



SansView: A new platform for SANS data analysis

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Introduction

A new small angle neutron scattering (SANS) data analysis package based on an open source model is being developed as part of the DANSE software project. The newly released beta version of the software includes most of the functionalities currently supported by the NIST IgorPro SANS package as well as allowing fitting of 2D anisotropic scattering patterns. Some of the planned enhancements include support for experiment simulations, advanced constrained fitting, parametric analysis, and calculating the scattering from MC and MD outputs.

The infrastructure is modular and flexible and is designed to allow plug-ins for easy extension by expert users, particularly for new models or polydispersity functions. Currently, both the simple SciPy optimization engine and the much more powerful PARK optimization engine, also being developed as part of the DANSE project, are supported.

<http://danse.chem.utk.edu/sansview.html>

Goal

Our mission is to provide a user friendly, freely distributed, open source framework for SANS analysis in order to help optimize the information extracted from SANS data. Our aim is to provide all the standard tools used today as well as new and more advanced features while encouraging the community contributions necessary for long term viability of the package as an engine for continuously advancing the state of the art in analysis.

Features

- ✓ **Ease of use for novice**
- ✓ **Power for expert users**
- ✓ **Easily extended by power users**
- ✓ **Loading data:**
Formats: 1D) ASCII (.txt, .abs) and CANSASxml.
2D) ASCII (from NIST IgorPro reduction package).
- ✓ **Data fitting:**
1D and 2D fitting
MC optimizer (PARK) and Scipy optimizer for fitting
Single and combined constrained fitting
Instrumental smearing (using dQ) supports pinhole and slit resolutions.
Polydispersity and angular distribution (2D)
- ✓ **Modeling:**
1D and 2D modeling
- ✓ **User defined functions:**
Support user functions written in python code
- ✓ **Saving data:**
Formats: ASCII and CANSAS xml

Model functions

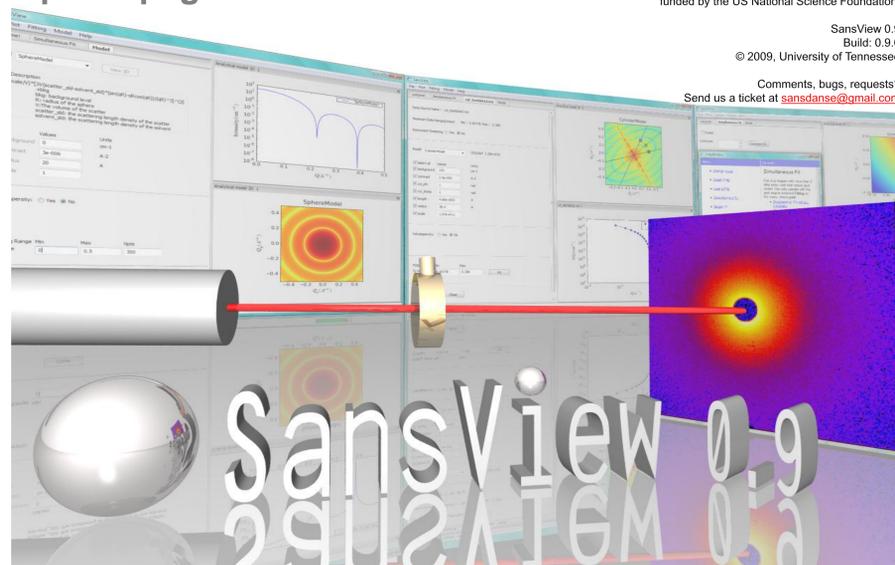
- **Shapes:** sphere, cylinder, ellipsoid, core shell sphere, core shell cylinder, and elliptical cylinder
- **Shape independent:** Debye, Guinier, Porod, fractal, power law, Teubner Stray, Lorentz, DBA, and BE polyelectrolyte
- **Structure factors:** hard sphere, square well, sticky hard sphere, and Hayter Penfold MSA
- **Customized models:** write your own model functions

Splash page

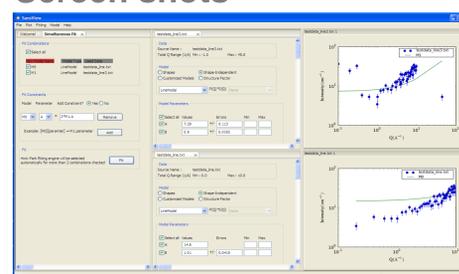
This software was developed by the University of Tennessee as part of the Distributed Data Analysis of Neutron Scattering Experiments (DANSE) project funded by the US National Science Foundation.

SansView 0.9
Build: 0.9.0
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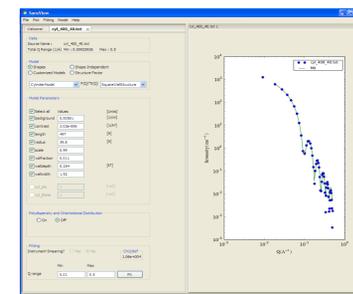
Comments, bugs, requests?
Send us a ticket at sansdanse@gmail.com



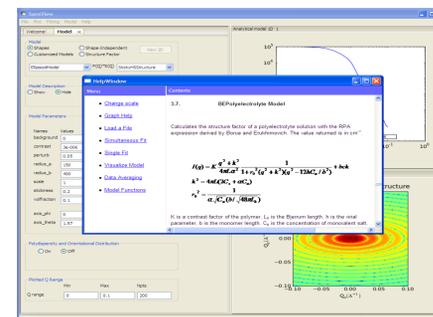
Screen shots



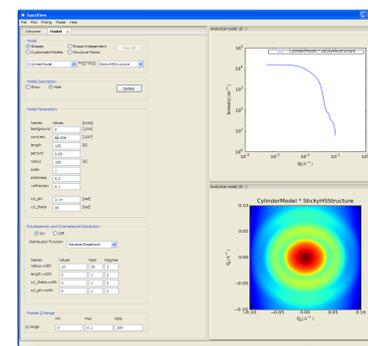
Simultaneously constrained fitting



Fitting with P(Q)*S(Q)



Function descriptions in the help menu



1D and 2D modeling

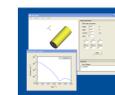
Distribution of software

- ✓ **Stand alone Windows application:**
Easy to install
User friendly graphical interface
- ✓ **Downloadable source code (python and C)**

Visit us to download at <http://danse.chem.utk.edu/sansview.html>

Other prototype applications

- **SimView:** 2D simulation of I(Q) for oriented systems.
- **PrView:** Compute P(r) from a measured I(Q) distribution.



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Release plan

- Feb 2010: Analysis application v2.0
- Integrated instrument simulation with 1D and 2D models
 - Parametric analysis
 - P(r) inversion
 - Ab-initio fitting (shape reconstruction)

Acknowledgement

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