

SANS and USANS Practical

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Science. Ingenuity. Sustainability.

The Basic Scattering Equation

For an ensemble of identical, randomly oriented particles, the intensity of coherently, elastically scattered radiation is dependant only upon the magnitude of q , and can be expressed as:

$$I(q) = N(\Delta\bar{\rho}V)^2 P(q)S(q)$$

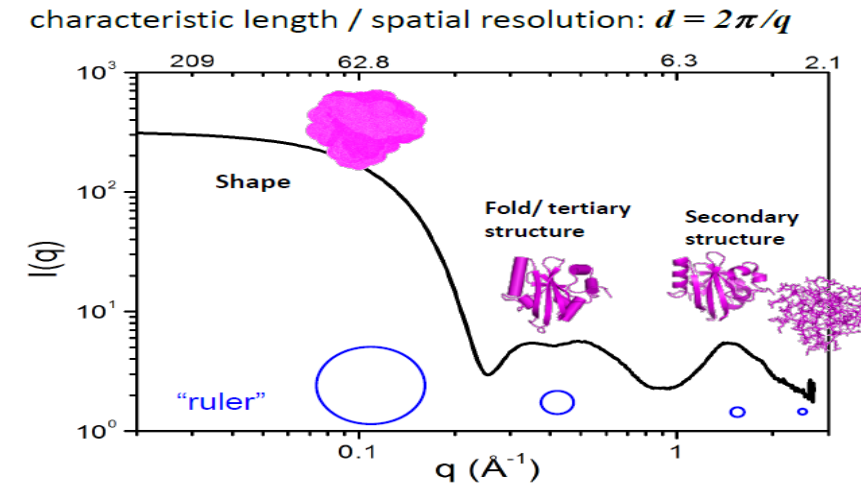
N = molecules/unit volume

V = molecular volume

$\Delta\bar{\rho} = \langle \rho(\mathbf{r}) \rangle - \bar{\rho}_s$ = contrast, the scattering density difference
between the scattering particle and solvent

$P(q)$ = form factor $\Rightarrow$ particle shape

$S(q)$ = structure factor $\Rightarrow$ inter-particle correlation distances



Analysis

- Data Collection
 - Good plan, good sample preparation, best use of beamtime
 - Strategy
- Data Reduction
 - Instrumental parameters
 - At facility
- Data Analysis
 - Basic information
 - Software

Data Analysis

- Scattering Length Density (SLD)
 - [NIST Calculator](https://www.ncnr.nist.gov/resources/activation/) (<https://www.ncnr.nist.gov/resources/activation/>)
 - [ISIS Biomolecular SLD calculator](http://psldc.isis.rl.ac.uk/Psldc/) (<http://psldc.isis.rl.ac.uk/Psldc/>)
- Reading
 - [NIST SANS tutorials](#)
 - [SANS toolbox](#)
- Analysis software
 - [IGOR macros](#)
 - [SasView](#)
 - [ATSAS](#)
 - [SASfit](#)

Data Analysis

- Scattering Length Density (SLD)

- [NIST Calculator](https://www.ncnr.nist.gov/resources/activation/) (<https://www.ncnr.nist.gov/resources/activation/>)

Neutron Activation and Scattering Calc: X

ncnr.nist.gov/resources/activation/

Apps ★ Bookmarks Imported From Firefox

NIST Center for Neutron Research

Home Instruments Science

Material
Co

Neutron Activation

For rabbit system

Thermal flux: 1e8 Cd ratio: 0 Thermal/fast ratio: 0
Mass: Time on beam: 10 Time off beam: 1 y

Absorption and Scattering

Density: Thickness:
Source neutrons: Source X-rays:
1 Ang Cu Ka

Neutron activation and scattering calculator

This calculator uses neutron cross sections to compute activation on the sample given the mass in the sample and the time the sample.

1. Enter the sample formula in the material panel.
2. To perform activation calculations, fill in the thermal flux, the mass, the time on and off the beam, then press the calculate button.
3. To perform scattering calculations, fill in the wavelength of the neutron and/or x-rays, the thickness and the density (if applicable).

Chemical formula

The chemical formula parser allows you to specify materials and mixtures. Formulas are parsed with [periodictable](#) python module.

NIST Center for Neutron Research

Home Instruments

Material
H2O

Thickness
Units: cm
The material thickness in cm is

Neutron Activation

For rabbit system

Thermal flux: 1e8 Cd ratio: 0 Thermal/fast ratio: 0
Mass: Time on beam: 10 Time off beam: 1 y

Absorption and Scattering

Density: Thickness:
Source neutrons: Source X-rays:
1 Ang Cu Ka

Source neutrons
Units: Ang, meV or m/s
The energy of the source neutrons in m/s.
Neutron cross sections are tabulated for many materials.

