write
  • data – data2D

Module contents

sas.sascalc.fit package

Submodules

sas.sascalc.fit.AbstractFitEngine module

class sas.sascalc.fit.AbstractFitEngine.FResult (model=None, param_list=None, data=None)
  Bases: object
  Storing fit result

  print_summary()
  set_fitness (fitness)
  set_model (model)

exception sas.sascalc.fit.AbstractFitEngine.FitAbort
  Bases: exceptions.Exception
  Exception raise to stop the fit

class sas.sascalc.fit.AbstractFitEngine.FitArrange

  add_data (data)
    add_data fill a self.data_list with data to fit

    Parameters data – Data to add in the list

  get_data ()
    Returns list of data data_list

  get_model ()
Returns  saved model

```python
def get_to_fit()
    return self.selected value
```

```python
remove_data(data)
    Remove one element from the list

Parameters  data – Data to remove from data_list
```

```python
def set_model(model)
    set_model save a copy of the model

Parameters  model – the model being set
```

```python
def set_to_fit(value=0)
    set self.selected to 0 or 1 for other values raise an exception

Parameters  value – integer between 0 or 1
```

```python
class sas.sascalc.fit.AbstractFitEngine.FitData1D(x, y, dx=None, dy=None, smearer=None, data=None, lam=None, dlam=None)
```

```text
Bases: sas.sascalc.dataloader.data_info.Data1D
```

Wrapper class for SAS data FitData1D inherits from DataLoader.data_info.Data1D. Implements a way to get residuals from data.

```python
def get_fit_range()
    Return the range of data.x to fit
```

```python
def residuals(fn)
    Compute residuals.
    If self.smearer has been set, use if to smear the data before computing chi squared.

Parameters  fn – function that return model value

Returns  residuals
```

```python
def residuals_deriv(model, pars=[])
    Returns  residuals derivatives .

Note  in this case just return empty array
```

```python
def set_fit_range(qmin=None, qmax=None)
    to set the fit range
```

```python
def size()
    Number of measurement points in data set after masking, etc.
```

```python
class sas.sascalc.fit.AbstractFitEngine.FitData2D(sas_data2d, data=None, err_data=None)
```

```text
Bases: sas.sascalc.dataloader.data_info.Data2D
```

Wrapper class for SAS data

```python
def get_fit_range()
    return the range of data.x to fit
```

```python
def residuals(fn)
    return the residuals
```

```python
def residuals_deriv(model, pars=[])
    Returns  residuals derivatives .

Note  in this case just return empty array
```

```python
def set_data(sas_data2d, qmin=None, qmax=None)
    Determine the correct qx_data and qy_data within range to fit
```

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set_fit_range (qmin=None, qmax=None)
To set the fit range

set_smearer (smearer)
Set smearer

size()
Number of measurement points in data set after masking, etc.

class sas.sascalc.fit.AbstractFitEngine.FitEngine

get_model (id)

Parameters
id – id is key in the dictionary containing the model to return

Returns
a model at this id or None if no FitArrange element was created with this id

get_problem_to_fit (id)
return the self.selected value of the fit problem of id

Parameters
id – the id of the problem

remove_fit_problem (id)
remove fitarrange in id

select_problem_for_fit (id, value)
select a couple of model and data at the id position in dictionary and set in self.selected value to value

Parameters
value – the value to allow fitting. can only have the value one or zero

set_data (data, id, smearer=None, qmin=None, qmax=None)
Receives plottable, creates a list of data to fit,set data in a FitArrange object and adds that object in a dictionary with key id.

Parameters
• data – data added
• id – unique key corresponding to a fitArrange object with data

set_model (model, id, pars=[], constraints=[], data=None)
set a model on a given in the fit engine.

Parameters
• model – sas.models type
• id – is the key of the fitArrange dictionary where model is saved as a value
• pars – the list of parameters to fit
• constraints – list of tuple (name of parameter, value of parameters) the value of parameter must be a string to constraint 2 different parameters. Example: we want to fit 2 model M1 and M2 both have parameters A and B. constraints can be constraints = [(M1.A, M2.B+2), (M1.B= M2.A *5),...,

Note pars must contains only name of existing model’s parameters

class sas.sascalc.fit.AbstractFitEngine.FitHandler
Bases: object

Abstract interface for fit thread handler.

The methods in this class are called by the optimizer as the fit progresses.

Note that it is up to the optimizer to call the fit handler correctly, reporting all status changes and maintaining the ‘done’ flag.

abort ()
Fit was aborted.
done = False
True when the fit job is complete

error (msg)
Model had an error; print traceback

finalize()
Fit is complete; best results are reported

improvement()
Called when a result is observed which is better than previous results from the fit.
result is a FitResult object, with parameters, #calls and fitness.

progress (current, expected)
Called each cycle of the fit, reporting the current and the expected amount of work. The meaning of these values is optimizer dependent, but they can be converted into a percent complete using (100*current)//expected.

Progress is updated each iteration of the fit, whatever that means for the particular optimization algorithm. It is called after any calls to improvement for the iteration so that the update handler can control I/O bandwidth by suppressing intermediate improvements until the fit is complete.

result = None
The current best result of the fit

set_result (result=None)

update_fit (last=False)

class sas.sascalc.fit.AbstractFitEngine.Model (sas_model, sas_data=None, **kw)
Fit wrapper for SAS models.

eval (x)
Override eval method of model.

Parameters x -- the x value used to compute a function

eval_derivs (x, pars=[])
Evaluate the model and derivatives wrt pars at x.

pars is a list of the names of the parameters for which derivatives are desired.

This method needs to be specialized in the model to evaluate the model function. Alternatively, the model can implement its own version of residuals which calculates the residuals directly instead of calling eval.

get_params (fitparams)
return a list of value of parameter to fit

Parameters fitparams -- list of parameters name to fit

set (**kw)

set_params (paramlist, params)
Set value for parameters to fit

Parameters params -- list of value for parameters to fit

sas.sascalc.fit.BumpsFitting module

BumpsFitting module runs the bumps optimizer.

class sas.sascalc.fit.BumpsFitting.BumpsFit
Bases: sas.sascalc.fit.AbstractFitEngine.FitEngine

Fit a model using bumps.
**fit** (msg_q=None, q=None, handler=None, curr_thread=None, ftol=1.49012e-08, reset_flag=False)

```python
class sas.sascalc.fit.BumpsFitting.BumpsMonitor (handler, max_step, pars, dof)
Bases: object
config_history (history)
```

**BumpsMonitor** contains population summary statistics to show progress of the fit. This is a list [(best, 0%, 25%, 50%, 75%, 100%)] or just a list [(best,)] if population size is 1.

```python
convergence_monitor (history)
```

**ConvergenceMonitor** contains population summary statistics to show progress of the fit. This is a list [(best, 0%, 25%, 50%, 75%, 100%)] or just a list [(best,)] if population size is 1.

```python
class sas.sascalc.fit.BumpsFitting.ConvergenceMonitor
Bases: object
```

ConvergenceMonitor contains population summary statistics to show progress of the fit. This is a list [(best, 0%, 25%, 50%, 75%, 100%)] or just a list [(best,)] if population size is 1.

```python
config_history (history)
```

**ParameterExpressions** (models)

```python
class sas.sascalc.fit.BumpsFitting.ParameterExpressions (models)
Bases: object
```

**ParameterExpressions** wraps SAS model as a bumps fitness object

```python
nllf()
npoints()
parameters()
residuals()
set_fitted(param_list)
    Flag a set of parameters as fitted parameters.
theory()
update()
```

**get_fitter()**

```python
sas.sascalc.fit.BumpsFitting.get_fitter()
```

**run_bumps** (problem, handler, curr_thread)

```python
sas.sascalc.fit.BumpsFitting.run_bumps (problem, handler, curr_thread)
```

**sas.sascalc.fit.Loader module**

```python
class sas.sascalc.fit.Loader.Load (x=None, y=None, dx=None, dy=None)
This class is loading values from given file or value giving by the user
```

**Load** (x=None, y=None, dx=None, dy=None)

```python
get_filename ()
    return the file’s path
get_values ()
    Return x, y, dx, dy
load_data (data)
    Return plottable
set_filename (path=None)
    Store path into a variable. If the user doesn’t give a path as a parameter a pop-up window appears to select the file.

    Parameters path -- the path given by the user
set_values ()
    Store the values loaded from file in local variables
```
**SasView Documentation, Release 4.2.1**

**sas.sascalc.fit.MultiplicationModel module**

```python
class sas.sascalc.fit.MultiplicationModel.MultiplicationModel(p_model, s_model):
    Bases: sas.sascalc.calculator.BaseComponent.BaseComponent

    Use for P(Q)*S(Q); function call must be in the order of P(Q) and then S(Q): The model parameters are combined from both models, P(Q) and S(Q), except 1) ’radius_effective’ of S(Q) which will be calculated from P(Q) via calculate_ER(), and 2) ‘scale’ in P model which is synchronized w/ volfraction in S then P*S is multiplied by a new parameter, ‘scale_factor’. The polydispersion is applicable only to P(Q), not to S(Q).

    Note: P(Q) refers to ‘form factor’ model while S(Q) does to ‘structure factor’.
```

**evalDistribution**(x=[])
Evaluate the model in cartesian coordinates

**Parameters**
- **x** – input q[] or [qx[], qy[]]

**Returns** scattering function P(q[])

**fill_description**(p_model, s_model)
Fill the description for P(Q)*S(Q)

**getProfile**()
Get SLD profile of p_model if exists

    **Returns** (r, beta) where r is a list of radius of the transition points beta is a list of the corresponding SLD values

**Note:** This works only for func_shell num = 2 (exp function).

**run**(x=0.0)
Evaluate the model

**Parameters**
- **x** – input q-value (float or [float, float] as [r, theta])

**Returns** (scattering function value)

**runXY**(x=0.0)
Evaluate the model

**Parameters**
- **x** – input q-value (float or [float, float] as [qx, qy])

**Returns** scattering function value

**setParam**(name, value)
Set the value of a model parameter

**Parameters**
- **name** – name of the parameter
- **value** – value of the parameter

**set_dispersion**(parameter, dispersion)
Set the dispersion object for a model parameter

**Parameters**
- **parameter** – name of the parameter [string]
- **dispersion** dispersion object of type DispersionModel
$sas.sascalc.fit.expression$ module

Parameter expression evaluator.

For systems in which constraints are expressed as string expressions rather than python code, $compile_constraints()$ can construct an expression evaluator that substitutes the computed values of the expressions into the parameters.

The compiler requires a symbol table, an expression set and a context. The symbol table maps strings containing fully qualified names such as ‘M1.c[3].full_width’ to parameter objects with a ‘value’ property that can be queried and set. The expression set maps symbol names from the symbol table to string expressions. The context provides additional symbols for the expressions in addition to the usual mathematical functions and constants.

The expressions are compiled and interpreted by python, with only minimal effort to make sure that they don’t contain bad code. The resulting constraints function returns 0 so it can be used directly in a fit problem definition.

Extracting the symbol table from the model depends on the structure of the model. If fitness.parameters() is set correctly, then this should simply be a matter of walking the parameter data, remembering the path to each parameter in the symbol table. For compactness, dictionary elements should be referenced by .name rather than ["name"]. Model name can be used as the top level.

Getting the parameter expressions applied correctly is challenging. The following monkey patch works by over-riding model_update in FitProblem so that after setp(p) is called and, the constraints expression can be applied before telling the underlying fitness function that the model is out of date:

```python
# Override model update so that parameter constraints are applied
problem._model_update = problem.model_update

def model_update():
    constraints()
    problem._model_update()
problem.model_update = model_update
```

Ideally, this interface will change

$sas.sascalc.fit.expression.compile_constraints$($symtab$, $exprs$, $context={}$)

Build and return a function to evaluate all parameter expressions in the proper order.

Input:
- $symtab$ is the symbol table for the model: { ‘name’: parameter }
- $exprs$ is the set of computed symbols: { ‘name’: ‘expression’ }
- $context$ is any additional context needed to evaluate the expression

Return:
- updater function which sets parameter.value for each expression

Raises:
- AssertionError - model, parameter or function is missing
- SyntaxError - improper expression syntax
- ValueError - expressions have circular dependencies

This function is not terribly sophisticated, and it would be easy to trick. However it handles the common cases cleanly and generates reasonable messages for the common errors.

This code has not been fully audited for security. While we have removed the builtins and the ability to import modules, there may be other vectors for users to perform more than simple function evaluations. Unauthenticated users should not be running this code.

Parameter names are assumed to contain only _a-zA-Z0-9#[]

Both names are provided for inverse functions, e.g., acos and arccos.

Should try running the function to identify syntax errors before running it in a fit.
Use `help(fn)` to see the code generated for the returned function `fn`. `dis.dis(fn)` will show the corresponding python vm instructions.

```python
sas.sascalc.fit.expression.no_constraints()
# This parameter set has no constraints between the parameters.
```

```python
sas.sascalc.fit.expression.order_dependencies(pairs)
# Order elements from pairs so that b comes before a in the ordered list for all pairs (a,b).
```

```python
sas.sascalc.fit.expression.test_deps()
sas.sascalc.fit.expression.test_expr()
```

### sas.sascalc.fit.models module

Utilities to manage models

```python
class sas.sascalc.fit.models.ModelManager
    Bases: object
    manage the list of available models

    base = None
    cat_model_list()
    composable_models()
    get_model_dictionary()
    get_model_list()
    plugins_reset()
    update()

class sas.sascalc.fit.models.ModelManagerBase
    Bases: object
    Base class for the model manager

    composable_models()
    return list of standard models that can be used in sum/multiply
    get_model_list()
    return dictionary of classified models
    Structure Factors are the structure factor models Multi-Functions are the multiplicity models Plugin Models are the plugin models
    Note that a model can be both a plugin and a structure factor or multiplicity model.
    last_time_dir_modified = 0
    timestamp on the plugin directory at the last plugin update
    model_dictionary = None
    mutable dictionary of models, continually updated to reflect the current set of plugins
    plugin_models = None
    list of plugin models reset each time the plugin directory is queried
    plugins_reset()
    return a dictionary of model
    plugins_update()
    return a dictionary of model if new models were added else return empty dictionary
    standard_models = None
    constant list of standard models
```
class sas.sascalc.fit.models.ReportProblem
    Bases: object
    
    Class to check for problems with specific values

sas.sascalc.fit.models.compile_file(dir)
    Compile a py file

sas.sascalc.fit.models.find_plugin_models()
    Find custom models

sas.sascalc.fit.models.find_plugins_dir()
    Find path of the plugins directory. The plugin directory is located in the user’s home directory.

sas.sascalc.fit.models.initialize_plugins_dir(path)

sas.sascalc.fit.models.plugin_log(message)
    Log a message in a file located in the user’s home directory

sas.sascalc.fit.pagestate module

Class that holds a fit page state

class sas.sascalc.fit.pagestate.PageState(model=None, data=None)
    Bases: object
    
    Contains information to reconstruct a page of the fitpanel.

    clone()
        Create a new copy of the current object

    from_xml(file=None, node=None)
        Load fitting state from a file

        Parameters

            • file – .fitv file
            • node – node of a XML document to read from

    static param_remap_from_sasmodels_convert(params)
        Converts [name : value] map back to [] param list :param params: parameter map returned from sasmodels :return: None

    static param_remap_to_sasmodels_convert(params, is_string=False)
        Remaps the parameters for sasmodels conversion

        Parameters params – list of parameters (likely self.parameters)

        Returns remapped dictionary of parameters

    report(fig_urls)
        Invoke report dialog panel

        :param figs: list of pylab figures [list]

    to_xml(file='fitting_state.fitv', doc=None, entry_node=None, batch_fit_state=None)
        Writes the state of the fit panel to file, as XML.

        Compatible with standalone writing, or appending to an already existing XML document. In that case, the XML document is required. An optional entry node in the XML document may also be given.

        Parameters

            • file – file to write to
            • doc – XML document object [optional]
            • entry_node – XML node within the XML document at which we will append the data [optional]
class sas.sascalc.fit.pagestate.BatchFitPageState
Bases: object
State of the simultaneous fit page for saving purposes

sas.sascalc.fit.pagestate.parse_entry_helper(node, item)
Create a numpy list from value extracted from the node

Parameters

• node – node from each the value is stored
• item – list name of three strings. the two first are name of data attribute and the third one is the type of the value of that attribute. type can be string, float, bool, etc.

: return: numpy array

sas.sascalc.fit.pluginmodel module

class sas.sascalc.fit.pluginmodel.Model1DPlugin(name='Plugin Model')
Bases: sas.sascalc.calculator.BaseComponent.BaseComponent

function(x)
Function to be implemented by the plug-in writer

is_multiplicity_model = False

run(x=0,0)
Evaluate the model

Parameters x – input x, or [x, phi] [radian]

Returns function value
runXY \( (x=0,0) \)
Evaluate the model

**Parameters**
- \( x \) – input x, or [x, y]

**Returns**
- function value

set_details()
Set default details

```python
class sas.sascalc.fit.qsmearing.PySmear (resolution, model, offset=None)
    Bases: object
    Wrapper for pure python sasmodels resolution functions.

    apply (iq_in, first_bin=0, last_bin=None)
    Apply the resolution function to the data. Note that this is called with iq_in matching data.x, but
    with iq_in[first_bin:last_bin] set to theory values for these bins, and the remainder left undefined. The
    first_bin, last_bin values should be those returned from get_bin_range. The returned value is of the
    same length as iq_in, with the range first_bin:last_bin set to the resolution smeared values.

    get_bin_range (q_min=None, q_max=None)
    For a given q_min, q_max, find the corresponding indices in the data. Returns first, last. Note that
    these are indexes into q from the data, not the q_calc needed by the resolution function. Note also that
    these are the indices, not the range limits. That is, the complete range will be q[first:last+1].

class sas.sascalc.fit.qsmearing.PySmear2D (data=None, model=None)
    Bases: object
    Q smearing class for SAS 2d pinhole data

    get_value ()
    Over sampling of r_nbins times phi_nbins, calculate Gaussian weights, then find smeared intensity

    set_accuracy (accuracy='Low')
    Set accuracy.

    Parameters accuracy – string

    set_data (data=None)
    Set data.

    Parameters data – DataLoader.Data_info type

    set_index (index=None)
    Set index.

    Parameters index – 1d arrays

    set_model (model=None)
    Set model.

    Parameters model – sas.models instance

    set_smearer (smearer=True)
    Set whether or not smearer will be used

    Parameters smearer – smear object
```

sas.sascalc.fit.qsmearing.pinhole_smear (data, model=None)
sas.sascalc.fit.qsmearing.slit_smear (data, model=None)
sas.sascalc.fit.qsmearing.smear_selection(data, model=None)

Creates the right type of smearer according to the data. The canSAS format has a rule that either slit smearing data OR resolution smearing data is available.

For the present purpose, we choose the one that has non-zero data. If both slit and resolution smearing arrays are filled with good data (which should not happen), then we choose the resolution smearing data.

Parameters

- **data** – Data1D object
- **model** – sas.model instance

Module contents

sas.sascalc.invariant package

Submodules

sas.sascalc.invariant.invariant module

This module implements invariant and its related computations.

author Gervaise B. Alina/UTK
author Mathieu Doucet/UTK
author Jae Cho/UTK

class sas.sascalc.invariant.invariant.Extrapolator(data, model=None)

Bases: object

Extrapolate I(q) distribution using a given model

fit (power=None, qmin=None, qmax=None)

Fit data for y = ax + b return a and b

Parameters

- **power** – a fixed, otherwise None
- **qmin** – Minimum Q-value
- **qmax** – Maximum Q-value

class sas.sascalc.invariant.invariant.Guinier(scale=1, radius=60)

Bases: sas.sascalc.invariant.invariant.Transform

class of type Transform that performs operations related to guinier function

evaluate_model (x)

return F(x)= scale* e-((radius*x)**2/3)

evaluate_model_errors (x)

Returns the error on I(q) for the given array of q-values

Parameters **x** – array of q-values

evaluate_model_parameters (constant, slope, dconstant=0, dslope=0)

assign new value to the scale and the radius

linearize_q_value (value)

Transform the input q-value for linearization

Parameters **value** – q-value

Returns **q**^2
class sas.sascalc.invariant.invariant.InvariantCalculator(data, background=0, scale=1)

Bases: object

Compute invariant if data is given. Can provide volume fraction and surface area if the user provides Porod constant and contrast values.

Precondition: the user must send a data of type DataLoader.Data1D the user provide background and scale values.

Note: Some computations depends on each others.

def get_data()
    Returns self._data

def get_extra_data_high(npts_in=None, q_end=10, npts=20)
    Returns the extrapolated data used for the high-Q invariant calculation. By default, the distribution will cover the data points used for the extrapolation. The number of overlap points is a parameter (npts_in). By default, the maximum q-value of the distribution will be Q_MAXIMUM, the maximum q-value used when extrapolating for the purpose of the invariant calculation.

    Parameters
    • npts_in – number of data points for which the extrapolated data overlap
    • q_end – is the maximum value to uses for extrapolated data
    • npts – the number of points in the extrapolated distribution

def get_extra_data_low(npts_in=None, q_start=None, npts=20)
    Returns the extrapolated data used for the low-Q invariant calculation. By default, the distribution will cover the data points used for the extrapolation. The number of overlap points is a parameter (npts_in). By default, the maximum q-value of the distribution will be the minimum q-value used when extrapolating for the purpose of the invariant calculation.

    Parameters
    • npts_in – number of data points for which the extrapolated data overlap
    • q_start – is the minimum value to uses for extrapolated data
    • npts – the number of points in the extrapolated distribution

def get_extrapolation_power(range='high')
    Returns the fitted power for power law function for a given extrapolation range

def get_qstar(extrapolation=None)
    Compute the invariant of the local copy of data.

    Parameters extrapolation – string to apply optional extrapolation

    Return q_star invariant of the data within data’s q range

    Warning: When using setting data to Data1D, the user is responsible of checking that the scale and the background are properly apply to the data

def get_qstar_high()
    Compute the invariant for extrapolated data at high q range.

    Implementation: data = self._get_extra_data_high() return self._get_qstar()

    Return q_star the invariant for data extrapolated at high q.

def get_qstar_low()
    Compute the invariant for extrapolated data at low q range.

    Implementation: data = self._get_extra_data_low() return self._get_qstar()
Return \texttt{q\_star} the invariant for data extrapolated at low q.

\texttt{get\_qstar\_with\_error}(\texttt{extrapolation=None})

Compute the invariant uncertainty. This uncertainty computation depends on whether or not the data is smeared.

\textbf{Parameters}\extrapolation – string to apply optional extrapolation

\textbf{Returns} \invariant, the invariant uncertainty

\texttt{get\_surface}(\texttt{contrast, porod\_const, extrapolation=None})

Compute the specific surface from the data.

\textbf{Implementation}:

\begin{verbatim}
V = self.get_volume_fraction(contrast, extrapolation)

Compute the surface given by:
    surface = (2*pi *V(1- V)*porod\_const)/ q\_star
\end{verbatim}

\textbf{Parameters}

\begin{itemize}
  \item \texttt{contrast} – contrast value to compute the volume
  \item \texttt{porod\_const} – Porod constant to compute the surface
  \item \texttt{extrapolation} – string to apply optional extrapolation
\end{itemize}

\textbf{Returns} \specific\_surface

\texttt{get\_surface\_with\_error}(\texttt{contrast, porod\_const, extrapolation=None})

Compute uncertainty of the surface value as well as the surface value. The uncertainty is given as follow:

\begin{verbatim}
dS = porod\_const *2*pi[( dV -2*V*dV)/q\_star
   + dq\_star(v-v**2)

q\_star: the invariant value
dq\_star: the invariant uncertainty
V: the volume fraction value
dV: the volume uncertainty
\end{verbatim}

\textbf{Parameters}

\begin{itemize}
  \item \texttt{contrast} – contrast value
  \item \texttt{porod\_const} – porod constant value
  \item \texttt{extrapolation} – string to apply optional extrapolation
\end{itemize}

\textbf{Return} S, dS the surface, with its uncertainty

\texttt{get\_volume\_fraction}(\texttt{contrast, extrapolation=None})

Compute volume fraction is deduced as follow:

\begin{verbatim}
q\_star = 2*(pi*contrast)**2* volume( 1- volume)
for k = 10^{(-8)}*q\_star/(2*(pi*|contrast|)**2)
we get 2 values of volume:
    with \ 1 - 4 * k >= 0
    volume1 = (1- sqrt(1- 4*k))/2
    volume2 = (1+ sqrt(1- 4*k))/2

q\_star: the invariant value included extrapolation is applied
    unit \ 1/A^{(3)}*1/cm
q\_star = self.get\_qstar()
\end{verbatim}

(continues on next page)
the result returned will be $0 \leq \text{volume} \leq 1$

Parameters

- **contrast** – contrast value provides by the user of type float. contrast unit is $1/A^2 = 10^{16}\text{cm}^2$
- **extrapolation** – string to apply optional extrapolation

Returns \ volume fraction

Note \ volume fraction must have no unit

**get_volume_fraction_with_error** (contrast, extrapolation=None)

Compute uncertainty on volume value as well as the volume fraction. This uncertainty is given by the following equation:

\[
dV = 0.5 \times (4 \times k \times dq_{\text{star}}) / (2 \times \sqrt{1 - k \times q_{\text{star}}})
\]

\[
\text{for } k = 10^{(-8)} \times q_{\text{star}} / (2 \times \pi \times |\text{contrast}|) \times 2
\]

$q_{\text{star}}$: the invariant value including extrapolated value if existing

$dq_{\text{star}}$: the invariant uncertainty

$dV$: the volume uncertainty

The uncertainty will be set to -1 if it can’t be computed.

Parameters

- **contrast** – contrast value
- **extrapolation** – string to apply optional extrapolation

Returns \ V, dV = volume fraction, error on volume fraction

**set_extrapolation** (range, npts=4, function=None, power=None)

Set the extrapolation parameters for the high or low Q-range. Note that this does not turn extrapolation on or off.

Parameters

- **range** – a keyword set the type of extrapolation. type string
- **npts** – the numbers of q points of data to consider for extrapolation
- **function** – a keyword to select the function to use for extrapolation. of type string.
- **power** – an power to apply power_low function

**class** sas.sascalc.invariant.invariant.PowerLaw (scale=1, power=4)

Bases: sas.sascalc.invariant.invariant.Transform

class of type transform that perform operation related to power_law function

**evaluate_model** (x)

given a scale and a radius transform x, y using a power_law function

**evaluate_model_errors** (x)

Returns the error on I(q) for the given array of q-values :param x: array of q-values

**extract_model_parameters** (constant, slope, dconstant=0, dslope=0)

Assign new value to the scale and the power

**linearize_q_value** (value)

Transform the input q-value for linearization

Parameters **value** – q-value
Returns \( \log(q) \)

class sas.sascalc.invariant.invariant.Transform

Bases: object

Define interface that need to compute a function or an inverse function given some \( x, y \)

evaluate_model \((x)\)

Returns an array \( f(x) \) values where \( f \) is the Transform function.

evaluate_model_errors \((x)\)

Returns an array of \( I(q) \) errors

extract_model_parameters \((constant, slope, dconstant=0, dslope=0)\)

set private member

get_allowed_bins \((data)\)

Goes through the data points and returns a list of boolean values to indicate whether each points is allowed by the model or not.

Parameters data – Data1D object

linearize_data \((data)\)

Linearize data so that a linear fit can be performed. Filter out the data that can’t be transformed.

Parameters data – LoadData1D instance

linearize_q_value \((value)\)

Transform the input q-value for linearization

sas.sascalc.invariant.invariant_mapper module

This module is a wrapper to a map function. It allows to loop through different invariant objects to call the same function

sas.sascalc.invariant.invariant_mapper.get_qstar \((inv, extrapolation=None)\)

Get invariant value (Q*)

sas.sascalc.invariant.invariant_mapper.get_qstar_with_error \((inv, extrapolation=None)\)

Get invariant value with uncertainty

sas.sascalc.invariant.invariant_mapper.get_surface \((inv, contrast, porod_const, extrapolation=None)\)

Get surface with uncertainty

sas.sascalc.invariant.invariant_mapper.get_surface_with_error \((inv, contrast, porod_const, extrapolation=None)\)

Get surface with uncertainty

sas.sascalc.invariant.invariant_mapper.get_volume_fraction \((inv, contrast, extrapolation=None)\)

Get volume fraction

sas.sascalc.invariant.invariant_mapper.get_volume_fraction_with_error \((inv, contrast, extrapolation=None)\)

Get volume fraction with uncertainty
Module contents

**sas.sascalc.pr package**

**Submodules**

**sas.sascalc.pr.distance_explorer module**

Module to explore the P(r) inversion results for a range of D_max value. User picks a number of points and a range of distances, then get a series of outputs as a function of D_max over that range.

```python
class sas.sascalc.pr.distance_explorer.DistExplorer(pr_state)
    Bases: object
    
The explorer class

class sas.sascalc.pr.distance_explorer.Results
    Bases: object
    
Class to hold the inversion output parameters as a function of D_max
```

**sas.sascalc.pr.invertor module**

Module to perform P(r) inversion. The module contains the Invertor class.

FIXME: The way the Invertor interacts with its C component should be cleaned up

```python
class sas.sascalc.pr.invertor.Invertor
    Bases: Cinvertor
    
Invertor class to perform P(r) inversion

    The problem is solved by posing the problem as Ax = b, where x is the set of coefficients we are looking for.

    Npts is the number of points.

    In the following i refers to the ith base function coefficient. The matrix has its entries j in its first Npts rows set to

    \[ A[j][i] = \text{(Fourier transformed base function for point j)} \]

    We then choose a number of r-points, n_r, to evaluate the second derivative of P(r) at. This is used as our regularization term. For a vector r of length n_r, the following n_r rows are set to

    \[ A[j+Npts][i] = \text{(2nd derivative of P(r), d^2(P(r))/d(r)^2, evaluated at r[j])} \]

    The vector b has its first Npts entries set to

    \[ b[j] = \text{(I(q) observed for point j)} \]

    The following n_r entries are set to zero.

    The result is found by using scipy.linalg.basic.lstsq to invert the matrix and find the coefficients x.
```

Methods inherited from Cinvertor:

- `get_peaks(pars)`: returns the number of P(r) peaks
- `oscillations(pars)`: returns the oscillation parameters for the output P(r)
- `get_positive(pars)`: returns the fraction of P(r) that is above zero
- `get_pos_err(pars)`: returns the fraction of P(r) that is 1-sigma above zero

---

2.1. Contents
background = 0
chi2 = 0
clone()
Return a clone of this instance
cov = None
elapsed = 0

estimate_alpha(nfunc)
Returns a reasonable guess for the regularization constant alpha

Parameters nfunc – number of terms to use in the expansion.

Returns alpha, message, elapsed

where alpha is the estimate for alpha, message is a message for the user, elapsed is the computation time

estimate_numterms(isquit_func=None)
Returns a reasonable guess for the number of terms

Parameters isquit_func – reference to thread function to call to check whether the computation needs to be stopped.

Returns number of terms, alpha, message

from_file(path)
Load the state of the Invertor from a file, to be able to generate P(r) from a set of parameters.

Parameters path – path of the file to load

info = {}
i

invert(nfunc=10, nr=20)
Perform inversion to P(r)

The problem is solved by posing the problem as Ax = b, where x is the set of coefficients we are looking for.

Npts is the number of points.

In the following i refers to the ith base function coefficient. The matrix has its entries j in its first Npts rows set to

A[i][j] = (Fourier transformed base function for point j)

We then choose a number of r-points, n_r, to evaluate the second derivative of P(r) at. This is used as our regularization term. For a vector r of length n_r, the following n_r rows are set to

A[i+Npts][j] = (2nd derivative of P(r), d²P(r)/dr², evaluated at r[j])

The vector b has its first Npts entries set to

b[j] = (I(q) observed for point j)

The following n_r entries are set to zero.

The result is found by using scipy.linalg.basic.lstsq to invert the matrix and find the coefficients x.

Parameters

• nfunc – number of base functions to use.

• nr – number of r points to evaluate the 2nd derivative at for the reg. term.

Returns c_out, c_cov - the coefficients with covariance matrix
invert_optimize \((nfunc=10, nr=20)\)

Slower version of the \(P(r)\) inversion that uses scipy.optimize.leastsq.

This probably produce more reliable results, but is much slower. The minimization function is set to
\[
\text{sum}_i \left( \frac{I_{\text{obs}}(q_i) - I_{\text{theo}}(q_i)}{\text{err}_i} \right)^2 + \alpha \cdot \text{reg term},
\]
where the reg term is given by Svergun: it is the integral of the square of the first derivative of \(P(r)\), \(d(P(r))/dr\), integrated over the full range of \(r\).

**Parameters**

- \(nfunc\) – number of base functions to use.
- \(nr\) – number of \(r\) points to evaluate the 2nd derivative at for the reg. term.

**Returns** \(c_{\text{out}}, c_{\text{cov}}\) - the coefficients with covariance matrix

\(iq(out, q)\)

Function to call to evaluate the scattering intensity

**Parameters** \(args\) – \(c\)-parameters, and \(q\)

**Returns** \(I(q)\)

\(\text{lstsq}(nfunc=5, nr=20)\)

The problem is solved by posing the problem as \(Ax = b\), where \(x\) is the set of coefficients we are looking for.

\(Npts\) is the number of points.

In the following \(i\) refers to the \(i\)th base function coefficient. The matrix has its entries \(j\) in its first \(Npts\) rows set to
\[
A[i][j] = (\text{Fourier transformed base function for point } j)
\]

We then choose a number of \(r\)-points, \(n_r\), to evaluate the second derivative of \(P(r)\) at. This is used as our regularization term. For a vector \(r\) of length \(n_r\), the following \(n_r\) rows are set to
\[
A[i+Npts][j] = (2\text{nd derivative of } P(r), \frac{d^2P(r)}{dr^2}, \text{evaluated at } r[j])
\]

The vector \(b\) has its first \(Npts\) entries set to
\[
b[j] = (I(q) \text{ observed for point } j)
\]

The following \(n_r\) entries are set to zero.

The result is found by using scipy.linalg.basic.lstsq to invert the matrix and find the coefficients \(x\).

**Parameters**

- \(nfunc\) – number of base functions to use.
- \(nr\) – number of \(r\) points to evaluate the 2nd derivative at for the reg. term.

If the result does not allow us to compute the covariance matrix, a matrix filled with zeros will be returned.

\(nfunc = 10\)

\(out = None\)

\(\text{pr_err}(c, c_{\text{cov}}, r)\)

Returns the value of \(P(r)\) for a given \(r\), and base function coefficients, with error.

**Parameters**

- \(c\) – base function coefficients
- \(c_{\text{cov}}\) – covariance matrice of the base function coefficients
- \(r\) – \(r\)-value to evaluate \(P(r)\) at
Returns P(r)

pr_fit (nfunc=5)

This is a direct fit to a given P(r). It assumes that the y data is set to some P(r) distribution that we are trying to reproduce with a set of base functions.

This method is provided as a test.

suggested_alpha = 0
to_file (path, npts=100)

Save the state to a file that will be readable by SliceView.

Parameters

• path – path of the file to write
• npts – number of P(r) points to be written

sas.sascalc.pr.invertor.help()

Provide general online help text Future work: extend this function to allow topic selection

sas.sascalc.pr.num_term module

class sas.sascalc.pr.num_term.NTermEstimator (invertor)
Bases: object

compare_err()
get0_out()
is_odd(n)
ls_osc()
median_osc()
num_terms (isquit_func=None)
sort_osc()
sas.sascalc.pr.num_term.load(path)

Module contents

P(r) inversion for SAS
Module contents

sas.sasgui package

Subpackages

sas.sasgui.guiframe package

Subpackages

sas.sasgui.guiframe.local_perspectives package

Subpackages

sas.sasgui.guiframe.local_perspectives.data_loader package

Submodules

sas.sasgui.guiframe.local_perspectives.data_loader.data_loader module

Plugin DataLoader responsible of loading data

class sas.sasgui.guiframe.local_perspectives.data_loader.data_loader.Plugin
    Bases: sas.sasgui.guiframe.plugin_base.PluginBase

    can_load_data()
        if return True, then call handler to load data

    get_data(path, format=None)

    get_file_path(path)
        Receive a list containing folder then return a list of file

    load_complete(output, message=", info='warning'
        post message to status bar and return list of data

    load_data(event)
        Load data

    load_error(error=None)
        Pop up an error message.

        Parameters error – details error message to be displayed

    load_update(message=", info='warning'
        print update on the status bar

    populate_file_menu()
        get a menu item and append it under file menu of the application add load file menu item and load folder item

sas.sasgui.guiframe.local_perspectives.data_loader.load_thread module

Loading thread

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class sas.sasgui.guiframe.local_perspectives.data_loader.load_thread.DataReader:

    path, loader, flag=True, transform_data=None, completefn=None, updatefn=None, yieldtime=0.01, worktime=0.01)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Load a data given a filename

compute()
    read some data

isquit()
    Raises KeyboardInterrupt – when the thread is interrupted

Module contents

sas.sasgui.guiframe.local_perspectives.plotting package

Submodules

sas.sasgui.guiframe.local_perspectives.plotting.AnnulusSlicer module

class sas.sasgui.guiframe.local_perspectives.plotting.AnnulusSlicer.AnnulusInteractor:

    base, axes, color='black', zorder=3

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Select an annulus through a 2D plot. This interactor is used to average 2D data with the region defined by 2 radius. this class is defined by 2 Ringinteractors.

clear()
    Clear the slicer and all connected events related to this slicer

draw()

freeze_axes()

get_params()
    Store a copy of values of parameters of the slicer into a dictionary.

    Return params the dictionary created

move(x, y, ev)
    Process move to a new position, making sure that the move is allowed.

moveend(ev)
    Called when any dragging motion ends. Post an event (type=SlicerParameterEvent) to plotter 2D with a copy slicer parameters Call _post_data method

restore()
    Restore the roughness for this layer.
save (ev)
Remember the roughness for this layer and the next so that we can restore on Esc.

set_cursor (x, y)

set_layer (n)
Allow adding plot to the same panel

Parameters n – the number of layer

set_params (params)
Receive a dictionary and reset the slicer with values contained in the values of the dictionary.

Parameters params – a dictionary containing name of slicer parameters and values the user assigned to the slicer.

thaw_axes ()

update ()
Respond to changes in the model by recalculating the profiles and resetting the widgets.

class sas.sasgui.guiframe.local_perspectives.plotting.AnnulusSlicer.CircularMask (base, axes, color='grey', zorder=3, side=None)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Draw a ring Given a radius

clear ()
Clear the slicer and all connected events related to this slicer

draw ()

freeze_axes ()

get_params ()
Store a copy of values of parameters of the slicer into a dictionary.

Return params the dictionary created

move (x, y, ev)
Process move to a new position, making sure that the move is allowed.

moveend (ev)
Called when any dragging motion ends. Post an event (type = SlicerParameterEvent) to plotter 2D with a copy slicer parameters Call _post_data method

restore ()
Restore the roughness for this layer.

save (ev)
Remember the roughness for this layer and the next so that we can restore on Esc.

set_cursor (x, y)

set_layer (n)
Allow adding plot to the same panel

Parameters n – the number of layer

set_params (params)
Receive a dictionary and reset the slicer with values contained in the values of the dictionary.

Parameters params – a dictionary containing name of slicer parameters and values the user assigned to the slicer.

thaw_axes ()
update()

Respond to changes in the model by recalculating the profiles and resetting the widgets.

class sas.sasgui.guiframe.local_perspectives.plotting.AnnulusSlicer.RingInteractor (base, axes, color='black', zorder=5, r=1.0, sign=1)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Draw a ring Given a radius

clear()

Clear the slicer and all connected events related to this slicer

get_params()

Store a copy of values of parameters of the slicer into a dictionary.

   Return params the dictionary created

get_radius()

   Return self._inner_mouse_x the current radius of the ring

move(x, y, ev)

Process move to a new position, making sure that the move is allowed.

moveend(ev)

Called after a dragging motion

restore()

Restore the roughness for this layer.

save(ev)

Remember the roughness for this layer and the next so that we can restore on Esc.

set_cursor(x, y)

draw the ring given x, y value

set_layer(n)

Allow adding plot to the same panel

   Parameters n – the number of layer

set_params(params)

Receive a dictionary and reset the slicer with values contained in the values of the dictionary.

