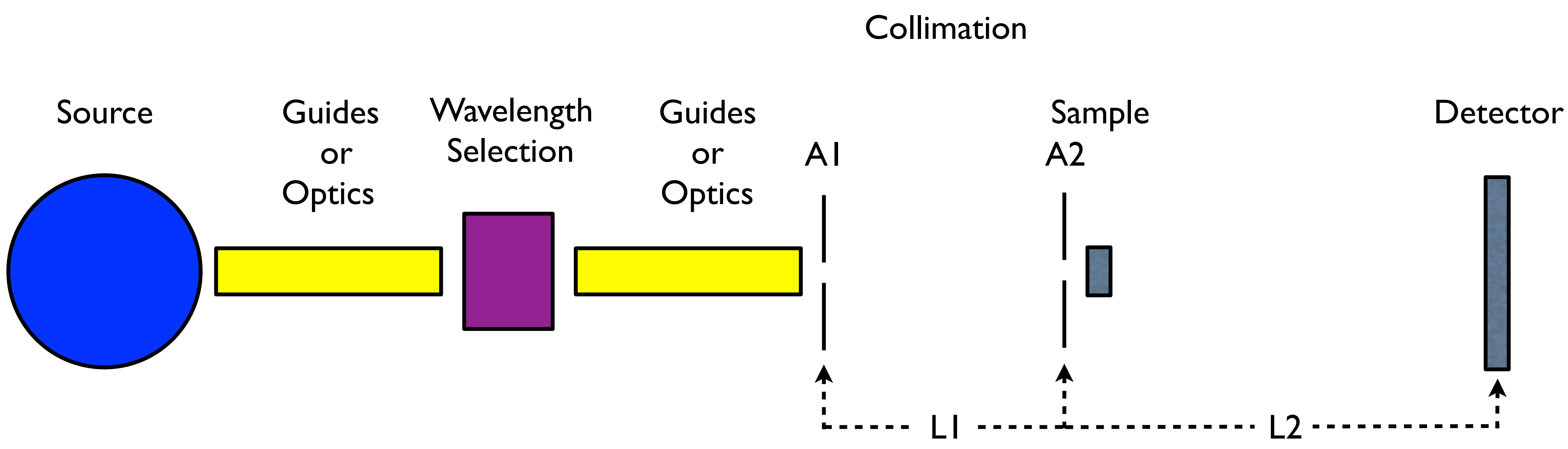
SasView : A Small Angle Scattering Analysis Software Package

Andrew Jackson, European Spallation Source
on behalf of the SasView Collaboration