Scattering from H2O

Source neutrons: $1.000 \text{ \AA} = 81.80 \text{ meV} = 3956 \text{ m/s}$

Source X-rays: $1.542 \text{ \AA} = 8.042 \text{ keV}$

Sample in beam: H2O at 1.00 g/cm^3

1/e penetration depth (cm)	Scattering length density ($10^{-6}/\text{\AA}^2$)	Scattering cross section (1/cm)	X-ray SLD ($10^{-6}/\text{\AA}^2$)
abs	80.836	real	-0.561
abs+incoh	0.178	imag	-0.000
abs+incoh+coh	0.177	incoh	21.180
		coh	0.004
		abs	0.012
		incoh	5.621
		real	9.469
		imag	-0.032

Neutron transmission is 56.93% for 0.1 cm of sample (after absorption and incoherent scattering).
Transmitted flux is $5.693 \times 10^7 \text{ n/cm}^2/\text{s}$ for a $1 \times 10^8 \text{ n/cm}^2/\text{s}$ beam.

Questions?

Neutron activation: NCNR Health Physics <hp@nist.gov>

Scattering calculations: Paul Kienzie <paul.kienzie@nist.gov>



Biomolecular Scattering Length Density Calculator

TITLE:

- Type of biomolecule :
- ☒ Protein / Peptide
 - ☐ RNA (A,U,G,C)
 - ☐ DNA (A,T,G,C)

Primary structure:

Submit

Reset

OPTIONS:

1. Solution D₂O% *¹

100

2. Deuteration % *²

0

3. Exchange % *³

90

4. Concentration of sample (mg/mL) *⁴

0

*¹ Default is 100% D₂O - assumes scattering is taking place in 100% D₂O

*² This value is the percentage deuteration of the non-labile hydrogens covalently bonded to carbon atoms.

*³ This is the percentage of labile hydrogens (bonded either to the side chains or amide backbone) that can exchange with the solution - please refer to the manual for a full description. For example, if we have 100% exchange in a 100% D₂O solution, all labile hydrogens will be deuterium. If we have 100% exchange in a 50% H₂O : D₂O solution, 50% of the labile hydrogens would be deuterium.

The exchange box is set to a default of 90% labile hydrogen exchange, this is an estimate for proteins.

*⁴ This allows an estimate of the intensity of theoretical scattering at zero angle I(0) to be determined.

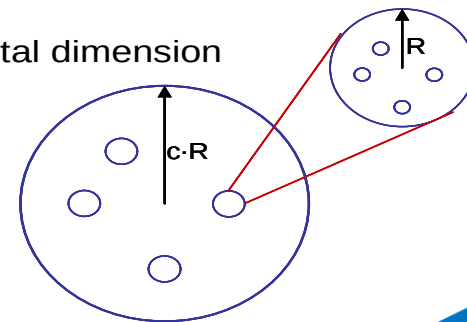
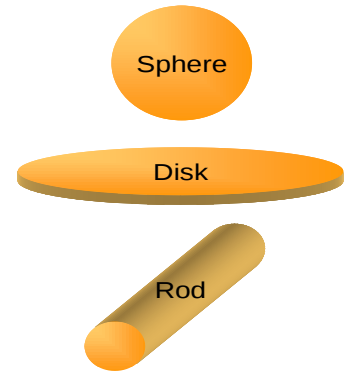
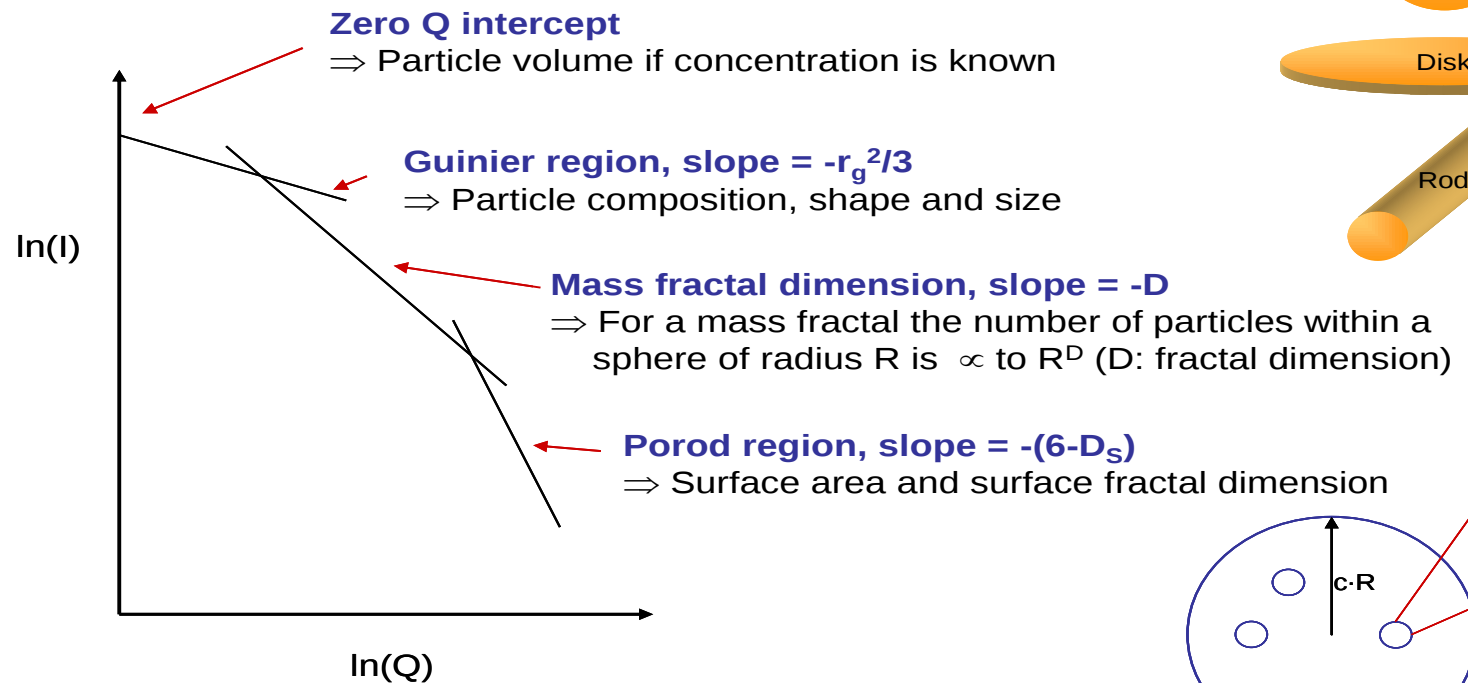
[The Protein Scattering length density calculator licence](#)
[The Protein Scattering length density calculator manual](#)