   Parameters params – a dictionary containing name of slicer parameters and values the user assigned to the slicer.

update()

Draw the new roughness on the graph.

sas.sasgui.guiframe.local_perspectives.plotting.Arc module

Arc slicer for 2D data

class sas.sasgui.guiframe.local_perspectives.plotting.Arc.ArcInteractor (base, axes, color='black', zorder=5, r=1.0, theta1=0.39269908169872414, theta2=0.7853981633974483)
Select an annulus through a 2D plot

```python
clear()
```
Clear this slicer and its markers

```python
get_params()
```

```python
get_radius()
```
Return arc radius

```python
move(x, y, ev)
```
Process move to a new position, making sure that the move is allowed.

```python
moveend(ev)
```
After a dragging motion reset the flag self.has_move to False 

```python
restore()
```
Restore the roughness for this layer.

```python
save(ev)
```
Remember the roughness for this layer and the next so that we can restore on Esc.

```python
set_cursor(radius, phi_min, phi_max, nbins)
```

```python
set_layer(n)
```
Allow adding plot to the same panel

```python
set_params(params)
```

```python
update(theta1=None, theta2=None, nbins=None, r=None)
```
Update the plotted arc

```python
sas.sasgui.guiframe.local_perspectives.plotting.AzimutSlicer module
```

```python
class sas.sasgui.guiframe.local_perspectives.plotting.AzimutSlicer.SectorInteractor
```

Bases: `sas.sasgui.guiframe.local_perspectives.plotting.AzimutSlicer.SectorInteractor`

Select an annulus through a 2D plot

```python
clear()
```

draw()

```python
freeze_axes()
```

```python
get_params()
```

```python
move(x, y, ev)
```
Process move to a new position, making sure that the move is allowed.

```python
moveend(ev)
```

```python
post_data(new_sector)
```
post data averaging in Q

```python
restore()
```
Restore the roughness for this layer.

```python
save(ev)
```
Remember the roughness for this layer and the next so that we can restore on Esc.
```
set_cursor(x, y)
set_layer(n)
set_params(params)
thaw_axes()
update()
    Respond to changes in the model by recalculating the profiles and resetting the widgets.

class sas.sasgui.guiframe.local_perspectives.plotting.AzimutSlicer.SectorInteractorPhi(base, axes, color='black', zorder=3)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.AzimutSlicer.SectorInteractor

class sas.sasgui.guiframe.local_perspectives.plotting.AzimutSlicer.SectorInteractorQ(base, axes, color='black', zorder=3)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.AzimutSlicer.SectorInteractor

sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor module

sas.sasgui.guiframe.local_perspectives.plotting.Edge module

class sas.sasgui.guiframe.local_perspectives.plotting.Edge.RadiusInteractor(base, axes, color='black', zorder=5, arc1=None, arc2=None, theta=0.39269908169872414)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Select an annulus through a 2D plot

clear()
get_angle()
get_params()
move(x, y, ev)
    Process move to a new position, making sure that the move is allowed.
moveend(ev)
restore(ev)
    Restore the roughness for this layer.
save(ev)
    Remember the roughness for this layer and the next so that we can restore on Esc.
set_cursor(r_min, r_max, theta)
set_layer(n)
set_params(params)
update(r1=None, r2=None, theta=None)
    Draw the new roughness on the graph.
```
class sas.sasgui.guiframe.local_perspectives.plotting.Plotter1D.ModelPanel1D (parent, id=-1, color=None, dpi=None, style=0, **kwargs)


Plot panel for use with the GUI manager

ALWAYS_ON = True

createAppDialog (event)
    Create the custom dialog for fit appearance modification
cursor_line (event)
    Move the cursor line to write Q range
draw_plot ()
    Draw plot

get_color_label ()
    Associates label to a specific color

get_data_xy_vals (xval)
    Get x, y data values near x = x_val

group_id = None

modifyGraphAppearance (event)
    On Modify Graph Appearance

onContextMenu (event)
    1D plot context menu

    Parameters event – wx context event

onFreeze (event)
    on Freeze data

onLeftDown (event)
    left button down and ready to drag Display the position of the mouse on the statusbar

onSetRange (event)

on_AppDialog_close (event)
    on_Modify Plot Property_close

on_close (event)
    On Close Event

on_graphApp_close (event)
    Gets values from graph appearance dialog and sends them off to modify the plot

on_plot_qrange (event=None)
    On Qmin Qmax vertical line event

plot_data (data)
    Data is ready to be displayed

    Parameters event – data event
remove_data_by_id(id)
Remove data from plot

schedule_full_draw(func='append')
Put self in schedule to full redraw list

set_data(list=None)

set_resizing(resizing=False)
Set the resizing (True/False)

window_caption = 'Graph'
window_name = 'plotpanel'
sas.sasgui.guiframe.local_perspectives.plotting.Plotter1D.find_key(dic, val)
return the key of dictionary dic given the value

sas.sasgui.guiframe.local_perspectives.plotting.Plotter2D module

class sas.sasgui.guiframe.local_perspectives.plotting.Plotter2D (parent, id=-
1, data2d=None, color=None, dpi=None, style=0, **kwargs)

Plot panel for use with the GUI manager

ALWAYS_ON = True
add_toolbar()
add toolbar
freeze_axes()
group_id = None
modifyGraphAppearance(e)
On Modify Graph Appearance
onBoxSum(event)
onBoxavgX(event)
Perform 2D data averaging on Qx Create a new slicer.
Parameters event – wx.menu event
onBoxavgY(event)
Perform 2D data averaging on Qy Create a new slicer.
Parameters event – wx.menu event
onCircular(event, ismask=False)
perform circular averaging on Data2D
Parameters event – wx.menu event
onClearSlicer(event)
Clear the slicer on the plot
onContextMenu(event)
2D plot context menu
Parameters event – wx context event

onEditLabels(event)
  Edit legend label

onLeftDown(event)
  left button down and ready to drag

onMaskedCircular(event)
  perform circular averaging on Data2D with mask if it exists

Parameters event – wx.menu event

onMouseMotion(event)

onSectorPhi(event)
  Perform sector averaging on Phi and draw annulus slicer

onSectorQ(event)
  Perform sector averaging on Q and draw sector slicer

onWheel(event)

on_graphApp_close(e)
  Gets values from graph appearance dialog and sends them off to modify the plot

on_plot_qrange(event=None)
  On Qmin Qmax vertical line event

plot_data(data)
  Data is ready to be displayed

  TODO  this name should be changed to something more appropriate Don’t forget that changing this name will mean changing code in plotting.py

Parameters event – data event

thaw_axes()

update(draw=True)
  Respond to changes in the model by recalculating the profiles and resetting the widgets.

window_caption = 'Plot Panel'

window_name = 'plotpanel'

class sas.sasgui.guiframe.local_perspectives.plotting.Plotter2D.NavigationToolBar2D(canvas, parent=None):

  Bases: sas.sasgui.plottools.toolbar.NavigationToolBar

  add_option()
    add item to the toolbar

  delete_option()
    remove default toolbar item

sas.sasgui.guiframe.local_perspectives.plotting.Plotter2D.find_key(dic, val)

  return the key of dictionary dic given the value

sas.sasgui.guiframe.local_perspectives.plotting.SectorSlicer module

  Sector interactor
class sas.sasgui.guiframe.local_perspectives.plotting.SectorSlicer.LineInteractor(base, axes, color='black', zorder=5, r=1.0, theta=0.7853981633974483)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Select an annulus through a 2D plot

clear()

get_params()

move(x, y, ev)

Process move to a new position, making sure that the move is allowed.

moveend(ev)

restore()

Restore the roughness for this layer.

save(ev)

Remember the roughness for this layer and the next so that we can restore on Esc.

set_cursor(x, y)

set_layer(n)

set_params(params)

update(theta=None)

Draw the new roughness on the graph.

class sas.sasgui.guiframe.local_perspectives.plotting.SectorSlicer.SectorInteractor(base, axes, color='black', zorder=3)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Draw a sector slicer. Allow to perform Q averaging on data 2D

clear()

Clear the slicer and all connected events related to this slicer

draw()

freeze_axes()

get_params()

Store a copy of values of parameters of the slicer into a dictionary.

Return params the dictionary created

move(x, y, ev)

Process move to a new position, making sure that the move is allowed.

moveend(ev)

Called a dragging motion ends. Get slicer event

restore()

Restore the roughness for this layer.

save(ev)

Remember the roughness for this layer and the next so that we can restore on Esc.

set_cursor(x, y)

set_layer(n)
Allow adding plot to the same panel

**Parameters**

- `n` – the number of layer

**set_params** *(params)*

Receive a dictionary and reset the slicer with values contained in the values of the dictionary.

**Parameters**

- `params` – a dictionary containing name of slicer parameters and values the user assigned to the slicer.

**thaw_axes** *

Respond to changes in the model by recalculating the profiles and resetting the widgets.

**thaw_axes** *

**update** *

**update** *

Bases: `sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor`

**SideInteractor** *(base, axes, color='black', zorder=5, r=1.0, phi=0.7853981633974483, theta2=1.0471975511965976)*

**Bases:**

- `sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor`

**_BaseInteractor**

Draw an oblique line

**Parameters**

- `phi` – the phase between the middle line and one side line
- `theta2` – the angle between the middle line and x-axis

**clear** *

Clear the slicer and all connected events related to this slicer

**get_params** *

**move** *(x, y, ev)*

Process move to a new position, making sure that the move is allowed.

**moveend** *(ev)*

**restore** *

**restore** *

**save** *(ev)*

Remember the roughness for this layer and the next so that we can restore on Esc.

**set_cursor** *(x, y)*

**set_layer** *(n)*

Allow adding plot to the same panel

**Parameters**

- `n` – the number of layer

**set_params** *(params)*

**update** *(phi=None, delta=None, mline=None, side=False, left=False, right=False)*

Draw oblique line

**Parameters**

- `phi` – the phase between the middle line and the current line
- `delta` – phi/2 applied only when the mline was moved
sas.sasgui.guiframe.local_perspectives.plotting.SimplePlot module

Simple Plot Frame: supporting only copy, print, scale

```python
class sas.sasgui.guiframe.local_perspectives.plotting.SimplePlot.PlotFrame (parent, id, title, scale='log_{10}', size=wx.Size(550, 470), show_menu_icons=True)
```

Bases: `wx._windows.Frame`

Frame for simple plot

```python
add_plot(plot)
```

Add Image

```python
disable_app_menu(panel)
```

```python
get_current_context_menu(plotpanel)
```

```python
im_show(img)
```

Show background image. Param img: [imread(path) from matplotlib.pyplot]

```python
on_close(event)
```

On Close

```python
on_copy_image(event)
```

Save image

```python
on_print_image(event)
```

Save image

```python
on_print_preview(event)
```

Save image

```python
on_save_file(event)
```

Save image

```python
set_plot_unfocus()
```

un focusing

```python
set_schedule(schedule=False)
```

```python
set_schedule_full_draw(panel, func)
```

```python
class sas.sasgui.guiframe.local_perspectives.plotting.SimplePlot.SimplePlotPanel (parent, id=-1, color=None, dpi=None, style=0, **kwargs)
```

Bases: `sas.sasgui.guiframe.local_perspectives.plotting.Plotter2D.ModelPanel2D`

PlotPanel for 1d and 2d

```python
add_toolbar()
```

```python
draw()
```

```python
onContextMenu(event)
```

2D plot context menu

Parameters event – wx context event
```python
onLeftDown(event)
    left button down and ready to drag

on_grid_onoff(event)
    On grid on/off

on_kill_focus(event)
    Reset the panel color

on_set_focus(event)
    By pass default boundary blue color drawing

show_plot(plot)
    Show the plot
```

`sas.sasgui.guiframe.local_perspectives.plotting.appearanceDialog` module

Dialog for appearance of plot symbols, color, size etc.

This software was developed by Institut Laue-Langevin as part of Distributed Data Analysis of Neutron Scattering Experiments (DANSE).

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```python
class sas.sasgui.guiframe.local_perspectives.plotting.appearanceDialog:
    Bases: wx._windows.Frame

    Appearance dialog

    close_dlg(event)
        On Close Dlg

    combo_click(event)
        Combox on click

    custom_size(event)
        On custom size

    static find_key(dic, val)
        Find key

    get_current_values()
        Get Current Values :returns : (size, color, symbol, dataname)

    init_ui()
        Create spacing needed

    on_ok(event)
        On OK button clicked

    populate_color()
        Populate Colors

    populate_size()
        Populate Size

    populate_symbol()
        Populate Symbols

    set_defaults(size, color, symbol, label)
        Set Defaults
```
Extension to MPL to support the binding of artists to key/mouse events.

```python
class sas.sasgui.guiframe.local_perspectives.plotting.binder.Binder (figure)
    Bases: object
    Track keyboard modifiers for events. TODO: Move keyboard modifier support into the backend. We cannot
    TODO: properly support it from outside the windowing system since there TODO: is no way to recognized
    whether shift is held down when the mouse TODO: first clicks on the the application window.
    alt = False
clear (h1, h2, ...)
    Remove connections for artists h1, h2, ...
    Use clearall() to reset all connections.
clearall ()
    Clear connections to all artists.
    Use clear(h1,h2,...) to reset specific artists.
    control = False
dclick_threshold = 0.25
disconnect ()
    In case we need to disconnect from the canvas...
    events = ['enter', 'leave', 'motion', 'click', 'dclick', 'drag', 'release', 'scroll', 'key', 'keyup']
    meta = False
    shift = False
    trigger (actor, action, ev)
    Trigger a particular event for the artist. Fallback to axes, to figure, and to ‘all’ if the event is not
    processed.
```

```python
class sas.sasgui.guiframe.local_perspectives.plotting.binder.Selection (artist=None, prop={})
    Bases: object
    Store and compare selections.
    artist = None
    prop = {}
```

SasView Documentation, Release 4.2.1
Parameters

- **zorder** – Artists with lower zorder values are drawn first.
- **x_min** – the minimum value of the x coordinate
- **x_max** – the maximum value of the x coordinate
- **y_min** – the minimum value of the y coordinate
- **y_max** – the maximum value of the y coordinate

**clear()**
Clear the slicer and all connected events related to this slicer

**draw()**

**freeze_axes()**

**get_mask()**
Return mask as a result of boxcut

**get_params()**
Store a copy of values of parameters of the slicer into a dictionary.

**Return params** the dictionary created

**move(x, y, ev)**
Process move to a new position, making sure that the move is allowed.

**moveend(ev)**
After a dragging motion this function is called to compute the error and the sum of pixel of a given data 2D

**restore()**
Restore the roughness for this layer.

**save(ev)**
Remember the roughness for this layer and the next so that we can restore on Esc.

**set_cursor(x, y)**

**set_params(params)**
Receive a dictionary and reset the slicer with values contained in the values of the dictionary.

**Parameters params** – a dictionary containing name of slicer parameters and values the user assigned to the slicer.

**thaw_axes()**

**update()**
Respond to changes in the model by recalculating the profiles and resetting the widgets.

```python
class sas.sasgui.guiframe.local_perspectives.plotting.boxMask.inner_BoxMask(base, axes, color='black', zorder=3, side=None, x_min=0.008, x_max=0.008, y_min=0.0025, y_max=0.0025)
```

Bases: `sas.sasgui.guiframe.local_perspectives.plotting.boxMask.BoxMask`
sas.sasgui.guiframe.local_perspectives.plotting.boxSlicer module

class sas.sasgui.guiframe.local_perspectives.plotting.boxSlicer.BoxInteractor(base, axes, color='black', zorder=3)


_BaseInteractor

BoxInteractor defines a rectangle that returns data1D average of Data2D in a rectangle area defined by -x, x, y, -y

clear()

Clear the slicer and all connected events related to this slicer
draw()

freeze_axes()

get_params()

Store a copy of values of parameters of the slicer into a dictionary.

Return params the dictionary created

move(x, y, ev)

Process move to a new position, making sure that the move is allowed.

moveend(ev)

Called after a dragging event. Post the slicer new parameters and creates a new Data1D corresponding to the new average

post_data(new_slab=None, nbins=None, direction=None)

Post data averaging in Qx or Qy given new_slab type

Parameters

• new_slab – slicer that determines direction to average
• nbins – the number of points plotted when averaging
• direction – the direction of averaging

restore()

Restore the roughness for this layer.

save(ev)

Remember the roughness for this layer and the next so that we can restore on Esc.

set_cursor(x, y)

set_layer(n)

Allow adding plot to the same panel

Parameters n – the number of layer

set_params(params)

Receive a dictionary and reset the slicer with values contained in the values of the dictionary.

Parameters params – a dictionary containing name of slicer parameters and values the user assigned to the slicer.

thaw_axes()

update()

Respond to changes in the model by recalculating the profiles and resetting the widgets.

update_and_post()

Update the slicer and plot the resulting data
class sas.sasgui.guiframe.local_perspectives.plotting.boxSlicer.BoxInteractorX (base, axes, color='black', zorder=3)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.boxSlicer.BoxInteractor

Average in Qx direction

class sas.sasgui.guiframe.local_perspectives.plotting.boxSlicer.BoxInteractorY (base, axes, color='black', zorder=3)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.boxSlicer.BoxInteractor

Average in Qy direction

class sas.sasgui.guiframe.local_perspectives.plotting.boxSlicer.HorizontalLines (base, axes, color='black', zorder=5, x=0.5, y=0.5)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Draw 2 Horizontal lines centered on (0,0) that can move on the x- direction and in opposite direction

clear ()

Clear this slicer and its markers

move (x, y, ev)

Process move to a new position, making sure that the move is allowed.

moveend (ev)

Called after a dragging this edge and set self.has_move to False to specify the end of dragging motion

restore ()

Restore the roughness for this layer.

save (ev)

Remember the roughness for this layer and the next so that we can restore on Esc.

set_layer (n)

Allow adding plot to the same panel

Parameters n – the number of layer

update (x=None, y=None)

Draw the new roughness on the graph.

Parameters

• x – x-coordinates to reset current class x

• y – y-coordinates to reset current class y

class sas.sasgui.guiframe.local_perspectives.plotting.boxSlicer.VerticalLines (base, axes, color='black', zorder=5, x=0.5, y=0.5)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Select an annulus through a 2D plot

2.1. Contents
clear()
Clear this slicer and its markers

move (x, y, ev)
Process move to a new position, making sure that the move is allowed.

moveend (ev)
Called after a dragging this edge and set self.has_move to False to specify the end of dragging motion

restore()
Restore the roughness for this layer.

save (ev)
Remember the roughness for this layer and the next so that we can restore on Esc.

set_layer (n)
Allow adding plot to the same panel

Parameters
n – the number of layer

update (x=None, y=None)
Draw the new roughness on the graph.

Parameters
• x – x-coordinates to reset current class x
• y – y-coordinates to reset current class y

sas.sasgui.guiframe.local_perspectives.plotting.boxSum module

Boxsum Class: determine 2 rectangular area to compute the sum of pixel of a Data.

class sas.sasgui.guiframe.local_perspectives.plotting.boxSum.BoxSum (base,
axes,
color='black',
zorder=3,
x_min=0.008,
x_max=0.008,
y_min=0.0025,
y_max=0.0025)

_BaseInteractor

Boxsum Class: determine 2 rectangular area to compute the sum of pixel of a Data. Uses PointerInteractor,
VerticalDoubleLine,HorizontalDoubleLine. @param zorder: Artists with lower zorder values are drawn
first. @param x_min: the minimum value of the x coordinate @param x_max: the maximum value of the
x coordinate @param y_min: the minimum value of the y coordinate @param y_max: the maximum value
of the y coordinate

clear()
Clear the slicer and all connected events related to this slicer

draw()

freeze_axes()

get_params()
Store a copy of values of parameters of the slicer into a dictionary. :return params: the dictionary
created

get_result()
return the result of box summation

move (x, y, ev)
Process move to a new position, making sure that the move is allowed.
moveend (ev)
After a dragging motion this function is called to compute the error and the sum of pixel of a given data 2D

restore()
Restore the roughness for this layer.

save (ev)
Remember the roughness for this layer and the next so that we can restore on Esc.

set_cursor (x, y)

set_layer (n)
Allow adding plot to the same panel @param n: the number of layer

set_panel_name (name)
Store the name of the panel associated to this slicer @param name: the name of this panel

set_params (params)
Receive a dictionary and reset the slicer with values contained in the values of the dictionary. :param params: a dictionary containing name of slicer parameters and values the user assigned to the slicer.

thaw_axes ()

update ()
Respond to changes in the model by recalculating the profiles and resetting the widgets.

class sas.sasgui.guiframe.local_perspectives.plotting.boxSum.HorizontalDoubleLine (base, axes, color='black', zorder=5, x=0.5, y=0.5, center_x=0, center_y=0)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Select an annulus through a 2D plot

clear ()
Clear this figure and its markers

move (x, y, ev)
Process move to a new position, making sure that the move is allowed.

moveend (ev)
After a dragging motion reset the flag self.has_move to False

restore ()
Restore the roughness for this layer.

save (ev)
Remember the roughness for this layer and the next so that we can restore on Esc.

set_cursor (x, y)
Update the figure given x and y

set_layer (n)
Allow adding plot to the same panel @param n: the number of layer

update (x1=None, x2=None, y1=None, y2=None, width=None, height=None, center=None)
Draw the new roughness on the graph. :param x1: new maximum value of x coordinates :param x2: new minimum value of x coordinates :param y1: new maximum value of y coordinates :param y2:
new minimum value of y coordinates
: param width: is the width of the new rectangle
: param height:
is the height of the new rectangle
: param center: provided x, y coordinates of the center point

class sas.sasgui.guiframe.local_perspectives.plotting.boxSum.PointInteractor
(base, axes, color='black', zorder=5, center_x=0.0, center_y=0.0)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Draw a point that can be dragged with the marker. this class controls the motion the center of the BoxSum

```
clear()
    Clear this figure and its markers
move(x, y, ev)
    Process move to a new position, making sure that the move is allowed.
moveend(ev)
restore()
    Restore the roughness for this layer.
save(ev)
    Remember the roughness for this layer and the next so that we can restore on Esc.
set_cursor(x, y)
set_layer(n)
    Allow adding plot to the same panel @param n: the number of layer
update(center_x=None, center_y=None)
    Draw the new roughness on the graph.
```

class sas.sasgui.guiframe.local_perspectives.plotting.boxSum.VerticalDoubleLine
(base, axes, color='black', zorder=5, x=0.5, y=0.5, center_x=0.0, center_y=0.0)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Draw 2 vertical lines moving in opposite direction and centered on a point (PointInteractor)

```
clear()
    Clear this slicer and its markers
move(x, y, ev)
    Process move to a new position, making sure that the move is allowed.
moveend(ev)
    After a dragging motion reset the flag self.has_move to False
restore()
    Restore the roughness for this layer.
save(ev)
    Remember the roughness for this layer and the next so that we can restore on Esc.
```
set_cursor \((x, y)\)
Update the figure given \(x\) and \(y\)

set_layer \((n)\)
Allow adding plot to the same panel :param \(n\): the number of layer

update \((x1=None, x2=None, y1=None, y2=None, width=None, height=None, center=None)\)
Draw the new roughness on the graph. :param \(x1\): new maximum value of \(x\) coordinates :param \(x2\): new minimum value of \(x\) coordinates :param \(y1\): new maximum value of \(y\) coordinates :param \(y2\): new minimum value of \(y\) coordinates :param \(width\): is the width of the new rectangle :param \(height\): is the height of the new rectangle :param \(center\): provided \(x, y\) coordinates of the center point

sas.sasgui.guiframe.local_perspectives.plotting.detector_dialog module

Widget to display a 2D map of the detector

class sas.sasgui.guiframe.local_perspectives.plotting.detector_dialog.DetectorDialog (parent, id=1, base=None, dpi=None, cmap=matplotlib.colors.LinearSegmentedColormap object, reset_zmin_ctl=None, reset_zmax_ctl=None, *args, **kwds)

Bases: wx._windows.Dialog

Dialog box to let the user edit detector settings

class Event
    Bases: object

    beam = 0
    cmap = None
    qpax = 0
    sym4 = False
    xnpts = 0
    ynpts = 0
    zmax = 0
    zmin = 0

checkValues (event)
    Check the validity of \(zmin\) and \(zmax\) value \(zmax\) should be a float and \(zmin\) less than \(zmax\)

getContent ()
    return event containing value to reset the detector of a given data

onSetFocus (event)
    Highlight the txtctrl

resetValues (event)
    reset detector info

setContent \((xnpts, ynpts, qmax, beam, zmin=None, zmax=None, sym=False)\)
    received value and displayed them
Parameters

- `xnpts` – the number of point of the x_bins of data
- `ynpts` – the number of point of the y_bins of data
- `qmax` – the maximum value of data pixel
- `beam` – the radius of the beam
- `zmin` – the value to get the minimum color
- `zmax` – the value to get the maximum color
- `sym`

`sas.sasgui.guiframe.local_perspectives.plotting.graphAppearance` module

Dialog for general graph appearance

This software was developed by Institut Laue-Langevin as part of Distributed Data Analysis of Neutron Scattering Experiments (DANSE).

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```python
class sas.sasgui.guiframe.local_perspectives.plotting.graphAppearance
    Bases: wx._windows.Frame

    InitUI()
    fillLegendLocs()
    get_legend_loc()
    get_loc_label()
    Associates label to a specific legend location
    get_togglegrid()
    get_togglelegend()
    get_xcolor()
    get_xfont()
    get_xlab()
    get_xtick_check()
    get_xunit()
    get_ycolor()
    get_yfont()
    get_ylab()
    get_ytick_check()
    get_yunit()
    on_cancel(e)
    on_ok(e)
    on_x_font(e)
    on_y_font(e)
```

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```python
setDefaults(grid, legend, xlab, ylab, xunit, yunit, xaxis_font, yaxis_font, legend_loc, xcolor, ycolor, is_xtick, is_ytick)
xfill_colors()
yfill_colors()
```

**sas.sasgui.guiframe.local_perspectives.plotting.masking module**

Mask editor

```python
class sas.sasgui.guiframe.local_perspectives.plotting.masking.CalcPlot(id=-1, panel=None, image=None, completefn=None, updatefn=None, elapsed=0, yieldtime=0.01, worktime=0.01)
```

Bases: `sas.sascalc.data_util.calcthread.CalcThread`

Compute Resolution

```python
compute()
```

executing computation

```python
class sas.sasgui.guiframe.local_perspectives.plotting.masking.FloatPanel(parent=None, base=None, data=None, dimension=1, id=139, *args, **kwds)
```

Bases: `wx._windows.Dialog`

Provides the Mask Editor GUI.

**CENTER_PANE = False**

**ID = 139**

```python
OnClose(event)
```

```python
complete(panel, image, elapsed=None)
```

Plot image

Parameters

- **image** — newplot [plotpanel]

- **freeze_axes()**
  freeze axes

- **get_plot()**
  Get Plot panel

- **set_plot_unfocus()**
  Not implemented

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thaw_axes()
    thaw axes

window_caption = 'Plot'
window_name = 'Plot'

class sas.sasgui.guiframe.local_perspectives.plotting.masking.MaskPanel(parent=None, base=None, data=None, id=-1, *args, **kwds)

Bases: wx._windows.Dialog

Provides the Mask Editor GUI.

CENTER_PANE = True

OnClose (event)
    Processing close event

ShowMessage (msg="")
    Show error message when mask covers whole data area

freeze_axes()
    freeze axes

onMouseMotion (event)
    onMotion event

onWheel (event)
    on wheel event

set_plot unfocus()
    Not implemented

thaw_axes()
    thaw axes

update (draw=True)
    Respond to changes in the model by recalculating the profiles and resetting the widgets.

window_caption = 'Mask Editor'
window_name = 'Mask Editor'

class sas.sasgui.guiframe.local_perspectives.plotting.masking.Maskplotpanel(
    parent, id=-1, dimension=2, color=None, dpi=None, **kwargs)

Bases: sas.sasgui.plottools.PlotPanel.PlotPanel

PlotPanel for Quick plot and masking plot

add_image (plot)
    Add Image

add_toolbar ()
    Add toolbar

draw ()
    Draw
onContextMenu (event)
    Default context menu for a plot panel

onLeftDown (event)
    Disables LeftDown

onMouseMove (event)
    Disable dragging 2D image

onPick (event)
    Disables OnPick

onWheel (event)

on_set_focus (event)
    send to the parent the current panel on focus

class sas.sasgui.guiframe.local_perspectives.plotting.masking.ViewApp (redirect=False, filename=None, useBestVisual=False, clearSigInt=True)

Bases: wx._core.App

OnInit ()

class sas.sasgui.guiframe.local_perspectives.plotting.masking.ViewerFrame (parent, id, title)

Bases: wx._windows.Frame

Add comment

sas.sasgui.guiframe.local_perspectives.plotting.parameters_panel_boxsum module

class sas.sasgui.guiframe.local_perspectives.plotting.parameters_panel_boxsum.SlicerPanel

Bases: wx._windows.Panel, sas.sasgui.guiframe.panel_base.PanelBase

Panel class to show the slicer parameters

CENTER_PANE = False

on_close (event)
    On Close Event

on_set_focus (evt)
    Highlight the txtctrl

on_text_enter (evt)
    Parameters have changed

set_slicer (type, params)
    Rebuild the panel

window_caption = 'Slicer Panel'
window_name = 'Slicer panel'

sas.sasgui.guiframe.local_perspectives.plotting.parameters_panel_slicer module

class sas.sasgui.guiframe.local_perspectives.plotting.parameters_panel_slicer.SlicerParameterPanel:

    Bases: wx._windows.Dialog

    Panel for dynamically changing slicer parameters and apply the same slicer to multiple 2D plot panels

    apply_params_list_and_process(evt=None)

        Event based parameter setting.

        Parameters

        evt -- Event triggered to apply parameters to a list of plots evt should have
                attrs plot_list and params

    check_item_and_children(data_ctrl, check_value=True)

    on_auto_save_checked(evt=None)

        Enable/Disable auto append when checkbox is checked :param evt: Event

    on_batch_slicer(evt=None)

        Event triggered when batch slicing button is pressed :param evt: Event triggering the batch slicing

    on_change_slicer(evt)

        Event driven slicer change when self.type_select changes :param evt: Event triggering this change

    on_check_box_list(evt=None)

        Prevent a checkbox item from being unchecked :param evt: Event triggered when a checkbox list item
        is checked

    on_evt_slicer(event)

        Process EVT_SLICER events When the slicer changes, update the panel

        Parameters

        event -- EVT_SLICER event

    on_help(event=None)

        Opens a help window for the slicer parameters/batch slicing window :param event: :return:

    on_param_change(evt)

        receive an event end reset value text fields inside self.parameters

    on_text_enter(evt)

        Parameters have changed

    process_list()

        Populate the check list from the currently plotted 2D data

    save_files(evt=None)

        Automatically save the sliced data to file. :param evt: Event that triggered the call to the method

    send_to_fitting(fit='No fitting', file_list=None)

        Send a list of data to the fitting perspective :param fit: fit type desired :param file_list: list of loaded
        file names to send to fit

    set_slicer(type, params)

        Rebuild the panel

    update_file_append(params=None)

        Update default_value when any parameters are changed :param params: dictionary of parameters
sas.sasgui.guiframe.local_perspectives.plotting.plotting module

class sas.sasgui.guiframe.local_perspectives.plotting.plotting.Plugin
Bases: sas.sasgui.guiframe.plugin_base.PluginBase
Plug-in class to be instantiated by the GUI manager

  clear_panel()
  Clear and Hide all plot panels, and remove them from menu

  clear_panel_by_id(group_id)
  clear the graph

  create_1d_panel(data, group_id)

  create_2d_panel(data, group_id)

  create_panel_helper(new_panel, data, group_id, title=None)

  delete_panel(group_id)

  get_panels(parent)
  Create and return a list of panel objects

  hide_panel(group_id)
  hide panel with group ID = group_id

  is_always_active()
  return True is this plugin is always active even if the user is switching between perspectives

  populate_menu(parent)
  Create a ‘Plot’ menu to list the panels available for displaying

  Parameters
  • id – next available unique ID for wx events
  • parent – parent window

  remove_plot(group_id, id)
  remove plot of ID = id from a panel of group ID = group_id

  set_panel_on_focus(panel)

  update_panel(data, panel)
  update the graph of a given panel

sas.sasgui.guiframe.local_perspectives.plotting.profile_dialog module

SLD Profile Dialog for multifunctional models

class sas.sasgui.guiframe.local_perspectives.plotting.profile_dialog.SLDPanel
Bases: wx._windows.Dialog
Provides the SLD profile plot panel.

  CENTER_PANE = True

  disable_app_menu(panel)
  Disable menu bar

  Parameters
  • parent=None, base=None, data=None, axes=[‘Radius’], id=-1, *args, **kwds)
get_current_context_menu(graph=None)

When the context menu of a plot is rendered, the get_context_menu method will be called to give you a chance to add a menu item to the context menu.

:param graph: the Graph object to which we attach the context menu

Returns a list of menu items with call-back function

on_change_caption(name, old_caption, new_caption)

set_plot_unfocus()

Set_plot unfocus

set_schedule(schedule=False)

Set schedule for redraw

set_schedule_full_draw(panel=None, func=None)

Set_schedule for full draw

show_data1d(data, name)

Show data dialog

window_caption = 'Scattering Length Density Profile'

window_name = 'Scattering Length Density Profile'

class sas.sasgui.guiframe.local_perspectives.plotting.profile_dialog.SLDplotpanel(parent, axes=[], id=-1, color=None, dpi=None, **kwargs)

Bases: sas.sasgui.guiframe.local_perspectives.plotting.Plotter1D.ModelPanel1D

add_image(plot)

Add image(Theory1D)

onChangeCaption(event)

Not implemented

on_kill_focus(event)

reset the panel color

on_set_focus(event)

send to the parent the current panel on focus

class sas.sasgui.guiframe.local_perspectives.plotting.profile_dialog.ViewApp(redirect=False, filename=None, useBestVisual=False, clearSigInt=True)

Bases: wx._core.App

OnInit()

class sas.sasgui.guiframe.local_perspectives.plotting.profile_dialog.ViewerFrame(parent, id, title)

Bases: wx._windows.Frame

Add comment
sas.sasgui.guiframe.local_perspectives.plotting.sector_mask module

Sector mask interactor

```python
class sas.sasgui.guiframe.local_perspectives.plotting.sector_mask.SectorMask(base, axes, color='gray', zorder=3, side=False)
```

**Bases:** sas.sasgui.guiframe.local_perspectives.plotting.BaseInteractor._BaseInteractor

Draw a sector slicer. Allow to find the data 2D inside of the sector lines

- `clear()` Clear the slicer and all connected events related to this slicer
- `draw()`
- `freeze_axes()`
- `get_params()` Store a copy of values of parameters of the slicer into a dictionary.
  
  **Return params** the dictionary created
- `move(x, y, ev)` Process move to a new position, making sure that the move is allowed.
- `moveend(ev)` Called a dragging motion ends. Get slicer event
- `restore()` Restore the roughness for this layer.
- `save(ev)` Remember the roughness for this layer and the next so that we can restore on Esc.
- `set_cursor(x, y)`
- `set_params(params)` Receive a dictionary and reset the slicer with values contained in the values of the dictionary.
  
  **Parameters params** – a dictionary containing name of slicer parameters and values the user assigned to the slicer.
- `thaw_axes()`
- `update()` Respond to changes in the model by recalculating the profiles and resetting the widgets.

Module contents

**Module contents**

Submodules

sas.sasgui.guiframe.CategoryInstaller module

Class for making sure all category stuff is installed and works fine.

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@author kieranrcampbell@gmail.com @modified by NIST/MD sasview team
class sas.sasgui.guiframe.CategoryInstaller.CategoryInstaller
    Bases: object
    Class for making sure all category stuff is installed
    Note - class is entirely static!
    static check_install(homedir=None, model_list=None)
    Makes sure categories.json exists and if not compile it and install.
    This is the main method of this class.
    Parameters
    • homefile – Override the default home directory
    • model_list – List of model names except those in Plugin Models which are user supplied.
    static get_default_file()
    static get_user_file()
    returns the user data file, eg .sasview/categories.json

sas.sasgui.guiframe.CategoryManager module

This software was developed by Institut Laue-Langevin as part of Distributed Data Analysis of Neutron Scattering Experiments (DANSE).
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class sas.sasgui.guiframe.CategoryManager.CategoryManager (parent, win_id, title)
    Bases: wx._windows.Frame
    A class for managing categories
    dial_ok(dialog=None, model=None)
    modify_dialog onclose

class sas.sasgui.guiframe.CategoryManager.ChangeCat (parent, title, cat_list, current_cats)
    Bases: wx._windows.Dialog
    dialog for changing the categories of a model
    get_category()
    Returns a list of categories applying to this model
    on_add(event)
    Callback for new category added
    on_existing(event)
    Callback for existing category selected
    on_newcat(event)
    Callback for new category added
    on_ok_mac(event)
    On OK pressed (MAC only)
    on_remove(event)
    Callback for a category removed

class sas.sasgui.guiframe.CategoryManager.CheckListCtrl (parent, call-back_func)
Taken from http://zetcode.com/wxpython/advanced/

**OnCheckItem** *(index, flag)*

When the user checks the item we need to save that state

```python
sas.sasgui.guiframe.CategoryManager.logger = <logging.Logger object>
```

Notes The category manager mechanism works from 3 data structures used:
- `self.master_category_dict`: keys are the names of categories, the values are lists of tuples, the first being the model names (the models belonging to that category), the second a boolean of whether or not the model is enabled
- `self.by_model_dict`: keys are model names, values are a list of categories belonging to that model
- `self.model_enabled_dict`: keys are model names, values are bools of whether the model is enabled

Use `self._regenerate_model_dict()` to create the latter two structures from the former
Use `self._regenerate_master_dict()` to create the first structure from the latter two

The need for so many data structures comes from the fact sometimes we need fast access to all the models in a category (eg user selection from the gui) and sometimes we need access to all the categories corresponding to a model (eg user modification of model categories)

### sas.sasgui.guiframe.aboutbox module

```python
class sas.sasgui.guiframe.aboutbox.DialogAbout(*args, **kwds)
    Bases: wx._windows.Dialog

    “About” Dialog
    Shows product name, current version, authors, and link to the product page. Current version is taken from version.py
    onAnstoLogo(event)
    onBamLogo(event)
    onDanseLogo(event)
    onDlsLogo(event)
    onEssLogo(event)
    onIllLogo(event)
    onIsisLogo(event)
    onNistLogo(event)
    onNsflLogo(event)
    onOrnlLogo(event)
    onSnsLogo(event)
    onTudelftLogo(event)
    onUTLogo(event)
    onUmdLogo(event)
```  

```python
class sas.sasgui.guiframe.aboutbox.MyApp(redirect=False, filename=None, useBestVisual=False, clearSigInt=True)
    Bases: wx._core.App

    OnInit()

    sas.sasgui.guiframe.aboutbox.launchBrowser(url)
    Launches browser and opens specified url
    In some cases may require BROWSER environment variable to be set up.
    Parameters url – URL to open
```
class sas.sasgui.guiframe.acknowledgebox.DialogAcknowledge(*args, **kwds)
   Bases: wx._windows.Dialog
   “Acknowledgement” Dialog Box
   Shows the current method for acknowledging SasView in scholarly publications.

class sas.sasgui.guiframe.acknowledgebox.MyApp(redirct=False, filename=None, useBestVisual=False, clearSig-Int=True)
   Bases: wx._core.App
   Class for running module as stand alone for testing
   OnInit()
       Defines an init when running as standalone

sas.sasgui.guiframe.config module

Application settings
sas.sasgui.guiframe.config.printEVT(message)

sas.sasgui.guiframe.custom_pstats module

class sas.sasgui.guiframe.custom_pstats.CustomPstats(*args, **kwds)
   Bases: pstats.Stats
   write_stats(*amount)
sas.sasgui.guiframe.custom_pstats.f8(x)
sas.sasgui.guiframe.custom_pstats.func_std_string(func_name)
sas.sasgui.guiframe.custom_pstats.profile(fn, name='profile.txt', *args, **kw)

sas.sasgui.guiframe.dataFitting module

Adapters for fitting module
class sas.sasgui.guiframe.dataFitting.Data1D(x=None, y=None, dx=None, dy=None, lam=None, dlam=None, isSesans=False)
   Bases: sas.sasgui.plottools.plottables.Data1D, sas.sascalc.dataloader.data_info.Data1D
   copy_from_datainfo(dataId)
       copy values of Data1D of type DataLaoder.Data_info

class sas.sasgui.guiframe.dataFitting.Data2D(image=None, err_image=None, qx_data=None, qy_data=None, q_data=None, mask=None, dqx_data=None, dqy_data=None, d_data=None, xmin=None, xmax=None, ymin=None, ymax=None, zmin=None, zmax=None)
Bases: `sas.sasgui.plottools.plottables.Data2D`, `sas.sascalc.dataloader.data_info.Data2D`

```python
copy_from_datainfo(data2d)
```
copy value of Data2D of type DataLoader.data_info

class sas.sasgui.guiframe.dataFitting.Theory1D(x=None, y=None, dy=None)
Bases: `sas.sasgui.plottools.plottables.Theory1D`, `sas.sascalc.dataloader.data_info.Data1D`

```python
copy_from_datainfo(data1d)
```
copy values of Data1D of type DataLaoder.Data_info

```python
sas.sasgui.guiframe.dataFitting.check_data_validity(data)
```
Return True is data is valid enough to compute chisqr, else False

### `sas.sasgui.guiframe.data_manager` module

This module manages all data loaded into the application. Data_manager makes available all data loaded for the current perspective.

All modules “creating Data” posts their data to data_manager. Data_manager make these new data available for all other perspectives.