SANS Refresher

Anatomy of a SAS Instrument

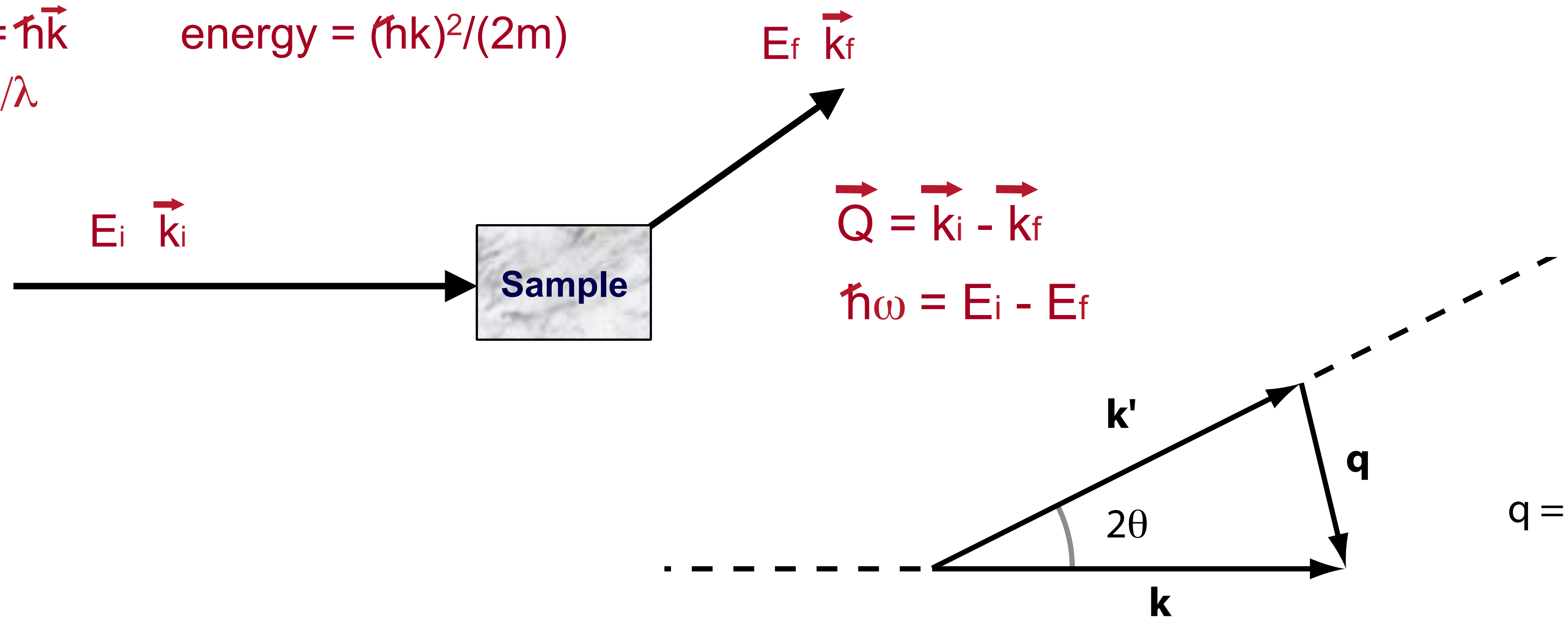


What do we measure?

momentum $= \hbar \vec{k}$

$k = 2\pi/\lambda$

energy $= (\hbar k)^2/(2m)$



$\vec{Q} = \vec{k}_i - \vec{k}_f$

$\hbar\omega = E_i - E_f$

$$\sin\theta = \frac{|\mathbf{q}|}{2}\frac{1}{|\mathbf{k}|}$$

$$q = 2k\sin\theta = \frac{4\pi}{\lambda}\sin\theta$$

Measure number of neutrons scattered as function of Q and ω

Intensity of scattering as function of Q is related to the Fourier transform of the spatial arrangement of matter in the sample => Correlations in **Space**

Intensity of scattering as function of ω is related to the Fourier transform of the temporal arrangement of matter in the sample => Correlations in **Time**

Small Angle Scattering

Having determined that we can use scattering length density to describe our samples, we can replace the sum in

$$\frac{d\sigma}{d\Omega}(\mathbf{q}) = \frac{1}{N}\left|\sum_{i}^{N} b_i e^{i\mathbf{q}\cdot\mathbf{r}}\right|^2$$

with the integral of the SLD distribution across the whole sample and normalize by the sample volume thus:

$$\frac{d\Sigma}{d\Omega}(\mathbf{q}) = \frac{N}{V}\frac{d\sigma}{d\Omega}(\mathbf{q}) = \frac{1}{V}\left|\int_V \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r}\right|^2$$

This is the "Rayleigh-Gans Equation" and shows us that small angle scattering arises as a result of **inhomogeneities in scattering length density.**

Form and Structure Factors

In small angle scattering we confuse terminology by often splitting the scattering structure factor into a **Form Factor**, P(q) and a **Structure Factor**, S(q) when considering particulate systems :