If you have any comments / questions please email either [Dr Daniel Myatt](#) or [Dr Luke Clifton](#)

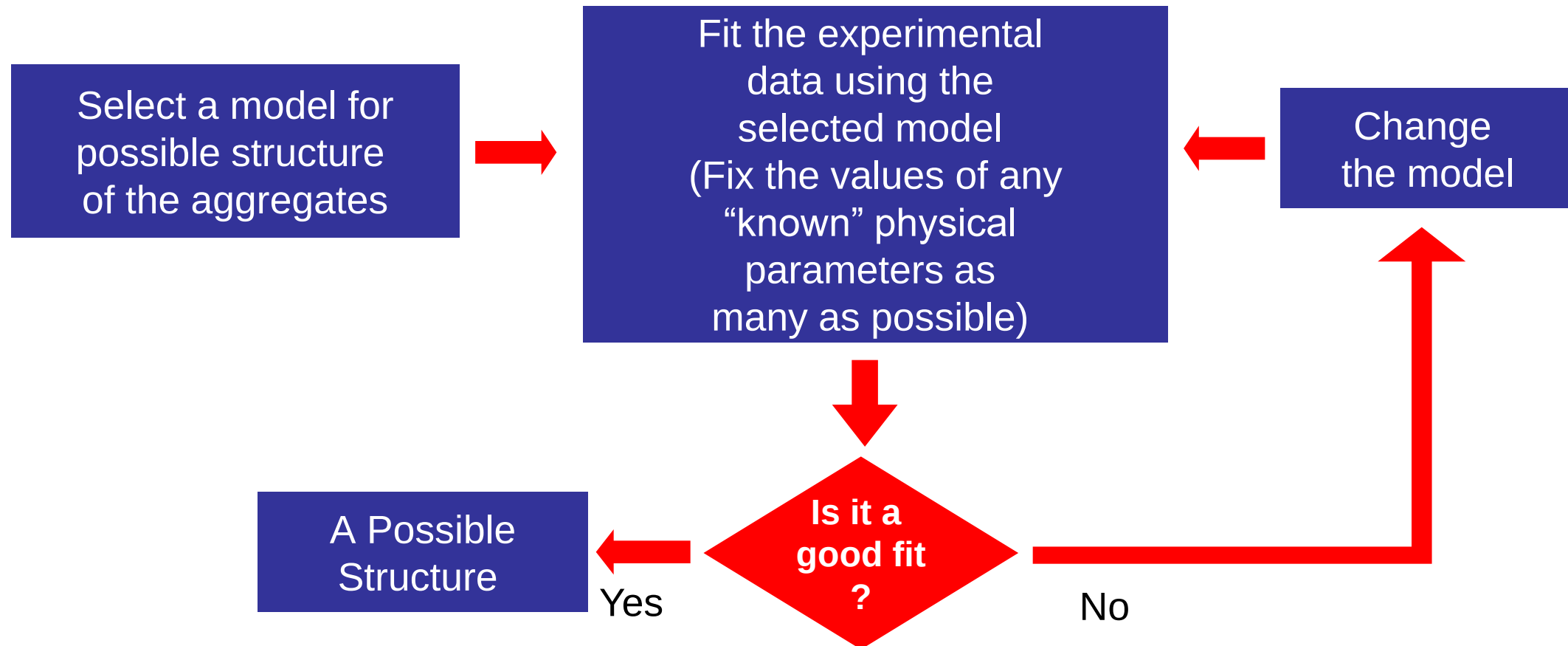
This website has been tested on Mozilla Firefox v21.0, Google Chrome v27.0 & IE v10.0. IE v8.0 and below may not display the images correctly.