```python
class sas.sasgui.guiframe.data_manager.DataManager
    Bases: object
    Manage a list of data
    add_data(data_list)
    receive a list of
    create_gui_data(data, path=None)
    Receive data from loader and create a data to use for guiframe
    delete_by_id(id_list=None)
    save data and path
    delete_by_name(name_list=None)
    save data and path
    delete_data(data_id, theory_id=None, delete_all=False)
    delete_theory(data_id, theory_id)
    freeze(theory_id)
    freeze_theory(data_id, theory_id)
    get_all_data()
    return list of all available data
    get_by_id(id_list=None)
    get_by_name(name_list=None)
    return a list of data given a list of data names
    get_data_state(data_id)
    Send list of selected data
    get_message()
    return message
    rename(name)
    rename data
    update_data(prev_data, new_data)
    update_theory(theory, data_id=None, state=None)
```

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**sas.sasgui.guiframe.data_panel module**

This module provides Graphic interface for the data_manager module.

```python
class sas.sasgui.guiframe.data_panel.DataDialog(data_list, parent=None, text='', *args, **kwds):
    Bases: wx._windows.Dialog
    Allow file selection at loading time
    get_data() -> return the selected data

class sas.sasgui.guiframe.data_panel.DataFrame(parent=None, owner=None, manager=None, size=(300, 800), list_of_perspective=[], list=[], *args, **kwds):
    Bases: wx._windows.Frame
    Data Frame
    ALWAYS_ON = True
    load_data_list(list=[]) -> Fill the list inside its panel
    window_caption = 'Data Panel'
    window_name = 'Data Panel'

class sas.sasgui.guiframe.data_panel.DataPanel(parent, list=None, size=(255, 750), id=-1, list_of_perspective=None, manager=None, *args, **kwds):
    Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase
    This panel displays data available in the application and widgets to interact with data.
    append_theory(state_id, theory_list) -> append theory object under data from a state of id = state_id replace that theory if already displayed
    append_theory_helper(tree, root, state_id, theory_list) -> Append theory helper
    check_theory_to_freeze() -> Check_theory_to_freeze
    define_panel_structure() -> Define the skeleton of the panel
    disable_app_combo(enable) -> Disable app combo box
    do_layout() -> Create the panel layout
    enable_append() -> enable or disable append button
    enable_freeze() -> enable or disable the freeze button
    enable_import() -> enable or disable send button
    enable_plot() -> enable or disable plot button
```

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enable_remove()  
enable or disable remove button

enable_remove_plot()  
enable remove plot button if there is a plot panel on focus

enable_selection()  
enable or disable combo box selection

fill_cbox_analysis(plugin)  
fill the combobox with analysis name

get_frame()  

layout_batch()  
Set up batch mode options

layout_button()  
Layout widgets related to buttons

layout_data_list()  
Add a listctrl in the panel

layout_selection()  
Create selection option combo box

load_data_list(list)  
add need data with its theory under the tree

load_error(error=None)  
Pop up an error message.

Parameters error – details error message to be displayed

onContextMenu(event)  
Retrieve the state selected state

on_append_plot(event=None)  
append plot to plot panel on focus

on_batch_mode(event)  
Change to batch mode :param event: UI event

on_check_item(event)  
On check item

on_close(event)  
On close event

on_close_page(event=None)  
On close

on_close_plot(event)  
close the panel on focus

on_data_info(event)  
Data Info panel

on_edit_data(event)  
Pop Up Data Editor

on_freeze(event)  
On freeze to make a theory to a data set

on_help(event)  
Bring up the data manager Documentation whenever the HELP button is clicked.

Calls DocumentationWindow with the path of the location within the documentation tree
(after /doc/ . . . .” Note that when using old versions of Wx (before 2.9) and thus not the

2.1. Contents
release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file:///...”

Parameters

- **event** – Triggers on clicking the help button

```python
on_import (event=None)
   Get all select data and set them to the current active perspective

on_plot (event=None)
   Send a list of data names to plot

on_plot_3d (event)
   Frozen image of 3D

on_quick_plot (event)
   Frozen plot

on_remove (event, prompt=True)
   Get a list of item checked and remove them from the treectrl Ask the parent to remove reference to this item

on_right_click_data (event)
   Allow Editing Data

on_right_click_theory (event)
   On click theory data

on_save_as (event)
   Save data as a file

on_single_mode (event)
   Change to single mode :param event: UI event

remove_by_id (id)
   Remove dat by id

set_active_perspective (name)
   set the active perspective

set_data_helper ()
   Set data helper

set_frame (frame)

set_panel_on_focus (name=None)
   set the plot panel on focus

set_plot_unfocus ()
   Unfocus plot

set_schedule_full_draw (panel=None, func='del')
   Send full draw to guimanager

show_data_button ()
   show load data and remove data button if dataloader on else hide them
```

**window_caption = 'Data Explorer'**

**window_name = 'Data Panel'**

**window_type = 'Data Panel'**

```python
class sas.sasgui.guiframe.data_panel.DataTreeCtrl (parent, root, *args, **kwds)
Bases: wx.lib.agw.customtreectrl.CustomTreeCtrl

Check list control to be used for Data Panel
```

OnCompareItems (**item1, item2**)
   Overrides OnCompareItems in wx.TreeCtrl. Used by the SortChildren method.
class sas.sasgui.guiframe.data_panel.State
    DataPanel State
sas.sasgui.guiframe.data_panel.set_data_state(data=None, path=None, theory=None, state=None)
    Set data state

sas.sasgui.guiframe.data_processor module

Implement grid used to store results of a batch fit.

This is in Guiframe rather than fitting which is probably where it should be. Actually could be a generic framework implemented in fit gui module. At this point however there this grid behaves independently of the fitting panel and only knows about information sent to it but not about the fits or fit panel and thus cannot feed back to the fitting panel. This could change in the future.

The organization of the classes goes as:

Note: Path to this is: /sasview/src/sas/sasgui/guiframe/data_processor.py

Note: Path to image is: /sasview/src/sas/sasgui/guiframe/media/BatchGridClassLayout.png
**GridPage Class** = the actual grid
* **GridCellEditor**: overrides class of same name in the wx.CSheet module
* **BatchCell**: class defines a cell within within the grid

**Notebook class** (nb, PanelBase)
contains all the GridPages

grid page 1

Plotting area = a standard gridsizer layout managed by the GridPanel class directly

**GridPanel class** (SPanel(ScrolledPanel))
contains the GridPage and the 'plotting area' below it

**GridFrame class** (wx.Frame)

class sas.sasgui.guiframe.data_processor.BatchCell
Bases: object

Object describing a cell in the grid.

class sas.sasgui.guiframe.data_processor.BatchOutputFrame
Bases: wx._windows.Frame

Allow to select where the result of batch will be displayed or stored

**on_apply** (event)
Get the user selection and display output to the selected application

**on_close** (event)
close the Window

**onselect** (event=None)
Receive event and display data into third party application or save data to file.

```python
class sas.sasgui.guiframe.data_processor.GridCellEditor (grid)
Bases: wx.lib.sheet.CCellEditor

Custom cell editor

This subclasses the sheet.CCellEditor (itself a subclass of grid.GridCellEditor) in order to override two of its methods: PaintBackground and EndEdit.

This is necessary as the sheet module is broken in wx 3.0.2 and improperly subclasses grid.GridCellEditor

**EndEdit** *(row, col, grid, previous)*

Commit editing the current cell. Returns True if the value has changed.

**Parameters** previous – previous value in the cell

**PaintBackground** *(dc, rect, attr)*

Overrides wx.sheet.CCellEditor.PaintBackground which incorrectly calls the base class method.

In wx3.0 all paint objects must explicitly have a wxPaintDC (Device Context) object. Thus the paint event which generates a call to this method provides such a DC object and the base class in grid expects to receive that object. sheet was apparently not updated to reflect this and hence fails. This could thus become obsolete in a future bug fix of wxPython.

Apart from adding a dc variable in the list of arguments in the def and in the call to the base class the rest of this method is copied as is from sheet.CCellEditor.PaintBackground

From original GridCellEditor docs:

Draws the part of the cell not occupied by the edit control. The base class version just fills it with background colour from the attribute.

**Note:** There is no need to override this if you don’t need to do something out of the ordinary.

**Parameters** dc – the wxDC object for the paint

```python
class sas.sasgui.guiframe.data_processor.JFrame (parent=None, data_inputs=None, data_outputs=None, id=-1, title='Batch Fitting Results Panel', size=(800, 500))

Bases: wx._windows.Frame

The main wx.Frame for the batch results grid

**GetLabelText** *(id)*

Get Label Text

**add_edit_menu** *(menubar)*

populates the edit menu on the menubar. Not activated as of SasView 3.1.0

**add_table** *(event)*

Add a new table

**on_append_column** *(event)*

Append a new column to the grid

**on_clear** *(event)*

On Clear from the Edit menu item on the menubar

**on_close** *(event)*

On Copy from the Edit menu item on the menubar

**on_copy** *(event)*
on_menu_open(event)
  On menu open

on_open(event)
  Open file containing batch result

on_paste(event)
  On Paste from the Edit menu item on the menubar

on_remove_column(event)
  On remove column from the Edit menu Item on the menubar

on_save_page(event)
  Saves data in grid to a csv file.
  At this time only the columns displayed get saved. Thus any error bars not inserted before saving will
  not be saved in the file

open_with_excel(event)
  open excel and display batch result in Excel

set_data(data_inputs, data_outputs, details="", file_name=None)
  Set data

class sas.sasgui.guiframe.data_processor.GridPage(parent, panel=None)
  Bases: wx.lib.sheet.CSheet
  Class that receives the results of a batch fit.
  GridPage displays the received results in a wx.grid using sheet. This is then used by GridPanel and Grid-
  Frame to present the full GUI.

OnCellChange(event)
  Processes when a cell has been edited by a cell editor. Checks for the edited row being outside the
  max row to use attribute and if so updates the last row. Then calls the base handler using skip.

OnLeftClick(event)
  Overrides sheet.CSheet.OnLeftClick.
  Processes when a cell is selected by left clicking on that cell. First process the base Sheet method then
  the current class specific method

get_grid_view()
  Return value contained in the grid

get_nofrows()
  Return number of total rows

insert_after_col_menu(menu, label, window)
  Method called to populate the ‘insert column after current column’ submenu

insert_col_menu(menu, label, window)
  method called to populate the ‘insert column before current column’ submenu.

insert_column(col, col_name)
  Insert column at position col with data[col_name] into the current grid.

onContextMenu(event)
  Method to handle cell right click context menu.
  THIS METHOD IS NOT CURRENTLY USED. It is designed to provide a cell pop up context by
  right clicking on a cell and gives the option to cut, paste, and clear. This will probably be removed in
  future versions and is being superseded by more traditional cut and paste options.

on_clear(event)
  Called when clear cell is chosen from cell right click context menu
THIS METHOD IS NOT CURRENTLY USED. it is part of right click cell context menu which is being removed. This will probably be removed in future versions and is being superseded by more traditional cut and paste options

**on_copy** *(event)*  
Called when copy is chosen from cell right click context menu

THIS METHOD IS NOT CURRENTLY USED. it is part of right click cell context menu which is being removed. This will probably be removed in future versions and is being superseded by more traditional cut and paste options

**on_insert_after_column** *(event)*  
Called when user chooses insert ‘column after’ submenu of the column context menu obtained when right clicking on a given column header.

Sets up to insert column into the current grid after the current highlighted column location and sets up what to populate that column with. Then calls insert_column method to actually do the insertion.

**on_insert_column** *(event)*  
Called when user chooses insert ‘column before’ submenu of the column context menu obtained when right clicking on a given column header.

Sets up to insert column into the current grid before the current highlighted column location and sets up what to populate that column with. Then calls insert_column method to actually do the insertion.

**on_left_click** *(event)*  
Is triggered when the left mouse button is clicked while the mouse is hovering over the column ‘label.’

This processes the information on the selected column: the column name (in row 0 of column) and the range of cells with a valid value to be used by the GridPanel set_axis methods.

**on_paste** *(event)*  
Called when paste is chosen from cell right click context menu

THIS METHOD IS NOT CURRENTLY USED. it is part of right click cell context menu which is being removed. This will probably be removed in future versions and is being superseded by more traditional cut and paste options

**on_remove_column** *(event=None)*  
Called when user chooses remove from the column right click menu Checks the columnn exists then calls the remove_column method

**on_right_click** *(event)*  
Is triggered when the right mouse button is clicked while the mouse is hovering over the column ‘label.’

This brings up a context menu that allows the deletion of the column, or the insertion of a new column either to the right or left of the current column. If inserting a new column can insert a blank column or choose a number of hidden columns. By default all the error parameters are in hidden columns so as to save space on the grid. Also any other intrinsic variables stored with the data such as Temperature, pressure, time etc can be used to populate this menu.

**on_selected_cell** *(event)*  
Handler catching cell selection.

Called after calling base ‘on left click’ method.

**on_set_x_axis** *(event)*  
Just calls the panel version of the method

**on_set_y_axis** *(event)*  
Just calls the panel version of the method

**remove_column** *(col, numCols=1)*  
Remove the col column from the current grid

**set_data** *(data_inputs, data_outputs, details, file_name)*  
Add data to the grid
Parameters

- **data_inputs** – data to use from the context menu of the grid
- **data_outputs** – default columns displayed

```python
set_grid_values()
```
Set the values in grids

```python
class sas.sasgui.guiframe.data_processor.GridPanel(parent, data_inputs=None, data_outputs=None, *args, **kwds)
```
Bases: `sas.sasgui.guiframe.data_processor.SPanel`

A ScrolledPanel class that contains the grid sheet as well as a number of widgets to create interesting plots and buttons for help etc.

```python
add_column()
```

```python
create_axis_label(cell_list)
```
Receive a list of cells and create a string presenting the selected cells.

Parameters
**cell_list** – list of tuple

```python
edit_axis_helper(tctrl_label, tctrl_title, label, title)
```
get controls to modify

```python
get_plot_axis(col, list)
```

```python
get_sentence(dict, sentence, column_names)
```
Get sentence from dict

```python
layout_grid()
```
Draw the area related to the grid by adding it as the first element in the panel’s grid_sizer

```python
layout_plotting_area()
```
Add the area containing all the plot options, buttons etc to a plotting area sizer to later be added to the top level grid_sizer

```python
on_edit_axis(event)
```
Get the selected column on the visible grid and set values for axis

```python
on_help(event)
```
Bring up the Batch Grid Panel Usage Documentation whenever the HELP button is clicked.

Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file:///…”

Parameters
**evt** – Triggers on clicking the help button

```python
on_plot(event)
```
Evaluate the contains of textctrl and plot result

```python
on_remove_column(event)
```
Get object represented by the given cells and plot them. Basically plot the column in y vs the column in x.

```python
set_dyaxis(label=", dy=None)
```

```python
set_xaxis(label=", x=None)
```

```python
set_yaxis(label=", y=None)
```

```python
class sas.sasgui.guiframe.data_processor.Notebook(parent, manager=None, data=None, *args, **kwargs)
```
Bases: `wx.aui.AuiNotebook, sas.sasgui.guiframe.panel_base.PanelBase`

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## Internal name for the AUI manager

```python
window_name = "Fit panel"
```

## Title to appear on top of the window

```python
add_column()
```

Append a new column to the grid

```python
add_empty_page()
```

## Title to appear on top of the window

```python
create_axis_label(cell_list)
```

Receive a list of cells and create a string presenting the selected cells that can be used as data for one axis of a plot.

**Parameters**

- `cell_list` – list of tuple

```python
enable_close_button()
```

Display the close button on the tab if more than 1 tab exits. Otherwise remove the close button

```python
get_column_labels()
```

Return dictionary of columns labels on the current page

```python
get_highlighted_row(is_number=True)
```

Add highlight rows

```python
get_odered_results(inputs, outputs=None)
```

Order a list of ‘inputs.’ Used to sort rows and columns to present in batch results grid.

```python
on_close_page(event)
```

Close the page

```python
on_edit_axis()
```

Return the selected cell range from a given selected column. Checks that all cells are from the same column

```python
on_remove_column()
```

Remove the selected column from the grid

```python
set_data(data_inputs, data_outputs, details="", file_name=None)
```

## Title to appear on top of the window

```python
window_caption = 'Notebook'
```

```python
class sas.sasgui.guiframe.data_processor.SPanel(parent, *args, **kwds)
```

Bases: `wx.lib.scrolledpanel.ScrolledPanel`

Ensure proper scrolling of GridPanel

Adds a SetupScrolling call to the normal ScrolledPanel init. GridPanel then subclasses this class

```python
class sas.sasgui.guiframe.data_state.parse_string(sentence, list)
```

Return a dictionary of column label and index or row selected

**Parameters**

- `sentence` – String to parse
- `list` – list of columns label

**Returns**

`col_dict`

## Title to appear on top of the window

```python
class sas.sasgui.guiframe.data_state.DataState(data=None, parent=None)
```

Bases: `object`

Store information about data

```python
clone()
```

```python
get_data()
```

## Title to appear on top of the window
SasView Documentation, Release 4.2.1

get_message()
return message

get_name()

get_path()
return the path of the loaded data

get_theory()

set_data(data)

set_name(name)

set_path(path)
Set the path of the loaded data

set_theory(theory_data, theory_state=None)

sas.sasgui.guiframe.documentation_window module

documentation module provides a simple means to add help throughout the application. It checks for the existence
of html2 package needed to support fully html panel which supports css. The class defined here takes a title for
the particular help panel, a pointer to the html documentation file of interest within the documentation tree along
with a ‘command’ string such as a page anchor or a query string etc. The path to the doc directory is retrieved
automatically by the class itself. Thus with these three pieces of information the class generates a panel with the
appropriate title bar and help file formatted according the style sheets called in the html file. Finally, if an old
version of Python is running and the html2 package is not available the class brings up the default browser and
passes the file:/// string to it. In this case however the instruction portion is usually not passed for security reasons.

class sas.sasgui.guiframe.documentation_window.DocumentationWindow(parent, dummy_id, path, url_instruction, title, size=(850, 540))

Bases: wx._windows.Frame

DocumentationWindow inherits from wx.Frame and provides a centralized coherent framework for all help
documentation. Help files must be html files stored in an properly organized tree below the top ‘doc’ folder.
In order to display the appropriate help file from anywhere in the gui, the code simply needs to know the
location below the top level where the help file resides along with the name of the help file. called (self, parent, dummy_id, path, url_instruction, title, size=(850, 540))

Parameters

• path – path to html file beginning AFTER /doc/ and ending in the file.html.
• url_instructions – anchor string or other query e.g. ‘#MyAnchor’
• title – text to place in the title bar of the help panel

OnError(evt)

sas.sasgui.guiframe.documentation_window.main()
main loop function if running alone for testing.
sas.sasgui.guiframe.documentation_window.start_documentation_server(doc_root, port)
sas.sasgui_guiframe_dummyapp module

Dummy application. Allows the user to set an external data manager

```python
class sas.sasgui_guiframe_dummyapp.DummyView(redirect=False, filename=None, useBestVisual=False, clearSignature=True):
    Bases: sas.sasgui_guiframe_gui_manager.SasViewApp
class sas.sasgui_guiframe_dummyapp.SasView
class sas.sasgui_guiframe_dummyapp.TestPlugin(name='Test_plugin'):
    Bases: sas.sasgui_guiframe_plugin_base.PluginBase
```

get_context_menu (graph=None)
This method is optional.

When the context menu of a plot is rendered, the get_context_menu method will be called to give you
a chance to add a menu item to the context menu.

A ref to a Graph object is passed so that you can investigate the plot content and decide whether you
need to add items to the context menu.

This method returns a list of menu items. Each item is itself a list defining the text to appear in the
menu, a tool-tip help text, and a call-back method.

**Parameters**

- `graph` – the Graph object to which we attach the context menu

**Returns**
a list of menu items with call-back function

get_panels (parent)
Create and return the list of wx.Panels for your plug-in. Define the plug-in perspective.

Panels should inherit from DefaultPanel defined below, or should present the same interface. They
must define “window_caption” and “window_name”.

**Parameters**

- `parent` – parent window

**Returns**
list of panels

get_tools ()
Returns a set of menu entries for tools

populate_menu (parent)
Create and return the list of application menu items for the plug-in. :param parent: parent window

**Returns**
plug-in menu

sas.sasgui_guiframe_events module

sas.sasgui_guiframe_gui_manager module

Gui manager: manages the widgets making up an application

```python
class sas.sasgui_guiframe_gui_manager.DefaultPanel(parent, *args, **kwds):
    Bases: wx._windows.Panel, sas.sasgui_guiframe_panel_base.PluginBase
```

Defines the API for a panels to work with the GUI manager

```
CENTERPane = True

window_caption = 'Welcome panel'
window_name = 'default'
```
class sas.sasgui.guiframe.gui_manager.MDIFrame (parent, panel, title='Untitled', size=(300, 200))

Bases: wx._windows.Frame

Frame for panels

OnClose (event)
  On Close event

set_panel (panel)

set_panel_focus (event)

show_data_panel (action)
  Turns on the data panel

  The data panel is optional. Most of its functions can be performed from the menu bar and from the plots.

class sas.sasgui.guiframe.gui_manager.SasViewApp (redirect=False, filename=None, useBestVisual=False, clearSigInt=True)

Bases: wx._core.App

SasView application

OnInit ()
  When initialised

add_perspective (perspective)
  Manually add a perspective to the application GUI

build_gui ()
  Build the GUI

clean_plugin_models (path)
  Delete plugin models in app folder

  Parameters path – path of the plugin_models folder in app

display_splash_screen (parent, path='/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasview/images/SVwelcome_mini.png')

  Displays the splash screen. It will exactly cover the main frame.

maximize_win ()
  Maximize the window after the frame shown

on_close_splash_screen (event)
  When the splash screen is closed.

open_file ()
  open a state file at the start of the application

set_manager (manager)
  Sets a reference to the application manager of the GUI manager (Frame)

set_welcome_panel (panel_class)
  Set the welcome panel

  Parameters panel_class – class of the welcome panel to be instantiated

window_placement (size)
  Determines the position and size of the application frame such that it fits on the user’s screen without obstructing (or being obstructed by) the Windows task bar. The maximum initial size in pixels is bounded by WIDTH x HEIGHT. For most monitors, the application will be centered on the screen; for very large monitors it will be placed on the left side of the screen.
class sas.sasgui.guiframe.gui_manager.ViewerFrame(parent, title, size=(-1, -1), gui_style=381, style=541072960, pos=wx.Point(-1, -1))

Bases: wx._windows.Frame

Main application frame

Close (event=None)
    Quit the application

PopStatusText (*args, **kwds)

PushStatusText (*args, **kwds)

SetStatusText (*args, **kwds)

WindowClose (event=None)
    Quit the application from x icon

add_data (data_list)
    receive a dictionary of data from loader store them its data manager if possible send to data the current active perspective if the data panel is not active. :param data_list: dictionary of data’s ID and value

Data

add_data_helper (data_list)

add_icon ()
    get list of child and attempt to add the default icon

add_perspective (plugin)
    Add a perspective if it doesn’t already exist.

append_bookmark (event=None)
    Bookmark available information of the panel on focus

build_gui ()
    Build the GUI by setting up the toolbar, menu and layout.

check_multimode (perspective=None)
    Check the perspective have batch mode capability

create_gui_data (data, path=None)

delete_data (data)
    Delete the data.

delete_panel (uid)
    delete panel given uid

disable_app_menu (p_panel=None)
    Disables all menus in the menubar

enable_add_data (new_plot)
    Enable append data on a plot panel

enable_bookmark ()
    Bookmark

enable_copy ()
    enable copy related control

enable_drag (event=None)
    drag

enable_edit_menu ()
    enable menu item under edit menu depending on the panel on focus

enable_paste ()
    enable paste
enable_preview()
    preview

enable_print()
    print

enable_redo()
    enable redo

enable_reset()
    reset the current panel

enable_save()
    save

enable_undo()
    enable undo related control

enable_zoom()
    zoom

enable_zoom_in()
    zoom in

enable_zoom_out()
    zoom out

freeze(data_id, theory_id)
    Saves theory/model and passes to data loader.
    .. warning:: This seems to be the exact same code as the next function called simply freeze. This
                probably needs fixing

full_draw()
    Draw the panels with axes in the schedule to full dwar list

get_client_size()
    return client size tuple

get_context_menu(plotpanel=None)
    Get the context menu items made available by the different plug-ins. This function is used by the
    plotting module

get_current_context_menu(plotpanel=None)
    Get the context menu items made available by the current plug-in. This function is used by the plotting
    module

get_current_perspective()
    return the current perspective

get_data(path)

get_data_manager()
    return the data manager.

get_paneinfo(name)
    Get pane Caption from window_name
    Parameters name – window_name in AuiPaneInfo
    Returns AuiPaneInfo of the name

get_save_location()
    return the _default_save_location

get_schedule()
    Get schedule

get_style()
    Return the gui style
get_toolbar()
    return the toolbar.

get_toolbar_height()

get_window_size()
    Get window size
    Returns size
    Return type tuple

load_data(path)
    load data from command line

load_folder(path)
    Load entire folder

load_from_cmd(path)
    load data from cmd or application

load_state(path, is_project=False)
    load data from command line or application

on_batch_selection(event=None)
    Parameters event – contains parameter enable. When enable is set to True the application
    is in Batch mode otherwise the application is in Single mode.

on_bookmark_panel(event=None)
    bookmark panel

on_category_panel(event)
    On cat panel

on_change_caption(name, old_caption, new_caption)
    Change the panel caption
    Parameters
    • name – window_name of the pane
    • old_caption – current caption [string]
    • new_caption – new caption [string]

on_change_categories(evt)

on_close_welcome_panel()
    Close the welcome panel

on_color_selection(event)
    Parameters event – contains parameters for id and color

on_copy_panel(event=None)
    copy the last panel on focus if possible

on_drag_panel(event=None)
    drag apply to the panel on focus

on_load_data(event)
    received an event to trigger load from data plugin

on_panel_close(event)
    Gets called when the close event for a panel runs. This will check which panel has been closed and
    delete it.

on_paste_panel(event=None)
    paste clipboard to the last panel on focus
on_preview_panel (event=None)
    preview information on the panel on focus
on_print_panel (event=None)
    print available information on the last panel on focus
on_read_batch_tofile (base)
    Open a file dialog, extract the file to read and display values into a grid
on_redo_panel (event=None)
    redo the last cancel action done on the last panel on focus
on_reset_panel (event=None)
    reset the current panel
on_save_helper (doc, reader, panel, path)
    Save state into a file
on_save_panel (event=None)
    save possible information on the current panel
on_set_batch_result (data_outputs, data_inputs=None, plugin_name="")
    Display data into a grid in batch mode and show the grid
on_set_plot_focus (panel)
    Set focus on a plot panel
on_undo_panel (event=None)
    undo previous action of the last panel on focus if possible
on_view (evt)
    A panel was selected to be shown. If it’s not already shown, display it.
    Parameters
evt – menu event
on_zoom_in_panel (event=None)
    zoom in of the panel on focus
on_zoom_out_panel (event=None)
    zoom out on the panel on focus
on_zoom_panel (event=None)
    zoom on the current panel if possible
onfreeze (theory_id)
    Saves theory/model and passes to data loader.
    ..warning:: This seems to be the exact same code as the next function called simply freeze. This
    probably needs fixing
open_with_externalapp (data, file_name, details="")
    Display data in the another application, by default Excel
open_with_localapp (data_inputs=None, details="", file_name=None, data_outputs=None)
    Display value of data into the application grid
    :param data_inputs: dictionary of string and list of items
    :param details: descriptive string
    :param file_name: file name
    :param data_outputs: Data outputs
plot_data (state_id, data_id=None, theory_id=None, append=False)
    send a list of data to plot
popup_panel (p)
    Add a panel object to the AUI manager
    Parameters
    p – panel object to add to the AUI manager
    Returns
    ID of the event associated with the new panel [int]
post_init ()
    This initialization method is called after the GUI has been created and all plug-ins loaded. It calls the
    post_init() method of each plug-in (if it exists) so that final initialization can be done.
**put_icon** *(frame)*
Put icon on the tap of a panel

**quit_guiframe** ()
Pop up message to make sure the user wants to quit the application

**read_batch_tofile** *(file_name)*
Extract value from file name and Display them into a grid

**remove_data** *(data_id, theory_id=None)*
Delete data state if data_id is provided. Delete theory created with data of id data_id if theory_id is provided. If delete all is true: delete the all state else delete theory

**reset_bookmark_menu** *(panel)*
Reset Bookmark menu list
: param panel: a control panel or tap where the bookmark is

**save_data1d** *(data, fname)*
Save data dialog

**save_data2d** *(data, fname)*
Save data2d dialog

**send_focus_to_datapanel** *(name)*
Send focusing on ID to data explorer

**set_current_perspective** *(perspective)*
Set the current active perspective

**set_custom_default_perspective** ()
Set default starting perspective

**set_data** *(data_id, theory_id=None)*
Set data to current perspective

**set_input_file** *(input_file)*
Parameters

**set_manager** *(manager)*
Sets the application manager for this frame
: Parameters

**set_panel_on_focus** *(event)*
Store reference to the last panel on focus update the toolbar if available update edit menu if available

**set_panel_on_focus_helper** ()
Helper for panel on focus with data_panel

**set_perspective** *(panels)*
Sets the perspective of the GUI. Opens all the panels in the list, and closes all the others.
: Parameters

**set_plot_unfocus** ()
Un focus all plot panels

**set_schedule** *(schedule=False)*
Set schedule

**set_schedule_full_draw** *(panel=None, func='del')*
Add/subtract the schedule full draw list with the panel given
: Parameters

- **panel** – plot panel
- **func** – append or del [string]
set_theory(state_id, theory_id=None)

setup_custom_conf()

    Set up custom configuration if exists

show_batch_frame(event=None)

    show the grid of result

data1d(data, name)

    Show data dialog

data2d(data, name)

    Show data dialog

data_panel(event=None, action=True)

    show the data panel

show_welcome_panel(event)

    Display the welcome panel

update_data(prev_data, new_data)

    Update the data.

update_theory(data_id, theory, state=None)

update_theory()

write_batch_tofile(data, file_name, details="")

    Helper to write result from batch into csv file

sas.sasgui.guiframe.gui_manager.custom_value(name, default=None)

    Fetch a config value from custom_config. Fallback to config, and then to default if it doesn’t exist in config.

sas.sasgui.guiframe.gui_statusbar module

Defines and draws the status bar that should appear along the bottom of the main SasView window.

class sas.sasgui.guiframe.gui_statusbar.Console(parent=None, status='', *args, **kwargs)

    The main class defining the Console window.

    Close(event)

    Calling close on the panel will hide the panel.

    Parameters

    event – A wx event.

set_message(status, event=None)

    Exposing the base ConsolePanel set_message

    Parameters

    • status – A status message to be sent to the console log.

    • event – A wx event.

    set_multiple_messages(messages=[])

    Method to send an arbitrary number of messages to the console log

    Parameters

    messages – A list of strings to be sent to the console log.

class sas.sasgui.guiframe.gui_statusbar.ConsolePanel(parent, *args, **kwargs)

    Interaction class for adding messages to the Console log.

    set_message(status='', event=None)

    Adds a message to the console log as well as the main sasview.log
Parameters

- **status** – A status message to be sent to the console log.
- **event** – A wx event.

```python
class sas.sasgui.guiframe.gui_statusbar.SPageStatusBar(parent, timeout=None, *args, **kwds)
```

Bases: `wx._windows.StatusBar`

```python
class sas.sasgui.guiframe.gui_statusbar.StatusBar(parent, id)
```

Bases: `wx._windows.StatusBar`

Application status bar

```python
PopStatusText (*args, **kwds)
```

Override status bar

```python
PushStatusText (*args, **kwds)
SetStatusText (text='', number=1, event=None)
```

Set the text that will be displayed in the status bar.

```python
clear_gauge (msg='')
```

Hide the gauge

```python
enable_clear_gauge ()
```

clear the progress bar

```python
get_msg_position ()
```

Get the last known message that was displayed on the console window.

```python
on_idle (event)
```

When the window is idle, check if the window has been resized

```python
on_size (evt)
```

If the window is resized, redraw the window.

```python
reposition ()
```

Place the various fields in their proper position

```python
set_dialog (event)
```

Display dialogbox

```python
set_gauge (event)
```

change the state of the gauge according the state of the current job

```python
set_icon (event)
```

Display icons related to the type of message sent to the statusbar when available. No icon is displayed if the message is empty

```python
set_message (event)
```

display received message on the statusbar

```python
set_status (event)
```

Update the status bar.

**Parameters**

- **type** – type of message send. type must be in ["start", "progress", "update", "stop"]
- **msg** – the message itself as string
- **thread** – if updatting using a thread status

sas.sasgui.guiframe.gui_style module

Provide the style for guiframe
class sas.sasgui.guiframe.gui_style.GUFRAME

CALCULATOR_ON = 256
DATALOADER_ON = 16
DEFAULT_STYLE = 92
FIXED_PANEL = 4
FLOATING_PANEL = 2
MANAGER_ON = 1
MULTIPLE_APPLICATIONS = 92
PLOTTING_ON = 8
SINGLE_APPLICATION = 64
TOOLBAR_ON = 32
WELCOME_PANEL_ON = 128

class sas.sasgui.guiframe.gui_style.GUFRAME_ICON

BOOKMARK_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x2f16d70>
BOOKMARK_ICON_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/bookmark.png'
COPY_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x2fcc300>
COPY_ICON_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/copy.png'
DRAG_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x26ffd20>
DRAG_ID_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/drag_hand.png'
FRAME_ICON_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/ball.ico'
HIDE_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x30aaf10>
HIDE_ID_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/hide.png'
PASTE_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x32d0a20>
PASTE_ICON_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/paste.png'
PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images'
PREVIEW_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x34b5d40>
PREVIEW_ID_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/report.png'
PRINT_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x30e7bd0>
PRINT_ID_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/printer.png'
REDO_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x26047d0>
REDO_ICON_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/redo.png'
RESET_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x3543cd0>
RESET_ID_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/reset.png'
SAVE_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x2e99d60>
SAVE_ICON_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/save.png'
UNDO_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x268f6b0>
UNDO_ICON_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/undo.png'
ZOOM_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x3531970>
ZOOM_ID_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/search_pan.png'
ZOOM_IN_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x2f30ad0>
ZOOM_IN_ID_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/zoom_in.png'
ZOOM_OUT_ICON = <wx._core.Image; proxy of <Swig Object of type 'wxImage *' at 0x2e26490>
ZOOM_OUT_ID_PATH = '/home/sasview/Jenkins/workspace/SasView_Ubuntu14.10/sasview/build/lib.linux-x86_64-2.7/sas/sasgui/guiframe/images/zoom_out.png'

class sas.sasgui.guiframe.gui_style.GUIFRAME_ID

BOOKMARK_ID = 104
COPYAS_ID = 116
COPYEX_ID = 114
COPYLAT_ID = 115
COPY_ID = 102
CURRENT_APPLICATION = 113
CURVE_SYMBOL_NUM = 13
DRAG_ID = 109
PASTE_ID = 103
PREVIEW_ID = 111
PRINT_ID = 112
REDO_ID = 101
RESET_ID = 110
SAVE_ID = 105
UNDO_ID = 100
ZOOM_ID = 108
ZOOM_IN_ID = 106
ZOOM_OUT_ID = 107

sas.sasgui.guiframe.gui_toolbar module

class sas.sasgui.guiframe.gui_toolbar.GUIToolBar (parent, *args, **kwds)
Bases: wx._controls.ToolBar
Implement toolbar for guiframe

ID_BOOKMARK = 138

add_bookmark_default ()
    Add default items in bookmark menu

append_bookmark (event)
    receive item to append on the toolbar button bookmark

append_bookmark_item (id, label)
    Append a item in bookmark

do_layout ()

enable_bookmark (panel)
enable_copy(panel)
enable_paste(panel)
enable_preview(panel)
enable_print(panel)
enable_redo(panel)
enable_reset(panel)
enable_save(panel)
enable_undo(panel)
enable_zoom(panel)
enable_zoom_in(panel)
enable_zoom_out(panel)
get_bookmark_items()
    Get bookmark menu items
on_bind_button()
    Bind the buttons
on_bookmark(event)
    add book mark
remove_bookmark_item(item)
    Remove a bookmark item
update_button(application_name="", panel_name="")
update_toolbar(panel=None)
sas.sasgui.guiframe.gui_toolbar.clear_image(image)

sas.sasgui.guiframe.panel_base module

class sas.sasgui.guiframe.panel_base.PanelBase(parent=None)
    Defines the API for a panels to work with the ViewerFrame toolbar and menu bar
    get_bookmark_flag()
        Get the bookmark flag to update appropriately the tool bar
    get_copy_flag()
        Get the copy flag to update appropriately the tool bar
    get_data()
        return list of current data
    get_drag_flag()
        Get the drag flag to update appropriately the tool bar
    get_frame()
    get_manager()
    get_paste_flag()
        Get the copy flag to update appropriately the tool bar
    get_preview_flag()
        Get the preview flag to update appropriately the tool bar
    get_print_flag()
        Get the print flag to update appropriately the tool bar
get_redo_flag()
    Get the redo flag to update appropriately the tool bar

get_reset_flag()
    Get the reset flag to update appropriately the tool bar

get_save_flag()
    Get the save flag to update appropriately the tool bar

get_state()
    return the current state

group_id = None

has_changed()

on_batch_selection(event)
    Parameters event – contains parameter enable. When enable is set to True the application
    is in Batch mode otherwise the application is in Single mode.

on_bookmark(event)
    The derivative class is on bookmark mode if implemented

on_close(event)
    Close event. Hide the whole window.

on_copy(event)
    The copy action if possible

on_drag(event)
    The derivative class allows dragging motion if implemented

on_kill_focus(event=None)
    The derivative class is on unfocus if implemented

on_paste(event)
    The paste action if possible

on_preview(event)
    Display a printable version of the class derivative

on_redo(event)
    The previous action is restored if possible

on_reset(event)
    The derivative class state is restored

on_save(event)
    The state of the derivative class is restored

on_set_focus(event=None)
    The derivative class is on focus if implemented

on_tap_focus()
    Update menu on clicking the panel tap
on_undo (event)
    The current action is canceled

on_zoom (event)
    The derivative class is on zoom mode (using pane) if zoom mode is implemented

on_zoom_in (event)
    The derivative class is on zoom in mode if implemented

on_zoom_out (event)
    The derivative class is on zoom out mode if implemented

save_project (doc=None)
    return an xml node containing state of the panel that guiframe can write to file

set_manager (manager)
    uid = None

sas.sasgui.guiframe.pdfview module

class sas.sasgui.guiframe.pdfview.PDFFrame (parent, id, title, path)
    Bases: wx._windows.Frame
    Frame for PDF panel

class sas.sasgui.guiframe.pdfview.PDFPanel (parent, path=None)
    Bases: wx._windows.Panel
    Panel that contains the pdf reader

OnClose (event)
    Close panel

OnLoad (event=None, path=None)
    Load a pdf file
    : Param path: full path to the file

OnNextPageButton (event)
    Goes to Next page

OnOpenButton (event)
    Open file button

OnPrevPageButton (event)
    Goes to Previous page

class sas.sasgui.guiframe.pdfview.TextFrame (parent, id, title, text)
    Bases: wx._windows.Frame
    Frame for PDF panel

class sas.sasgui.guiframe.pdfview.TextPanel (parent, text=None)
    Bases: wx.lib.scrolledpanel.ScrolledPanel
    Panel that contains the text

OnClose (event)
    Close panel

class sas.sasgui.guiframe.pdfview.ViewApp (redirect=False, filename=None, useBestVisual=False, clearSigInt=True)
    Bases: wx._core.App
    OnInit ()
sas.sasgui.guiframe.plugin_base module

Defines the interface for a Plugin class that can be used by the gui_manager.

class sas.sasgui.guiframe.plugin_base.PluginBase(name='Test_plugin')
    Bases: object

This class defines the interface for a Plugin class that can be used by the gui_manager.

Plug-ins should be placed in a sub-directory called “perspectives”. For example, a plug-in called Foo should be place in “perspectives/Foo”. That directory contains at least two files:

1. perspectives/Foo/__init__.py contains two lines:
   
   ```python
   PLUGIN_ID = "Foo plug-in 1.0"
   from Foo import *
   ```

2. perspectives/Foo/Foo.py contains the definition of the Plugin class for the Foo plug-in. The interface of that Plugin class should follow the interface of the class you are looking at.

See dummyapp.py for a plugin example.