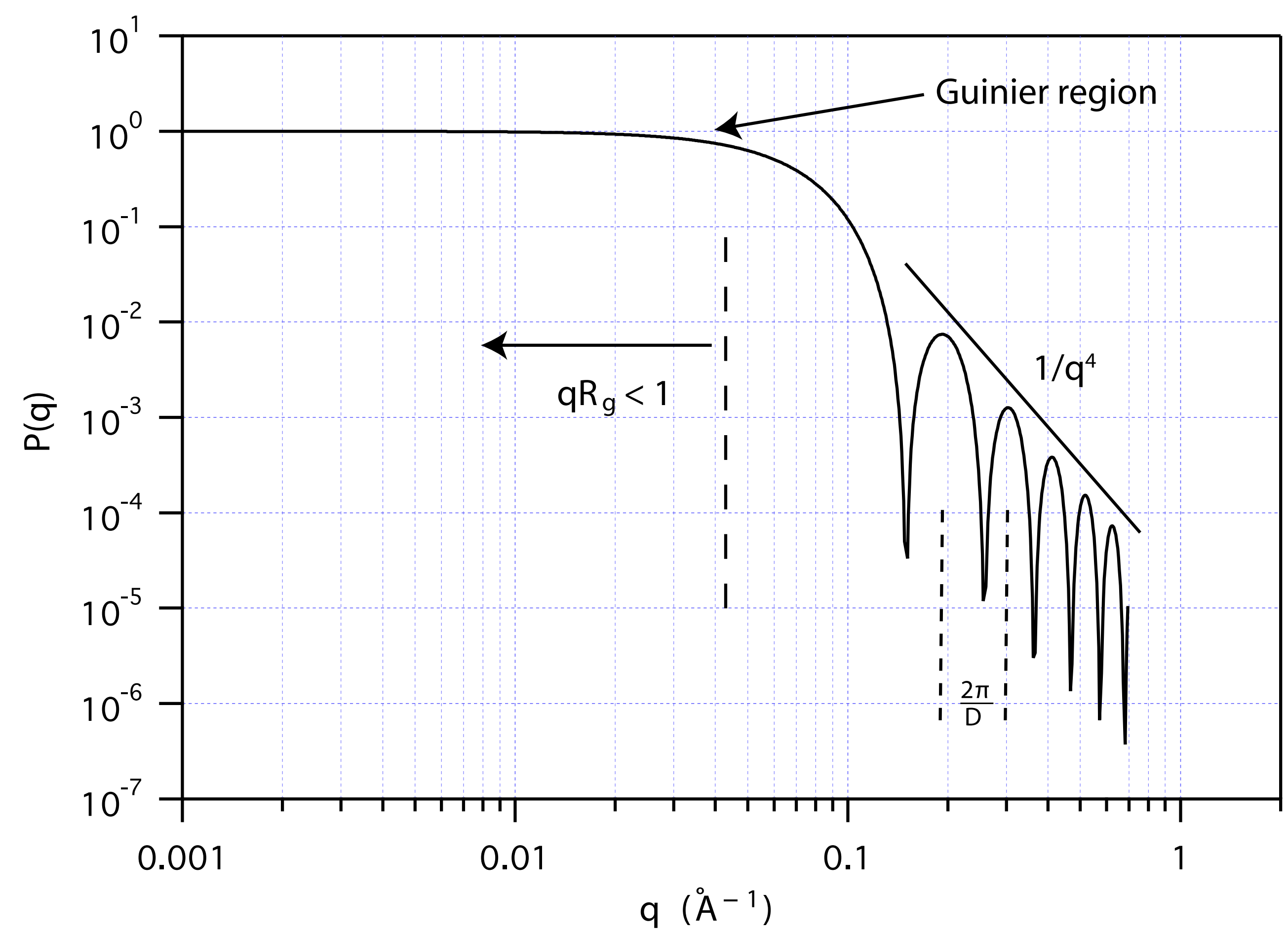
$$\frac{d\Sigma}{d\Omega}(q) = \frac{N}{V}(\rho_1 - \rho_2)^2 V_p^2 P(q) S(q)$$

P(q) represents the interference of neutrons scattered from different parts of the same object, while S(q) represents interference between neutrons scattered from different objects. If there is no interparticle correlation (e.g. it is a dilute solution) then S(q) = 1.

If we have an isotropic solution then

$$S(q) = 1 + 4\pi N_p \int_0^\infty [g(r) - 1] \frac{\sin(qr)}{qr} r^2 dr$$

where g(r) is the particle pair correlation function and is related to the interaction potential between particles.