Typical Intensity Plot for SAS

Porod Exponent D	
4	Particles with smooth surfaces
3	Very rough surfaces, also "collapsed" polymer chains (in a bad solvent)
5/3	"Fully swollen" chains (in a good solvent)
2	Gaussian polymer chains or two-dimensional structure (such as lamellae or platelets)
1	Stiff rod (or thin cylinder)
< 3	"Mass fractals"
$3 \leq D \leq 4$	"Surface fractals"



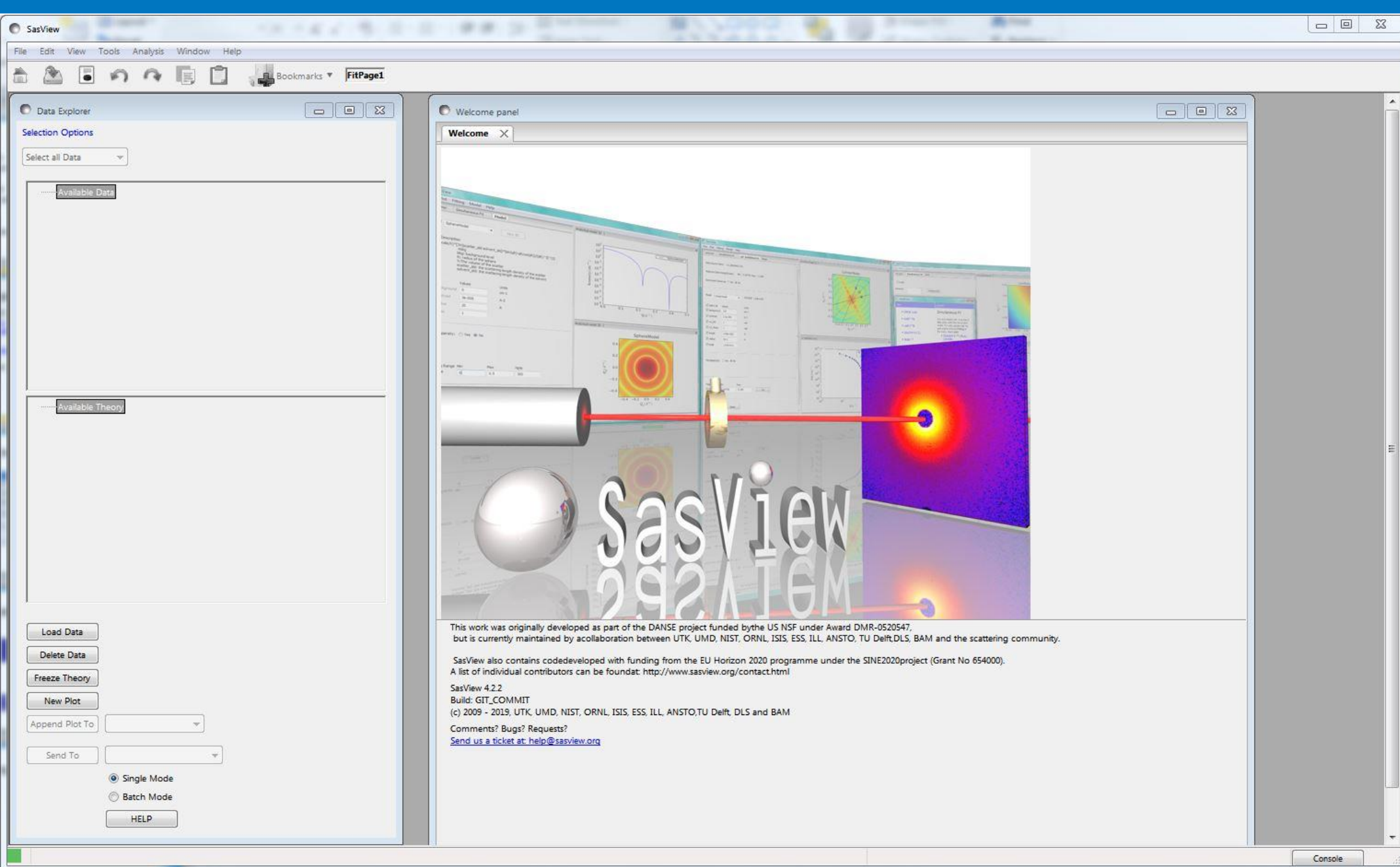
SAS Analysis

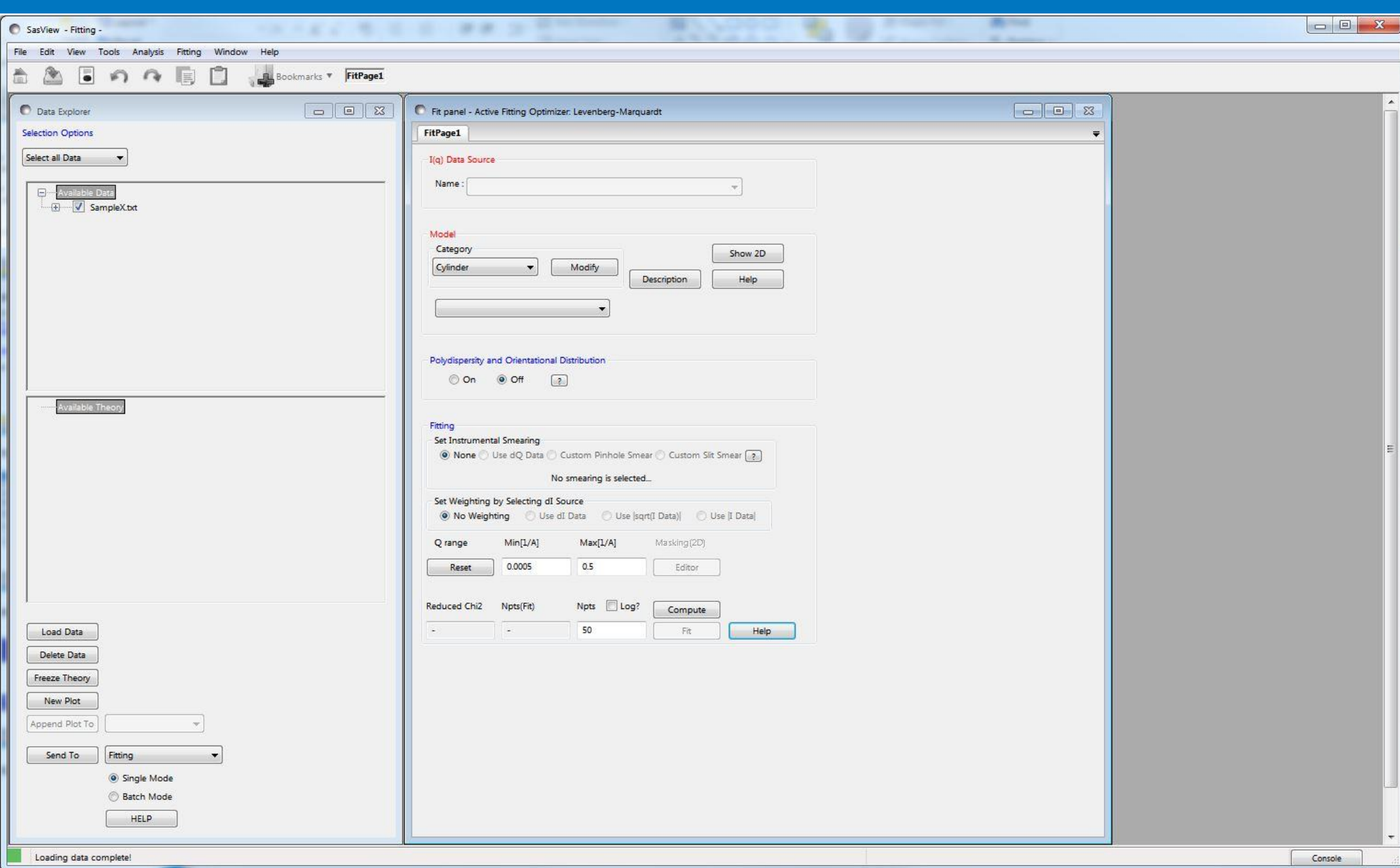