```python
add_color(color, id)
    Adds color to a plugin

can_load_data()
    if return True, then call handler to load data

clear_panel()
    clear all related panels

delete_data(data_id)
    Delete all references of data which id are in data_list.

get_batch_capable()
    Check if the plugin has a batch capability

get_context_menu(plotpanel=None)
    This method is optional.
    When the context menu of a plot is rendered, the get_context_menu method will be called to give you a chance to add a menu item to the context menu.
    A ref to a plotpanel object is passed so that you can investigate the plot content and decide whether you need to add items to the context menu.
    This method returns a list of menu items. Each item is itself a list defining the text to appear in the menu, a tool-tip help text, and a call-back method.
    
    Parameters graph – the Graph object to which we attach the context menu
    
    Returns a list of menu items with call-back function

get_extensions()
    return state reader and its extensions

get_frame()
    Returns MDIChildFrame

get_panels(parent)
    Create and return the list of wx.Panels for your plug-in. Define the plug-in perspective.
    Panels should inherit from DefaultPanel defined below, or should present the same interface. They must define “window_caption” and “window_name”.
    
    Parameters parent – parent window
    
    Returns list of panels
```
**get_perspective()**
Get the list of panel names for this perspective

**get_tools()**
Returns a set of menu entries for tools

**is_always_active()**
return True is this plugin is always active and it is local to guiframe even if the user is switching between perspectives

**is_in_use(data_id)**
get a data id a list of data name if data data is currently used by the plugin and the name of the plugin

data_name = ‘None’ in_use = False example [(data_name, self.sub_menu)]

**load_data(event)**
Load data

**load_folder(event)**
Load entire folder

**on_batch_selection(flag)**
need to be overwritten by the derivated class

**on_perspective(event=None)**
Call back function for the perspective menu item. We notify the parent window that the perspective has changed.

Parameters event – menu event

**on_set_state_helper(event)**
update state

**populate_file_menu()**
Append menu item under file menu item of the frame

**populate_menu(parent)**
Create and return the list of application menu items for the plug-in.

Parameters parent – parent window

Returns plug-in menu

**post_init()**
Post initialization call back to close the loose ends

**set_batch_selection(flag)**
the plugin to its batch state if flag is True

**set_data(data_list=None)**
receive a list of data and use it in the current perspective

**set_is_active(active=False)**
Set if the perspective is always active

**set_state(state=None, datainfo=None)**
update state

**set_theory(theory_list=None)**

Parameters theory_list – list of information related to available theory state

**use_data()**
return True if these plugin use data
sas.sasgui.guiframe.proxy module

```python
class sas.sasgui.guiframe.proxy.Connection(url, timeout)
    Bases: object
    connect()
        Performs the request and gets a response from self.url
        @return: response object from urllib2.urlopen

class sas.sasgui.guiframe.proxy.logger = <logging.Logger object>

HTTP Proxy parser and Connection

connect() function:
- auto detects proxy in windows, osx
- in ux systems, the http_proxy environment variable must be set
- if it fails, try to find the proxy.pac address. - parses the file, and looks up for all possible proxies
```

sas.sasgui.guiframe.report_dialog module

Base class for reports. Child classes will need to implement the onSave() method.

```python
class sas.sasgui.guiframe.report_dialog.BaseReportDialog(report_list, imgRAM, fig_urls, *args, **kwds)
    Bases: wx._windows.Dialog
    HTML2PDF (data, filename)
        Create a PDF file from html source string. Returns True is the file creation was successful. : data:
        html string : filename: name of file to be saved
    onClose (event=None)
        Close the Dialog : event: Close button event
    onPreview (event=None)
        Preview : event: Preview button event
    onPrint (event=None)
        Print : event: Print button event
```

sas.sasgui.guiframe.report_image_handler module

```python
class sas.sasgui.guiframe.report_image_handler.ReportImageHandler

    static check_for_empty_instance()
    instance = None
    static remove_figure()
    static set_figs (bitmaps, perspective)
```

sas.sasgui.guiframe.startup_configuration module

```python
sas.sasgui.guiframe.startup_configuration.PANEL_HEIGHT = 215
    Dialog to set Appication startup configuration
```
**class** sas.sasgui.guiframe.startup_configuration.StartupConfiguration

**Bases:** wx._windows.Dialog

Dialog for Startup Configuration

**OnCurrent** (event=None)

Set to current setup

**OnDefault** (event=None)

Set to default

**write_custom_config()**

Write custom configuration

---

**sas.sasgui.guiframe.utils module**

Contains common classes and functions

**class** sas.sasgui.guiframe.utils.IdList

Create a list of wx ids that can be reused.

Ids for items need to be unique within their context. In a dynamic application where the number of ids needed different each time the form is created, depending for example, on the number of items that need to be shown in the context menu, you cannot preallocate the ids that you are going to use for the form. Instead, you can use an IdList, which will reuse ids from context to context, adding new ones if the new context requires more than a previous context.

IdList is set up as an iterator, which returns new ids forever or until it runs out. This makes it pretty useful for defining menus:

```python
class Form(wx.Dialog):
    _form_id_pool = IdList()

def __init__(self):
    ...
    menu = wx.Menu()
    for item, wx_id in zip(menu_items, self._form_id_pool):
        name, description, callback = item
        menu.Append(wx_id, name, description)
        wx.EVT_MENU(self, wx_id, callback)
    ...
```

It is a little unusual to use an iterator outside of a loop, but it is supported. For example, when defining a form, your class definition might look something like:

```python
class Form(wx.Dialog):
    _form_id_pool = IdList()

def __init__(self, pairs, ...):
    ids = iter(_form_id_pool)
    ...
    wx.StaticText(self, ids.next(), "Some key-value pairs")
    for name, value in pairs:
        label = wx.StaticText(self, ids.next(), name)
        input = wx.TextCtrl(self, ids.next(), value=str(value))
    ...
```
If the dialog is really dynamic, and not defined all in one place, then save the id list iterator as `self._ids = iter(_form_id_pool)` in the constructor.

The wx documentation is not clear on whether ids need to be unique. Clearly different dialogs can use the same ids, as this is done for the standard button ids such as wx.ID_HELP. Presumably each widget on the form needs its own id, but whether these ids can match the ids of menu items is not indicated, or whether different submenus need their own ids. Using different id lists for menu items and widgets is safest, but probably not necessary. And what about notebook tabs. Do the ids need to be unique across all tabs?

```python
class sas.sasgui.guiframe.utils.PanelMenu(*args, **kwargs)
    Bases: wx._core.Menu
    graph = None
    plots = None
    set_graph(graph)
    set_plots(plots)
sas.sasgui.guiframe.utils.check_float(item)
    Parameters item -- txtctrl containing a value
sas.sasgui.guiframe.utils.check_int(item)
    Parameters item -- txtctrl containing a value
sas.sasgui.guiframe.utils.format_number(value, high=False)
    Return a float in a standardized, human-readable formatted string
sas.sasgui.guiframe.utils.look_for_tag(string1, begin, end=None)
    this method remove the begin and end tags given by the user from the string .
    Parameters
    * begin -- the initial tag
    * end -- the final tag
    * string -- the string to check
    Returns begin_flag==True if begin was found, end_flag==if end was found else return false, false
sas.sasgui.guiframe.utils.parse_name(name, expression)
    remove “_” in front of a name
sas.sasgui.guiframe.utils.split_list(separator, mylist, n=0)
    returns a list of string without white space of separator
    Parameters separator -- the string to remove
sas.sasgui.guiframe.utils.split_text(separator, string1, n=0)
    return a list of string without white space of separator
    Parameters separator -- the string to remove
```

Module contents

- `sas.sasgui.guiframe.data_files()`
  Return the data files associated with guiframe images .
  The format is a list of (directory, [files...]) pairs which can be used directly in setup(..., data_files=...) for setup.py.
- `sas.sasgui.guiframe.get_data_path(media)`
- `sas.sasgui.guiframe.get_media_path(media)`

2.1. Contents
SasView Documentation, Release 4.2.1

sas.sasgui.perspectives package

Subpackages

sas.sasgui.perspectives.calculator package

Submodules

sas.sasgui.perspectives.calculator.aperture_editor module

```python
class sas.sasgui.perspectives.calculator.aperture_editor.ApertureDialog (parent=None, manager=None, aperture=None, *args, **kwds)
```

Bases: wx._windows.Dialog

- `get_aperture()`
  return the current aperture

- `get_notes()`
  return notes

- `on_change_distance()`
  Change distance of the aperture

- `on_change_name()`
  Change name

- `on_change_size()`
  Change aperture size

- `on_change_size_name()`
  Change the size’s name

- `on_change_type()`
  Change aperture type

- `on_click_apply(event)`
  Apply user values to the aperture

- `on_click_cancel(event)`
  reset the current aperture to its initial values

- `reset_aperture()`
  put the default value of the detector back to the current aperture

- `set_manager(manager)`
  Set manager of this window

- `set_values()`
  take the aperture values of the current data and display them through the panel

sas.sasgui.perspectives.calculator.calculator module

Calculator Module

```python
class sas.sasgui.perspectives.calculator.calculator.Plugin
Bases: sas.sasgui.guiframe.plugin_base.PluginBase
```

This class defines the interface for a Plugin class for calculator perspective
get_python_panel (filename=None)
    Get the python shell panel

    Parameters filename – file name to open in editor

get_tools ()
    Returns a set of menu entries for tools

on_calculate_dv (event)
    Compute the mass density or molar voulme

on_calculate_kiessig (event)
    Compute the Kiessig thickness

on_calculate_resoltuion (event)
    Estimate the instrumental resolution

on_calculate_sld (event)
    Compute the scattering length density of molecula

on_calculate_slit_size (event)
    Compute the slit size a given data

on_data_operation (event)
    Data operation

on_edit_data (event)
    Edit meta data

on_gen_model (event)
    On Generic model menu event

on_image_viewer (event)
    Get choose an image file dialog

    Parameters event – menu event

on_python_console (event)
    Open Python Console

    Parameters event – menu event

on_show_orientation (event)
    Make sasmodels orientation & jitter viewer available

put_icon (frame)
    Put icon in the frame title bar

sas.sasgui.perspectives.calculatorcalculator_widgets module

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class sas.sasgui.perspectives.calculatorcalculator_widgets.InputTextCtrl (parent=None, *args, **kwds)

    Bases: wx._controls.TextCtrl

    Text control for model and fit parameters. Binds the appropriate events for user interactions.

class sas.sasgui.perspectives.calculatorcalculator_widgets.InterActiveOutputTextCtrl (*args, **kwds)

    Bases: wx._controls.TextCtrl
Text control used to display outputs. No editing allowed. The background is grayed out. User can’t select text.

```python
class sas.sasgui.perspectives.calculator.calculator_widgets.OutputTextCtrl(*args, **kwds)

Bases: sas.sasgui.perspectives.calculator.calculator_widgets.InterActiveOutputTextCtrl
```

Text control used to display outputs. No editing allowed. The background is grayed out. User can’t select text.

`sas.sasgui.perspectives.calculator.collimation_editor` module

```python
class sas.sasgui.perspectives.calculator.collimation_editor.CollimationDialog(parent=None, manager=None, collimation=[], *args, **kwds)
```

Bases: `wx._windows.Dialog`

```python
add_aperture(event)
    Append empty aperture to data’s list of aperture

add_collimation(event)
    Append empty collimation to data’s list of collimation

edit_aperture(event)
    Edit the selected aperture

enable_aperture()
    Enable /disable widgets crelated to aperture

enable_collimation()
    Enable /disable widgets related to collimation

fill_aperture_combox()
    fill the current comboxbox with the available aperture

fill_collimation_combox()
    fill the current comboxbox with the available collimation

get_collimation()
    return the current collimation

get_current_collimation()

get_notes()
    return notes

on_change_length()
    Change the length

on_change_name()
    Change name

on_click_apply(event)
    Apply user values to the collimation

on_click_cancel(event)
    leave the collimation as it is and close
```
on_select_collimation(event)
    fill the control on the panel according to the current selected collimation

remove_aperture(event)
    Remove aperture to data’s list of aperture

remove_collimation(event)
    Remove collimation to data’s list of collimation

reset_aperture_combobox(edited_aperture)
    take all edited editor and reset clientdata of aperture combo box

reset_collimation_combobox(edited_collimation)
    take all edited editor and reset clientdata of collimation combo box

set_aperture(aperture)
    set aperture for data

set_manager(manager)
    Set manager of this window

set_values()
    take the collimation values of the current data and display them through the panel

sas.sasgui.perspectives.calculator.console module

Console Module display message of a dialog

class sas.sasgui.perspectives.calculator.console.ConsoleDialog(parent=None, manager=None, data=None, title='Data Summary', size=(530, 560))

Bases: wx._windows.Dialog

Data summary dialog

set_manager(manager)
    Set the manager of this window

set_message(msg="")
    Display the message received

sas.sasgui.perspectives.calculator.data_editor module

class sas.sasgui.perspectives.calculator.data_editor.DataEditorPanel(parent, data=[], *args, **kwds)

Bases: wx._windows.ScrolledWindow

Parameters data – when not empty the class can same information into a dat object and post
event containing the changed data object to some other frame

choose_data_file(location=None)
    Open a file dialog to allow loading a file

complete_loading(data=None, filename="")
    Complete the loading and compute the slit size
edit_collimation()
    Edit the selected collimation

edit_detector()
    Edit the selected detector

detector_selection()
    Select the detector from a list

edit_sample()
    Open the dialog to edit the sample of the current data

equipments_selection()
    Select the equipment from a list

edit_source()
    Open the dialog to edit the source of the current data

definition_selection()
    Select the definition from a list

enable_data_cbox()
fill_data_combobox()
fill the current combobox with the available data

current_data_selection()
    Select the current data from a list

g_current_data()
    Return the current data

g_notes()
    Return notes

change_run(event=None)
    Change run

change_title(event=None)
    Change title

change_apply(event)
    Changes are saved in data object imported to edit

change_browse(event)
    Open a file dialog to allow the user to select a given file. Display the loaded data if available.

change_reset(event)

change_save(event)
    Save change into a file

change_view(event)
    Display data info

change_close(event)
    Leave data as it is and close

change_edit(event)

change_select_data(event=None)

reset_panel()

reset_radiobox()

set_collimation(collimation, notes=None)
    Set collimation for data

set_detector(detector, notes=None)
    Set detector for data

set_sample(sample, notes=None)
    Set sample for data

set_source(source, notes=None)
    Set source for data

set_values()
    Take the aperture values of the current data and display them through the panel
```
class sas.sasgui.perspectives.calculator.data_editor.DataEditorWindow 
  (parent, manager, data=None, *args, **kwds)

Bases: wx._windows.Frame

get_data ()
  return the current data

sas.sasgui.perspectives.calculator.data_editor.load_error (error=None)

  Pop up an error message.
  @param error: details error message to be displayed

sas.sasgui.perspectives.calculator.data_operator module

GUI for the data operations panel (sum and multiply)
class sas.sasgui.perspectives.calculator.data_operator.DataOperPanel 
  (parent, *args, **kwds)

Bases: wx._windows.ScrolledWindow

check_data_inputs ()
  Check data1 and data2 whether or not they are ready for operation
disconnect_panels ()
draw_output (output)
  Draw output data(temp)
fill_data_combox ()
  fill the current combobox with the available data
fill_operator_combox ()
  fill the current combobox with the operator
get_datalist ()
make_data_out (data1, data2)
  Make a temp. data output set
on_click_apply (event)
  changes are saved in data object imported to edit
on_close (event)
  leave data as it is and close
on_help (event)
  Bring up the Data Operations Panel Documentation whenever the HELP button is clicked.
  Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file://...”

Parameters 
  evt – Triggers on clicking the help button

on_name (event=None)
  On data name typing

on_number (event=None, control=None)
  On selecting Number for Data2
```
on_select_data1 (event=None)
    On select data1

on_select_data2 (event=None)
    On Selecting Data2

on_select_operator (event=None)
    On Select an Operator

put_text_pic (pic=None, content='')
    Put text to the pic

send_warnings (msg='', info='info')
    Send warning to status bar

set_panel_on_focus (event)
    On Focus at this window

set_plot_unfocus ()
    Unfocus on right click

class sas.sasgui.perspectives.calculator.data_operator.DataOperatorWindow (parent, manager, *args, **kwds)

    Bases: wx._windows.Frame

OnClose (event=None)
    On close event

class sas.sasgui.perspectives.calculator.data_operator.SmallPanel (parent, id=-1, is_number=False, content='?', **kwargs)

    Bases: sas.sasgui.plottools.PlotPanel.PlotPanel

PlotPanel for Quick plot and masking plot

add_image (plot)
    Add Image

add_text ()
    Text in the plot

add_toolbar ()
    Add toolbar

draw ()
    Draw

erase_legend ()
    Remove Legend

onContextMenu (event)
    Default context menu for a plot panel

onLeftDown (event)
    Disables LeftDown

onMouseMotion (event)
    Disable dragging 2D image

onPick (event)
    Remove Legend

onWheel (event)
on_set_focus (event)
    send to the parent the current panel on focus

ontogglescale (event)
    On toggle 2d scale

set_content (content="")
    Set text content

**sas.sasgui.perspectivescalculator.density_panel module**

This module provide GUI for the mass density calculator

```python
class sas.sasgui.perspectivescalculatordensity_panel.DensityPanel (parent,
    base=None,
    *args,
    **kwds)
```

Bases: `wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase`

Provides the mass density calculator GUI.

**CENTERPane** = True

calculate (event)
    Calculate the mass Density/molar Volume of the molecules

check_inputs ()
    Check validity user inputs

clear_outputs ()
    Clear the outputs textctrl

get_input ()
    Return the current input and output combobox values

on_close (event)
    close the window containing this panel

on_help (event)
    Bring up the density/volume calculator Documentation whenever the HELP button is clicked.

    Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file:///...”

    Parameters
    evt – Triggers on clicking the help button

on_select_input (event)
    On selection of input combobox, update units and output combobox

on_select_output (event)
    On selection of output combobox, update units and input combobox

set_values ()
    Sets units and combobox values

window_caption = 'Mass Density Calculator'

window_name = 'Mass Density Calculator'
class sas.sasgui.perspectives.calculator.density_panel.DensityWindow (parent=None, title='Density/Volume Calculator', base=None, manager=None, size=(483.0, 296.7741935483871), *args, **kwds)

Bases: wx._windows.Frame

on_close (event)
    On close event

class sas.sasgui.perspectives.calculator.density_panel.ViewApp (redirect=False, filename=None, useBestVisual=False, clearSigInt=True)

Bases: wx._core.App

OnInit()

sas.sasgui.perspectives.calculator.detector_editor module

class sas.sasgui.perspectives.calculator.detector_editor.DetectorDialog (parent=None, manager=None, detector=None, title='Detector Editor', size=(550, 480))

Bases: wx._windows.Dialog

add_detector (event)
    Append empty detector to data's list of detector

enable_detector()
    Enable /disable widgets crelated to detector

fill_detector_combobox()
    fill the current combobox with the available detector

gcet_current_detector()

gcet_detector()
    return the current detector
get_notes()
    return notes

on_change_beam_center()
    Change the detector beam center

on_change_distance()
    Change distance of the sample to the detector

on_change_instrument()
    Change instrument

on_change_offset()
    Change the detector offset

on_change_orientation()
    Change the detector orientation

on_change_pixel_size()
    Change the detector pixel size

on_change_slit_length()
    Change slit length of the detector

on_click_apply(event)
    Apply user values to the detector

on_click_cancel(event)
    reset the current detector to its initial values

remove_detector(event)
    Remove detector to data’s list of detector

reset_detector()
    put the default value of the detector back to the current detector

reset_detector_combobox(edited_detector)
    take all edited editor and reset clientdata of detector combo box

set_detector(detector)
    set detector for data

set_manager(manager)
    Set manager of this window

set_values()
    take the detector values of the current data and display them through the panel

sas.sasgui.perspectives/calculator.gen_scatter_panel module

Generic Scattering panel. This module relies on guiframe manager.

class sas.sasgui.perspectives/calculator.gen_scatter_panel.CalcGen(id=-1, input=None, completefn=None, updatefn=None, yiel
time=0.01, worktime=0.01)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Computation

2.1. Contents
compute()
  executing computation

class sas.sasgui.perspectives.calculator.gen_scatter_panel.OmfPanel (parent, *args, **kwds)

Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase

Provides the sas gen calculator GUI.

check_inputs()
  check if the inputs are valid

display_npts(nap)
  Displays Npts ctrl

get_pix_volumes()
  Get the pixel volume

get_sld_val()
  Set sld_n of slddata on sld input

on_save(event)
  Close the window containing this panel

on_sld_draw(event)
  Draw sld profile as scattered plot

set_npts_from_slddata()
  Set total n. of points form the sld data

set_sld_ctr(sld_data)
  Set sld textctrls

set_slddata(slddata)
  Set sld data related items

window_caption = 'SLD Pixel Info '
window_name = 'SLD Pixel Info'

class sas.sasgui.perspectives.calculator.gen_scatter_panel.SasGenPanel (parent, *args, **kwds)

Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase

Provides the sas gen calculator GUI.

choose_data_file(location=None)
  Choosing a data file

complete(input, update=None)
  Gen compute complete function :Param input: input list [qx_data, qy_data, i_out]

complete_loading(data=None, filename=")
  Complete the loading

estimate_ctime()
  Calculation time estimation

load_update()
  print update on the status bar

on_compute(event)
  Compute I(qx, qy)

on_help(event)
Bring up the General scattering Calculator Documentation whenever the HELP button is clicked.

Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file:///...”

**Parameters**

- **evt** – Triggers on clicking the help button

  **on_load_data** *(event)*
  
  Open a file dialog to allow the user to select a given file. The user is only allow to load file with extension .omf, .txt, .sld. Display the slit size corresponding to the loaded data.

  **on_panel_close** *(event)*
  
  close the window containing this panel

  **set_est_time** *
  
  Set text for est. computation time

  **set_input_params** *
  
  Set model parameters

  **set_scale2d** *(scale)*
  
  Set SLD plot scale

  **set_volume_ctl_val** *(val)*
  
  Set volume txtctrl value

  **sld_draw** *(event=None, has-arrow=True)*
  
  Draw 3D sld profile

  **window_caption = 'Generic SAS '**

  **window_name = 'Generic SAS Calculator'**

**class sas.sasgui.perspectives.calculator.gen_scatter_panel.SasGenWindow** *(parent=None, manager=None, title='Generic Scattering Calculator', size=(868.0, 610.5), *args, **kwargs)*

Bases: wx._windows.Frame

GEN SAS main window

**build_panels** *

**check_omfpanel_inputs** *

Check OMF panel inputs

**draw_graph** *(plot, title="")*

**get_npix** *

Get no. of pixels from omf panel
get_path()
    File location

get_pix_volumes()
    Get a pixel volume

get_sld_data()
    Return slddata

get_sld_data_from_omf()

get_sld_from_omf()

on_close(event)
    Close

on_open_file(event)
    On Open

on_panel_close(event)

on_save_file(event)
    On Close

set_etime()
    Sets est. computation time on panel

set_file_location(path)
    File location

set_main_panel_sld_data(sld_data)

set_omfpanel_default_shap(shape)
    Set default_shape in omfpanel

set_omfpanel_npts()
    Set Npts in omf panel

set_scale2d(scale)

set_schedule_full_draw(panel=None, func='del')
    Send full draw to gui frame

set_sld_data(data)
    Set omfdata

set_sld_n(sld)

set_volume_ctr_val(val)
    Set volume txtctl value

sld_draw()
    sld draw

sas.sasgui.perspectives.calculator.gen_scatter_panel.add_icon(parent, frame)
    Add icon in the frame

sas.sasgui.perspectives.calculator.image_viewer module

class sas.sasgui.perspectives.calculator.image_viewer.ImageFrame(parent,
    id, title, image=Non, scale='log_{10}', size=wx.Size(550, 470))

PlotFrame

Frame for simple plot

`on_help(event)`

Bring up Image Viewer Documentation from the image viewer window whenever the help menu item “how to” is clicked. Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ . . .”.

**Parameters**

- `evt` – Triggers on clicking “how to” in help menu

`on_set_data(event)`

Rescale the x y range, make 2D data and send it to data explore

**class** 

`sas.sasgui.perspectives.calculator.image_viewer.ImageView(parent=None)`

Open a file dialog to allow the user to select a given file. Display the loaded data if available.

`choose_data_file(location=None)`

Open a file dialog to allowing loading a file

`load()`

load image files

**class** 

`sas.sasgui.perspectives.calculator.image_viewer.SetDialog(parent, id=-1, title='Convert to Data', image=None, size=(480, 270))`

**Bases:** `wx._windows.Dialog`

Dialog for Data Set

`OnClose(event)`

Close event

`convert_image(rgb, xmin, xmax, ymin, ymax, zscale)`

Convert image to data2D

`on_set(event)`

Set image as data

`rgb2gray(rgb)`

RGB to Grey

**sas.sasgui.perspectives.calculator.kiessig_calculator_panel module**

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**class** 

`sas.sasgui.perspectives.calculator.kiessig_calculator_panel.KiessigThicknessCalculatorPanel(parent, *args, **kwds)`

**Bases:** `wx._windows.Panel, sas.sasgui.guiframe.panel_base.PanelBase`

Provides the Kiessig thickness calculator GUI.

```
CENTER_PANE = True
```

`format_number(value=None)`

Return a float in a standardized, human-readable formatted string
on_close (event)
  close the window containing this panel

on_compute (event)
  Execute the computation of thickness

on_help (event)
  Bring up the Kiessig fringe calculator Documentation whenever the HELP button is clicked. Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file://...”.

Parameters

- evt -- Triggers on clicking the help button

window_caption = 'Kiessig Thickness Calculator'
window_name = 'Kiessig Thickness Calculator'

class sas.sasgui.perspectives.calculator.kiessig_calculator_panel.KiessigWindow (parent=None, manager=None, title='Kiessig Thickness Calculator', size=(560, 230), *args, **kwds)

Bases: wx._windows.Frame

on_close (event)
  Close event

sas.sasgui.perspectives.calculator.load_thread module

Thread handler used to load data

class sas.sasgui.perspectives.calculator.load_thread.DataReader (path, completefn=None, updatelnf=None, yielddatefn=None, yieldtime=0.01, worktime=0.01)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Load a data given a filename

compute ()
  read some data

isquit ()
  @raise KeyboardInterrupt: when the thread is interrupted
class sas.sasgui.perspectives.calculator.load_thread.GenReader(path, louder, completefn=None, updatefn=None, yield-time=0.01, work-time=0.01)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Load a sld data given a filename

compute()
  read some data

isquit()
  @raise KeyboardInterrupt: when the thread is interrupted

*sas.sasgui.perspectives.calculator.model_editor module*

This module provides three model editor classes: the composite model editor, the easy editor which provides a simple interface with tooltip help to enter the parameters of the model and their default value and a panel to input a function of y (usually the intensity). It also provides a drop down of standard available math functions. Finally a full python editor panel for complete customization is provided.

:TODO the writing of the file and name checking (and maybe some other functions?) should be moved to a computational module which could be called from a python script. Basically one just needs to pass the name, description text and function text (or in the case of the composite editor the names of the first and second model and the operator to be used).

class sas.sasgui.perspectives.calculator.model_editor.EditorPanel(parent, base, path, title, *args, **kwds)

Bases: wx._windows.ScrolledWindow

Simple Plugin Model function editor

check_name()  
  Check name if exist already

get_notes()  
  return notes

get_param_helper(param_str)  
  yield a sequence of name, value pairs for the parameters in param_str

Parameters can be defined by one per line by name=value, or multiple on the same line by separating the pairs by semicolon or comma. The value is optional and defaults to “1.0”.

get_warning()  
  Get the warning msg

on_change_name(event=None)  
  Change name

on_click_apply(event)  
  Changes are saved in data object imported to edit.

checks firs for valid name, then if it already exists then checks that a function was entered and finally that if entered it contains at least a return statement. If all passes writes file then tries to compile. If
compile fails or import module fails or run method fails tries to remove any .py and pyc files that may have been created and sets error message.

todo this code still could do with a careful going over to clean up and simplify, the non GUI methods such as this one should be removed to computational code of SasView. Most of those computational methods would be the same for both the simple editors.

```python
on_close(event)
leave data as it is and close
```

```python
on_help(event)
Bring up the New Plugin Model Editor Documentation whenever the HELP button is clicked.

Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file:///…”

**Parameters**
- **evt** – Triggers on clicking the help button

```python
on_over_cb(event)
Set overwrite name flag on cb event
```

```python
set_function_helper(line)
Get string in line to define the local params

**Parameters**
- **line** – one line of string got from the param_str

```python
write_file(fname, name, desc_str, param_str, func_str)
Write content in file

**Parameters**
- **fname** – full file path
- **desc_str** – content of the description strings
- **param_str** – content of params; Strings
- **func_str** – content of func; Strings
```

```python
class sas.sasgui.perspectives.calculator.model_editor.EditorWindow(parent, base, path, title, size=(800, 735), *args, **kwds)

**Bases:** wx._windows.Frame

**Editor Window**

```python
on_close(event)
On close event
```

```python
class sas.sasgui.perspectives.calculator.model_editor.TextDialog(parent=None, base=None, id=None, title=", model_list=[], plugin_dir=None)

**Bases:** wx._windows.Dialog

**Dialog for easy custom composite models.** Provides a wx.Dialog panel to choose two existing models (including pre-existing Plugin Models which may themselves be composite models) as well as an operation
on those models (add or multiply) the resulting model will add a scale parameter for summed models and a
background parameter for a multiplied model.

The user also gives a brief help for the model in a description box and must provide a unique name which is
verified as unique before the new model is saved.

This Dialog pops up for the user when they press ‘Sum|Multi(p1,p2)’ under ‘Plugin Model Operations’
under ‘Fitting’ menu. This is currently called as a Modal Dialog.

:TODO the built in compiler currently balks at when it tries to import a model whose name contains spaces
or symbols (such as + ... underscore should be fine). Have fixed so the editor cannot save such a file
name but if a file is dropped in the plugin directory from outside this class will create a file that cannot be
compiled. Should add the check to the write method or to the on_model method.

• PDB:April 5, 2015

check_name (event=None)
Check that proposed new model name is a valid Python module name and that it does not already exist.
If not show error message and pink background in text box else call on_apply

:TODO this should be separated out from the GUI code. For that we need to pass it the name (or if
we want to keep the default name option also need to pass the self.operator attribute) We just need
the function to return an error code that the name is good or if not why (not a valid name, name exists
already). The rest of the error handling should be done in this module. so on_apply would then start
by checking the name and then either raise errors or do the deed.

compile_file (path)
Compile the file in the path

delete_file (path)
Delete file in the path

fill_explanation_helpstring (operator)
Choose the equation to use depending on whether we now have a sum or multiply model then create
the appropriate string

for the sum model the result will be: scale_factor * (scale1 * model_1 + scale2 * model_2) + back-
ground while for the multiply model it will just be: scale_factor * (model_1* model_2) + background

fill_operator_combox ()
fill the current combobox with the operator

get_textnames ()
Returns model name string as list

on_apply (path)
This method is a misnomer - it is not bound to the apply button event. Instead the apply button event
goes to check_name which then calls this method if the name of the new file is acceptable.

:TODO this should be bound to the apply button. The first line should call the check_name method
which itself should be in another module separated from the the GUI modules.

on_change_name (event=None)
Change name

on_help (event)
Bring up the Composite Model Editor Documentation whenever the HELP button is clicked.

Calls DocumentationWindow with the path of the location within the documentation tree
(after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the
release version of installers, the help comes up at the top level of the file as webbrowser does
not pass anything past the # to the browser when it is running “file://...”

Parameters evt – Triggers on clicking the help button
on_model1 (event)
   Set model1

on_model2 (event)
   Set model2

on_select_operator (event=None)
   On Select an Operator

update_cm_list ()
   Update custom model list

write_string (fname, model1_name, model2_name)
   Write and Save file

```
sas.sasgui.perspectives.calculator.pyconsole module

Console Module display Python console

class sas.sasgui.perspectives.calculator.pyconsole.PyConsole (parent=None, 
               base=None, 
               manager=None, 
               panel=None, 
               title='Python Shell/Editor', 
               filename=None, 
               size=(830, 730))
```

Bases: wx.py.editor.EditorNotebookFrame

CENTER_PANE = False

OnAbout (event)
   On About

OnCheckModel (event)
   Compile

OnHelp (event)
   Show a help dialog.

OnNewFile (event)
   OnFileOpen

OnOpenFile (event)
   OnFileOpen

OnRun (event)
   Run

OnSaveAsFile (event)
   OnFileSaveAs overwrite

OnSaveFile (event)
   OnFileSave overwrite

OnUpdateCompileMenu (event)
   Update Compile menu items based on current tap.

bufferOpen ()
   Open file in buffer, bypassing editor bufferOpen

bufferSaveAs ()
   Save buffer to a new filename: Bypassing editor bufferSaveAs
on_close(event)
    Close event

set_manager(manager)
    Set the manager of this window

window_caption = 'Plugin Model Editor'
window_name = 'Custom Model Editor'

class sas.sasgui.perspectives.calculator.pyconsole.ResizableScrolledMessageDialog(parent, msg, caption, pos=wx.Point(-1, -1), size=(500, 300), style=536877120)

Bases: wx._windows.Dialog
    Custom version of wx ScrolledMessageDialog, allowing border resize

sas.sasgui.perspectives.calculator.pyconsole.check_model(path)
    Check that the model on the path can run.

sas.sasgui.perspectives.calculator.pyconsole.show_model_output(parent, fname)

sas.sasgui.perspectives.calculator.resolcal_thread module

Thread for Resolution computation

class sas.sasgui.perspectives.calculator.resolcal_thread.CalcRes(id=-1, func=None, qx=None, qy=None, qx_min=None, qx_max=None, qy_min=None, qy_max=None, image=None, completefn=None, updatefn=None, elapsed=0, yieldtime=0.01, worktime=0.01)

Bases: sas.sascalc.data_util.calcthread.CalcThread
    Compute Resolution

compute()
    executing computation
sas.sasgui.perspectives.calculator.resolution_calculator_panel module

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class sas.sasgui.perspectives.calculator.resolution_calculator_panel.ResolutionCalculatorPanel

    Bases: wx.lib.scrolledpanel.ScrolledPanel

    Provides the Resolution calculator GUI.

    CENTER_PANE = True

    complete(image, elapsed=None)
        Call after complete: wx call after needed for stable output

    complete_cal(image, elapsed=None)
        Complete computation

    format_number(value=None)
        Return a float in a standardized, human-readable formatted string

    on_close(event)
        close the window containing this panel

    on_compute(event=None)
        Execute the computation of resolution

    on_compute_call(event=None)
        Execute the computation of resolution

    on_help(event)
        Bring up the Resolution calculator Documentation whenever the HELP button is clicked.
        Calls DocumentationWindow with the path of the location within the documentation tree
        (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the
        release version of installers, the help comes up at the top level of the file as webbrowser does
        not pass anything past the # to the browser when it is running “file://...”

        Parameters
        event – Triggers on clicking the help button

    on_reset(event)
        Execute the reset

    window_caption = ''

    window_name = 'Q Resolution Estimator'
class sas.sasgui.perspectives.calculator.resolution_calculator_panel.ResolutionWindow

Bases: wx._windows.Frame

Resolution Window

OnClose(event)

On close event

sas.sasgui.perspectives.calculator.sample_editor module

class sas.sasgui.perspectives.calculator.sample_editor.SampleDialog

Bases: wx._windows.Dialog

get_notes()
    return notes

get_sample()
    return the current sample

on_change_details()
    Change details

on_change_id()
    Change id of the sample

on_change_name()
    Change name

on_change_orientation()
    Change orientation

on_change_position()
    Change position

on_change_temperature()
    Change temperature
on_change_thickness()
    Change thickness

on_change_transmission()
    Change transmission

on_click_apply(event)
    Apply user values to the sample

on_click_cancel(event)
    leave the sample as it is and close

reset_sample()
    Put initial values of the sample back to the current sample

set_details(sample)
    print details on the current sample

set_manager(manager)
    Set manager of this window

set_values()
    take the sample values of the current data and display them through the panel

sas.sasgui.perspectives.calculator.sld_panel module

This module provide GUI for the neutron scattering length density calculator

class sas.sasgui.perspectives.calculator.sld_panel.SldPanel(parent, base=None, *args, **kwds)

    Bases: wx._windows.Panel, sas.sasgui.guiframe.panel_base.PanelBase

    Provides the SLD calculator GUI.

    CENTER_PANE = True

calculateSld(event)
    Calculate the neutron scattering density length of a molecule

calculate_sld_helper(element, density, molecule_formula)
    Get an element and compute the corresponding SLD for a given formula

        Parameters

        element – elements a string of existing atom

    calculate_xray_sld(element)
    Get an element and compute the corresponding SLD for a given formula

        Parameters

        element – elements a string of existing atom

check_inputs()
    Check validity user inputs

clear_outputs()
    Clear the outputs textctrl

fill_xray_cbox()
    fill the x-ray combobox with the sources

on_close(event)
    close the window containing this panel

on_help(event)
    Bring up the SLD Documentation whenever the HELP button is clicked.

    Calls DocumentationWindow with the path of the location within the documentation tree
    (after /doc/ …”). Note that when using old versions of Wx (before 2.9) and thus not the
release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file://...”

Parameters

- **evt** – Triggers on clicking the help button

```python
on_select_xray(event=None)

On Selecting a source
```

```python
window_caption = 'SLD Calculator'
window_name = 'SLD Calculator'
```

```python
class sas.sasgui.perspectives.calculator.sld_panel.SldWindow(
    parent=None,
    title='SLD Calculator',
    base=None,
    manager=None,
    size=(410, 410),
    *args,
    **kwds)
```

Bases: `wx._windows.Frame`

```python
on_close(event)
```

On close event

```python
class sas.sasgui.perspectives.calculator.sld_panel.ViewApp(
    redirect=False,
    filename=None,
    useBestVisual=False,
    clearSigInt=True)
```

Bases: `wx._core.App`

```python
OnInit()
```

**sas.sasgui.perspectives.calculator.slit_length_calculator_panel module**

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```python
class sas.sasgui.perspectives.calculator.slit_length_calculator_panel.SlitLengthCalculatorPanel(
    parent,
    *args,
    **kwds)
```

Bases: `wx._windows.Panel`, `sas.sasgui.guiframe.panel_base.PanelBase`

Provides the slit length calculator GUI.

**CENTER_PANE** = True

```python
choose_data_file(location=None)
```

```python
complete_loading(data=None, filename=“”)
```

Complete the loading and compute the slit size

```python
load_update()
```

print update on the status bar

```python
on_close(event)
```

close the window containing this panel

```python
on_help(event)
```

2.1. Contents 417
Bring up the slit length calculator Documentation whenever the HELP button is clicked. Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file://../”.

**Parameters**

- `evt` - Triggers on clicking the help button

```python
on_load_data(event)
Open a file dialog to allow the user to select a given file. The user is only allow to load file with extension .DAT or .dat. Display the slit size corresponding to the loaded data.

window_caption = 'Slit Size Calculator'
window_name = 'Slit Size Calculator'
class sas.sasgui.perspectives.calculator.slit_length_calculator_panel.SlitLengthCalculatorWindow(...)
```

Bases: `wx._windows.Frame`

- `on_close(event)`
  Close event

`sas.sasgui.perspectives.calculator.source_editor module`

```python
class sas.sasgui.perspectives.calculator.source_editor.SourceDialog(parent=None, manager=None, source=None, *args, **kwds)
```

Bases: `wx._windows.Dialog`

- `get_notes()`
  return notes
- `get_source()`
  return the current source
- `on_change_beam_shape()`
  Change beams shape
- `on_change_beam_size()`
  Change beam size
- `on_change_beam_size_name()`
  Change beam size name
- `on_change_name()`
  Change name
on_change_radiation()  
Change radiation of the sample

on_change_wavelength()  
Change the wavelength

on_change_wavelength_max()  
Change the wavelength maximum

on_change_wavelength_min()  
Change the wavelength minimum

on_change_wavelength_spread()  
Change the wavelength spread

on_click_apply(event)  
Apply user values to the source

on_click_cancel(event)  
reset the current source

reset_source()  
put back initial values of the source

set_manager(manager)  
Set manager of this window

set_values()  
take the source values of the current data and display them through the panel

Module contents

sas.sasgui.perspectives.calculator.data_files()  
Return the data files associated with media calculator.