The form factor for a sphere (shown above) is given by:

$$P(q) = \left[\frac{3(\sin(qr) - qr\cos(qr))}{(qr)^3}\right]^2$$

Form and Structure Factors

The form factor for a cylinder is given by:

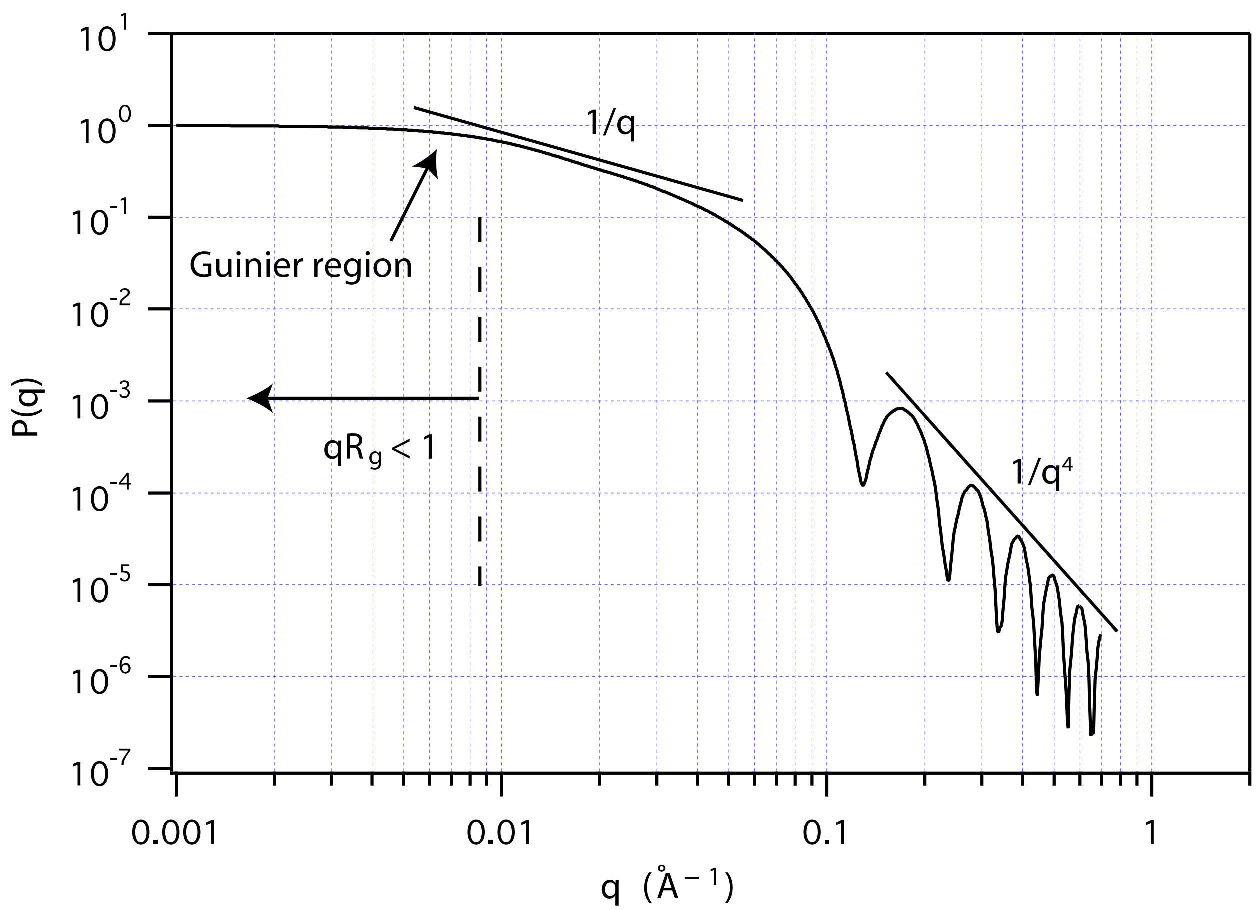
$$P(q) = \int_0^{\pi/2} f^2(q,\alpha)\sin\alpha d\alpha$$

$$f(q,\alpha) = j_0(qHcos\alpha)\frac{J_1(qr\sin\alpha)}{(qrsin\alpha)}$$

$$j_0(x) = sin(x)/x$$

$$V_{cyl} = \pi r^2 L$$

where J_1 is the first order Bessel function and α is defined as the angle between the cylinder axis and the scattering vector q.



The radius of gyration of a cylinder is given by

$$R_g^2 = \frac{R^2}{2} + \frac{L^2}{12}$$

where R is the radius and L the length of the cylinder.