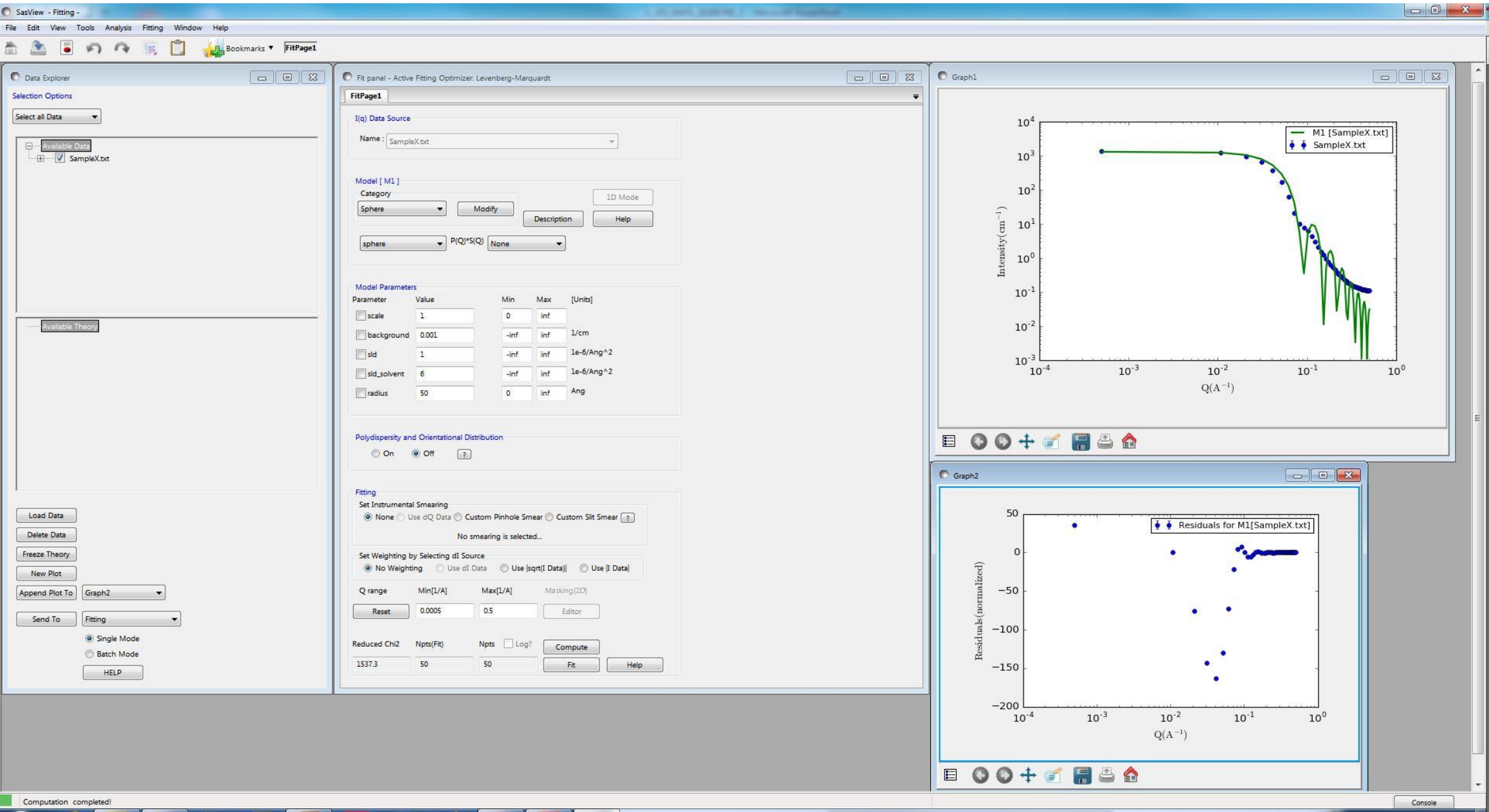
Data Fitting

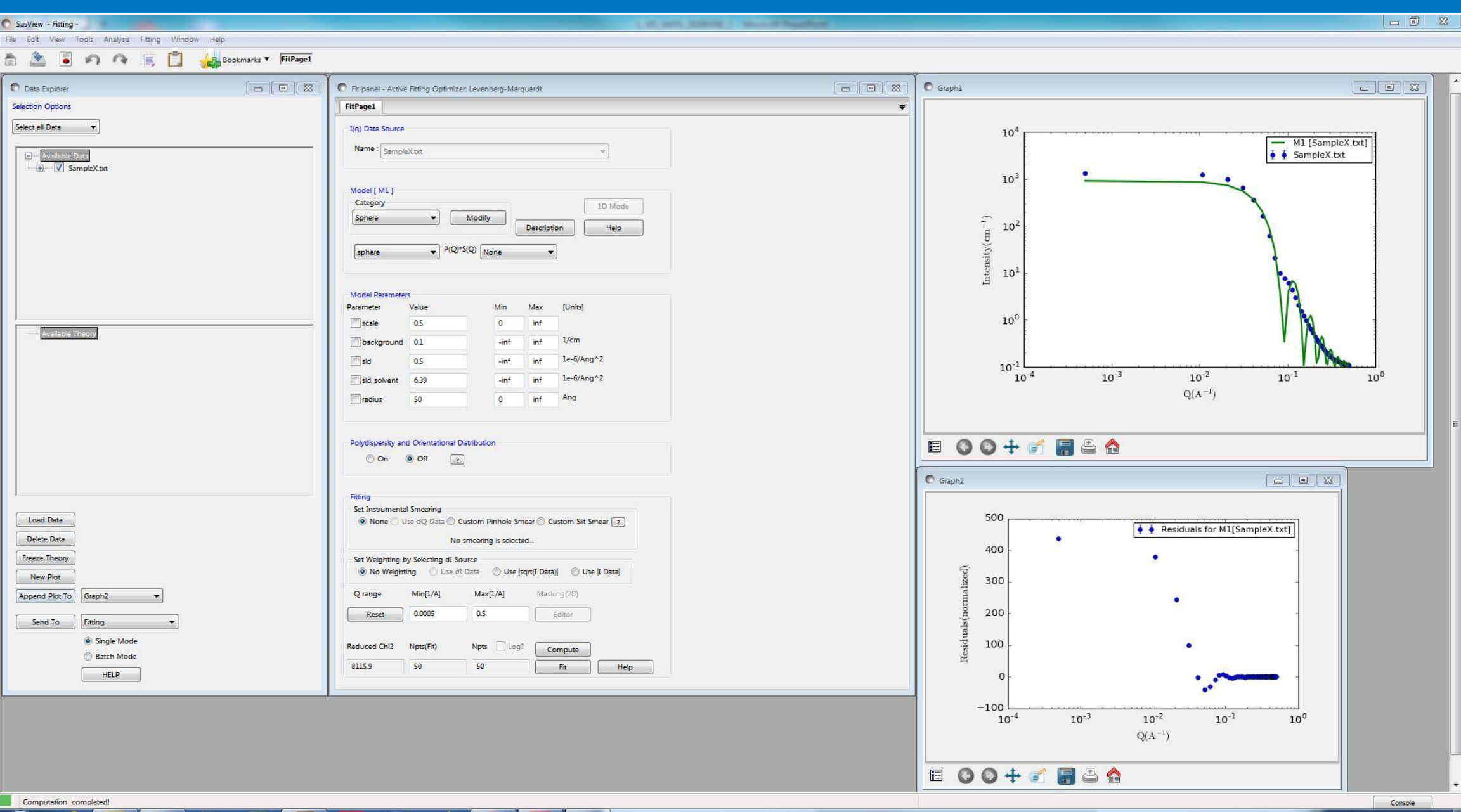
■ SasView

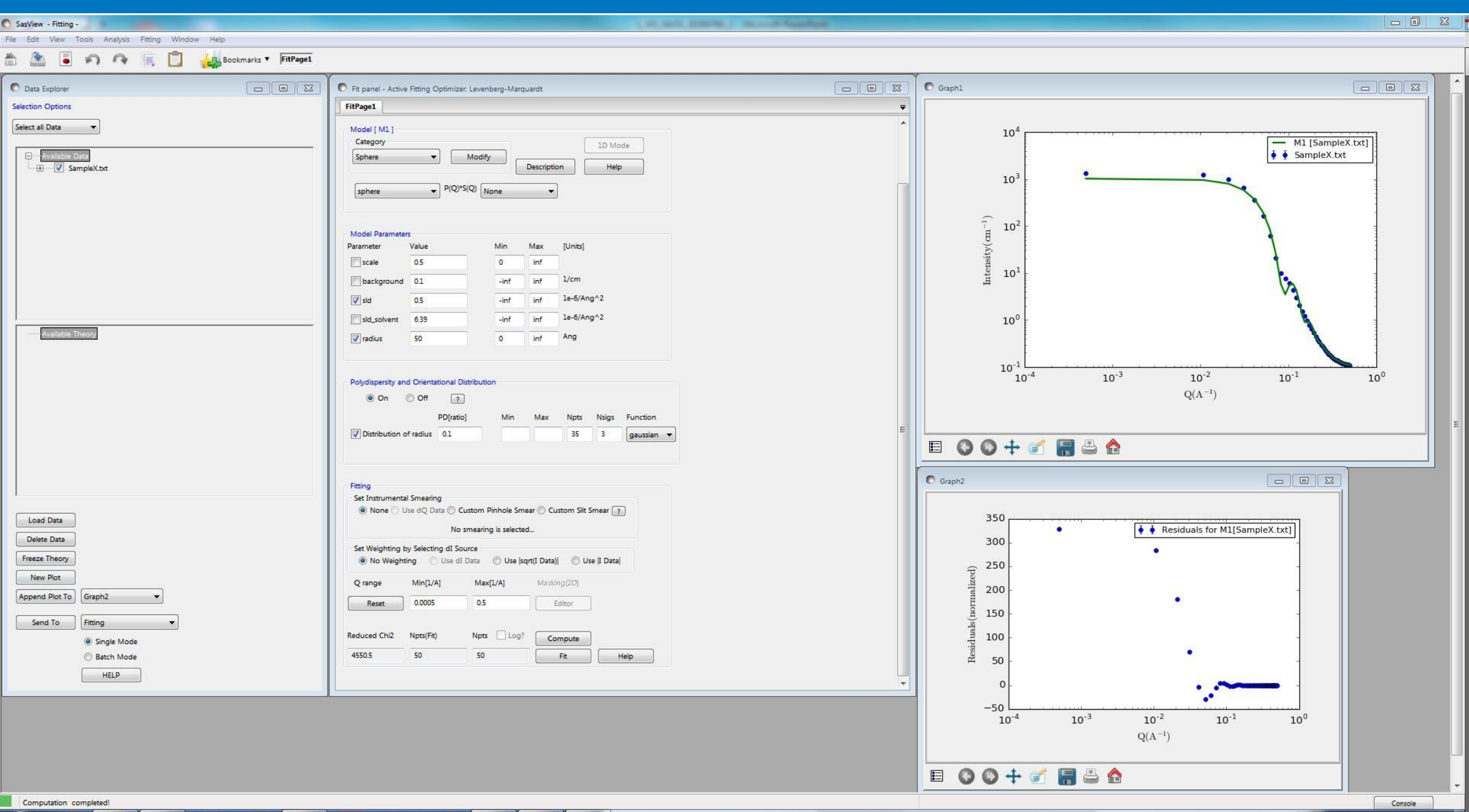
- Download software from <https://www.sasview.org/>
- “SasView is a Small Angle Scattering Analysis Software Package, originally developed as part of the NSF DANSE project under the name SansView, now managed by an international collaboration of facilities. Feedback and contributions are welcome and encouraged”.