The format is a list of (directory, [files...]) pairs which can be used directly in setup(...,data_files=...) for setup.py.

sas.sasgui.perspectives.calculator.get_data_path(media)

sas.sasgui.perspectives.corfunc package

Submodules

sas.sasgui.perspectives.corfunc.corfunc module

Corfunc perspective
class sas.sasgui.perspectives.corfunc.corfunc.Plugin  
Bases: sas.sasgui.guiframe.plugin_base.PluginBase

This class defines the interface for a plugin class for a correlation function perspective

clear_data()  
delete_data(data)  
Delete the data from the perspective

get_context_menu(plotpanel=None)  
Get the context menu items available for Corfunc.

Parameters  
plotpanel – A Plotter1D panel

Returns  
a list of menu items with call-back function

2.1. Contents
**Note** if Data1D was generated from Theory1D the fitting option is not allowed

```python
def get_panels(parent):
    # Define the GUI panels

def set_data(data_list=None):
    # Load the data that’s been selected

    Parameters:
    
    data_list -- The data to load in

    def set_state(state=None, datainfo=None):
        # Callback for CorfuncState reader. Called when a .crf file is loaded

    def show_data(data, label, reset=False, active_ctrl=None):
        # Show data read from a file

        Parameters:
        
        data -- The data to plot (Data1D)
        label -- What to label the plot. Also used as the plot ID
        reset -- If True, all other plottables will be cleared

class sas.sasgui.perspectives.corfunc.corfunc_panel.CorfuncPanel

    CENTER_PANE = True

    def compute_extrapolation(event=None):
        # Compute and plot the extrapolated data. Called when Extrapolate button is pressed.

    def compute_transform(event=None):
        # Compute and plot the transformed data. Called when Transform button is pressed.

    def extract_parameters(event=None):
        # Called when “Extract Parameters” is clicked

    def get_data():
        # return list of current data

    def get_save_flag():
        # Get the save flag to update appropriately the tool bar

    def get_state():
        # Return the state of the panel

    def onSetFocus(evt):

    def on_help(event=None):
        # Show the corfunc documentation

    def on_save(event=None):
        # Save corfunc state into a file

    def on_set_focus(event=None):
        # The derivative class is on focus if implemented

    def plot_qrange(active=None, leftdown=False):
```

**SasView Documentation, Release 4.2.1**
radio_changed (event=None)
Called when the “Transform type” radio button are changed

save_project (doc=None)
Return an XML node containing the state of the panel

Parameters doc – An xml node to attach the project state to (optional)

set_background (bg)

set_data (data=None, set_qrange=True)
Update the GUI to reflect new data that has been loaded in

Parameters data – The data that has been loaded

set_extracted_params (params=None, reset=False)
Displays the values of the parameters extracted from the Fourier transform

set_extrapolation_params (params=None)
Displays the value of the parameters calculated in the extrapolation

set_qmax (qmax)
set_qmin (qmin)

set_state (state=None, data=None)
Set the state of the panel. If no state is provided, the panel will be set to the default state.

Parameters

• state – A CorfuncState object
• data – A Data1D object

transform_complete (transforms=None)
Called from FourierThread when calculation has completed

transform_update (msg="")
Called from FourierThread to update on status of calculation

window_caption = 'Correlation Function'
window_name = 'Correlation Function'

sas.sasgui.perspectives.corfunc.corfunc_state module

class sas.sasgui.perspectives.corfunc.corfunc_state.CorfuncState
Bases: object
Stores information about the state of CorfuncPanel

fromXML (node)
Load corfunc states from a file

Parameters node – node of an XML document to read from (optional)

set_saved_state (name, value)
Set a value in the current state.

Parameters

• name – The name of the parameter to set
• value – The value to set the parameter to

toXML (filename='corfunc_state.crf', doc=None, entry_node=None)
Writes the state of the CorfuncPanel panel to file, as XML.

Compatible with standalone writing, or appending to an already existing XML document. In that case, the XML document is required. An optional entry node in the XML document may also be given.
Parameters

- **file** – file to write to
- **doc** – XML document object [optional]
- **entry_node** – XML node within the XML document at which we will append the data [optional]

Returns None if no doc is provided, modified XML document if doc!=None

class sas.sasgui.perspectives.corfunc.corfunc_state.Reader(callback)

Bases: sas.sascalc.dataloader.readers.cansas_reader.Reader

Reads a CanSAS file containing the state of a CorfuncPanel

`ext = ['*.crf', '*.CRF', '*.svs', '*.SVS']`

`get_state()`

`read(path)`

Load data and corfunc information from a CanSAS file.

Parameters **path** – The file path to read from

Returns Data1D object, a list of Data1D objects, or None

Raises

- IOError – When the file can’t be found
- IOError – When the file is an invalid file type
- ValueError – When the length of the data vectors are inconsistent

`type = ['Corfunc file (*.crf)|*.crf', 'SASView file (*.svs)|*.svs']`

`type_name = 'Corfunc'`

write (filename, datainfo=None, state=None)

Write the content of a Data1D as a CanSAS file.

: param filename: Name of the file to write : param datainfo: Data1D object : param state: Corfunc-State object

sas.sasgui.perspectives.corfunc.plot_labels module

Module contents

sas.sasgui.perspectives.file_converter package

Submodules

sas.sasgui.perspectives.file_converter.converter_panel module

This module provides a GUI for the file converter

class sas.sasgui.perspectives.file_converter.converter_panel.ConverterPanel(parent, base=None, *args, **kwargs)

Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase

This class provides the File Converter GUI
ask_frame_range \((n_{frames})\)
Display a dialog asking the user to input the range of frames they would like to export

**Parameters**
n_{frames} – How many frames the loaded data file has

**Returns**
A dictionary containing the parameters input by the user

colorbar

convert_1d_data \((qdata, iqdata)\)
Formats a 1D array of q_axis data and a 2D array of I axis data (where each row of iqdata is a separate row), into an array of Data1D objects

colorbar

convert_2d_data \((dataset)\)

colorbar

convert_to_cansas \((frame_{data}, filepath, single_{file})\)
Saves an array of Data1D objects to a single CanSAS file with multiple <SasData> elements, or to multiple CanSAS files, each with one <SasData> element.

**Parameters**

- **frame_{data}** – If single_{file} is true, an array of Data1D objects. If single_{file} is false, a dictionary of the form \([frame\_number: Data1D]\).
- **filepath** – Where to save the CanSAS file
- **single_{file}** – If true, array is saved as a single file, if false, each item in the array is saved to it’s own file

datatype_changed \((event)\)
Update the UI and self.data_type when a data type radio button is pressed

effect

extract_ascii_data \((filename)\)
Extracts data from a single-column ASCII file

**Parameters**
filename – The file to load data from

**Returns**
A numpy array containing the extracted data

effect

extract_bsl_data \((filename)\)
Extracts data from a 2D BSL file

**Parameters**
filename – The header file to extract the data from

Return x_data A 1D array containing all the x coordinates of the data

Return y_data A 1D array containing all the y coordinates of the data

Return frame_data A dictionary of the form \([frame\_number: data]\), where data is a 2D numpy array containing the intensity data

effect

extract_otoko_data \((filename)\)
Extracts data from a 1D OTOKO file

**Parameters**
filename – The OTOKO file to load the data from

**Returns**
A numpy array containing the extracted data

effect

generate_ascii

generate_cansas

generate_data

generate_graph

generate_html

generate_pdf

generate_plot

generate_table

generate_text

generate_visualization

generate_word

get_metadata ()

metadata_changed \((event)\)

on_collapsible_pane \((event)\)
Resize the scrollable area to fit the metadata pane when it’s collapsed or expanded

effect

on_convert \((event)\)
Called when the Convert button is clicked

effect

on_help \((event)\)
Show the File Converter documentation

effect

radiationtype_changed \((event)\)
Show the window for inputting Detector metadata

Show the window for inputting Sample metadata

Show the window for inputting Source metadata

validate_inputs()

class sas.sasgui.perspectives.file_converter.converter_panel.ConverterWindow (parent=None, title='File Converter', base=None, manager=None, size=(518.4, 486.0), *args, **kwargs)

Bases: wx._windows.Frame
Displays ConverterPanel

on_close (event)

sas.sasgui.perspectives.file_converter.converter_widgets module

This module provides some custom wx widgets for the file converter perspective

class sas.sasgui.perspectives.file_converter.converter_widgets.FileInput (parent, wildcard=' ')

Bases: object

GetCtrl ()

GetPath ()

SetWildcard (wildcard)

class sas.sasgui.perspectives.file_converter.converter_widgets.VectorInput (parent, control_name, callback=None, labels=['x:', 'y:', 'z:'], z_enabled=False)

Bases: object
An input field for inputting 2 (or 3) components of a vector.

GetNamex ()

GetSizer ()
    Get the control’s sizer
Return sizer a wx.BoxSizer object

GetValue()
Get the value of the vector input

Return v A Vector object

SetValue(vector)
Set the value of the vector input

Parameters vector – A Vector object

Validate()
Validate the contents of the inputs

Return all_valid Whether or not the inputs are valid

Return invalid_ctrl A control that is not valid (or None if all are valid)

sas.sasgui.perspectives.file_converter.file_converter module

File Converter Plugin

class sas.sasgui.perspectives.file_converter.file_converter.Plugin
Bases: sas.sasgui.guiframe.plugin_base.PluginBase

This class defines the interface for a Plugin class for File Converter perspective

going_tools()
Returns a set of menu entries

on_file_converter(event)

put_icon(frame)
Put icon in the frame title bar

sas.sasgui.perspectives.file_converter.frame_select_dialog module

class sas.sasgui.perspectives.file_converter.frame_select_dialog.FrameSelectDialog
Bases: wx._windows.Dialog

This class provides a wx.Dialog subclass for selecting which frames of a multi-frame file to export

sas.sasgui.perspectives.file_converter.meta_panels module

class sas.sasgui.perspectives.file_converter.meta_panels.DetectorPanel
parent, detector, base=None, *args, **kwargs)

Bases: sas.sasgui.perspectives.file_converter.meta_panels.MetadataPanel

on_close(event=None)
Close event. Hide the whole window.
class sas.sasgui.perspectives.file_converter.meta_panels.MetadataPanel (parent, metadata, base=None, *args, **kwargs)

Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase

A common base class to be extended by panels that deal with metadata input. Handles input validation and passing inputted data back to ConverterPanel.

get_property_string (name, is_float=False)
on_change (event)
on_close (event=None)

Close event. Hide the whole window.

class sas.sasgui.perspectives.file_converter.meta_panels.MetadataWindow (PanelClass, parent=None, title=", base=None, manager=None, size=(470, 376.0), metadata=None, *args, **kwargs)

Bases: wx._windows.Frame

on_close (event)

class sas.sasgui.perspectives.file_converter.meta_panels.SamplePanel (parent, sample, base=None, *args, **kwargs)

Bases: sas.sasgui.perspectives.file_converter.meta_panels.MetadataPanel

on_close (event=None)

Close event. Hide the whole window.

class sas.sasgui.perspectives.file_converter.meta_panels.SourcePanel (parent, source, base=None, *args, **kwargs)

Bases: sas.sasgui.perspectives.file_converter.meta_panels.MetadataPanel

on_close (event=None)

Close event. Hide the whole window.
Module contents

`sas.sasgui.perspectives.fitting` package

Subpackages

`sas.sasgui.perspectives.fitting.plugin_models` package

Module contents

Example plugin models to be added to the SasView plugin directory on startup if no plugins are present. This is currently empty.

Submodules

`sas.sasgui.perspectives.fitting.basepage` module

Base Page for fitting

```python
class sas.sasgui.perspectives.fitting.basepage.BasicPage(parent, color='blue', **kwargs):
    Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase

    This class provide general structure of the fitpanel page

    ID_BOOKMARK = 177
    ID_DISPERSER_HELP = 178

    check_invalid_panel()
        check if the user can already perform some action with this panel

    createMemento()
        return the current state of the page

    create_default_data()
        Given the user selection, creates a 1D or 2D data Only when the page is on theory mode.

    define_page_structure()
        Create empty sizer for a panel

    formfactor_combo_init()
        First time calls _show_combbox_helper

    get_all_checked_params()
        Found all parameters current check and add them to list of parameters to fit if implemented

    get_cat_combo_box_pos(state)
        Iterate through the categories to find the structurefactor :return: combo_box_position

    get_clipboard()
        Get strings in the clipboard

    get_copy()
        Get copy params to clipboard

    get_copy_excel()
        Get copy params to clipboard

    get_copy_latex()
        Get copy params to clipboard
```

2.1. Contents
get_copy_params()
Get the string copies of the param names and values in the tap

get_copy_params_excel()
Get the string copies of the param names and values in the tap

get_copy_params_latex()
Get the string copies of the param names and values in the tap

get_data()
return the current data

get_data_list()
return the current data

get_images()
Get the images of the plots corresponding this panel for report
: return graphs: list of figures : Need Move to guiFrame

generate_paste()
Paste params from the clipboard

generate_paste_params(text="")
Get the string copies of the param names and values in the tap

generate_state()
return the current page state

generate_weight_flag()
Get flag corresponding to a given weighting dI data if implemented

initialize_combobox()
put default value in the combo box

donContextMenu(event)
Retrieve the state selected state

donPinholeSmear(event)
Create a custom pinhole smear object if implemented

donRedo(event)
Restore the previous action cancelled

donResetModel(event)
Reset model state

donSetFocus(evt)
highlight the current textctrl and hide the error text control shown after fitting

donSlitSmear(event)
Create a custom slit smear object if implemented

donSmear(event)
Create a smear object if implemented

donUndo(event)
Cancel the previous action

don bookmark (event)
save history of the data and model

don_copy (event)
Copy Parameter values to the clipboard

don_function_help_clicked (event)
Function called when ‘Help’ button is pressed next to model of interest. This calls DocumentationWindow from documentation_window.py. It will load the top level of the html model help document if either a plugin model (which normally does not have an html help help file) is

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selected or if no model is selected. Otherwise, if a regula model is selected, the documentation for that model will be sent to a browser window.

todo the quick fix for no documentation in plugins is the if statment. However, the right way to do this would be to check whether the html file exists and load the model docs if it does and the general docs if it doesn’t - this will become important if we ever figure out how to build docs for plugins on the fly. Sep 9, 2018 -PDB

Parameters event – on Help Button pressed event

on_left_down(event)
Get key stroke event

on_model_help_clicked(event)
Function called when ‘Description’ button is pressed next to model of interest. This calls the Description embedded in the model. This should work with either Wx2.8 and lower or higher. If no model is selected it will give the message that a model must be chosen first in the box that would normally contain the description. If a badly behaved model is encountered which has no description then it will give the message that none is available.

Parameters event – on Description Button pressed event

on_paste(event)
Paste Parameter values to the panel if possible

on_pd_help_clicked(event)
Bring up Polydispersity Documentation whenever the ? button is clicked. Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ ....). Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file:///...”

Parameters event – Triggers on clicking ? in polydispersity box

on_preview(event)
Report the current fit results

on_reset_clicked(event)
On ‘Reset’ button for Q range clicked

on_save(event)
Save the current state into file

on_set_focus(event)
On Set Focus, update guimanger and menu

on_smear_helper(update=False)
Help for onSmear if implemented

Parameters update – force or not to update

on_tap_focus()
Update menu1 on clicking the page tap

populate_box(model_list_box)
Store list of model

Parameters model_list_box – dictionary containing categorized models

read_file(path)
Read two columns file

Parameters path – the path to the file to read

reset_page(state, first=False)
reset the state if implemented

reset_page_helper(state)
Use page_state and change the state of existing page
**Precondition** the page is already drawn or created

**Postcondition** the state of the underlying data changes as well as the state of the graphic interface

```python
save_current_state()
    Store current state

save_current_state_fit()
    Store current state for fit_page

select_log(event)
    Log checked to generate log spaced points for theory model

select_param(event)
    Select TextCtrl checked if implemented

set_clipboard(content=None)
    Put the string to the clipboard

set_data(data=None)
    Sets data if implemented

set_dispers_sizer()
    fill sizer containing dispersity info

set_index_model(index)
    Index related to this page

set_layout()
    layout

set_manager(manager)
    set panel manager

    Parameters
    manager – instance of plugin fitting

set_model_dictionary(model_dictionary)
    Store a dictionary linking model name -> model object

    Parameters
    model_dictionary – dictionary containing all models

set_model_state(state)
    reset page given a model state

set_owner(owner)
    set owner of fitpage

    Parameters
    owner – the class responsible of plotting

show_npts2fit()
    setValue Npts for fitting if implemented

update_pinhole_smear()
    Method to be called by sub-classes Moveit; This method doesn’t belong here

update_slit_smear()
    called by kill_focus on pinhole TextCntrl to update the changes if implemented

window_caption = 'Fit Page'
window_name = 'Fit Page'
```
class sas.sasgui.perspectives.fitting.basepage.ModelTextCtrl(parent, id=-1, value=u", pos=wx.Point(-1, -1), size=wx.Size(-1, -1), style=0, validator=<wx._core.Validator; proxy of <Swig Object of type 'wxValidator *'> >, name=u'text', kill_focus_callback=None, set_focus_callback=None, mouse_up_callback=None, text_enter_callback=None)

Bases: wx._controls.TextCtrl

Text control for model and fit parameters. Binds the appropriate events for user interactions. Default callback methods can be overwritten on initialization

Parameters

- **kill_focus_callback** – callback method for EVT_KILL_FOCUS event
- **set_focus_callback** – callback method for EVT_SET_FOCUS event
- **mouse_up_callback** – callback method for EVT_LEFT_UP event
- **text_enter_callback** – callback method for EVT_TEXT_ENTER event

full_selection = False

sas.sasgui.perspectives.fitting.batchfitpage module

Batch panel

class sas.sasgui.perspectives.fitting.batchfitpage.BGTextCtrl(*args, **kwds)

Bases: wx._controls.TextCtrl

Text control used to display outputs. No editing allowed. The background is grayed out. User can’t select text.

class sas.sasgui.perspectives.fitting.batchfitpage.BatchFitPage(parent, color=None)

Bases: sas.sasgui.perspectives.fitting.fitpage.FitPage

Batch Page

window_caption = 'BatchFit'

window_name = 'BatchFit'

sas.sasgui.perspectives.fitting.console module

class sas.sasgui.perspectives.fitting.console.ConsoleUpdate(parent, manager=None, quiet=False, progress_delta=60, improvement_delta=5)

Bases: sas.sascalc.fit.AbstractFitEngine.FitHandler
Print progress to the console.

```python
abort()
```

```python
error(msg)
    Model had an error; print traceback
```

```python
finalize()
```

```python
get_result()
```

```python
improvement()
    Called when a result is observed which is better than previous results from the fit.
```

```python
improvement_delta = 5
    Number of seconds between improvement updates
```

```python
isbetter = False
    Record whether results improved since last update
```

```python
print_result()
    Print result object
```

```python
progress(k, n)
    Report on progress.
```

```python
progress_delta = 60
    Number of seconds between progress updates
```

```python
set_result(result)
```

```python
starting_fit()
```

```python
stop(msg)
    Post event msg and stop
```

```python
update_fit(last=False)
```

**sas.sasgui.perspectives.fitting.fit_thread module**

```python
class sas.sasgui.perspectives.fitting.fit_thread.FitThread(fn, page_id, handler, batch_outputs, batch_inputs=None, pars=None, completefn=None, updatefn=None, yieldtime=0.03, worktime=0.03, reset_flag=False)
```

Bases: `sas.sascalc.data_util.calcthread.CalcThread`

Thread performing the fit

```python
compute()
    Perform a fit
```

```python
isquit()
    Raises KeyboardInterrupt – when the thread is interrupted
```

```python
sas.sasgui.perspectives.fitting.fit_thread.map_apply(arguments)
```

```python
sas.sasgui.perspectives.fitting.fit_thread.map_getattr(classInstance, classFunc, *args)
```

Take an instance of a class and a function name as a string. Execute class.function and return result.
sas.sasgui.perspectives.fitting.fitpage module

FitPanel class contains fields allowing to display results when fitting a model and one data

```python
class sas.sasgui.perspectives.fitting.fitpage.BGTextCtrl(*args, **kwds)
    Bases: wx._controls.TextCtrl
    Text control used to display outputs. No editing allowed. The background is grayed out. User can’t select text.

class sas.sasgui.perspectives.fitting.fitpage.FitPage(parent, color=None)
    Bases: sas.sasgui.perspectives.fitting.basepage.BasicPage
    FitPanel class contains fields allowing to display results when fitting a model and one data
```

Note
For Fit to be performed the user should check at least one parameter on fit Panel window.

```python
compute_data_range(data)
    compute the minimum and the maximum range of the data return the npts contains in data

compute_data_set_range(data_list)
    find the range that include all data in the set return the minimum and the maximum values

enable_datasource()
    Enable or disable data source control depending on existing data

enable_fit_button()
    Enable fit button if data is valid and model is valid

fill_data_combobox(data_list)
    Get a list of data and fill the corresponding combobox

get_all_checked_params()
    Found all parameters current check and add them to list of parameters to fit

get_chis2()
    return the current chis2

get_npts2fit()
    return numbers of data points within qrange

    Note This is to normalize chisq by Npts of fit

get_range()
    return the fitting range

get_view_mode()
    return True if the panel allow 2D or False if 1D

get_weight_flag()
    Get flag corresponding to a given weighting dI data.

onPinholeSmear(event)
    Create a custom pinhole smear object that will change the way residuals are compute when fitting

    Note accuracy is given by strings ‘High’, ‘Med’, ‘Low’ FOR 2d, None for 1D

onSlitSmear(event)
    Create a custom slit smear object that will change the way residuals are compute when fitting

onSmear(event)
    Create a smear object that will change the way residuals are computed when fitting

onWeighting(event)
    On Weighting radio button event, sets the weightbt_string

on_complete_chisqr(event)
    Display result chisqr on the panel :event: activated by fitting/ complete after draw
on_key (event)
On Key down

on_qrange_text (event)
#On q range value updated. DO not combine with qrange_click().

on_right_down (event)
Get key stroke event

on_select_data (event=None)
On select_data

on_set_focus (event)
Override the basepage focus method to ensure the save flag is set properly when focusing on the fit page.

on_smear_helper (update=False)
Help for onSmear

Parameters
update – force or not to update

onsetValues (chisqr, p_name, out, cov)
Build the panel from the fit result

Parameters
• chisqr – Value of the goodness of fit metric
• p_name – the name of parameters
• out – list of parameter with the best value found during fitting
• cov – Covariance matrix

qrang_set_focus (event=None)
ON Qrange focus

qrange_click (event)
On Qrange textctrl click, make the qrange lines in the plot

rename_model ()
find a short name for model

reset_page (state, first=False)
reset the state

select_param (event=None)
Select TextCtrl checked for fitting purpose and stores them in self.param_toFit=[] list

set_data (data)
reset the current data

set_fitbutton ()
Set fit button label depending on the fit_started[bool]

set_model_param_sizer (model)
Build the panel from the model content

Parameters
model – the model selected in combo box for fitting purpose

show_npts2fit ()
setValue Npts for fitting

update_pinhole_smear ()
called by kill_focus on pinhole TextCntrl to update the changes

Returns
False when wrong value was entered

update_slit_smear ()
called by kill_focus on pinhole TextCntrl to update the changes
Returns False when wrong value was entered

sas.sasgui.perspectives.fitting.fitpanel module

FitPanel class contains fields allowing to fit models and data

    note For Fit to be performed the user should check at least one parameter on fit Panel window.

class sas.sasgui.perspectives.fitting.fitpanel.FitPanel (parent, manager=None, *args, **kwargs)
Bases: wx.aui.AuiNotebook, sas.sasgui.guiframe.panel_base.PanelBase

FitPanel class contains fields allowing to fit models and data

    note For Fit to be performed the user should check at least one parameter on fit Panel window.

CENTER_PANE = True
add_empty_page ()
    add an empty page
add_sim_page (caption='Const & Simul Fit')
    Add the simultaneous fit page
clear_panel ()
    Clear and close all panels, used by guimanager
close_all ()
    remove all pages, used when a svs file is opened
close_page_with_data (deleted_data)
    close a fit page when its data is completely remove from the graph
delete_data (data)
    Delete the given data
enable_close_button ()
    display the close button on tab for more than 1 tabs else remove the close button
get_current_page ()
    Returns the current page selected
get_data ()
    get the data in the current page
get_page_by_id (uid)
get_state ()
    return the state of the current selected page
helper_on_page_change ()
on_close_page (event=None)
    close page and remove all references to the closed page
on_closed (event)
on_page_changing (event)
    calls the function when the current event handler has exited. avoiding to call panel on focus on a panel
    that is currently deleted
on_set_focus (event)
reset_pmodel_list ()
save_project (doc=None)
    return an xml node containing state of the panel that guiframe can write to file
set_data(data_list)
Add a fitting page on the notebook contained by fitpanel

Parameters data_list – data to fit
:return panel : page just added for further used. is used by fitting module

set_data_on_batch_mode(data_list)
Add all data to a single tab when the application is on Batch mode. However all data in the set of data
must be either 1D or 2D type. This method presents option to select the data type before creating a

set_manager(manager)
set panel manager

Parameters manager – instance of plugin fitting

set_model_dictionary(model_dictionary)
copy a dictionary of model name -> model object

Parameters model_dictionary – dictionary linking model name -> model object

set_model_list(dict)
copy a dictionary of model into its own dictionary

Parameters dict – dictionnary made of model name as key and model class as value

set_model_state(state)
receive a state to reset the model in the current page

set_state(state)
Restore state of the panel

update_model_list()

window_caption = 'Fit Panel'
window_name = 'Fit panel'

sas.sasgui.perspectives.fitting.fitproblem module

Interface containing information to store data, model, range of data, etc... and retrieve this information. This is
an interface for a fitProblem i.e relationship between data and model.

class sas.sasgui.perspectives.fitting.fitproblem.FitProblem
    Bases: object

    Define the relationship between data and model, including range, weights, etc.

    clear_model_param()
    clear constraint info

    enable_smearing(flag=False)

    Parameters flag – bool.When flag is 1 get the computer smear value. When flag is 0
    ignore smear value.

    get_fit_data()

    Returns data associate with this class

    get_fit_tab_caption()

    get_graph_id()
    Get graph_id

    get_model()

    Returns saved model
get_model_param()  
return list of couple of parameter name and value

get_name()  
get_origin_data()  
get_param2fit()  
return the list param names to fit

get_range()  
Returns fitting range

get_residuals()  
Returns residuals

get_result()  
get result

get_scheduled()  
return true or false if a problem as being schedule for fitting

get_smearer()  
return smear object

get_theory_data()  
Returns theory generated with the current model and data of this class

get_weight()  
returns weight array

save_model_name(name)
schedule_tofit(schedule=0)  
set schedule to true to decide if this fit must be performed

set_fit_data(data)  
Store data associated with this class :param data: list of data selected

set_fit_tab_caption(caption)

set_graph_id(id)  
Set graph id (from data_group_id at the time the graph produced)

set_model(model)  
associates each model with its new created name :param model: model selected :param name: name created for model

set_model_param(name, value=None)  
Store the name and value of a parameter of this fitproblem’s model :param name: name of the given parameter :param value: value of that parameter

set_param2fit(list)  
Store param names to fit (checked) :param list: list of the param names

set_range(qmin=None, qmax=None)  
set fitting range :param qmin: minimum value to consider for the fit range :param qmax: maximum value to consider for the fit range

set_residuals(residuals)  
save a copy of residual :param data: data selected

set_result(result)

set_smearer(smearer)  
save reference of smear object on fitdata

Parameters smear – smear object from DataLoader
set_theory_data (data)
    save a copy of the data select to fit

Parameters data — data selected

set_weight (is2d, flag=None)
    Received flag and compute error on data. :param flag: flag to transform error of data. :param is2d: flag to distinguish 1D to 2D Data

class sas.sasgui.perspectives.fitting.fitproblem.FitProblemDictionary
    Bases: dict
    This module implements a dictionary of fitproblem objects

add_data (data)
    Add data to the current dictionary of fitproblem. if data id does not exist create a new fit problem. :note: only data changes in the fit problem

clear_model_param (fid=None)
    clear constraint info

enable_smearing (flag=False, fid=None)
    Parameters flag — bool. When flag is 1 get the computer smear value. When flag is 0 ignore smear value.

get_batch_result ()
    get result

get_fit_data (fid)
    return data for the given fitproblem id :param fid: key representing a fitproblem, usually extract from data id

get_fit_problem ()
    return fitproblem contained in this dictionary

get_fit_tab_caption ()
    Return the caption of the page associated with object

get_graph_id ()
    Get graph_id

get_model (fid)
    Returns saved model

get_model_param (fid)
    return list of couple of parameter name and value

get_name (fid=None)

get_param2fit ()
    return the list param names to fit

get_range (fid)
    Returns fitting range

get_residuals (fid)
    Returns residuals

get_result (fid)
    get result

get_scheduled ()
    return true or false if a problem as being schedule for fitting

get_smearer (fid=None)
    return smear object
get_theory_data (fid)
Returns list of data dList

get_weight (fid=None)
return fit weight

save_model_name (name, fid=None)

schedule_tofit (schedule=0)
set schedule to true to decide if this fit must be performed

set_batch_result (batch_inputs, batch_outputs)
set a list of result

set_fit_data (data)
save a copy of the data select to fit :param data: data selected

set_fit_tab_caption (caption)
store the caption of the page associated with object

set_graph_id (id)
Set graph id (from data_group_id at the time the graph produced)

set_model (model, fid=None)
associates each model with its new created name :param model: model selected :param name: name created for model

set_model_param (name, value=None, fid=None)
Store the name and value of a parameter of this fitproblem’s model :param name: name of the given parameter :param value: value of that parameter

set_param2fit (list)
Store param names to fit (checked) :param list: list of the param names

set_range (qmin=None, qmax=None, fid=None)
set fitting range

set_residuals (residuals, fid)
save a copy of residual :param data: data selected

set_result (result, fid)

set_smearer (smearer, fid=None)
save reference of smear object on fitdata :param smear: smear object from DataLoader

set_theory_data (fid, data=None)
save a copy of the data select to fit :param data: data selected

set_weight (is2d, flag=None, fid=None)
fit weight

sas.sasgui.perspectives.fitting.fitting module

Fitting perspective

class sas.sasgui.perspectives.fitting.fitting.Plugin
Bases: sas.sasgui.guiframe.plugin_base.PluginBase

Fitting plugin is used to perform fit

add_color (color, id)
adds a color as a key with a plot id as its value to a dictionary

add_fit_page (data)
given a data, ask to the fitting panel to create a new fitting page, get this page and store it into the page_finder of this plug-in :param data: is a list of data

2.1. Contents
clear_panel()

create_fit_problem(page_id)
Given an ID create a fitproblem container

create_theory_1D(x, y, page_id, model, data, state, data_description, data_id, dy=None)
Create a theory object associate with an existing Data1D and add it to the data manager. @param x: x-values of the data @param y: y_values of the data @param page_id: fit page ID @param model: model used for fitting @param data: Data1D object to create the theory for @param state: model state @param data_description: title to use in the data manager @param data_id: unique data ID

delete_custom_model(event)
Delete custom model file

delete_data(data)
delete the given data from panel

delete_fit_problem(page_id)
Given an ID create a fitproblem container

draw_model(model, page_id, data=None, smearer=None, enable1D=True, enable2D=False, state=None, fid=None, toggle_mode_on=False, qmin=None, qmax=None, update_chisqr=True, weight=None, source='model')
Draw model.

Parameters

- model – the model to draw
- name – the name of the model to draw
- data – the data on which the model is based to be drawn
- description – model’s description
- enable1D – if true enable drawing model 1D
- enable2D – if true enable drawing model 2D
- qmin – Range’s minimum value to draw model
- qmax – Range’s maximum value to draw model
- qstep – number of step to divide the x and y-axis
- update_chisqr – update chisqr [bool]

edit_custom_model(event)
Get the python editor panel

delete_batch_capable()
Check if the plugin has a batch capability

def get_context_menu(plotpanel=None)
Get the context menu items available for P(r).them allow fitting option for Data2D and Data1D only.

Parameters graph – the Graph object to which we attach the context menu

Returns a list of menu items with call-back function

Note if Data1D was generated from Theory1D the fitting option is not allowed

def get_graph_id(uid)
Set graph_id for fitprobelm

def get_page_finder()
return self.page_finder used also by simfitpage.py

def get_panels(parent)
Create and return a list of panel objects
load_plugin_models (event)
   Update of models in plugin_models folder

make_new_model (event)
   Make new model

make_sum_model (event)
   Edit summodel template and make one

onFit (uid)
   Get series of data, model, associates parameters and range and send then to series of fitters. Fit data
   and model, display result to corresponding panels. :param uid: id related to the panel currently calling
   this fit function.

on_add_new_page (event=None)
   ask fit panel to create a new empty page

on_add_sim_page (event)
   Create a page to access simultaneous fit option

on_batch_selection (flag)
   switch the the notebook of batch mode or not

on_bumps_options (event=None)
   Open the bumps options panel.

on_fit_results (event=None)
   Make the Fit Results panel visible.

on_fitter_changed (event)

on_gpu_options (event=None)
   Make the Fit Results panel visible.

on_help (algorithm_id)

on_reset_batch_flag (event)
   Set batch_reset_flag

on_set_batch_result (page_id, fid, batch_outputs, batch_inputs)

on_set_state_helper (event=None)
   Set_state_helper. This actually sets state after plotting data from state file.
   : event: FitStateUpdateEvent called by dataloader.plot_data from guiFrame

populate_menu (owner)
   Create a menu for the Fitting plug-in

   Parameters

   • id – id to create a menu

   • owner – owner of menu

   Returns list of information to populate the main menu

put_icon (frame)
   Put icon in the frame title bar

remove_plot (uid, fid=None, theory=False)
   remove model plot when a fit page is closed :param uid: the id related to the fitpage to close :param
   fid: the id of the fitproblem(data, model, range,etc)

save_fit_state (filepath, fitstate)
   save fit page state into file

schedule_for_fit (value=0, uid=None)
   Set the fit problem field to 0 or 1 to schedule that problem to fit. Schedule the specified fitproblem or
get the fit problem related to the current page and set value.

:param value: integer 0 or 1
:param uid: the id related to a page containing fitting information

**select_data**(panel)

**set_data**(data_list=None)
receive a list of data to fit

**set_edit_menu**(owner)
Set list of the edit model menu labels

**set_edit_menu_helper**(owner=None, menu=None)
help for setting list of the edit model menu labels

**set_fit_range**(uid, qmin, qmax, fid=None)
Set the fitting range of a given page for all its data by default. If fid is provide then set the range only for the data with fid as id.

:param uid: id corresponding to a fit page
:param fid: id corresponding to a fit problem (data, model)
:param qmin: minimum value of the fit range
:param qmax: maximum value of the fit range

**set_fit_weight**(uid, flag, is2d=False, fid=None)
Set the fit weights of a given page for all its data by default. If fid is provide then set the range only for the data with fid as id.

:param uid: id corresponding to a fit page
:param fid: id corresponding to a fit problem (data, model)
:param weight: current dy data

**set_graph_id**(uid, graph_id)
Set graph_id for fitproblem

**set_page_finder**(modelname, names, values)
Used by simfitpage.py to reset a parameter given the string constraint.

**Parameters**
- **modelname** – the name of the model for with the parameter has to reset
- **value** – can be a string in this case.
- **names** – the parameter name

**set_param2fit**(uid, param2fit)
Set the list of param names to fit for fitproblem

**set_smearer**(uid, smearer, fid, qmin=None, qmax=None, draw=True, enable_smearer=False)
Get a smear object and store it to a fit problem of fid as id. If proper flag is enable, will plot the theory with smearing information.

**Parameters**
- **smearer** – smear object to allow smearing data of id fid
- **enable_smearer** – Define whether or not all (data, model) contained in the structure of id uid will be smeared before fitting.
- **qmin** – the maximum value of the theory plotting range
- **qmax** – the maximum value of the theory plotting range
- **draw** – Determine if the theory needs to be plot

**set_state**(state=None, datainfo=None, format=None)
Call-back method for the fit page state reader. This method is called when a .fitv/.svs file is loaded.

:param state: PageState object
:param datainfo: data

**set_theory**(theory_list=None)

**split_string**(item)
receive a word containing dot and split it. used to split parameterset name into model name and parameter name example:
parameterset (item) = M1.A
Will return model_name = M1, parameter name = A

stop_fit (uid)
Stop the fit

store_data (uid, data_list=None, caption=None)
Receive a list of data and store them as well as a caption of the fit page where they come from.
:param uid: if related to a fit page
:param data_list: list of data to fit
:param caption: caption of the window related to these data

update_custom_combo()
Update custom model list in the fitpage combo box

update_fit (result=None, msg="")

sas.sasgui.perspectives.fitting.fitting_widgets module

class sas.sasgui.perspectives.fitting.fitting_widgets.BatchDataDialog (parent=None, *args, **kwds)

Bases: wx._windows.Dialog

The current design of Batch fit allows only of type of data in the data set. This allows the user to make a quick selection of the type of data to use in fit tab.

get_data()
return 1 if user requested Data1D, 2 if user requested Data2D

class sas.sasgui.perspectives.fitting.fitting_widgets.DataDialog (data_list, parent=None, text="", nb_data=4, *args, **kwds)

Bases: wx._windows.Dialog

Allow file selection at loading time

get_data()
return the selected data

class sas.sasgui.perspectives.fitting.fitting_widgets.DialogPanel (*args, **kwds)

Bases: wx.lib.scrolledpanel.ScrolledPanel

sas.sasgui.perspectives.fitting.gpu_options module

Module provides dialog for setting SAS_OPENCL variable, which defines device choice for OpenCL calculation

Created on Nov 29, 2016
@author: wpotrzebowski

class sas.sasgui.perspectives.fitting.gpu_options.CustomButtonBox (parent, msg, title)

Bases: wx._windows.Dialog

Custom message box for OpenCL results
class sas.sasgui.perspectives.fitting.gpu_options.GpuOptions(*args, **kwds)

Bases: wx._windows.Dialog

“OpenCL options” Dialog Box

Provides dialog for setting SAS_OPENCL variable, which defines device choice for OpenCL calculation

on_OK(event)
    Close window on acceptance

on_check(event)
    Action triggered when box is selected

on_help(event)
    Provide help on opencl options.

on_reset(event)
    Resets selected values

on_test(event)
    Run sasmodels check from here and report results from

sas.sasgui.perspectives.fitting.hint_fitpage module

This class provide general structure of fitpanel page

class sas.sasgui.perspectives.fitting.hint_fitpage.HelpWindow(parent, id, title)

Bases: wx._windows.Frame

class sas.sasgui.perspectives.fitting.hint_fitpage.HintFitPage(parent)

Bases: wx._windows.ScrolledWindow, sas.sasgui.guiframe.panel_base.PanelBase

This class provide general structure of fitpanel page

createMemento()

do_layout()
    Draw the page

    window_caption = 'Hint page '

    window_name = 'Hint Page'

sas.sasgui.perspectives.fitting.model_thread module

Calculation thread for modeling
class sas.sasgui.perspectives.fitting.model_thread.Calc1D(model, page_id, data, fid=None, qmin=None, qmax=None, weight=None, smearer=None, toggle_mode_on=False, state=None, completefn=None, updatefn=None, update_chisqr=True, source='model', yieldtime=0.01, worktime=0.01, exception_handler=None)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Compute 1D data

calculate()  
Compute model 1d value given qmin, qmax, x value

results()  
Send results of the computation

class sas.sasgui.perspectives.fitting.model_thread.Calc2D(data, model, smearer, qmin, qmax, page_id, state=None, weight=None, fid=None, toggle_mode_on=False, completefn=None, updatefn=None, update_chisqr=True, source='model', yieldtime=0.04, worktime=0.04, exception_handler=None)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Compute 2D model This calculation assumes a 2-fold symmetry of the model where points are computed for one half of the detector and I(qx, qy) = I(-qx, -qy) is assumed.

calculate()  
Compute the data given a model function

sas.sasgui.perspectives.fitting.report_dialog module

Dialog report panel to show and summarize the results of the fitting calculation.

class sas.sasgui.perspectives.fitting.report_dialog.ReportDialog(report_list, *args, **kwds)


The report dialog box.
FitPanel class contains fields allowing to fit models and data

Note For Fit to be performed the user should check at least one parameter on fit Panel window.

class sas.sasgui.perspectives.fitting.resultpanel.ResultPanel(parent, manager=None, *args, **kwargs)

Bases: wx.aui.AuiNotebook, sas.sasgui.guiframe.panel_base.PanelBase

FitPanel class contains fields allowing to fit models and data

Note For Fit to be performed the user should check at least one parameter on fit Panel window.

CENTER_PANE = True

get_frame()

on_close(event)
Close event. Hide the whole window.

on_plot_results(event)

window_caption = 'Result Panel'

window_name = 'Result panel'

sas.sasgui.perspectives.fitting.simfitpage module

Simultaneous or Batch fit page

class sas.sasgui.perspectives.fitting.simfitpage.ConstraintLine(model_cbox, param_cbox, egal_txt, constraint, btRemove, sizer)

Bases: tuple

btRemove
Alias for field number 4

c constraint
Alias for field number 3

egal_txt
Alias for field number 2

model_cbox
Alias for field number 0

param_cbox
Alias for field number 1

sizer
Alias for field number 5
class sas.sasgui.perspectives.fitting.simfitpage.SimultaneousFitPage(parent,  
  page_finder={},  
  id=-1,  
  batch_on=False,  
  *args,  
  **kwargs)

Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase

Simultaneous fitting panel All that needs to be defined are the two data members window_name and window_caption

ID_ADD = 182
ID_DOC = 179
ID_FIT = 181
ID_SET_ALL = 180

check_all_model_name(event=None)
  check all models names

check_model_name(event)
  Save information related to checkbox and their states

define_page_structure()
  Create empty sizers, their hierarchy and set the sizer for the panel

draw_page()
  Construct the Simultaneous/Constrained fit page. fills the first region (sizer1) with the list of available fit page pairs of data and models. Then fills sizer2 with the checkbox for adding constraints, and finally fills sizer3 with the fit button and instructions.

get_state()
  Return the state of the current page :return: self.state

load_from_save_state(sim_state)
  Load in a simultaneous/constrained fit from a save state :param fit: Fitpanel object :return: None

on_fit(event)
  signal for fitting

on_remove(event)
  Remove constraint fields

on_set_focus(event=None)
  The derivative class is on focus if implemented

set_fitbutton()
  Set fit button label depending on the fit_started

set_manager(manager)
  set panel manager

    Parameters
    ----------
    manager -- instance of plugin fitting

set_state()
  Define a set of state parameters for saving simultaneous fits.

window_caption = 'Simultaneous Fit Page'
window_name = 'Simultaneous Fit Page'
sas.sasgui.perspectives.fitting.simfitpage.get_fittableParam(model)
  return list of fittable parameters from a model

    Parameters
    ----------
    model -- the model used
sas.sasgui.perspectives.fitting.simfitpage.setComboBoxItems(cbox, items)

**sas.sasgui.perspectives.fitting.utils module**

Module contains functions frequently used in this package

`sas.sasgui.perspectives.fitting.utils.get_weight(data, is2d, flag=None)`

Received flag and compute error on data. :param flag: flag to transform error of data. :param is2d: flag to
distinguish 1D to 2D Data

**Module contents**

`sas.sasgui.perspectives.fitting.data_files()`

Return the data files associated with media.

The format is a list of (directory, [files...]) pairs which can be used directly in setup(...,data_files=...) for
setup.py.

`sas.sasgui.perspectives.fitting.get_data_path(media)`

**sas.sasgui.perspectives.invariant package**

**Submodules**

**sas.sasgui.perspectives.invariant.invariant module**

```python
class sas.sasgui.perspectives.invariant.invariant.Plugin
    Bases: sas.sasgui.guiframe.plugin_base.PluginBase

    This class defines the interface for invariant Plugin class that can be used by the gui_manager.

    clear_panel()

    compute_helper(data)

    delete_data(data_id)

    get_context_menu(plotpanel=None)

    This method is optional.