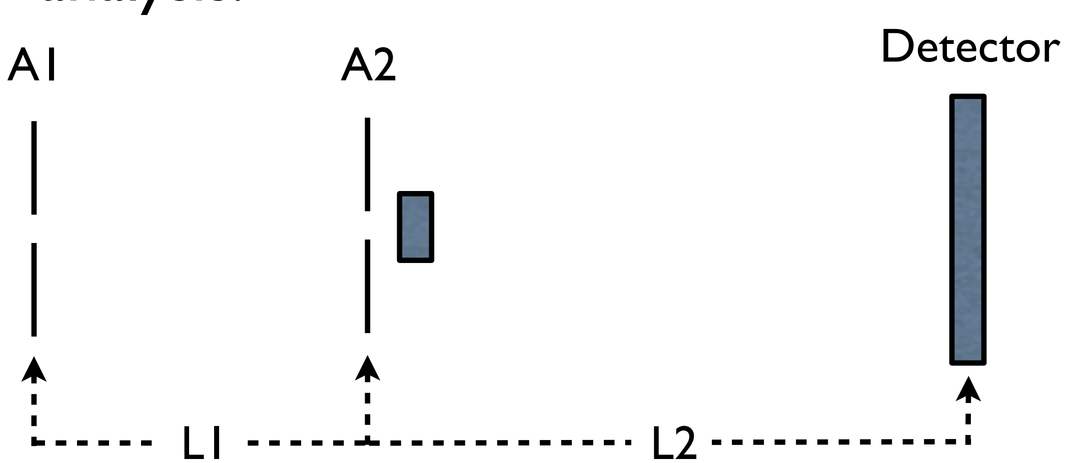
SANS Resolution

The intensity measured at each nominal Q value is, in fact, a sum of intensities from nearby Q vectors.

This is a result of the beam and the detector pixels having finite sizes, and the wavelength having a spread of values.

The effect is that the scattering that one would calculate is “**smeared**” by a **resolution function**.

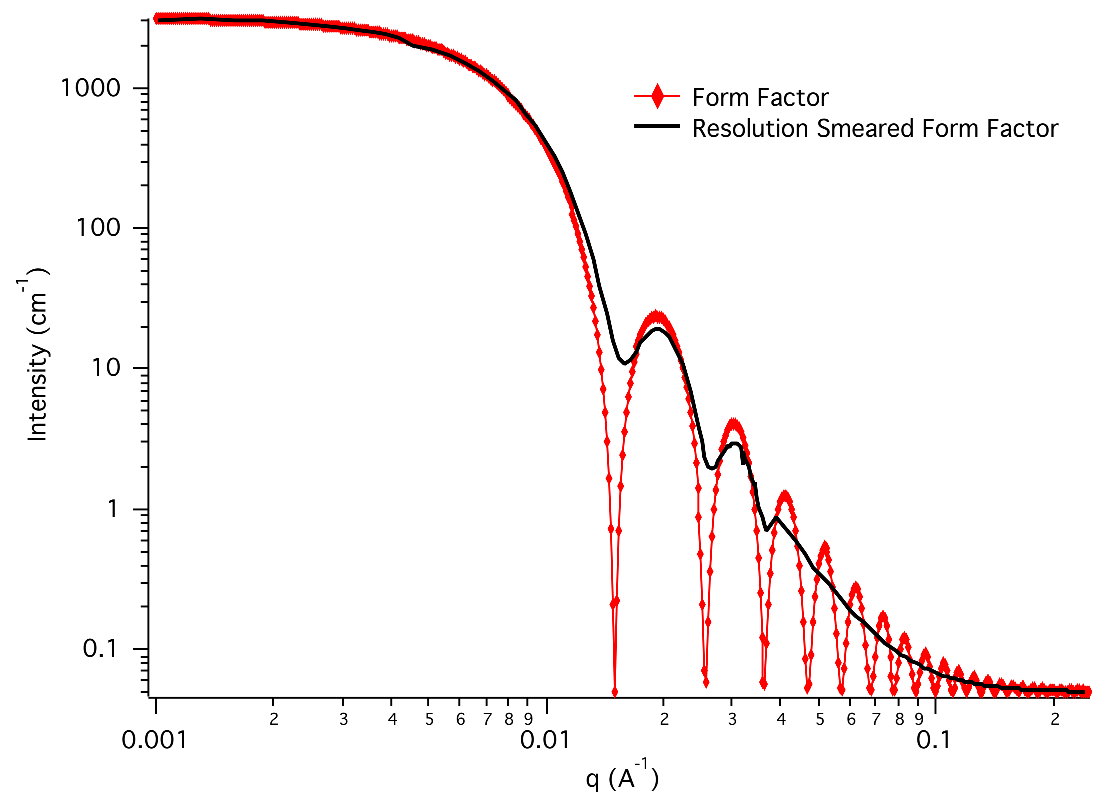
Difficult to “desmear” reliably, therefore smear model functions in analysis.