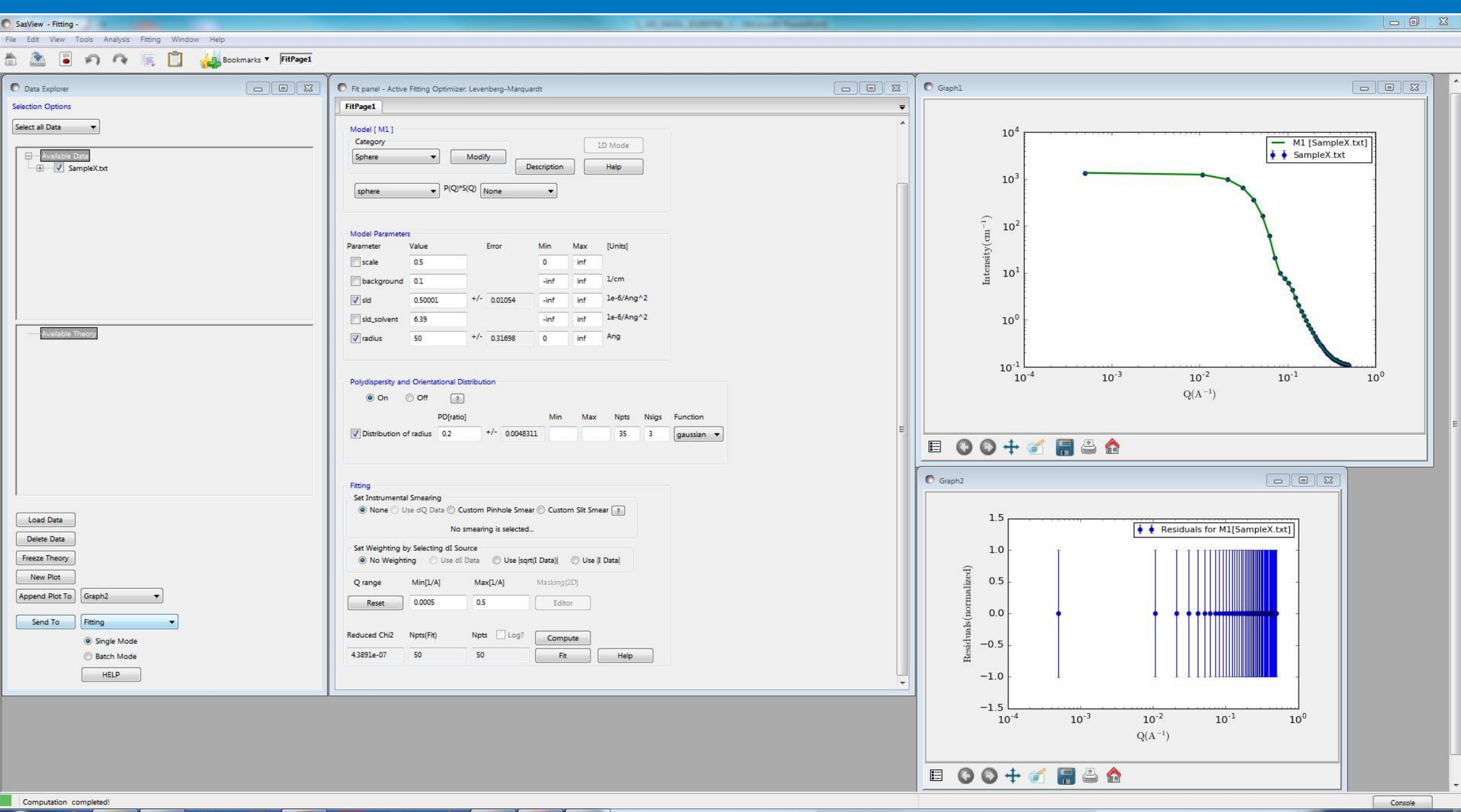












“Homework”

- Send me your answers as private chat (in zoom).
- Calculate neutron SLD and neutron transmission for the followings, (You need physical densities (google?). Samples are 1mm thick. Neutron $\lambda=5\text{\AA}$)
 - D_2O
 - $\text{C}_{12}\text{H}_{25}\text{NaSO}_4$ (Extra points for the name, and use)
 - $\text{C}_{16}\text{H}_{34}$ and $\text{C}_{16}\text{D}_{34}$
 - SiO_2

Questions?