    When the context menu of a plot is rendered, the get_context_menu method will be called to give you
    a chance to add a menu item to the context menu.

    A ref to a Graph object is passed so that you can investigate the plot content and decide whether you
    need to add items to the context menu.

    This method returns a list of menu items. Each item is itself a list defining the text to appear in the
    menu, a tool-tip help text, and a call-back method.

    Parameters graph -- the Graph object to which we attach the context menu

    Returns a list of menu items with call-back function

    get_data()

    get_panels(parent)

    Create and return the list of wx.Panels for your plug-in. Define the plug-in perspective.

    Panels should inherit from DefaultPanel defined below, or should present the same interface. They
    must define “window_caption” and “window_name”.

    Parameters parent -- parent window
```
Returns list of panels

**on_set_state_helper** *(event=None)*
Set the state when called by EVT_STATE_UPDATE event from guiframe after a .inv/.svs file is loaded

**plot_data** *(scale, background)*
replot the current data if the user enters a new scale or background

**plot_theory** *(data=None, name=None)*
Receive a data set and post a NewPlotEvent to parent.

Parameters

- **data** – extrapolated data to be plotted
- **name** – Data’s name to use for the legend

**save_file** *(filepath, state=None)*
Save data in provided state object.

Parameters

- **filepath** – path of file to write to
- **state** – invariant state

**set_data** *(data_list=None)*
receive a list of data and compute invariant

**set_state** *(state=None, datainfo=None)*
Call-back method for the state reader. This method is called when a .inv/.svs file is loaded.

Parameters **state** – State object

---

**sas.sasgui.perspectives.invariant.invariant_details module**

Invariant panel

**class** `sas.sasgui.perspectives.invariant.invariant_details.InvariantContainer`

Bases: `wx._core.Object`

This class stores some values resulting from invariant calculations. Given the value of total invariant, this class can also determine the percentage of invariants resulting from extrapolation.

**check_values** ()
check the validity if invariant

**compute_percentage** ()
Compute percentage of each invariant

**class** `sas.sasgui.perspectives.invariant.invariant_details.InvariantDetailsPanel`

Bases: `wx._windows.Dialog`

This panel describes proportion of invariants

**get_scale** *(percentage, scale_name='scale')*
Check scale receive in this panel.
SasView Documentation, Release 4.2.1

on_close(event)
Close the current window

on_paint(event)
Draw the chart

set_color_bar()
Change the color for low and high bar when necessary

set_values()
Set value of txtctrl

sas.sasgui.perspectives.invariant.invariant_panel module

This module provides the GUI for the invariant perspective panel

class sas.sasgui.perspectives.invariant.invariant_panel.InvariantDialog (parent=None, id=1, graph=None, data=None, title='Invariant', base=None)

Bases: wx._windows.Dialog
Invariant Dialog

class sas.sasgui.perspectives.invariant.invariant_panel.InvariantPanel (parent, data=None, manager=None, *args, **kwds)

Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase
Main class defining the sizers (wx “panels”) used to draw the Invariant GUI.

CENTER_PANE = True

clear_panel()  
Clear panel to defaults, used by set_state of manager

compute_invariant(event=None)  
compute invariant

display_details(event)  
open another panel for more details on invariant calculation

get_background()  
return the background textctrl value as a float

get_bookmark_by_num(num=None)  
Get the bookmark state given by number  
: param num: the given bookmark number

get_contrast()  
return the contrast textctrl value as a float

get_data()  

get_extrapolation_type(low_q, high_q)  
get extrapolation type

get_high_qstar(inv, high_q=False)  
get high qstar
get_low_qstar (inv, npts_low, low_q=False)
get low qstar

get_porod_const ()
return the porod constant textctrl value as a float

get_qstar (inv)
get qstar

get_scale ()
return the scale textctrl value as a float

get_state ()

get_state_by_num (state_num=None)
Get the state given by number
: param state_num: the given state number

get_surface (inv, contrast, porod_const, extrapolation)
get surface value

get_total_qstar (inv, extrapolation)
get total qstar

get_volume (inv, contrast, extrapolation)
get volume fraction

on_bookmark (event)
Save the panel state in memory and add the list on the popup menu on bookmark context menu event

on_help (event)
Bring up the Invariant Documentation whenever the HELP button is clicked.
Calls DocumentationWindow with the path of the location within the documentation tree (after /doc/ . . . .”. Note that when using old versions of Wx (before 2.9) and thus not the release version of installers, the help comes up at the top level of the file as webbrowser does not pass anything past the # to the browser when it is running “file:///. . . .”

Parameters evt – Triggers on clicking the help button

on_preview (event=None)
Invoke report dialog panel
: param event: report button event

on_redo (event=None)
Go forward to the previous state
: param event: redo button event

on_save (evt=None)
Save invariant state into a file

on_undo (event=None)
Go back to the previous state
: param event: undo button event

reset_panel ()
set the panel at its initial state.

save_project (doc=None)
return an xml node containing state of the panel that guiframe can write to file

set_data (data)
Set the data
**set_extrapolation_high** (*inv, high_q=False*)
return float value necessary to compute invariant a high q

**set_extrapolation_low** (*inv, low_q=False*)
return float value necessary to compute invariant a low q

**set_manager** (*manager*)
set value for the manager

**set_message**()
Display warning message if available

**set_state** (*state=None, data=None*)
set state when loading it from a .inv/.svs file

window_caption = 'Invariant'

window_name = 'Invariant'

class sas.sasgui.perspectives.invariant.invariant_panel.InvariantWindow (parent=None, id=1, graph=None, data=None, title='Invariant', base=None)

Bases: wx._windows.Frame

Invariant Window

class sas.sasgui.perspectives.invariant.invariant_panel.MyApp (redirect=False, filename=None, useBestVisual=False, clearSigInt=True)

Bases: wx._core.App

Test App

OnInit()

Init

**sas.sasgui.perspectives.invariant.invariant_state module**

State class for the invariant UI

class sas.sasgui.perspectives.invariant.invariant_state.InvariantState
Bases: object

Class to hold the state information of the InversionControl panel.

**clone_state**()
deeplcopy the state

**fromXML** (*file=None, node=None*)
Load invariant states from a file

: param file: .inv file : param node: node of a XML document to read from

**set_plot_state** (*extra_high=False, extra_low=False*)
Build image state that wx.html understand by plotting, putting it into wx.FileSystem image object

: extrap_high,extra_low: low/high extrapolations are possible extra-plots
set_report_string()
Get the values (strings) from __str__ for report

set_saved_state(name, value)
Set the state list
:param name: name of the state component :param value: value of the state component

toXML(file='inv_state.inv', doc=None, entry_node=None)
Writes the state of the InversionControl panel to file, as XML.
Compatible with standalone writing, or appending to an already existing XML document. In that case, the XML document is required. An optional entry node in the XML document may also be given.
:param file: file to write to :param doc: XML document object [optional] :param entry_node: XML node within the document at which we will append the data [optional]

class sas.sasgui.perspectives.invariant.invariant_state.Reader(call_back, canas=True)
Bases: sas.sascalc.dataloader.readers.cansas_reader.Reader
Class to load a .inv invariant file

ext = ['.inv', '.INV', '.svs', 'SVS']

get_state()

read(path)
Load a new invariant state from file
:param path: file path : return: None

type = ['Invariant file (*.inv)|*.inv', 'SASView file (*.svs)|*.svs']
type_name = 'Invariant'

write(filename, datainfo=None, invstate=None)
Write the content of a Data1D as a CanSAS XML file
:param filename: name of the file to write :param datainfo: Data1D object :param invstate: InvariantState object

write_toXML(datainfo=None, state=None)
Write toXML, a helper for write()
:return: xml doc

sas.sasgui.perspectives.invariant.invariant_widgets module

class sas.sasgui.perspectives.invariant.invariant_widgets.DataDialog(data_list, parent=None, *args, **kwds)
Bases: wx._windows.Dialog
Allow file selection at loading time

get_data()
return the selected data

class sas.sasgui.perspectives.invariant.invariant_widgets.DialogPanel(*args, **kwds)
Bases: wx.lib.scrolledpanel.ScrolledPanel

class sas.sasgui.perspectives.invariant.invariant_widgets.InvTextCtrl(*args, **kwds)
Bases: wx._controls.TextCtrl

2.1. Contents
Text control for model and fit parameters. Binds the appropriate events for user interactions.

```python
class sas.sasgui.perspectives.invariant.invariant_widgets.OutputTextCtrl(*args, **kwds)
```

Bases: `wx._controls.TextCtrl`

Text control used to display outputs. No editing allowed. The background is grayed out. User can’t select text.

`sas.sasgui.perspectives.invariant.report_dialog` module

Dialog report panel to show and summarize the results of the invariant calculation.

```python
class sas.sasgui.perspectives.invariant.report_dialog.ReportDialog(report_list, *args, **kwds)
```

Bases: `sas.sasgui.guiframe.report_dialog.BaseReportDialog`

The report dialog box.

```python
onSave(event=None)
Save
```

Module contents

```python
sas.sasgui.perspectives.invariant.data_files()
```

Return the data files associated with media invariant.

The format is a list of (directory, [files...]) pairs which can be used directly in setup(...,data_files=...) for setup.py.

```python
sas.sasgui.perspectives.invariant.get_data_path(media)
```

`sas.sasgui.perspectives.pr` package

Submodules

`sas.sasgui.perspectives.pr.explore_dialog` module

Dialog panel to explore the P(r) inversion results for a range of D_max value. User picks a number of points and a range of distances, then can toggle between inversion outputs and see their distribution as a function of D_max.

```python
class sas.sasgui.perspectives.pr.explore_dialog.ExploreDialog(pr_state, nfunc, *args, **kwds)
```

Bases: `wx._windows.Dialog`

The explorer dialog box. This dialog is meant to be invoked by the InversionControl class.

```python
class Event
```

Bases: `object`

Class that holds the content of the form

```python
dmax = 0
dmin = 0
npts = 0
```

```python
send_focus_to_datapanel(name)
```

The GUI manager sometimes calls this method TODO: refactor this
set_plot_unfocus()
  Not implemented

class sas.sasgui.perspectives.pr.explore_dialog.OutputPlot (d_min, d_max,
  parent, id=-1, color=None, dpi=None, style=0, **kwargs)

Bases: sas.sasgui.plottools.PlotPanel.PlotPanel
Plot panel used to show the selected results as a function of D_max

onContextMenu (event)
  Default context menu for the plot panel

    TODO  Would be nice to add printing and log/linear scales. The current version of plottools
  no longer plays well with plots outside of guiframe. Guiframe team needs to fix this.

window_caption = 'D Explorer'

class sas.sasgui.perspectives.pr.explore_dialog.Results
  Bases: object
  Class to hold the inversion output parameters as a function of D_max

sas.sasgui.perspectives.pr.inversion_panel module

class sas.sasgui.perspectives.pr.inversion_panel.InversionControl (parent,
  id=-1, plots=None, **kwargs)

Bases: wx.lib.scrolledpanel.ScrolledPanel, sas.sasgui.guiframe.panel_base.PanelBase

CENTER_PANE = True

clear_panel()

get_data()

get_state()
  Get the current state
  : return: state object

on_help (event)
  Bring up the P(r) Documentation whenever the HELP button is clicked.
  Calls DocumentationWindow with the path of the location within the documentation tree
  (after /doc/ ...”). Note that when using old versions of Wx (before 2.9) and thus not the
  release version of installers, the help comes up at the top level of the file as webbrowser does
  not pass anything past the # to the browser when it is running “file:///...”

Parameters  evt  – Triggers on clicking the help button

on_reset (event=None)
  Resets inversion parameters

on_save (evt=None)
  Method used to create a memento of the current state

Returns  state object

oscillation_max = 1.5
save_project \( (doc=\text{None}) \)

return an xml node containing state of the panel that guiFrame can write to file

set_manager \( (\text{manager}) \)

set_state \( (\text{state}) \)

Set the state of the panel and inversion problem to the state passed as a parameter. Execute the inversion immediately after filling the controls.

Parameters state – InversionState object

window_caption = 'P(r) control panel'

window_name = 'pr_control'

class sas.sasgui.perspectives.pr.inversion_panel.PrDistDialog \( (parent, id) \)

Bases: wx._windows.Dialog

Property dialog to let the user change the number of points on the P(r) plot.

get_content ()

Return the content of the dialog. At this point the values have already been checked.

set_content \( (\text{npts}) \)

Initialize the content of the dialog.

sas.sasgui.perspectives.pr.inversion_state module

Handling of P(r) inversion states

class sas.sasgui.perspectives.pr.inversion_state.InversionState

Bases: object

Class to hold the state information of the InversionControl panel.

fromXML \( (\text{file=\text{None}}, \text{node=\text{None}}) \)

Load a P(r) inversion state from a file

Parameters

• file – .prv file

• node – node of a XML document to read from

toXML \( (\text{file='pr_state.prv'}, \text{doc=\text{None}}, \text{entry_node=\text{None}}) \)

Writes the state of the InversionControl panel to file, as XML.

Compatible with standalone writing, or appending to an already existing XML document. In that case, the XML document is required. An optional entry node in the XML document may also be given.

Parameters

• file – file to write to

• doc – XML document object [optional]

• entry_node – XML node within the XML document at which we will append the data [optional]

class sas.sasgui.perspectives.pr.inversion_state.Reader \( (\text{call\_back, canساس=True}) \)

Bases: sas.sascalc.dataloader.readers.cansas_reader.Reader

Class to load a .prv P(r) inversion file

ext = ['.prv', '.PRV', '.svs', '.SVS']

read \( (\text{path}) \)

Load a new P(r) inversion state from file
Parameters `path` – file path

Returns None

type = ['P(r) files (*.prv)|*.prv', 'SASView files (*.svs)|*.svs']

type_name = 'P(r)'

write (filename, datainfo=None, prstate=None)
    Write the content of a Data1D as a CanSAS XML file

Parameters

    • filename – name of the file to write
    • datainfo – Data1D object
    • prstate – InversionState object

write_toXML (datainfo=None, state=None)
    Write toXML, a helper for write()

    : return: xml doc

sas.sasgui.perspectives.pr.pr module

P(r) perspective for SasView

class sas.sasgui.perspectives.pr.pr.Plugin
    Bases: sas.sasgui.guiframe.plugin_base.PluginBase

    P(r) inversion perspective

    DEFAULT_ALPHA = 0.0001
    DEFAULT_DMAX = 140.0
    DEFAULT_NFUNC = 10

delete_data (data_id)
    delete the data association with prview

estimate_file_inversion (alpha, nfunc, d_max, data, path=None, q_min=None, q_max=None, bck=False, height=0, width=0)
    Estimate parameters for inversion

estimate_plot_inversion (alpha, nfunc, d_max, q_min=None, q_max=None, est_bck=False, bck_val=0, height=0, width=0)
    Estimate parameters from plotted data

get_context_menu (plotpanel=None)
    Get the context menu items available for P(r)

    Parameters `graph` – the Graph object to which we attach the context menu

    Returns a list of menu items with call-back function

get_data ()
    Returns the current data

get_npts ()
    Returns the number of points in the I(q) data

get_panels (parent)
    Create and return a list of panel objects

help (evt)
    Show a general help dialog.

    TODO replace the text with a nice image
load(data)
Load data. This will eventually be replaced by our standard DataLoader class.

load_abs(path)
Load an IGOR .ABS reduced file

Parameters path – file path

Returns x, y, err vectors

load_columns(path='sphere_60_q0_2.txt')
Load 2- or 3-column ascii

perform_estimate()
Perform parameter estimation

perform_estimateNT()
Perform parameter estimation

perform_inversion()
Perform inversion

post_init()
Post initialization call back to close the loose ends [Somehow openGL needs this call]

pr_theory(r, R)
Return P(r) of a sphere for a given R For test purposes

save_data(filepath, prstate=None)
Save data in provided state object.

TODO move the state code away from inversion_panel and move it here. Then remove the
“prstate” input and make this method private.

Parameters

• filepath – path of file to write to

• prstate – P(r) inversion state

set_data(data_list=None)
receive a list of data to compute pr

set_state(state=None, datainfo=None)
Call-back method for the inversion state reader. This method is called when a .prv file is loaded.

Parameters

• state – InversionState object

• datainfo – Data1D object [optional]

setup_file_inversion(alpha, nfunc, d_max, data, path=None, q_min=None, q_max=None, bck=False, height=0, width=0)
Set up inversion

setup_plot_inversion(alpha, nfunc, d_max, q_min=None, q_max=None, est_bck=False, bck_val=0, height=0, width=0)
Set up inversion from plotted data

show_data(path=None, data=None, reset=False)
Show data read from a file

Parameters

• path – file path

• reset – if True all other plottables will be cleared

show_Iq(out, pr, q=None)
Display computed I(q)
show_pr (out, pr, cov=None)

show_shpere (x, radius=70.0, x_range=70.0)

start_thread()

Start a calculation thread

### sas.sasgui.perspectives.pr.pr_thread module

**class** sas.sasgui.perspectives.pr.pr_thread.CalcPr (pr, nfunc=5, error_func=None, completefn=None, updatefn=None, yieldtime=0.01, worktime=0.01)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Compute P(r)

**compute()**

Perform P(r) inversion

**class** sas.sasgui.perspectives.pr.pr_thread.EstimateNT (pr, nfunc=5, error_func=None, completefn=None, updatefn=None, yieldtime=0.01, worktime=0.01)

Bases: sas.sascalc.data_util.calcthread.CalcThread

compute()

Calculates the estimate

isquit()

**class** sas.sasgui.perspectives.pr.pr_thread.EstimatePr (pr, nfunc=5, error_func=None, completefn=None, updatefn=None, yieldtime=0.01, worktime=0.01)

Bases: sas.sascalc.data_util.calcthread.CalcThread

Estimate P(r)

**compute()**

Calculates the estimate

### sas.sasgui.perspectives.pr.pr_widgets module

Text controls for input/output of the main PrView panel

**class** sas.sasgui.perspectives.pr.pr_widgets.DataDialog (data_list, parent=None, text=", *args, **kwds)

Bases: wx._windows.Dialog

Allow file selection at loading time

**get_data()**

return the selected data

**class** sas.sasgui.perspectives.pr.pr_widgets.DataFileTextCtrl (*args, **kwds)

Bases: sas.sasgui.perspectives.pr.pr_widgets.OutputTextCtrl

Text control used to display only the file name given a full path.
TODO now that we no longer choose the data file from the panel, it’s no longer necessary to pass around the file path. That code should be refactored away and simplified.

GetValue()
Return the full path

SetValue(value)
Sets the file name given a path

class sas.sasgui.perspectives.pr.pr_widgets.DialogPanel(*args,**kwds)
Bases: wx.lib.scrolledpanel.ScrolledPanel

class sas.sasgui.perspectives.pr.pr_widgets.OutputTextCtrl(*args,**kwds)
Bases: wx._controls.TextCtrl
Text control used to display outputs. No editing allowed. The background is grayed out. User can’t select text.

class sas.sasgui.perspectives.pr.pr_widgets.PrTextCtrl(*args,**kwds)
Bases: wx._controls.TextCtrl
Text control for model and fit parameters. Binds the appropriate events for user interactions.
sas.sasgui.perspectives.pr.pr_widgets.load_error(error=None)
Pop up an error message.

Parameters error – details error message to be displayed

Module contents

Module contents

sas.sasgui.plottools package

Submodules

sas.sasgui.plottools.BaseInteractor module
sas.sasgui.plottools.LabelDialog module

class sas.sasgui.plottools.LabelDialog.LabelDialog(parent, id, title, label)
Bases: wx._windows.Dialog
getText()

sas.sasgui.plottools.LineModel module

Provide Line function (y=Ax + B). Until July 10, 2016 this function provided (y= A + Bx). This however was contrary to all the other code using it which assumed (y= mx+b) or in this nomenclature (y=Ax + B). This lead to some contortions in the code and worse incorrect calculations until now for at least some of the functions. This seemed the easiest to fix particularly since this function should disappear in a future iteration (see notes in fitDialog)
PDB July 10, 2016

class sas.sasgui.plottools.LineModel.LineModel
Bases: object

Class that evaluates a linear model.

f(x) = Ax + B
List of default parameters: A = 1.0 B = 1.0

**getParam**(name)
Return parameter value

**run**(x=0.0)
Evaluate the model

Parameters x – simple value

Returns (Line value)

**Note:** This is the function called by fitDialog to calculate the y(xmin) and y(xmax), but the only difference between this and runXY is when the if statement is true. I however cannot see what that function is for. It needs to be documented here or removed. PDB 7/10/16

**runXY**(x=0.0)
Evaluate the model.

Parameters x – simple value

Returns Line value

**Note:** This is to be what is called by fitDialog for the actual fit the only difference between this and run is when the if statement is true. I however cannot see what that function is for. It needs to be documented here or removed. PDB 7/10/16

**setParam**(name, value)
Set parameter value

---

**sas.sasgui.plottools.PlotPanel module**

Plot panel.

**class** sas.sasgui.plottools.PlotPanel.NoRepaintCanvas(*args, **kwargs)
Bases: matplotlib.backends.backend_wxagg.FigureCanvasWxAgg

We subclass FigureCanvasWxAgg, overriding the _onPaint method, so that the draw method is only called for the first two paint events. After that, the canvas will only be redrawn when it is resized.

**class** sas.sasgui.plottools.PlotPanel.PlotPanel(parent, id=-1, xtransform=None, ytransform=None, scale='log_{10}', color=None, dpi=None, **kwargs)
Bases: wx._windows.Panel

The PlotPanel has a Figure and a Canvas. OnSize events simply set a flag, and the actually redrawing of the figure is triggered by an Idle event.

**ChangeLegendLoc**(label)
Changes legend loc based on user input

**OnCopyFigureMenu**(evt)
Copy the current figure to clipboard

**On_Paint**(event)

**SetColor**(rgbtuple)
Set figure and canvas colours to be the same

**add_toolbar**( )
add toolbar

---

---

2.1. Contents
clear()
    Reset the plot

curve(x, y, dy=None, color=0, symbol=0, label=None)
    Draw a line on a graph, possibly with confidence intervals.

cursor_line(event)

draw()
    Where the actual drawing happens

get_loc_label()
    Associates label to a specific legend location

get_xscale()
    Returns x-axis scale

get_yscale()
    Returns Y-axis scale

image(data, qx_data, qy_data, xmin, xmax, ymin, ymax, zmin, zmax, color=0, symbol=0, markersize=0, label='data2D', cmap=<matplotlib.colors.LinearSegmentedColormap object>)
    Render the current data

interactive_curve(x, y, dy=None, name='', color=0, symbol=0, zorder=1, id=None, label=None)
    Draw markers with error bars

interactive_points(x, y, dx=None, dy=None, name='', color=0, symbol=0, markersize=5, zorder=1, id=None, label=None, hide_error=False)
    Draw markers with error bars

is_zoomed

legend_picker(legend, event)
    Pick up the legend patch

linear_plottable_fit(plot)
    when clicking on linear Fit on context menu, display Fitting Dialog
    Parameters plot – PlotPanel owning the graph

onChangeCaption(event)

onChangeLegendLoc(event)
    Changes legend loc based on user input

onContextMenu(event)
    Default context menu for a plot panel

onFitDisplay(tempx, tempy, xminView, xmaxView, xmin, xmax, func)
    Add a new plottable into the graph. In this case this plottable will be used to fit some data
    Parameters
    • tempx – The x data of fit line
    • tempy – The y data of fit line
    • xminView – the lower bound of fitting range
    • xmaxView – the upper bound of fitting range
    • xmin – the lowest value of data to fit to the line
    • xmax – the highest value of data to fit to the line

onFitting(event)
    when clicking on linear Fit on context menu, display Fitting Dialog
onGridOnOff (gridOnOff)
   Allows ON/OFF Grid

onLeftDown (event)
   left button down and ready to drag

onLeftUp (event)
   Dragging is done

onLegend (legOnOff)
   Toggles whether legend is visible/not visible

onMouseMotion (event)
   check if the left button is press and the mouse in moving. computer delta for x and y coordinates and then calls draghelper to perform the drag

onPick (event)
   On pick legend

onPrint (event=None)

onPrinterPreview (event=None)
   Matplotlib canvas can no longer print itself. Thus need to do everything ourselves: need to create a printpreview frame to to see the preview but needs a parent frame object. Also needs a printout object (just as any printing task).

onPrinterSetup (event=None)

onResetGraph (event)
   Reset the graph by plotting the full range of data

onSaveImage (evt)
   Implement save image

onToolContextMenu (event)
   ContextMenu from toolbar

   Parameters event – toolbar event

onWheel (event)
   Process mouse wheel as zoom events

   Parameters event – Wheel event

on_kill_focus (event)
   Reset the panel color

on_set_focus (event)
   Send to the parent the current panel on focus

plottable_selected (id)
   Called to register a plottable as selected

points (x, y, dx=None, dy=None, color=0, symbol=0, marker_size=5, label=None, id=None, hide_error=False)
   Draw markers with error bars

properties (prop)
   Set some properties of the graph. The set of properties is not yet determined.

remove_legend (ax=None)
   Remove legend for ax or the current axes.

render()
   Commit the plot after all objects are drawn

resetFitView()
   For fit Dialog initial display
returnTrans()
    Return values and labels used by Fit Dialog

schedule_full_draw(func='append')
    Put self in schedule to full redraw list

setTrans(xtrans, ytrans)
    Parameters
    • xtrans – set x transformation on Property dialog
    • ytrans – set y transformation on Property dialog

set_legend_alpha(alpha=1)
    Set legend alpha

set_resizing(resizing=False)
    Set the resizing (True/False)

set_selected_from_menu(menu, id)
    Set selected_plottable from context menu selection
    Parameters
    • menu – context menu item
    • id – menu item id

set_xscale(scale='linear')
    Set the scale on x-axis
    Parameters scale – the scale of x-axis

set_yscale(scale='linear')
    Set the scale on Y-axis
    Parameters scale – the scale of y-axis

xaxis(label, units, font=None, color='black', t_font=None)
    xaxis label and units.
    We need to do this so that we can detect when axes are not commesurate. Currently this is ignored
    other than for formatting purposes.

yaxis(label, units, font=None, color='black', t_font=None)
    yaxis label and units.
sas.sasgui.plottools.PlotPanel.show_tree(obj, d=0)
    Handy function for displaying a tree of graph objects

sas.sasgui.plottools.PropertyDialog module

class sas.sasgui.plottools.PropertyDialog.Properties(parent, id=-1, title='Select the scale of the graph')
    Bases: wx._windows.Dialog

getValues()

setValues(x, y, view)

viewChanged(event)
sas.sasgui.plottools.RangeDialog module

class sas.sasgui.plottools.RangeDialog.RangeDialog(parent, id, title='Set Graph Range')
    Bases: wx._windows.Dialog
    GetXRange()
    GetYRange()
    SetXRange(x_range)
    SetYRange(y_range)

sas.sasgui.plottools.SimpleFont module

This software was developed by Institut Laue-Langevin as part of Distributed Data Analysis of Neutron Scattering Experiments (DANSE).

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class sas.sasgui.plottools.SimpleFont.SimpleFont(parent, id, title)
    Bases: wx._windows.Dialog
    InitUI()
    get_font()
    get_ticklabel_check()
        Get tick label check value
    set_default_font(font)
    set_ticklabel_check(check=False)
        Set tick label check value

sas.sasgui.plottools.SizeDialog module

class sas.sasgui.plottools.SizeDialog.SizeDialog(parent, id, title)
    Bases: wx._windows.Dialog
    getText()
        Get text typed

sas.sasgui.plottools.TextDialog module

class sas.sasgui.plottools.TextDialog.TextDialog(parent, id, title, label=", unit=None)
    Bases: wx._windows.Dialog
    getColor()
        Returns font size for the text box
    getFamily()
        Returns font family for the text box
    getSize()
        Returns font size for the text box
    getStyle()
        Returns font tyle for the text box
    getText()
        Returns text string as input by user.
getTickLabel()
    Bool for use on tick label

getUnit()
    Returns unit string as input by user.

getWeight()
    Returns font weight for the text box

on_color (event)
    Set the color

on_family (event)
    Set the family

on_size (event)
    Set the size

on_style (event)
    Set the style

on_tick_label (event)
    Set the font for tick label

on_weight (event)
    Set the weight

sas.sasgui.plottools.arrow3d module

Module that draws multiple arrows in 3D coordinates

class sas.sasgui.plottools.arrow3d.Arrow3D (base, xs, ys, zs, colors, *args, **kwargs)
    Bases: matplotlib.patches.FancyArrowPatch

    Draw 3D arrow

draw (renderer, rasterized=True)
    Drawing actually happens here

on_left_down (event)
    Mouse left-down event

on_left_up (event)
    Mouse left up event

sas.sasgui.plottools.binder module

Extension to MPL to support the binding of artists to key/mouse events.

class sas.sasgui.plottools.binder.BindArtist (figure)
    Bases: object

    alt = False

    clear (h1, h2, ...)
        Remove connections for artists h1, h2, ...
        Use clearall() to reset all connections.

    clearall ()
        Clear connections to all artists.
        Use clear(h1,h2,...) to reset specific artists.

    control = False

dclick_threshold = 0.25
disconnect()
In case we need to disconnect from the canvas...

events = ['enter', 'leave', 'motion', 'click', 'dclick', 'drag', 'release', 'scroll']
meta = False
shift = False

toggle
actor, action, ev)
    Trigger a particular event for the artist. Fallback to axes, to figure, and to 'all' if the event is not
    processed.

class sas.sasgui.plottools.binder.Selection (artist=None, prop={})
    Bases: object
    Store and compare selections.
    artist = None
    prop = {}

sas.sasgui.plottools.canvas module

This module implements a faster canvas for plotting. it overwrites some matplotlib methods to allow printing on
sys.platform=='win32'

class sas.sasgui.plottools.canvas.FigureCanvas (*args, **kw)
    Bases: matplotlib.backends.backend_wxagg.FigureCanvasWxAgg
    Add features to the wx agg canvas for better support of AUI and faster plotting.
    draw (drawDC=None)
        Render the figure using agg.
    draw_idle (*args, **kwargs)
        Render after a delay if no other render requests have been made.
    scroll_event (x, y, step=1, guiEvent=None)
        Backend derived classes should call this function on any scroll wheel event. x,y are the canvas coords:
        0,0 is lower, left. button and key are as defined in MouseEvent
    set_panel (panel)
        Set axes
    set_resizing (resizing=False)
        Setting the resizing
    sas.sasgui.plottools.canvas.OnPrintPage (self, page)
        override printPage of matplotlib
    sas.sasgui.plottools.canvas.draw_image (self, x, y, im, bbox, clippath=None, clip path_trans=None)
        Draw the image instance into the current axes;
    Parameters
        • x – is the distance in pixels from the left hand side of the canvas.
        • y – the distance from the origin. That is, if origin is upper, y is the distance from top. If
          origin is lower, y is the distance from bottom
        • im – the class 'matplotlib._image.Image' instance
        • bbox – a class matplotlib.transforms.Bbox instance for clipping, or None
    sas.sasgui.plottools.canvas.select (self)
    sas.sasgui.plottools.canvas.unselect (self)
sas.sasgui.plottools.config module

sas.sasgui.plottools.convert_units module

Convert units to strings that can be displayed. This is a cleaned up version of unitConverter.py.

sas.sasgui.plottools.convert_units.convert_unit(power, unit)

Convert units to strings that can be displayed.

sas.sasgui.plottools.fitDialog module

class sas.sasgui.plottools.fitDialog.LinearFit(parent, plottable, push_data, transform, title)

Bases: wx._windows.Dialog

checkFitValues(item)

Check the validity of input values.

floatForwardTransform(x)

transform a float.

floatInvTransform(x)

transform a float. It is used to determine the x.View min and x.View max for values not in x. Also used to properly calculate RgQmin, RgQmax and to update qmin and qmax in the linear range boxes on the panel.

floatTransform(x)

transform a float. It is used to determine the x. View min and x. View max for values not in x

layout()

Sets up the panel layout for the linear fit including all the labels, text entry boxes, and buttons.

register_close(owner)

Method to register the close event to a parent window that needs notification when the dialog is closed.

Parameters
owner – parent window

setFitRange(xmin, xmax, xminTrans, xmaxTrans)

Set fit parameters.

set_fit_region(xmin, xmax)

Set the fit region: param xmin: minimum x-value to be included in fit; param xmax: maximum x-value to be included in fit.

class sas.sasgui.plottools.fitDialog.MyApp(redirect=False, filename=None, useBestVisual=False, clearSigInt=True)

Bases: wx._core.App

Test application

OnInit()

Test application initialization

onFitDisplay(tempx, tempy, xminView, xmaxView, xmin, xmax, func)

Test application dummy method

returnTrans()

Test application dummy method

sas.sasgui.plottools.fitDialog.format_number(value, high=False)

Return a float in a standardized, human-readable formatted string. This is used to output readable (e.g. x.xxxe-y) values to the panel.
sas.sasgui.plottools.fittings module

This module is used to fit a set of x,y data to a model passed to it. It is used to calculate the slope and intercepts for the linearized fits. Two things should be noted:

First, this fitting module uses the NLLSQ module of SciPy rather than a linear fit. This along with a few other modules could probably be removed if we move to a linear regression approach.

Second, this infrastructure does not allow for resolution smearing of the the models. Hence the results are not that accurate even for pinhole collimation of SANS but may be good for SAXS. It is completely wrong for slit smeared data.