$$(\sigma_Q)^2 = \frac{1}{12}\left(\frac{2\pi}{\lambda}\right)\left[3\frac{R_1^2}{L_1^2} + 3\frac{R_2^2}{L'^2} + \frac{(\Delta R)^2}{L_2^2} + \frac{R^2}{L_2^2}\left(\frac{\Delta\lambda}{\lambda}\right)\right]$$

$$Q = \frac{2\pi\theta}{\lambda} = \frac{2\pi R}{\lambda L_2} \qquad L' = \frac{1}{L_1} + \frac{1}{L_2}$$

$$\left(\frac{\sigma_Q}{Q}\right)^2 = \left(\frac{R_1 L_2}{2RL_1}\right)^2 + \left(\frac{R_2(L_1+L_2)}{2RL_1}\right)^2 + \frac{1}{12}\left(\frac{\Delta R}{R}\right)^2 + \frac{1}{12}\left(\frac{\Delta\lambda}{\lambda}\right)^2$$



See Mildner & Carpenter, J. Appl. Cryst. 17, 1984 for the gory details.

SAS Data Analysis

Model Independent

We can use an approximation from Guinier

$$I(Q) = I(0)e^{-\frac{(QR_g)^2}{3}}$$

$$ln(I(Q)) = ln(I(0)) - \frac{R_g^2}{3}Q^2$$

to obtain the radius of gyration of the scattering objects assuming particulate scatterers and S(q) = 1.

Similar approximations can be made to get the cross section of cylinders or the thickness of disks. Various other model independent approaches exist to extract information from the data without a scattering model.

Indirect Fourier Transform

Since we are missing the phase information as a result of the differential cross section being related to the square of the amplitude of the fourier transform, we cannot simply take the fourier transform of our data to get back to ρ(**r**). Thus we must use an indirect method.

A popular implementation of this method is found in the *ATSAS suite* of software from Prof. Svergun's group. *SasView* also has an implementation of this method.

Model Dependent

We calculate the form and structure factors for a given scattering system and compare that with the measured scattering data. The model is fitted to the data to obtain the parameters that describe the scattering. We can simultaneously fit multiple contrasts to be able to study complex structures.

The software we will be using for this workshop is called *SasView* (http://www.sasview.org) and is being jointly developed by NIST, ILL, ISIS, SNS, ANSTO and ESS.
Other software packages for this kind of analysis include the *NIST Igor Macros* developed at the NCNR and *SasFit* developed at the Paul Scherrer Institute.

Ab-inito Structure Generation

An approach that is popular for bio-macromolecules in solution is to generate a structure from many sub-resolution spheres and calculate what the scattering would be. That is then compared with the data and the spheres redistributed. This is repeated until agreement is found.
The *ATSAS suite* is the primary example of software using this method

