Software Design for SANS Data Analysis-Simulation

SANS group
Overview

• SANS Data Analysis Package
  – Model-independent analysis
  – Modeling

• SANS modeling
  – Predict the shape of the target molecule that is measured in SANS
  – Simulation & Optimization

• Simulation
  – Theoretical SANS scattering profiles calculations from various models
    • Analytical models
    • Geometric shaped simple and complex space-filling models
    • High-resolution structures
WBS task list coverage

- 8.2.2  1D model fitting
- 8.3.1  Rotationally averaged 2-D scattering pattern
- 8.3.2  Build single-shaped real-space models in 3D
  Build oriented complex models from single-shaped models in 3D
- 8.3.3  Constrained fitting by use of data from other experimental techniques
- 8.4.1.3 Advanced analysis interface design (partially)
Use Case Diagram

User

Get I(Q)

extend

Build Analytical Models

extend

Build Space Filling Models

extend

Import PDB files
Required components

Rotation & shifts

Space-filling single geometric model builder

Space-filling complex model builder

The Cartesian coordinates from PDB file

If incomplete

Coarse graining model for high-resolution structures

If complete

$I(Q)$ calculation through Fourier transform of $P(r)$

Analytical form factor calculation

$I(Q)$
Details of Components

I(Q) calculation through fourier transform of P(r)

INTERFACE:

METHODS:

IQ = getIQ(coor, qmax, numI)

INPUT:

coor is a 2D array with 4 columns, Cartesian coordinates X Y Z & SLD
dmax is a double, is required for I(Q) calculation
numI is a int, is required for I(Q) calculation

OUTPUT:

IQ is a 2D array with 2 columns Q vs I.

IMPLEMENTATION:

DESCRIPTION:

Will calculate distance distribution function from a set of points with Cartesian coordinates, and do the fourier transform to get I(Q) (arbitrary unit)

ERRORS:
Get $I(Q)$ from three different models for protein apoferritin:

$$P(q) = \frac{\text{scale}}{V_s} \left[ \frac{3V_s(\rho_s - \rho_e)j_l(qr_c)}{qr_c} + \frac{3V_s(\rho_s - \rho_{\text{sol}})j_l(qr_s)}{qr_s} \right]^2 + \text{bkg}$$

**Space-filling shell**

**Crystal structure**
Results Validation

• Reproduce the results from program IGOR & LORES
• IGOR test cases for each shape
• Examples for LORES:
  – Protein apoferritin (hollow sphere)
  – Protein ribonuclease S. (ellipsoid)
  – A 10-mer DNA duplex (double helix)