```python
class sas.sasgui.plottools.fittings.Parameter(model, name, value=None)
Bases: object

    Class to handle model parameters - sets the parameters and their initial value from the model based to it.

    set (value)
    Set the value of the parameter
```

```python
sas.sasgui.plottools.fittings.calcCommandline(event)
```

```python
sas.sasgui.plottools.fittings.sasfit (model, pars, x, y, err_y, qmin=None, qmax=None)
Fit function

Parameters

- `model` – sas model object
- `pars` – list of parameters
- `x` – vector of x data
- `y` – vector of y data
- `err_y` – vector of y errors
```

sas.sasgui.plottools.plottable_interactor module

This module allows more interaction with the plot

```python
class sas.sasgui.plottools.plottable_interactor.PointInteractor (base, axes, color='black', zorder=3, id="")
Bases: sas.sasgui.plottools.BaseInteractor._BaseInteractor

clear ()

connect_markers (markers)
    Connect markers to callbacks

curve (x, y, dy=None, color=0, symbol=0, zorder=10, label=None, width=2.0)

points (x, y, dx=None, dy=None, color=0, symbol=0, zorder=1, markersize=5, label=None, hide_error=False)

step (x, y, dy=None, color=0, symbol=0, zorder=1, label=None, width=2.0)

update ()
    Update

vline (x, y, dy=None, color=0, symbol=0, zorder=1, label=None, width=2.0)
```
sas.sasgui.plottools.plottables module

Prototype plottable object support.

The main point of this prototype is to provide a clean separation between the style (plotter details: color, grids, widgets, etc.) and substance (application details: which information to plot). Programmers should not be dictating line colours and plotting symbols.

Unlike the problem of style in CSS or Word, where most paragraphs look the same, each line on a graph has to be distinguishable from its neighbours. Our solution is to provide parametric styles, in which a number of different classes of object (e.g., reflectometry data, reflectometry theory) representing multiple graph primitives cycle through a colour palette provided by the underlying plotter.

A full treatment would provide perceptual dimensions of prominence and distinctiveness rather than a simple colour number.

class sas.sasgui.plottools.plottables.Chisq(chisq=None)
    Bases: sas.sasgui.plottools.plottables.Plottable
    Chisq plottable plots the chisq
    render(plot, **kw)
    setChisq(chisq)
        Set the chisq value.

class sas.sasgui.plottools.plottables.Data1D(x, y, dx=None, dy=None, lam=None, dlam=None)
    Bases: sas.sasgui.plottools.plottables.Plottable
    Data plottable: scatter plot of x,y with errors in x and y.
    changed()
    classmethod labels(collection)
        Build a label mostly unique within a collection
    render(plot, **kw)
        Renders the plottable on the graph

class sas.sasgui.plottools.plottables.Data2D(image=None, qx_data=None, qy_data=None, err_image=None, xmin=None, xmax=None, ymin=None, ymax=None, zmin=None, zmax=None)
    Bases: sas.sasgui.plottools.plottables.Plottable
    2D data class for image plotting
    changed()
    classmethod labels(collection)
        Build a label mostly unique within a collection
    render(plot, **kw)
        Renders the plottable on the graph
    setValues(datainfo=None)
        Use datainfo object to initialize data2D
        Parameters datainfo – object
    set_zrange(zmin=None, zmax=None)
    xaxis(label, unit)
        set x-axis
        Parameters
            • label – x-axis label
unit – x-axis unit

\texttt{yaxis (label, unit)}

set y-axis

Parameters

\begin{itemize}
\item \texttt{label} – y-axis label
\item \texttt{unit} – y-axis unit
\end{itemize}

\texttt{zaxis (label, unit)}

set z-axis

Parameters

\begin{itemize}
\item \texttt{label} – z-axis label
\item \texttt{unit} – z-axis unit
\end{itemize}

class \texttt{sas.sasgui.plottools.plottables.Fit1D (data=None, theory=None)}

Bases: \texttt{sas.sasgui.plottools.plottables.Plottable}

Fit plottable: composed of a data line plus a theory line. This is treated like a single object from the perspective of the graph, except that it will have two legend entries, one for the data and one for the theory.

The color of the data and theory will be shared.

\texttt{render (plot, **kw)}

class \texttt{sas.sasgui.plottools.plottables.Graph (**kw)}

Bases: \texttt{object}

Generic plottables graph structure.

Plot styles are based on color/symbol lists. The user gets to select the list of colors/symbols/sizes to choose from, not the application developer. The programmer only gets to add/remove lines from the plot and move to the next symbol/color.

Another dimension is prominence, which refers to line sizes/point sizes.

Axis transformations allow the user to select the coordinate view which provides clarity to the data. There is no way we can provide every possible transformation for every application generically, so the plottable objects themselves will need to provide the transformations. Here are some examples from reflectometry:

\begin{verbatim}

def independent: x -> f(x)
def monitor scaling: y -> M+y
def log: y -> log(y if y > min else min)
def cos: y -> cos(y*pi/180)
def dependent: x -> f(x,y)
def Q4: y -> y*x^4
def fresnel: y -> y*fresnel(x)
def coordinated: x,y = f(x,y)
def Q: x,y = 2*pi/L (cos(x*pi/180) - cos(y*pi/180))
y,y = 2*pi/L (sin(x*pi/180) + sin(y*pi/180))
def reducing: x,y = f(x1,x2,y1,y2)
def spin asymmetry: x -> x1, y -> (y1 - y2)/(y1 + y2)
def vector net: x -> x1, y -> y1*cos(y2*pi/180)
\end{verbatim}

Multiple transformations are possible, such as Q4 spin asymmetry

Axes have further complications in that the units of what are being plotted should correspond to the units on the axes. Plotting multiple types on the same graph should be handled gracefully, e.g., by creating a separate tab for each available axis type, breaking into subplots, showing multiple axes on the same plot, or generating inset plots. Ultimately the decision should be left to the user.
Graph properties such as grids/crosshairs should be under user control, as should the sizes of items such as axis fonts, etc. No direct access will be provided to the application.

Axis limits are mostly under user control. If the user has zoomed or panned then those limits are preserved even if new data is plotted. The exception is when, e.g., scanning through a set of related lines in which the user may want to fix the limits so that user can compare the values directly. Another exception is when creating multiple graphs sharing the same limits, though this case may be important enough that it is handled by the graph widget itself. Axis limits will of course have to understand the effects of axis transformations.

High level plottable objects may be composed of low level primitives. Operations such as legend/hide/show copy/paste, etc. need to operate on these primitives as a group. E.g., allowing the user to have a working canvas where they can drag lines they want to save and annotate them.

Graphs need to be printable. A page layout program for entire plots would be nice.

```python
add(plottable, color=None)
    Add a new plottable to the graph
changed()
    Detect if any graphed plottables have changed
delete(plottable)
    Remove an existing plottable from the graph
get(key)
    Get the graph properties
get_plottable(name)
    Return the plottable with the given name if it exists. Otherwise return None
get_range()
    Return the range of all displayed plottables
isPlotted(plottable)
    Return True is the plottable is already on the graph
render(plot)
    Redraw the graph
replace(plottable)
    Replace an existing plottable from the graph
reset()
    Reset the graph.
reset_scale()
    Resets the scale transformation data to the underlying data
returnPlottable()
    This method returns a dictionary of plottables contained in graph It is just by Plotpanel to interact with the complete list of plottables inside the graph.
set(**kw)
    Set the graph properties
title(name)
    Graph title
xaxis(name, units)
    Properties of the x axis.
yaxis(name, units)
    Properties of the y axis.
class sas.sasgui.plottools.plottables.Plottable
    Bases: object
    check_data_PlottableX()
    Since no transformation is made for log10(x), check that no negative values is plot in log scale
```
check_data_PlottableY()
Since no transformation is made for log10(y), check that no negative values is plot in log scale

colors()
Return the number of colors need to render the object

custom_color = None
dx = None
dy = None

get_xaxis()
Return the units and name of x-axis

get_yaxis()
Return the units and name of y-axis

hidden = False

interactive = True

is_empty()
Returns True if there is no data stored in the plottable

classmethod labels(collection)
Construct a set of unique labels for a collection of plottables of the same type.
Returns a map from plottable to name.

markersize = 5

name = None

onFitRange(xmin=None, xmax=None)
It limits View data range to plot from min to max

Parameters
  • xmin – the minimum value of x to plot.
  • xmax – the maximum value of x to plot

onReset()
Reset x, y, dx, dy view with its parameters

render(plot)
The base class makes sure the correct units are being used for subsequent plottable.
For now it is assumed that the graphs are commensurate, and if you put a Qx object on a Temperature
graph then you had better hope that it makes sense.

reset_view()
Reload view with new value to plot

returnValuesOfView()
Return View parameters and it is used by Fit Dialog

setLabel(labelx, labely)
It takes a label of the x and y transformation and set View parameters

Parameters
  • transx – The label of x transformation is sent by Properties Dialog
  • transy – The label of y transformation is sent Properties Dialog

set_View(x, y)
Load View

set_data(x, y, dx=None, dy=None)

short_name = None
transformView()
It transforms x, y before displaying

transformX(transx, transdx)
Receive pointers to function that transform x and dx and set corresponding View pointers

Parameters

• transx – pointer to function that transforms x
• transdx – pointer to function that transforms dx

transformY(transy, transdy)
Receive pointers to function that transform y and dy and set corresponding View pointers

Parameters

• transy – pointer to function that transforms y
• transdy – pointer to function that transforms dy

x = None

xaxis(name, units)
Set the name and unit of x_axis

Parameters

• name – the name of x-axis
• units – the units of x_axis

y = None

yaxis(name, units)
Set the name and unit of y_axis

Parameters

• name – the name of y-axis
• units – the units of y_axis

class sas.sasgui.plottools.plottables.Text (text=None, xpos=0.5, ypos=0.9, name='text')
Bases: sas.sasgui.plottools.plottables.Plottable

getText (text)
Get the text string.

render (plot, **kw)

setText (text)
Set the text string.

set_x (x)
Set the x position of the text ACCEPTS: float

set_y (y)
Set the y position of the text ACCEPTS: float

class sas.sasgui.plottools.plottables.Theory1D (x, y, dy=None)
Bases: sas.sasgui.plottools.plottables.Plottable

Theory plottable: line plot of x,y with confidence interval y.

class sas.sasgui.plottools.plottables.Transform
Bases: object

Define a transform plugin to the plottable architecture.
transforms operate on axes. the plottable defines the set of transforms available for it, and the axes on which they operate. these transforms can operate on the x axis only, the y axis only or on the x and y axes together.

this infrastructure is not able to support transformations such as log and polar plots as these require full control over the drawing of axes and grids.

a transform has a number of attributes.

**name** user visible name for the transform. this will appear in the context menu for the axis and the transform menu for the graph.

**type** operational axis. this determines whether the transform should appear on x,y or z axis context menus, or if it should appear in the context menu for the graph.

**inventory** (not implemented) a dictionary of user settable parameter names and their associated types. these should appear as keyword arguments to the transform call. for example, fresnel reflectivity requires the substrate density: { 'rho': type.Value(10e-6/units.angstrom**2) }

supply reasonable defaults in the callback so that limited plotting clients work even though they cannot set the inventory.

class sas.sasgui.plottools.plottables.View(x=None, y=None, dx=None, dy=None)

    bases: object

    representation of the data that might include a transformation

current_data_logX()

    remove negative value in x vector to avoid plotting negative value of log10

current_data_logY()

    remove negative value in y vector to avoid plotting negative value of log10

dx = None

dy = None

onFitRangeView(xmin=None, xmax=None)

    it limits view data range to plot from min to max

parameters

    * xmin – the minimum value of x to plot.
    * xmax – the maximum value of x to plot

onResetView()

    reset x,y,dx and y in their full range and in the initial scale in case their previous range has changed

returnXview()

    return view x,y,dx,dy

setTransformX(funcx, funcdx)

    receive pointers to function that transform x and dx and set corresponding view pointers

parameters

    * transx – pointer to function that transforms x
    * transdx – pointer to function that transforms dx

setTransformY(funcy, funcdy)

    receive pointers to function that transform y and dy and set corresponding view pointers

parameters

    * transx – pointer to function that transforms y
    * transdx – pointer to function that transforms dy

transform(x=None, y=None, dx=None, dy=None)

    transforms the x,y,dx and dy vectors and stores the output in view parameters
Parameters

- \( x \) – array of x values
- \( y \) – array of y values
- \( dx \) – array of errors values on x
- \( dy \) – array of error values on y

\[
x = \text{None}
\]
\[
y = \text{None}
\]

sas.sasgui.plottools.plottables.all(L)
sas.sasgui.plottools.plottables.any(L)
sas.sasgui.plottools.plottables.demo_plotter(graph)
sas.sasgui.plottools.plottables.sample_graph()

sas.sasgui.plottools.toolbar module

This module overwrites matplotlib toolbar

```python
class sas.sasgui.plottools.toolbar.NavigationToolBar(canvas, parent=None):
    Bases: matplotlib.backends.backend_wxagg.NavigationToolbar2WxAgg

    context_menu(event)
    
    copy_figure(event)
    
    on_menu(event)
    
    print_figure(event)

class sas.sasgui.plottools.toolbar.PlotPrintout(canvas):
    Bases: wx._windows.Printout

    Create the wx.Printout object for matplotlib figure from the PlotPanel. Provides the required OnPrintPage and HasPage overrides. Other methods may be added/overridden in the future. :TODO: this needs LOTS of TLC .. but fixes immediate problem

    GetPageInfo()
    
    just sets the page to 1 - no flexibility for now

    OnPrintPage(page)
    
    Most rudimentary OnPrintPage override. instantiates a dc object, gets its size, gets the size of the figure object, scales it to the dc canvas size keeping the aspect ratio intact, then prints as bitmap

sas.sasgui.plottools.toolbar.bind(actor, event, action, **kw)
sas.sasgui.plottools.toolbar.copy_image_to_clipboard(canvas)
```

sas.sasgui.plottools.transform module

```python
sas.sasgui.plottools.transform.errFromX2(x, y=None, dx=None, dy=None)
```

calculate error of \( \sqrt{x} \)

Parameters

- \( x \) – float value
- \( dx \) – float value
sas.sasgui.plottools.transform.errFromX4(x, y=None, dx=None, dy=None)
   calculate error of \( x^{1/4} \)

   Parameters
   • x – float value
   • dx – float value

sas.sasgui.plottools.transform.errOneOverSqrtX(x, y=None, dx=None, dy=None)
   calculate error on \( 1/\sqrt{x} \)

sas.sasgui.plottools.transform.errOneOverX(x, y=None, dx=None, dy=None)
   calculate error of \( 1/x \)

sas.sasgui.plottools.transform.errToLog10X(x, y=None, dx=None, dy=None)
   calculate error of \( \log(x) \)

   Parameters
   • x – float value
   • dx – float value

sas.sasgui.plottools.transform.errToLogX(x, y=None, dx=None, dy=None)
   calculate error of \( \log(x) \)

   Parameters
   • x – float value
   • dx – float value

sas.sasgui.plottools.transform.errToLogXY(x, y, dx=None, dy=None)
   calculate error of \( \log(xy) \)

sas.sasgui.plottools.transform.errToLogYX2(y, x, dy=None, dx=None)
   calculate error of \( \log(yx^2) \)

sas.sasgui.plottools.transform.errToLogYX4(y, x, dy=None, dx=None)
   error for \( \ln(y*x^{4}) \)

   Parameters
   • x – float value

sas.sasgui.plottools.transform.errToX(x, y=None, dx=None, dy=None)
   calculate error of \( x^2 \)

   Parameters
   • x – float value
   • dx – float value

sas.sasgui.plottools.transform.errToX2(x, y=None, dx=None, dy=None)
   calculate error of \( x^2 \)

   Parameters
   • x – float value
   • dx – float value

sas.sasgui.plottools.transform.errToX4(x, y=None, dx=None, dy=None)
   calculate error of \( x^4 \)

   Parameters
   • x – float value
   • dx – float value

sas.sasgui.plottools.transform.errToX_pos(x, y=None, dx=None, dy=None)
   calculate error of \( x^2 \)
Parameters

- \( x \) – float value
- \( dx \) – float value

sas.sasgui.plottools.transform.errToYX2 \((y, x, dy=None, dx=None)\)
sas.sasgui.plottools.transform.errToYX4 \((y, x, dy=None, dx=None)\)

Error for \((y \cdot x^4)\)

Parameters \( x \) – float value

sas.sasgui.plottools.transform.fromX2 \((x, y=None)\)

This function is used to load value on Plottable.View Calculate square root of \( x \)

Parameters \( x \) – float value

sas.sasgui.plottools.transform.fromX4 \((x, y=None)\)

This function is used to load value on Plottable.View Calculate square root of \( x \)

Parameters \( x \) – float value

sas.sasgui.plottools.transform.toLogX \((x, y=None)\)

This function is used to load value on Plottable.View Calculate log \( x \)

Parameters \( x \) – float value

sas.sasgui.plottools.transform.toLogXY \((y, x)\)

This function is used to load value on Plottable.View Calculate log \( x \)

Parameters \( x \) – float value

sas.sasgui.plottools.transform.toLogX2 \((y, x)\)
sas.sasgui.plottools.transform.toLogX4 \((y, x)\)
sas.sasgui.plottools.transform.toOneOverSqrtX \((y, x=None)\)
sas.sasgui.plottools.transform.toOneOverX \((x, y=None)\)
sas.sasgui.plottools.transform.toX \((x, y=None)\)

This function is used to load value on Plottable.View

Parameters \( x \) – Float value

Returns \( x \)

sas.sasgui.plottools.transform.toX2 \((x, y=None)\)

This function is used to load value on Plottable.View

Calculate \( x^2 \)

Parameters \( x \) – float value

sas.sasgui.plottools.transform.toX4 \((x, y=None)\)

This function is used to load value on Plottable.View

Calculate \( x^4 \)

Parameters \( x \) – float value

sas.sasgui.plottools.transform.toX_pos \((x, y=None)\)

This function is used to load value on Plottable.View

Parameters \( x \) – Float value

Returns \( x \)

sas.sasgui.plottools.transform.toYX2 \((y, x)\)
sas.sasgui.plottools.transform.toYX4 \((y, x)\)
Module contents

sas.sasview package

Submodules

sas.sasview.custom_config module

Application appearance custom configuration

sas.sasview.local_config module

Application settings

sas.sasview.sasview module

Base module for loading and running the main SasView application.

```python
class sas.sasview.sasview.SasView
    Bases: object
    Main class for running the SasView application
    check_sasmodels_compiler()
        Checking c compiler for sasmodels and raises xcode command line tools for installation

sas.sasview.sasview.run_cli()

sas.sasview.sasview.run_gui()
    __main__ method for loading and running SasView

sas.sasview.sasview.setup_logging()

sas.sasview.sasview.setup_mpl(backend=None)

sas.sasview.sasview.setup_sasmodels()
    Prepare sasmodels for running within sasview.

sas.sasview.sasview.setup.wx()
```

sas.sasview.welcome_panel module

Welcome page

```python
class sas.sasview.welcome_panel.ViewApp
    Bases: wx._core.App
    Test application
    OnInit()

class sas.sasview.welcome_panel.WelcomeFrame
    Bases: wx._windows.Frame
    Test frame
```

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class sas.sasview.welcome_panel.WelcomePage(*args, **kwds)
    Bases: wx.lib.scrolledpanel.ScrolledPanel

    Panel created like about box as a welcome page Shows product name, current version, authors, and link to
    the product page.

    CENTER_PANE = True

    set_data(data=None)

    window_caption = 'Welcome panel'

    window_name = 'default'

class sas.sasview.welcome_panel.WelcomePanel(*args, **kwds)
    Bases: wx.aui.AuiNotebook, sas.sasgui.guiframe.panel_base.PanelBase

    Panel created like about box as a welcome page Shows product name, current version, authors, and link to
    the product page.

    CENTER_PANE = True

    get_frame()

    on_close_page(event)
        Called when the welcome panel is closed

    set_data(data=None)

    set_frame(frame)

    set_manager(manager)
        the manager of the panel in this case the application itself

    window_caption = 'Welcome panel'

    window_name = 'default'

sas.sasview.wxcruft module

class sas.sasview.wxcruft.CallLater(millis, callableObj, *args, **kwargs)
    A convenience class for wx.Timer, that calls the given callable object once after the given amount of mil-
    liseconds, passing any positional or keyword args. The return value of the callable is availbale after it has
    been run with the GetResult method.

    If you don’t need to get the return value or restart the timer then there is no need to hold a reference to this
    object.

    See wx.CallAfter

    GetInterval()

    GetResult()

    HasRun()

    Interval

    IsRunning()

    Notify()
        The timer has expired so call the callable.

    Restart(millis=None, *args, **kwargs)
        (Re)start the timer

    Result
SetArgs (*args, **kwargs)
(Re)set the args passed to the callable object. This is useful in conjunction with Restart if you want to schedule a new call to the same callable object but with different parameters.

Start (millis=None, *args, **kwargs)
(Re)start the timer

Stop()
Stop and destroy the timer.

class sas.sasview.wxcrutf.FutureCall (millis, callableObj, *args, **kwargs)
Bases: sas.sasview.wxcrutf.CallLater
A compatibility alias for CallLater.

sas.sasview.wxcrutf.NewId()

class sas.sasview.wxcrutf.PyTimer (notify, *args, **kw)
Bases: wx._misc.Timer

Notify (self)

sas.sasview.wxcrutf.callLaterFix()

sas.sasview.wxcrutf.traceNewId()

Module contents

Submodules

sas.logger_config module

class sas.logger_config.SetupLogger (logger_name)
Bases: object

Called at the beginning of run.py or sasview.py

config_development()

config_production()

Module contents

sas.getAppDir()
The directory where the sasview application is found.

Returns the path to sasview if running in place or installed with setup. If the application is frozen, returns the parent directory of the application resources such as test files and images.

sas.getUserDir()
The directory where the per-user configuration is stored.

Returns ~/.sasview, creating it if it does not already exist.

sas.getLocalConfig()
Loads the local config file.

sas.getCustomConfig()
Setup the custom config dir and cat file
2.1.2 Sasmodels Developers Guide

Code Overview

Computational kernels

- core
- modelinfo
- kernel
- product
- mixture

At the heart of sasmodels are the individual computational kernels. These functions take a particular \( q \) value and a set of parameter values and return the expected scattering for that \( q \). The instructions for writing a kernel are documented in Writing a Plugin Model. The source code for the kernels is stored in models.

The primary interface to the models is through core, which provides functions for listing available models, loading the model definition and compiling the model. Use core.load_model() to load in a model definition and compile it. This makes use of core.load_model_info() to load the model definition and core.build_model() to turn it into a computational kernel model kernel.KernelModel.

The modelinfo.ModelInfo class defines the properties of the model including the available model parameters modelinfo.ParameterTable with individual parameter attributes such as units and hard limits defined in modelinfo.Parameter.

The product.ProductModel and mixture.MixtureModel classes are derived models, created automatically for models with names like “hardsphere*sphere” and “cylinder+sphere”.

Data loaders

- data

In order to test models a minimal set of data management routines is provided in data. In particular, it provides mock data.Data1D and data.Data2D classes which mimic those classes in SasView. The functions data.empty_data1D() and data.empty_data2D() are handy for creating containers with a particular set of \( q, \Delta q \) points which can later be evaluated, and data.plot_theory() to show the result. If SasView is available on the path then data.load_data() can be used to load any data type defined in SasView. The function data.plot_data() can plot that data alone without the theory value.

Kernel execution

- resolution
- resolution2d
- sesans
- weights
- details
- direct_model
- bumps_model
- sasview_model

To execute a computational kernel at a particular set of \( q \) values, the use kernel.KernelModel.make_kernel(), which returns a callable kernel.Kernel for that \( q \) vector (or a pair of \( q_x, q_y \) for 2-D datasets).
The calculated $q$ values should include the measured data points as well as additional $q$ values required to properly compute the $q$ resolution function. The Resolution subclasses in resolution define the $q_{calc}$ attribute for this purpose. These are resolution.Perfect1D for perfect resolution, resolution.Pinhole1D for the usual SANS pinhole aperture, resolution.Slit1D for the usual USANS slit aperture and resolution2d.Pinhole2D for 2-D pinhole data. In addition, resolution2d.Slit2D defines 1-D slit smeared data for oriented samples, which require calculation at particular $q_x$ and $q_y$ values instead of $|q|$ as is the case for orientationally averaged USANS. The sesans.SesansTransform class acts like a 1-D resolution, having a $q_{calc}$ attribute that defines the calculated $q$ values for the SANS models that get converted to spin-echo values by the sesnas.SesansTransform.apply() method.

Polydispersity is defined by weights.Dispersion classes, weights.RectangleDispersion, weights.ArrayDispersion, weights.LogNormalDispersion, weights.GaussianDispersion, weights.SchulzDispersion. The weights.get_weights() function creates a dispersion object of the class matching weights.Dispersion.type, and calls it with the current value of the parameter. This returns a vector of values and weights for a weighted average polydispersity.

In order to call the kernel.Kernel, the values and weights for all parameters must be composed into a details.CallDetails object. This is a compact vector representation of the entire polydispersity loop that can be passed easily to the kernel. Additionally, the magnetic parameters must be converted from polar to cartesian coordinates. This work is done by the details.make_kernel_args() function, which returns values that can be sent directly to the kernel. It uses details.make_details() to set the details object and details.convert_magnetism() for the coordinate transform.

In the end, making a simple theory function evaluation requires a lot of setup. To make calling them a little easier, the DirectModel and BumpsModel interfaces are provided. See Scripting Interface for an example.

The direct_model.DirectModel interface accepts a data object and a kernel model. Within the class, the direct_model.DataMixin._interpret_data() method is called to query the data and set the resolution. The direct_model.DataMixin._calc_theory() takes a set of parameter values, builds the kernel arguments, calls the kernel, and applies the resolution function, returning the predicted value for the data $q$ values. The bumps_model.Experiment class is like the DirectModel class, but it defines a Fitness class that can be handed directly to the bumps optimization and uncertainty analysis program.

The sasview_model.SasviewModel class defines a SasView 4.x compatible interface to the sasmodels definitions, allowing sasmodels to be used directly from SasView. Over time the SasView shim should disappear as SasView access the modelinfo.ModelInfo and computational kernels directly.

### Kernel execution

- kernelcl
- kerneldll
- kernelpy
- generate

The kernel functions for the most part do not define polydispersity, resolution or magnetism directly. Instead sasmodels automatically applies these, calling the computation kernel as needed.

The outermost loop is the resolution calculation. For the 1-D case this computes a single vector of $I(q)$ values and applies the convolution to the resulting set. Since the same $I(q)$ vector is used to compute the convolution at each point, it can be precomputed before the convolution, and so the convolution is reasonably efficient. The 2-D case is not that efficient, and instead recomputes the entire shifted/scaled set of $q_x$, $q_y$ values many times, or very many times depending on the accuracy requested.

Polydispersity is handled as a mesh over the polydisperse parameters. This is the next level of the loop. For C kernels run in a DLL or using OpenCL, the polydispersity loop is generated separately for each model as C code. Inside the polydispersity loop there is a loop over the magnetic cross sections for magnetic models, updating the SLD parameters with the effective magnetic SLD for that particular $q$ value. For OpenCL, each $q$ value loops over the polydispersity mesh on a separate processor. For DLL, the outer loop cycles through polydispersity, and the inner loop distributes $q$ values amongst the processors. Like the DLL, the Python kernel execution cycles over the
polydisperse parameters and the magnetic cross sections, calling the computation kernel with a vector of \( q \) values. Assuming the kernel code accepts vectors, this can be fast enough (though it is painfully slow if not vectorized).

Further details are provided in the next section, *Calculator Interface*

**Orientation and Numerical Integration**

For 2d data from oriented anisotropic particles, the mean particle orientation is defined by angles \( \theta, \phi \) and \( \Psi \), which are not in general the same as similarly named angles in many form factors. The wikipedia page on Euler angles ([https://en.wikipedia.org/wiki/Euler_angles](https://en.wikipedia.org/wiki/Euler_angles)) lists the different conventions available. To quote: “Different authors may use different sets of rotation axes to define Euler angles, or different names for the same angles. Therefore, any discussion employing Euler angles should always be preceded by their definition.”

We are using the \( z-y-z \) convention with extrinsic rotations \( \Psi - \theta - \phi \) for the particle orientation and \( x-y-z \) convention with extrinsic rotations \( \Psi - \theta - \phi \) for jitter, with jitter applied before particle orientation.

When computing the orientation dispersity integral, the weights for the individual points depends on the map projection used to translate jitter angles into latitude/longitude. The choice of projection is set by `sasmodels.generate.PROJECTION`, with the default `PROJECTION=1` for equirectangular and `PROJECTION=2` for sinusoidal. The more complicated Guyou and Postel projections are not implemented. See jitter.draw_mesh for details.

For numerical integration within form factors etc. sasmodels is mostly using Gaussian quadrature with 20, 76 or 150 points depending on the model. It also makes use of symmetries such as calculating only over one quadrant rather than the whole sphere. There is often a U-substitution replacing \( \theta \) with \( \cos(\theta) \) which changes the limits of integration from 0 to \( \pi/2 \) to 0 to 1 and also conveniently absorbs the \( \sin(\theta) \) scale factor in the integration. This can cause confusion if checking equations to include in a paper or thesis! Most models use the same core kernel code expressed in terms of the rotated view \((q_a, q_b, q_c)\) for both the 1D and the 2D models, but there are also historical quirks such as the parallelepiped model, which has a useless transformation representing \( j_0(aq_a) \) as \( j_0(bq_a/a/b) \).

Useful testing routines include:

The `sascomp` utility is used to view and compare models with different parameters and calculation engines. The usual case is to simply plot a model that you are developing:

```python
python sascomp path/to/model.py
```

Once the obvious problems are addressed, check the numerical precision across a variety of randomly generated inputs:

```python
python sascomp -engine=single,double path/to/model.py -sets=10
```

You can compare different parameter values for the same or different models. For example when looking along the long axis of a cylinder (\( \theta = 0 \)), dispersity in \( \theta \) should be equivalent to dispersity in \( \phi \) when \( \phi = 90 \):

```python
python sascomp -2d cylinder theta=0 phi=0,90 theta_pd_type=rectangle \phi_pd_type=rectangle phi_pd=10,1 theta_pd=1,10 length=500 radius=10
```

It turns out that they are not because the equirectangular map projection weights the points by \( \cos(\theta) \) so \( \Delta \theta \) is not identical to \( \Delta \phi \). Setting `PROJECTION=2` in `sasmodels.generate` helps somewhat. Postel would help even more in this case, though leading to distortions elsewhere. See `sasmodels.compare` for many more details.

`sascomp -ngauss=n` allows you to set the number of quadrature points used for the 1D integration for any model. For example, a carbon nanotube with length 10 \( \mu \)m and radius 1 nm is not computed correctly at high \( q \):

```python
python sascomp cylinder length=100000 radius=10 -ngauss=76,500 -double -highq
```

Note: ticket 702 gives some forms for long rods and thin disks that may be used in place of the integration, depending on \( q \), radius and length; if the cylinder model is updated with these corrections then above call will show no difference.
explore/check1d.py uses sasmodels 1D integration and compares that with a rectangle distribution in $\theta$ and $\phi$, with $\theta$ limits set to $\pm 90/\sqrt{3}$ and $\phi$ limits set to $\pm 180/\sqrt{3}$ [The rectangle weight function uses the fact that the distribution width column is labelled sigma to decide that the 1-$\sigma$ width of a rectangular distribution needs to be multiplied by $\sqrt{3}$ to get the corresponding gaussian equivalent, or similar reasoning.] This should rotate the sample through the entire $\theta$-$\phi$ surface according to the pattern that you see in jitter.py when you use ‘rectangle’ rather than ‘gaussian’ for its distribution without changing the viewing angle. In order to match the 1-D pattern for an arbitrary viewing angle on triaxial shapes, we need to integrate over $\theta$, $\phi$ and $\Psi$.

sascomp -sphere=$n$ uses the same rectangular distribution as check1d to compute the pattern of the $q_x$-$q_y$ grid. This ought to produce a spherically symmetric pattern.

explore/precision.py investigates the accuracy of individual functions on the different execution platforms. This includes the basic special functions as well as more complex expressions used in scattering. In many cases the OpenCL function in sasmodels will use a polynomial approximation over part of the range to improve accuracy, as shown in:

```
python explore/precision.py 3j1/x
```

explore/realspace.py allows you to set up a Monte Carlo simulation of your model by sampling random points within and computing the 1D and 2D scattering patterns. This was used to check the core shell parallelepiped example. This is similar to the general sas calculator in sasview, though it uses different code.

sasmodels/jitter.py is for exploring different options for handling orientation and orientation dispersity. It uses sasmodels/guyou.py to generate the Guyou projection.

explore/asmint.py is a direct implementation of the 1D integration for a number of different models. It calculates the integral for a particular $q$ using several different integration schemes, including mpmath with 100 bits of precision (33 digits), so you can use it to check the target values for the 1D model tests. This is not a general purpose tool; you will need to edit the file to change the model parameters. It does not currently apply the $u = \cos(\theta)$ substitution that many models are using internally so the 76-point gaussian quadrature may not match the value produced by the equivalent model from sasmodels.

explore/symint.py is for rotationally symmetric models (just cylinder for now), so it can compute an entire curve rather than a single $q$ point. It includes code to compare the long cylinder approximation to cylinder.

explore/rpa.py is for checking different implementations of the RPA model against calculations for specific blends. This is a work in (suspended) progress.

There are a few modules left over in explore that can probably be removed. angular_pd.py was an early version of jitter.py. sc.py and sc.c was used to explore different calculations for paracrystal models; it has been absorbed into asymint.py. transform_angles.py translates orientation parameters from the SasView 3.x definition to sasmodels.

explore/angles.py generates code for the view and jitter transformations. Keep this around since it may be needed if we add new projections.

Testing

- model_test
- compare
- compare_many
- rst2html
- list_pars

Individual models should all have test values to make sure that the evaluation is correct. This is particularly important in the context of OpenCL since sasmodels doesn’t control the compiler or the hardware, and since GPUs are notorious for preferring speed over precision. The tests can be run as a group using model_test as main:

```
$ python -m sasmodels.model_test all
```

2.1. Contents
Individual models can be listed instead of all, which is convenient when adding new models.

The compare module, usually invoked using ./sascomp provides a rich interface for exploring model accuracy, execution speed and parameter ranges. It also allows different models to be compared. The compare_many module does batch comparisons, keeping a list of the particular random seeds which lead to large differences in output between different computing platforms.

The rst2html module provides tools for converting model docs to html and viewing the html. This is used by compare to display the model description, such as:

```
$ ./sascomp -html sphere
```

This makes debugging the latex much faster, though this may require Qt in order for mathjax to work correctly.

When run as main, it can display arbitrary ReStructuredText files. E.g.,

```
$ python -m sasmodels.rst2html doc/developer/overview.rst
```

This is handy for sorting out rst and latex syntax. With some work the results could be improved so that it recognizes sphinx roles such as mod, class and func, and so that it uses the style sheets from the sasmodels docs.

The list_pars module lists all instances of parameters across all models. This helps to make sure that similar parameters have similar names across the different models. With the verbose flag, the particular models which use each named parameter are listed.

### Model conversion

- convert
- conversion_table

Model definitions are not static. As needs change or problems are found, models may be updated with new model names or may be reparameterized with new parameter definitions. For example, in translating the Teubner-Strey model from SasView 3.x to sasmodels, the definition in terms of \( \text{drho}, k, c1, c2, a2 \) and prefactor was replaced by the definition in terms of \( \text{volfraction}_a, xi, d, \text{sld}_a \) and \( \text{sld}_b \). Within convert, the \_hand_convert_3_1_2_to_4_1 function must be called when loading a 3.x model definition to update it to 4.1, and then the model should be further updated to 4.2, 5.0, and so on. The convert.convert_model() function does this, using the conversion table in conversion_table (which handled the major renaming from SasView 3.x to sasmodels), and using the internal \_hand_convert function for the more complicated cases.

### Other

- exception
- alignment

The exception.annotate_exception() function annotates the current exception with a context string, such as “while opening myfile.dat” without adjusting the traceback.

The alignment module is unused.

### Calculator Interface

This document describes the layer between the form factor kernels and the model calculator which implements the dispersity and magnetic SLD calculations. There are three separate implementations of this layer, kernelcl for OpenCL, which operates on a single Q value at a time, kerneldll for the DLL, which loops over a vector of Q values, and kernelpy for python models which operates on vector Q values.

Each implementation provides three different calls \( I_q, I_{qxy} \) and Imagnetic for 1-D, 2-D and 2-D magnetic kernels respectively. The C code is defined in kernel_iq.c, with the minor differences between OpenCL and DLL handled by #ifdef statements.
The kernel call looks as follows:

```c
kernel void KERNEL_NAME(
    int nq,          // Number of q values in the q vector
    int pd_start,    // Starting position in the dispersity loop
    int pd_stop,     // Ending position in the dispersity loop
    ProblemDetails *details, // dispersity info
    double *values,  // Value and weights vector
    double *q,       // q or (qx,qy) vector
    double *result,  // returned I(q), with result[nq] = pd_weight
    double cutoff)   // dispersity weight cutoff
```

The details for OpenCL and the python loop are slightly different, but these data structures are common.

`nq` indicates the number of q values that will be calculated.

The `pd_start` and `pd_stop` parameters set the range of the dispersity loop to compute for the current kernel call. Give a dispersity calculation with 30 weights for length and 30 weights for radius for example, there are a total of 900 calls to the form factor required to compute the kernel. These might be done in chunks of 100, so the first call would start at zero and stop after 100 iterations. The second call would then have to set the length index to 3 and the radius index to 10 for a position of 3*30+10=100, and could then proceed to position 200. This allows us to interrupt the calculation in the middle of a long dispersity loop without having to do special tricks with the C code. More importantly, it stops the OpenCL kernel in a reasonable time; because the GPU is used by the operating system to show its windows, if a GPU kernel runs too long then it will be automatically killed and no results will be returned to the caller.

The `ProblemDetails` structure is a direct map of the `details.CallDetails` buffer. This indicates which parameters have dispersity, and where in the values vector the values and weights can be found. For each parameter with dispersity there is a parameter id, the length of the dispersity loop for that parameter, the offset of the parameter values in the pd value and pd weight vectors and the ‘stride’ from one index to the next, which is used to translate between the position in the dispersity loop and the particular parameter indices. The `num_eval` field is the total size of the dispersity loop. `num_weights` is the number of elements in the pd value and pd weight vectors. `num_active` is the number of non-trivial pd loops (parameters with dispersity should be ordered by decreasing pd vector length, with a length of 1 meaning no dispersity). Oriented objects in 2-D need a cos(theta) spherical correction on the angular variation in order to preserve the ‘surface area’ of the weight distribution. `theta_par` is the id of the polar coordinate parameter if there is one.

The `values` vector consists of the fixed values for the model plus pd value and pd weight vectors. There are `NUM_VALUES` fixed values for the model, which includes the initial two slots for scale and background, the `NUM_PARS` values for the kernel parameters, three slots for the applied magnetism, and three slots for each of the SLD parameters for the sample magnetiziation \((M_x, M_y, M_z)\). Sample magnetization is translated from \((M, \theta, \phi)\) to \((M_x, M_y, M_z)\) before the kernel is called. After the fixed values comes the pd value vector, with the dispersity values for each parameter stacked one after the other. The order isn’t important since the location for each parameter is stored in the `pd_offset` field of the `ProblemDetails` structure, but the values do need to be contiguous. After `num_weights` values, the pd weight vector is stored, with the same configuration as the pd value vector. Note that the pd vectors can contain values that are not in the dispersity loop; this is used by mixture. MixtureKernel to make it easier to call the various component kernels.

The `q` vector contains one value for each \(q\) for \(I_q\) kernels, or a pair of \((qx,qy)\) values for each \(q\) for \(I_{qxy}\) and \(I_{magnetic}\) kernels. OpenCL pads all vectors to 32 value boundaries just to be safe, including the `values` vector and the the `results` vector.

The `results` vector contains one slot for each of the `nq` values, plus one extra slot at the end for the weight normalization accumulated across all points in the dispersity mesh. This is required when the dispersity loop is broken across several kernel calls.

`cutoff` is a importance cutoff so that points which contribute negligibly to the total scattering can be skipped without calculating them.

generate.make_source() defines the following C macros:

- USE_OPENCCL is defined if running in opencl
- MAX_PD is the maximum depth of the dispersity loop [model specific]
• NUM_PARS is the number of parameter values in the kernel. This may be more than the number of parameters if some of the parameters are vector values.

• NUM_VALUES is the number of fixed values, which defines the offset in the value list to the dispersity value and weight vectors.

• NUM_MAGNETIC is the number of magnetic SLDs

• MAGNETIC_PARS is a comma separated list of the magnetic SLDs, indicating their locations in the values vector.

• KERNEL_NAME is the name of the function being declared

• PARAMETER_TABLE is the declaration of the parameters to the kernel:

  Cylinder:

  ```c
  #define PARAMETER_TABLE
  double length;
  double radius;
  double sld;
  double sld_solvent;
  ```

  Note: scale and background are never included

  Multi-shell cylinder (10 shell max):

  ```c
  #define PARAMETER_TABLE
  double num_shells;
  double length;
  double radius[10];
  double sld[10];
  double sld_solvent;
  ```

• CALL_IQ(q, i, var) is the declaration of a call to the kernel:

  Cylinder:

  ```c
  #define CALL_IQ(q, i, var) Iq(q[i],
  var.length, 
  var.radius,
  var.sld, 
  var.sld_solvent)
  ```

  Multi-shell cylinder:

  ```c
  #define CALL_IQ(q, i, var) Iq(q[i],
  var.num_shells, 
  var.length, 
  var.radius, 
  var.sld, 
  var.sld_solvent)
  ```

  Cylinder2D:

  ```c
  #define CALL_IQ(q, i, var) Iqxy(qa, qc, 
  var.length, 
  var.radius, 
  var.sld, 
  var.sld_solvent)
  ```

• CALL_VOLUME(var) is similar, but for calling the form volume:

  ```c
  #define CALL_VOLUME(var) 
  form_volume(var.length, var.radius)
  ```
There is an additional macro that can be defined within the model.c file:

- INVALID(var) is a test for model parameters in the correct range:

  Cylinder:
  ```c
  #define INVALID(var) 0
  ```

  BarBell:
  ```c
  #define INVALID(var) (var.bell_radius < var.radius)
  ```

  Model with complicated constraints:
  ```c
  inline bool constrained(p1, p2, p3) { return expression; }
  #define INVALID(var) constrained(var.p1, var.p2, var.p3)
  ```

Our design supports a limited number of dispersity loops, wherein we need to cycle through the values of the dispersity, calculate the I(q, p) for each combination of parameters, and perform a normalized weighted sum across all the weights. Parameters may be passed to the underlying calculation engine as scalars or vectors, but the dispersity calculator treats the parameter set as one long vector.

Let’s assume we have 8 parameters in the model, two of which allow dispersity. Since this is a 1-D model the orientation parameters won’t be used:

- 0: scale {scl = constant}
- 1: background {bkg = constant}
- 2: radius {r = vector of 10pts}
- 3: length {l = vector of 30pts}
- 4: sld {s1 = constant/(radius**2*length)}
- 5: sld_solvent {s2 = constant}
- 6: theta {not used}
- 7: phi {not used}

This generates the following call to the kernel. Note that parameters 4 and 5 are treated as having dispersity even though they don’t — this is because it is harmless to do so and simplifies the looping code:

```
MAX_PD = 4
NUM_PARS = 6  // kernel parameters only
NUM_VALUES = 17 // all values, including scale and background
NUM_MAGNETIC = 2 // two parameters might be magnetic
MAGNETIC_PARS = 4, 5 // they are sld and sld_solvent

details {
  pd_par = {3, 2, 4, 5}  // parameters *radius* and *length* vary
  pd_length = {30, 10, 1, 1}  // *length* has more, so it is first
  pd_offset = {10, 0, 31, 32}  // *length* starts at index 10 in weights
  pd_stride = {1, 30, 300, 300}  // cumulative product of pd length
  num_eval = 300  // 300 values in the dispersity loop
  num_weights = 42  // 42 values in the pd vector
  num_active = 2  // only the first two pd are active
  theta_var = 6  // spherical correction
}

values = { scl, bkg, r, l, s1, s2, theta, phi, mx s1, my s1, mz s1, mx s2, my s2, mz s2, r0, ..., r9, 10, ..., 129, s, s2, r0, ..., r9, 10, ..., 129, s, s2}  // pd values
   r0, ..., r9, 10, ..., 129, s, s2}  // pd weights

nq = 130
q = { q0, q1, ..., q130, x, x }  # pad to 8 element boundary
result = {r1, ..., r130, pd_norm, x }
```
The dispersity parameters are stored in as an array of parameter indices, one for each parameter, stored in pd_par[n]. Parameters which do not support dispersity do not appear in this array. Each dispersity parameter has a weight vector whose length is stored in pd_length[n]. The weights are stored in a contiguous vector of weights for all parameters, with the starting position for the each parameter stored in pd_offset[n]. The values corresponding to the weights are stored together in a separate weights[] vector, with offset stored in par_offset[pd_par[n]]. Dispersity parameters should be stored in decreasing order of length for highest efficiency.

We limit the number of dispersity dimensions to MAX_PD (currently 4), though some models may have fewer if they have fewer dispersity parameters. The main reason for the limit is to reduce code size. Each additional dispersity parameter requires a separate dispersity loop. If more than 4 levels of dispersity are needed, then we need to switch to a monte carlo importance sampling algorithm with better performance for high-dimensional integrals.

Constraints between parameters are not supported. Instead users will have to define a new model with the constraints built in by making a copy of the existing model. Mac provides OpenCL and we are supplying the tinycc compiler for Windows so this won’t be a complete limitation, but it is rather inconvenient. The process could perhaps be automated so that there is no code copying required, just an alternate CALL_IQ macro that implements the constraints. Think carefully about constraining theta since the polar coordinates normalization is tied to this parameter.

If there is no dispersity we pretend that we have a dispersity mesh over a single parameter with a single point in the distribution, giving pd_start=0 and pd_stop=1.

The problem details structure could be allocated and sent in as an integer array using the read-only flag. This would allow us to copy it once per fit along with the weights vector, since features such as the number of dispersity points per pd parameter won’t change between function evaluations. A new parameter vector must be sent for each I(q) evaluation. This is not currently implemented, and would require some restructuring of the sasview_model. SasviewModel interface.

The results array will be initialized to zero for dispersity loop entry zero, and preserved between calls to [start, stop] so that the results accumulate by the time the loop has completed. Background and scale will be applied when the loop reaches the end. This does require that the results array be allocated read-write, which is less efficient for the GPU, but it makes the calling sequence much more manageable.

For accuracy we may want to introduce Kahan summation into the integration:

```c
double accumulated_error = 0.0;
...
#else
    ret += next;
#endif
```

This will require accumulated error for each I(q) value to be preserved between kernel calls to implement this fully. The kernel_iq.c code, which loops over q for each parameter set in the dispersity loop, will also need the accumulation vector.

### 2.2 Indices and Search

- genindex
- modindex
- search
CHAPTER THREE

RELEASE NOTES

Note: In Windows use [Alt]-[Cursor left] to return to the previous page
4.1 New in Version 4.2.1

The major changes for this point release were to fix several problems with using the built in editor to create new models and to bring the NXcanSAS reader into compliance with the final published specification. The original reader was based on a draft version of the specification. As an early adopter, interpretation and implementation of the spec was iterated with all producers of NXcanSAS reduced data known to the SasView team in order to ensure compatibility and verify the implementation. A few other enhancements and bug fixed were also introduced such as cleaning up the resolution section of the fitting page GUI, increasing the max size range allowed in the corfunc analysis, and adding the incomplete gamma function to the python library.

4.1.1 Resolved Issues

- Fixes # 976: CanSas HDF reader will not read all valid CanSas HDF (NXcanSAS) files
- Fixes # 1074: Add incomplete gamma function to sasmodels
- Fixes # 1111: Convert all input Q units to 1/A
- Fixes # 1129: NXcanSAS writer not writing all meta data
- Fixes # 1142: Plugin framework is broken
- Fixes # 1183: Test from creating new model reset all parameters to default in all open FitPages
- Fixes # 1188: Colons removed from magnetic parameter names to address Python variable issue - done in 4.2. but documented in 4.2.1
- Fixes # 1205: 4.2 set weighting choice seems to be ignored.
- Fixes # 1206: Incorrect (and confusing) presentation of dQ from data in instrumental smearing section
- Fixes # 1212: Bug in Iqxqy plotting non rectangular / square matrices?
- Fixes # 1221: ABS reader does not read in USANS data properly GitHub
- Fixes # 1222: smearing options incorrect on show2D and show1D in fitpage14: Loading a saved project is really really slow
- Fixes # 1223: Expand permitted range of transformed data in Corfunc implementation

4.2 New in Version 4.2.0

This release heralds many improvements and a host of bug fixes, along with some significant changes from previous versions. Further, as promised, it marks the end of support for 32 bit operating systems and is only available for 64 bit operating systems.
With this version the change to the new model API and plugins infrastructure begun with 4.0 is essentially complete (though extensions are in the works, and more are likely, they should remain backwardly compatible with previous versions of SasView).

**Warning:** Old-style plugin models, including old sum|multiply models, continue to be supported (i.e. SasView will run them) in 4.x, although our automatic on-the-fly translation may not cope in all use cases (see Known Issues below). However, this backward compatibility will be removed in 5.0 and users are therefore strongly encouraged to convert their custom models to the new API.

Finally, the changes to orientation angles and orientational distribution definitions are now also complete.

### 4.2.1 Changes

- The infrastructure for calculating 2D patterns from 3D orientated objects has been totally re-factored. It is now more accurate and consistent across models.
- The way that SasView defines the orientation of anisometric and aligned objects has been completely overhauled. It now differs from previous versions.
- Plugin models, including sum|multiply models, have completely migrated to the new infrastructure. NOTE that 3.x type models as well as early, intermediate 4.x type models, including those generated by sum|multiply will continue to be supported in 4.x but will likely no longer be supported after the move to 5.0. Users are strongly encouraged to migrate any custom models.
- The NeXus loader has been removed as it is superseded by the NXcanSAS standard loader and SasView does not support the treatment of raw data.

### 4.2.2 Improvements

- The accuracy/speed of some numerical integrations have been improved.
- An orientation viewer tool has been introduced to assist in understanding the new orientation framework.
- Problems with the computation of magnetic scattering from some objects have been rectified. Some questions remain however.
- The known issue with the core_shell_parallelepiped model is now fixed.
- An error in the be_polyelectrolyte model was identified and rectified, but the fix is yet to be validated.
- (Added post-release) An error with the reporting of the scale parameter from the spinodal model was rectified.
- A number of issues and inconsistencies with the creation of sum|multiply models have been rectified.
- A Boltzmann distribution has been added for polydispersity/orientational distributions.
- Some batch slicing options have been introduced.
- Correlation function analysis now computes both the 1D and 3D functions.
- There are several data loading improvements.
- There are several improvements to Save/Load Project.
- The SasView version number now appears in Reports.
- The Release Notes are now available from the program Help menu.
- There have been numerous other bug fixes.
4.2.3 Documentation

Several sections of the help documentation have undergone significant checking and updating, particularly those relating to orientation, magnetic scattering, and polydispersity distributions.

Detailed advanced instructions for plugin writing and some scripting instructions have also been added.

Concerns about the intended versus implemented meaning of some parameters in the bcc_paracrystal, fcc_paracrystal, and sc_paracrystal models have been brought to our attention. These have yet to be resolved and so a Warning has been placed on each of these models. Anyone who feels they may have the requisite expertise to investigate these concerns is strongly encouraged to contact the Developers!

4.2.4 Other Work

- A Third-Party initiative has recently succeeded in getting SasView to run on Debian. More details at http://trac.sasview.org/wiki/DevNotes/Projects/Debian
- With this release we have started to prepare for the inevitable move to Python 3, which will occur with the release of 5.0
- SasView 5.0 is currently in development. The two most significant features of this version will be (i) a move away from the present WxPython GUIs to new, completely rewritten, Qt5 GUIs, and (ii) implementation of the Beta-approximation for S(Q). Subject to resources, some limited access to the latter functionality may be available in a future SasView 4.x release.

4.2.5 Bug Fixes

- Fixes # 14: Loading a saved project is really really slow
- Fixes # 260: Box integration does not update when entering values in dialog
- Fixes # 446: Saving plot as PGF (not PDF!) format throws error
- Fixes # 467: Extend batch functionality to slicer
- Fixes # 489: ABS reader (NIST 1D) does not handle negative dx properly (USANS slit smearing)
- Fixes # 499: create sin(x)/x, 2*J1(x)/x and 3*j1(x)/x functions
- Fixes # 510: Build PDF documentation along with HTML
- Fixes # 525: Add GUI category defaults to models in sasmodels
- Fixes # 579: clean up sasview directory
- Fixes # 597: Need to document Combine Batch Fit
- Fixes # 645: GUI logic problem in Batch vs single fit mode
- Fixes # 648: Need to allow user input background value in Pr perspective
- Fixes # 685: Fix data upload to marketplace
- Fixes # 695: linear slope in onion model
- Fixes # 735: Review new Corfunc documentation
- Fixes # 741: Recalculate P(Q) and S(Q) components on model update.
- Fixes # 767: Sum/Product Models don’t do what they should
- Fixes # 776: angular dispersity
- Fixes # 784: Add 3D integral to Correlation Function analysis
- Fixes # 786: core_shell_parallelepiped 1-D model is incorrect
- Fixes # 818: “report button” followed by “save” makes an empty pdf file???
• Fixes # 830: Check compliance of loader against NXcanSAS-1.0 release
• Fixes # 838: Fix model download from marketplace
• Fixes # 848: can’t save analysis when only one fit page
• Fixes # 849: Load Folder should ignore files starting with .
• Fixes # 852: More unit tests, especially for oriented or 2d models
• Fixes # 854: remove unnecessary sleep() in fitting perspective
• Fixes # 856: Reading SAS_OPENCL from custom_config sometimes raises an ERROR
• Fixes # 861: cannot defined a structure factor plugin
• Fixes # 864: New Model Editor (simple plugin editor) error parsing parameter line
• Fixes # 865: Plugin live discovery issues
• Fixes # 866: inform user when NaN is returned from compute
• Fixes # 869: fit page computation thread cleanup
• Fixes # 875: Possible weirdness with 1D NXcanSAS data
• Fixes # 876: Add check for HDF5 format in dataloader
• Fixes # 887: reorganize tree, separating the installed source from the build source
• Fixes # 889: Refactor dataloader error handling infrastructure
• Fixes # 890: use new orientation definition for asymmetric shapes
• Fixes # 891: update docs for oriented shapes with new orientation definition
• Fixes # 896: equations in core shell parallelepiped docs do not match code
• Fixes # 898: Image Viewer Tool file selector issue
• Fixes # 899: Igor Reader q calculation
• Fixes # 902: IgorReader Q calculation needs fixing/improving
• Fixes # 903: sasview - all non-gui tests should be converted to run in Python 3
• Fixes # 906: polydispersity not showing up in tabulated results
• Fixes # 912: About box points to misleading contributors page on Github
• Fixes # 913: Need to add Diamond developer and logo in relevant places
• Fixes # 915: load project issues
• Fixes # 916: Proper Logging
• Fixes # 920: Logarithmic binning option in the slice viewer
• Fixes # 921: Improve developer communication methods
• Fixes # 922: Remove support for all data formats that are not in q space
• Fixes # 923: Add CI and trac integrations to Slack
• Fixes # 930: fitting help says chisq is normalized to number of points
• Fixes # 931: Allow admins to edit all models and upload data etc on marketplace
• Fixes # 932: Need to fix upload of data files to marketplace
• Fixes # 934: Slurp tutorial repo for tutorials
• Fixes # 935: Build new tutorials as PDF
• Fixes # 943: Deep copy error on setting model after data is selected
• Fixes # 950: Most of the readers don’t close files properly.
• Fixes #954: cross check dll/opencl/python polydispersity and orientation results
• Fixes #956: Possible problem with new doc build process
• Fixes #961: sasmodels tests should fail if the parameter name does not exist
• Fixes #962: star polymer typo in docs
• Fixes #966: Inconsistent chi2 reporting
• Fixes #967: no uncertainties errors on fitting parameters
• Fixes #969: About Box not picking up dls_logo.png
• Fixes #970: ASCII loader doesn’t handle ISIS 2D ASCII
• Fixes #974: blacklist Intel HD 620/630 for double precision
• Fixes #978: load project fails for pages which have not been defined
• Fixes #983: Remove Nexus Loader
• Fixes #984: PDF reports are not being properly generated on Windows
• Fixes #985: Saving Project Fails
• Fixes #986: Send to fitting overwrites theory page even if blank FitPage has focus
• Fixes #990: uctest_sasview.py giving different results than run_one.py
• Fixes #993: Windows x64 versions not installing to correct folder
• Fixes #994: Error changing fit engine
• Fixes #995: OpenCL required on Linux even if turned off in GUI
• Fixes #1006: multiplicity models don’t work with SQ
• Fixes #1007: spherical_sld model freezes SasView
• Fixes #1008: plugin model scaling not working?
• Fixes #1010: Win64 build script not creating working executable
• Fixes #1011: sld_test failing on ubuntu
• Fixes #1013: FileReaderBaseClass output[] not reset - same file loaded multiple times
• Fixes #1018: add Boltzmann distribution
• Fixes #1021: add PDF documentation to website and document in wiki release process
• Fixes #1024: Update version numbers in master
• Fixes #1025: Sum/multiply editor hangs
• Fixes #1030: volume normalization for hollow shapes is different from solvent-filled shapes
• Fixes #1032: convert C++ modules to C
• Fixes #1035: Order of combining P(Q) and S(Q) in Plugins seems to matter
• Fixes #1037: data loader crop not working? & all fits crashing
• Fixes #1043: problem compiling marketplace models
• Fixes #1044: Unable to upload c file to marketplace
• Fixes #1046: convert non builtin models in the marketplace to new API
• Fixes #1050: fix appveyor test for sasmodels win 64 python 3
• Fixes #1052: Can’t use a user-created plugin model in a plugin model
• Fixes #1054: Check plugin & orientation descriptions in full docs once SasModels PR #57 is merged
• Fixes #1057: phi rotation issue for elliptical cylinder
• Fixes #1060: incorrect default for rectangle dispersion
• Fixes #1062: win32 build not installing correctly
• Fixes #1064: “Fitting did not converge!!!” error with a Sum|Multi plugin model
• Fixes #1068: 2d data (from NG7) not loading - strange format?
• Fixes #1069: GUI problem when using polydispersity/orientation distributions
• Fixes #1070: Parameter error boxes should not be editable
• Fixes #1072: Orientation distributions seem to depend on initial angle
• Fixes #1079: Remove save button in report dialog on Mac
• Fixes #1081: GUI problem with new orientation distribution
• Fixes #1083: Magnetic models not being computed
• Fixes #1099: Erratic behaviour of Sum|Multi model in 4.1.2
• Fixes #1101: Batch results page not displaying polydispersity values
• Fixes #1128: AutoPlot generation for model documentation does not include background
• Fixes #1131: OpencCl dialog does not open
• Fixes #1132: Slit Size Calculator Tool not working
• Fixes #1139: Missing Docs and Help for new Batch Slicing
• Fixes #1141: Intro to scripting.rst needs improvement
• Fixes #1142: Plugin framework is broken
• Fixes #1145: Update models in model marketplace to 4.2 when 4.2 is released.
• Fixes #1155: BE Polyelectrolyte errors
• Fixes #1160: fix VR for core_shell_cylinder, fractal_core_shell and hollow_cylinder
• Fixes #1163: Fix help note in sum of sumxyinterface
• Fixes #1164: Sphinx doc build does not support superscript or substitution
• Fixes #1166: No longer able to report from multiple fit pages
• Fixes #1167: Clarify the documentation for the Spinodal Model
• Fixes #1173: more problems with math in plugins
• Fixes #1176: Make Release Notes/Known Issues available from Help in Menu Bar
• Fixes #1179: PDF Report should contain SasView Version Number
• Fixes #1183: Test from creating new model reset all parameters to default in all open FitPages
• Fixes #1188: fitpage hangs if change model while magnetism is on
• Fixes #1191: Correct erroneous Scale reported by Spinodal model

It is recommended that all users upgrade to this version, but your attention is drawn to the Changes section above.

4.3 New in Version 4.2.0-Beta

This is a beta pre-release version of 4.2.0. A number of fixes and changes have been made in the year since the previous release. Full release notes will be compiled prior to the full release 4.2.0.

Highlights are:

• Infrastructure for calculating 2D patterns from 3D orientated objects has now been totally refactored
• Plugins have completely migrated to the new infrastructure now, including sum/multiply models
• Some batch slicing options have been introduced
• The known issue with the core_shell_parallelepiped is now fixed
• Several data loading improvements
• Several save Project improvements (though there are more to come)
• Numerous bug fixes
• Lots of documentation enhancement

In the meantime please report any bugs or issues found while using this beta

4.4 New in Version 4.1.2

This point release is a bug-fix release addressing:
• Fixes #984: PDF Reports Generate Empty PDFs
• Fixes a path typo
• 64 bit and 32 bit Windows executables now available

It is recommended that all users upgrade to this version

4.5 New in Version 4.1.1

This point release is a bug-fix release addressing:
• Fixes #948: Mathjax CDN is going away
• Fixes #938: Cannot read canSAS1D file output by SasView
• Fixes #960: Save project throws error if empty fit page
• Fixes #929: Problem deleting data in first fit page
• Fixes #918: Test folders not bundled with release
• Fixes an issue with the live discovery of plugin models
• Fixes an issue with the NXcanSAS data loader
• Updated tutorials for SasView 4.x.y

4.6 New in Version 4.1.0

This incremental release brings a series of new features and improvements, and a host of bug fixes. Of particular note are:

4.6.1 Correlation Function Analysis (Corfunc)

This performs a correlation function analysis of one-dimensional SAXS/SANS data, or generates a model-independent volume fraction profile from the SANS from an adsorbed polymer/surfactant layer.

A correlation function may be interpreted in terms of an imaginary rod moving through the structure of the material. \( G_1(R) \) is the probability that a rod of length \( R \) moving through the material has equal electron/neutron scattering length density at either end. Hence a frequently occurring spacing within a structure manifests itself as a peak.
A volume fraction profile $\Phi(z)$ describes how the density of polymer segments/surfactant molecules varies with distance from an (assumed locally flat) interface. *This is not yet implemented.*

### 4.6.2 Fitting of SESANS Data

Data from Spin-Echo SANS measurements can now be loaded and fitted. The data will be plotted against the correct axes and models will automatically perform a Hankel transform in order to calculate SESANS from a SANS model.

### 4.6.3 Documentation

The documentation has undergone significant checking and updating.

### 4.6.4 Improvements

- Correlation function (corfunc) analysis of 1D SAS data added from CCP13
- File converter tool for multi-file single column data sets
- SESANS data loading and direct fitting using the Hankel transformation
- Saving and loading of simultaneous and constrained fits now supported
- Save states from SasView v3.x.y now loaded using sasmodel model names
- Saving and loading of projects with 2D fits now supported
- Loading a project removes all existing data, fits, and plots
- Structure factor and form factor can be plotted independently
- OpenCL is disabled by default and can be enabled through a fit menu
- Data and theory fields are now independently expandable

### 4.6.5 Bug Fixes

- Fixes #667: Models computed multiple times on parameters changes
- Fixes #673: Custom models override built in models of same name
- Fixes #678: Hard crash when running complex models on GPU
- Fixes #774: Old style plugin models unloadable
- Fixes #789: stacked disk scale doesn’t match cylinder model
- Fixes #792: core_shell_fractal uses wrong effective radius
- Fixes #800: Plot range reset on plot redraws
- Fixes #811 and #825: 2D smearing broken
- Fixes #815: Integer model parameter handling
- Fixes #824: Cannot apply sector averaging when no detector data present
- Fixes #830: Canas HDF5 reader fully compliant with NXCanSAS v1.0 format
- Fixes #835: Fractal model breaks with negative Q values
- Fixes #843: Multilayer vesicle does not define effective radius
- Fixes #858: Hayter MSA S(Q) returns errors
- Numerous grammatical and contextual errors in documentation
4.7 New in Version 4.0.1

This release fixes the critical bug #750 in P(Q)xS(Q). Most damaging it appears that the background term was being added to S(Q) prior to multiplication by P(Q).

4.8 New in Version 4.0

This release fixes the various bugs found during the alpha and beta testing

4.8.1 Improvements

• Support for reading data files from Anton Paar Saxess instruments
• Adds documentation on how to write custom models in the new framework

4.8.2 Bug Fixes

• Fixes #604: Pringle model questions
• Fixes #472: Reparameterize Teubner-Strey
• Fixes #530: Numerical instabilities in Teubner Strey model
• Fixes #658: ASCII reader very broken

4.9 New in Version 4.0 beta 1

This beta adds support for the magnetic and multilevel models of 3.1.2 and along with a host of bug fixes found in the alpha.

4.9.1 Model package changes and improvements

• All 3.1.2 models now available in new interface
• Old custom models should now still work
• Custom model editor now creates new style models
• Custom model editor supports better error checking

Note: Old custom models should be converted to the new model format which is now the same as the built-in models and offers much better support. The old custom model format will be deprecated in a future version.

4.9.2 Documentation improvements

• Continued general cleanup
4.9.3 Other improvements/additions

- Support for new canSAS 2D data files added
- Plot axes range can now be set manually as well as by zooming
- Plot annotations can now be moved around after being placed on plot.
- The active optimizer is now listed on the top of the fit panel.
- Linear fits now update qmin and max when the x scale limits are changed. Also the plot range no longer resets after a fit.

4.9.4 Bug fixes

- Fixes #511: Errors in linearized fits and clean up of interface including Kratky representation
- Fixes #186: Data operation Tool now executes when something is entered in the text box and does not wait for the user to hit enter
- Fixes #459: plot context menu bug
- Fixes #559: copy to clipboard in graph menu broken
- Fixes #466: cannot remove a linear fit from graph
- Numerous bugs introduced in the alpha

4.10 New in Version 4.0.0-alpha

This alpha release brings a major overhaul of the model system. The new model package allows rapid integration of custom models and access to polydispersity without requiring a compiler.

4.10.1 Model package changes and improvements

- Separation of GUI and calculations for future GUI enhancements
- Model interface moved to independent sasmodels package.
- Most models converted to new interface.
- Allows rapid integration of user-written models.
- OpenCL GPU utilization for faster fitting.
- Improved numerical integration of Bessel functions.

4.10.2 SESANS integration and implementation

- Scripting interface added for analysis of SESANS data.
- Hankel transformation now accepts finite acceptance angles.
- 2D cosine transformation added for TOF SESANS analysis.
4.10.3 Documentation improvements

- The documentation tree was restructured for a better end user experience.
- The documentation for each model was revamped and verified by at least two people following the conversion of the model.
- Theoretical 1D (and 2D if applicable) scattering curves are auto-generated and added to the model documentation for each model.

4.10.4 Bug fixes

- Fixes #411: No stop button on simultaneous fit page
- Fixes #410: Error with raspberry model
- Fixes #364: Possible inconsistency in Poly_GausCoil model
- Fixes #439: Hayter Penfold MSA code needs checking
- Fixes #484: lammellerPC is precision limited
- Fixes #498: $HOME/.matplotlib conflicts
- Fixes #348: Control order in which fit parameters appear in the gui
- Fixes #456: Provide DREAM Results Panel with something to identify data and age of results
- Fixes #556: Build script improvements for developers

4.11 New in Version 3.1.2

This release is a major stability improvement, having fixed a serious bug that came to light since release 3.1.1. All users should upgrade.

- Fixes #468: broken remove constraint buttons in simultaneous/constrained fitting panel
- Fixes #474: resulting from changes in 3.1.1 that had introduced an error in the high-Q of slit-smeared models.
- Fixes #478: which would cause wx to run out of IDs and result in SasView crashing even if left alone.
- Fixes #479: missing help button on simultaneous/constrained fit page
- Fixes #480: GUI resizing issues on simultaneous fit page
- Fixes #486: broken Report Results
- Fixes #488: redraw issues in fit page

4.12 New in Version 3.1.1

Fixes #457 that prevented SasView from starting if the user was not connected to the internet, or was behind a proxy server.

4.13 New in Version 3.1.0

The documentation/help has had a complete overhaul including:

- A completely new presentation interface (Sphinx).
- Proof reading!
• Updating for latest features.

• A Help (or sometimes ?) button has been added to every panel, and some sub panels if appropriate, linking to the appropriate section in the documentation.

• The model help has been split so that the Details button now brings up a very short pop-up giving the equation being used while HELP goes to the section in the full documentation describing the model.

• Extensive help has also been added for the new optimizer engine (see below) including rules of thumb on how and when to choose a given optimizer and what the parameters do.

The optimizer engine has been completely replaced. The new optimizer still defaults to the standard Levenberg-Marquardt algorithm. However 4 other optimizers are now also available. Each starts with a set of default parameters which can be tuned. The DREAM optimizer takes the longest but is the most powerful and yields rich information including full parameter correlation and uncertainty plots. A results panel has been added to accommodate this. The five new optimizers are:

• A Levenberg-Marquardt optimizer
• A Quasi-Newton BFGS optimizer
• A Nelder-Mead Simplex optimizer
• A Differential Evolution optimizer
• A Monte Carlo optimizer (DREAM)

New models were added:
• MicelleSphCoreModel (currently residing in the Uncategorized category)

Existing models were updated:
• LamellarPS (bug in polydispersity integration fixed)
• RectangularPrismModel
• RectangularHollowPrismModel
• RectangularHollowPrismInfThinWallsModel

Other work:
• Infrastructure to allow SESANS data to be fit with models was added. This will become available in a future release but can currently be used from the command line with some caveats.

• A number of bugs were fixed including a thread crashing issue and an incorrect slit smearing resolution calculation.

• Implemented much more robust error logging to enable much easier debugging in general but particularly the debugging of issues reported by SasView users.

• A number of infrastructure tasks under the hood to enhance maintainability

• Upgrade from Wx 2.8 to Wx 3.0.2 which allows several new features but required significant additional rework as well.

• Fully implemented Sphinx to the build process to produce both better user documentation and developer documentation.

• Restructuring of the code base to more unified nomenclature and structure so that the source installation tree more closely matches the installer version tree.

• Code cleanup (an ongoing task).

• Migration of the repository to github simplifying contributions from non-project personnel through pull requests.
4.14 New in Version 3.0.0

- The GUI look and feel has been refactored to be more familiar for Windows users by using MDI frames. Graph windows are also now free-floating.
- Five new models have been added: PringlesModel, CoreShellEllipsoidXTModel, RectangularPrismModel, RectangularHollowPrismModel and RectangularHollowPrismInfThinWallsModel.
- The data loader now supports ILL DAT data files and reads the full meta information from canSAS file formats.
- Redefined convention for specifying angular parameters for anisotropic models.
- A number of minor features have been added such as permitting a log distribution of points when using a model to simulate data, and the addition of a Kratky plot option to the linear plots.
- A number of bugs have also been fixed.
- Save Project and Save Analysis now work more reliably.
- BETA: Magnetic contrast supporting full polarization analysis has been implemented for some spherical and cylindrical models.
- BETA: Two new tools have been added:
  - A generic scattering calculator which takes an atomic, magnetic or SLD distribution in space and generates the appropriate 2D scattering pattern. In some cases the orientationally averaged (powder) 1D scattering can also be computed. Supported formats include: SLD or text, PDB, and OMF magnetic moment distribution file.
  - An image viewer/converter for data in image format; this reads in an image file and will attempt to convert the image pixels to data. Supported formats include: TIFF, TIF, PNG, BMP, JPG.

4.15 New in Version 2.2.1

- Minor patch to support CanSAS XML v1.1 file format
- Added DataInfo for data in the DataExplorer and plots
- Added Maximize/Restore button in the title bar of the graphs
- Added a hide button in the toolbar of the graph panel
- The ‘x’ button now deletes a graph
- Edit SUM Model from the menubar can now generate and save more than one sum model
- Reports can now be saved in pdf format on WIN and MAC
- Made significant improvements to the batch/grid panel and fixed several bugs
- Fixed a number of other minor bugs

4.16 New in Version 2.2.0

- Application name changed to SasView
- New fully customizable Category Manager added for better management of increasing number of models
- Improved the Grid Window functionality in the batch fitting mode
- Added a simpler Graph/Plot modification interface
- Added a new ‘Data Operation’ tool for addition, subtraction, multiplication, division, of two data sets.
- The ‘Sum Model’ editor was extended and renamed ‘Summation and Multiplication’ editor
• Added more plot symbols options for 1d plots
• Added improved trapping of compiling errors to the ‘New model editor’
• Added some intelligent outputs (e.g., Rg, background, or rod diameter depending on the choice of axis scale of the plot) to the linear fits
• Added more models

4.17 Feature set from previous versions

4.17.1 Perspectives Available

• Invariant calculator: Calculates the invariant, volume fraction, and specific surface area.
• P(r) inversion calculator: Indirect Fourier transformation method.
• Fitting: the tool used for modeling and fitting 1D and 2D data to analytical model functions
• Tools: provides a number of useful supplementary tools such as SLD calculation

4.17.2 Fitting

• Includes a large number of model functions, both form factors and structure factors.
• Support P(Q)*S(Q) for form factors that flag they can be so multiplied.
• Supports Gaussian, lognormal, Shulz, rectangular and custom distribution functions for models that need to include polydispersity or for orientational distributions if appropriate.
• Anisotropic shapes and magnetic moment modeling in 2D allow for a non-uniform distribution of orientations of a given axis leading to modeling and fitting capabilities of non azimuthaly symmetric data.
• User can choose to weight fits or not. If using weights, the user can choose the error bar on each point if provided in the file, the square root of the intensity or the intensity itself.
• Instrumental resolution smearing of model or fits is provided with several options: read the resolution/point from the file. Input a pinhole resolution or a slit resolution.
• Users can define the Qrange (Qmin and Qmax) for both 1D and 2D data for fitting and modeling, but not graphically. The range can be reset to the defaults (limits of q in data set for a fit) with the reset button.
• A mask can be applied to 2D calculation and fitting.
• Normalized residual plots are provided with every fit.
• Model function help available through detail button or from the fitting panel.
• Simultaneous/(advanced)constrained fitting allows for fitting a single data set or several different sets simultaneously with the application of advanced constraints relating fit parameters to functions of other parameters (including from a different set). For example thickness of shell = sin(30) times the length.
• Models that are the sum of two other models can be easily generated through the SUM Model menubar item.
• New Python models can be added on the fly by creating an appropriate Python file in the model plugin directory. Two tools are provided to help: An easy to use custom model editor allows the quick generation of new Python models by supplying only the parameters and their default value (box 1) and the mathematical function of the model (box 2) and generating the necessary .py file. A separate advanced model editor provides a full Python file editor. Either way once saved the model becomes immediately available to the application.
• A batch fitting capability allows for the analysis of a series of data sets to a single model and provides the results in a tabular form suitable for saving or plotting the evolution of the fit parameters with error bars (from within the application).
### 4.17.3 Tools

- A scattering length density calculator, including some X-ray information is provided.
- A density to vol. fraction converter is provided
- In application access to a Python shell/editor (PyCrust) is provided
- An instrument resolution calculator, including possible gravitational and TOF effects is provided
- A slit size calculator optimized for Anton Paar Saxess is provided.
- A kiessig fringe thickness calculator is provided

### 4.17.4 Plots and plot management

- A 3D graphing option (for 2d data/results) is provided with the view controlled by the mouse
- 2D plots are shown with an intensity color bar. 2D Color map can be user adjusted.
- Supports output of plot to a variety of graphic formats. Supported formats include: png, eps, emf, jpg/jpeg, pdf, ps, tif/tiff, rawRGBbitmap(raw, rgba), and scalable vector graphic (svg/svgz)
- Supports output of data in plot (1 or 2D) to limited data formats
- Multiple data sets can be loaded into a single graph for viewing (but a fit plot can currently only have a single plot).
- Extensive context sensitive plot/fitting/manipulation options are available through a right mouse click pop-up menu on plots.

### 4.17.5 Data management

- Supports 2 + column 1D ASCII data, NIST 1D and 2D data, and canSAS data via plug-in mechanism which can easily allow other readers as appropriate.
- 2D data is expected in Q space but for historical reasons accepts the NIST 2D raw pixel format and will do conversion internally.
- The full data and metadata available to SasView is viewable in ASCII via right clicking on a data set and choosing Data Info in the DataExplorer or on the plots
- Supports loading a single file, multiple files, or a whole folder
- An optional Data Explorer is provided (default) which simplifies managing, plotting, deleting, or setup for computation. Most functions however do not require access to the explorer/manager and can be accessed through right click menus and the toolbar. The data explorer can be re-started from the menu bar.

### 4.17.6 Data manipulation

- Support various 2D averaging methods: Circular, sectors, annular, boxsum, boxQx and boxQy.
- A 2D data maks editor is provided
- 2D mask can be applied to the circular averaging.

### 4.17.7 Miscellaneous features

- Limited reports can be generated in pdf format
- Provides multiprocessor support (Windows only)
- Limited startup customization currently includes default startup data folder and choice of default starting with data manager
• Limited support for saving(opening) a SasView project or a SasView analysis (subproject) is provided.

• SasView can be launched and loaded with a file of interest by double-clicking on that file (recognized extension)

• A data file or data folder can be passed to SasView when launched from the command line.

• Limited bookmarking capability to later recall the results of a fit calculation is provided.

• Extensive help is provided through context sensitive mouse roll-over, information bar (at the bottom of the panel), the console menu, and access to the help files in several different ways.
5.1 System Requirements

- Python version $\geq 2.5$ and $< 3.0$ should be running on the system
- We currently use Python 2.7

5.2 Package Dependencies

- Ensure the required dependencies are installed
- For the latest list of dependencies see the appropriate yml file in the SasView repo at sasview/build_tools/conda/ymls

5.3 Installing from Source

- Get the source code
- Create a folder to contain the source code; if working with multiple versions you might want to use versioned folder names like ‘sasview-x.x.x’
- Open a command line window in the source code folder
- To get the CURRENT DEVELOPMENT VERSION from source control use git clone https://github.com/SasView/sasview.git sasview git clone https://github.com/SasView/sasmodels.git sasmodels git clone https://github.com/bumps/bumps.git bumps
- To get a SPECIFIC RELEASE VERSION from source control go to https://github.com/SasView/sasview/releases and download the required zip or tar.gz file. Unzip/untar it to the source code folder.
5.4 Building and Installing

- To build the code use ‘python setup.py build’
- To build the documentation use ‘python setup.py docs’

5.5 Running SasView

- use ‘python run.py’; this runs from the source directories, so you don’t have to rebuild every time you make a change, unless you are changing the C model files.
- if using Conda the above command will also build SasView, but you must issue ‘activate sasview’ first.
A full list of known bugs and feature requests by release version that users may wish to be aware of can be viewed at http://trac.sasview.org/report/3

6.1 4.2.0 - All systems

The refactoring of the plugin model architecture means that some issues may be encountered if Save Project/Analysis files using plugin models created in earlier versions of SasView are loaded in version 4.2.0. For example:

- on loading an old project file an error window appears with the error *This model state has missing or outdated information* or *dictionary changed size during iteration*.
  - if this occurs, try restarting SasView and reloading the project.
- on loading an old project file all the FitPages and Graphs appear, but only the SasView default model parameters appear in the FitPages.
  - this has happened because plugin model parameter names have changed. There are two possible workarounds:
    - Install the version of SasView that the project was created in, recreate the plugin in that version, then run 4.2.0 and re-load the project. All being well, 4.2.0 will still compile the old plugin.
    - If 4.2.0 cannot compile the old plugin, the more tedious solution is to use a text editor to do global search & replace operations to change all the parameter names in the project file by hand. The quickest way to see the existing parameter names is simply to scroll to the bottom of the project file. To see what the new parameter names should be, simply create the equivalent plugin in SasView 4.2.0. In most instances, what was \texttt{p1\_parameter} will become \texttt{A\_parameter}, \texttt{p2\_parameter} will become \texttt{B\_parameter}, and so on.

6.2 4.1.x - All systems

The conversion to sasmodels infrastructure is ongoing and should be completed in the next release. In the meantime this leads to a few known issues:

- The way that orientation is defined is being refactored to address long standing issues and comments. In release 4.1 however only models with symmetry (e.g. \texttt{a=b}) have been converted to the new definitions. The rest (\texttt{a <> b <> c} - e.g. parellelepiped) maintain the same definition as before and will be converted in 4.2. Note that orientational distribution also makes much more sense in the new framework. The documentation should indicate which definition is being used for a given model.
- The infrastructure currently handles internal conversion of old style models so that user created models in previous versions should continue to work for now. At some point in the future such support will go away. Everyone is encouraged to convert to the new structure which should be relatively straight forward and provides a number of benefits.
• In that vein, the distributed models and those generated by the new plugin model editor are in the new format, however those generated by sum|multiply models are the old style sum|multiply models. This should also disappear in the near future.

• The on the fly discovery of plugin models and changes thereto behave inconsistently. If a change to a plugin model does not seem to register, the Load Plugin Models (under fitting -> Plugin Model Operations) can be used. However, after calling Load Plugin Models, the active plugin will no longer be loaded (even though the GUI looks like it is) unless it is a sum|multiply model which works properly. All others will need to be recalled from the model dropdown menu to reload the model into the calculation engine. While it might be annoying it does not appear to prevent SasView from working.

• The model code and documentation review is ongoing. At this time the core shell parallelepiped is known to have the C shell effectively fixed at 0 (noted in documentation) while the triaxial ellipsoid does not seem to reproduce the limit of the oblate or prolate ellipsoid. If errors are found and corrected, corrected versions will be uploaded to the marketplace.

• (Added after Release 4.2.0) The scale parameter reported from the spinodal model is the square root of the true value.

### 6.3 3.1- All systems

• The documentation window may take a few seconds to load the first time it is called. Also, an internet connection is required before equations will render properly. Until then they will show in their original TeX format.

• If the documentation window remains stubbornly blank, try installing a different browser and set that as your default browser. Issues have been noted with Internet Explorer 11.

• Check for Updates may fail (with the status bar message ‘Cannot connect to the application server’) if your internet connection uses a proxy server. Tested resolutions for this are described on the website FAQ.

• The copy and paste functions (^C, ^V) in the batch mode results grid require two clicks: one to select the cell and a second to select the contents of the cell.

• The tutorial has not yet been updated and is somewhat out of date.

• Very old computers may struggle to run the 3.x and later releases.

• Polydispersity on multiple parameters included in a simultaneous/ constrained fit will likely not be correct.

• Constrained/simultaneous fit page does not have a stop button.

• Constrained/simultaneous fit do not accept min/max limits.

• Save project does not store the state of all the windows.

• Loading projects can be very slow.

• Save Project only works once a data set has been associated with a model. Error is reported on status bar.

• There is a numerical precision problem with the multishell model when the inner radius gets large enough (ticket #288).

• The angular distribution angles are not clearly defined and may in some cases lead to incorrect calculations (ticket #332).

### 6.4 3.1 - Windows

• If installed to same directory as old version without first removing the old version, the old desktop icon will remain but point to the new exe version. Likewise all the start menu folders and items will have the old name even though pointing to the new version. Usually safest to uninstall old version prior to installing new version anyway.
6.5 3.1 - MAC

- Application normally starts up hidden. Click icon in Dock to view/use application.
- Multiprocessing does not currently work on MAC OS

6.6 3.1 - Linux

- Not well tested
http://www.sasview.org

This main project site is the gateway to all information about the sasview project. It includes information about the project, a FAQ page and links to all developer and user information, tools and resources.
FREQUENTLY ASKED QUESTIONS

http://www.sasview.org/faq.html
CHAPTER NINE

INSTALLER DOWNLOAD WEBSITE

Latest release Version https://github.com/SasView/sasview/releases
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