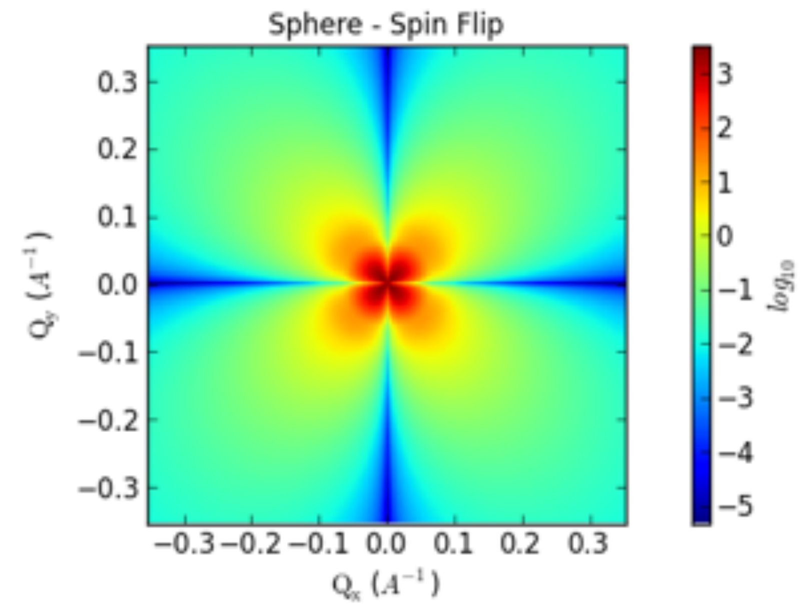
What is SasView?

SasView

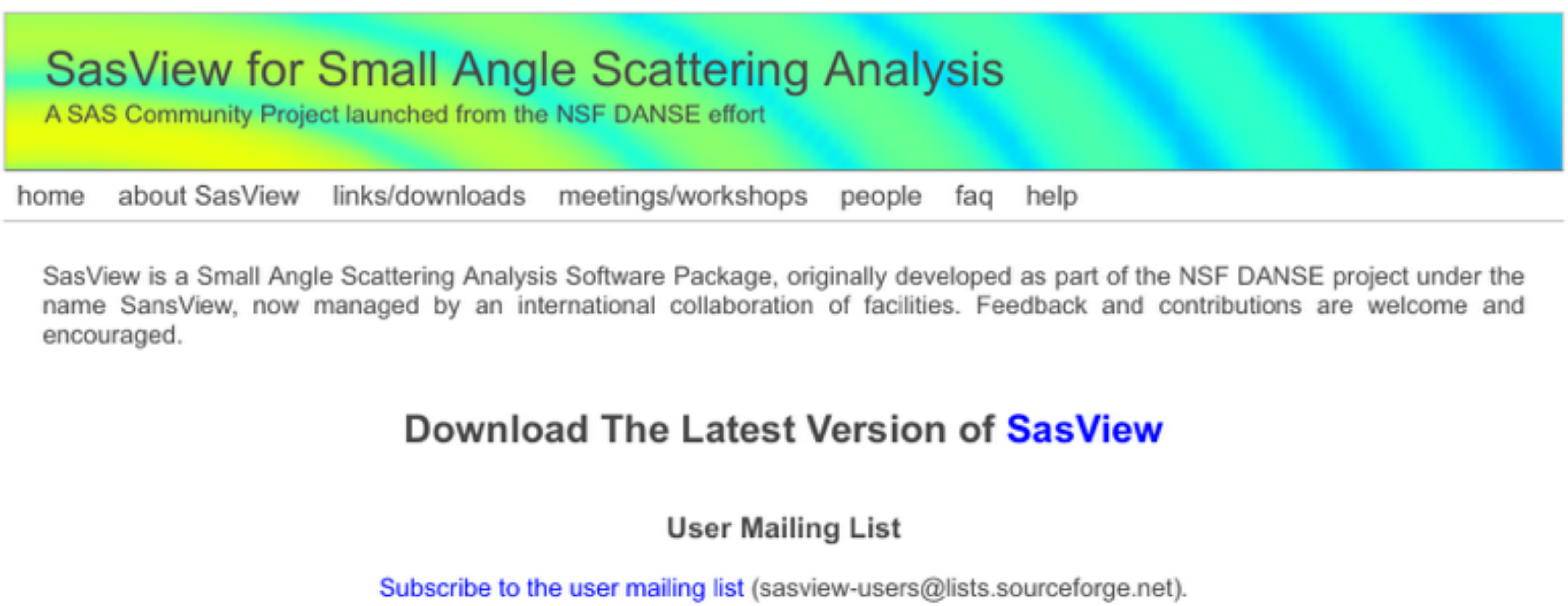
User friendly, open source analytical modeling of SAS data.

Current Release (3.1.2) Includes:

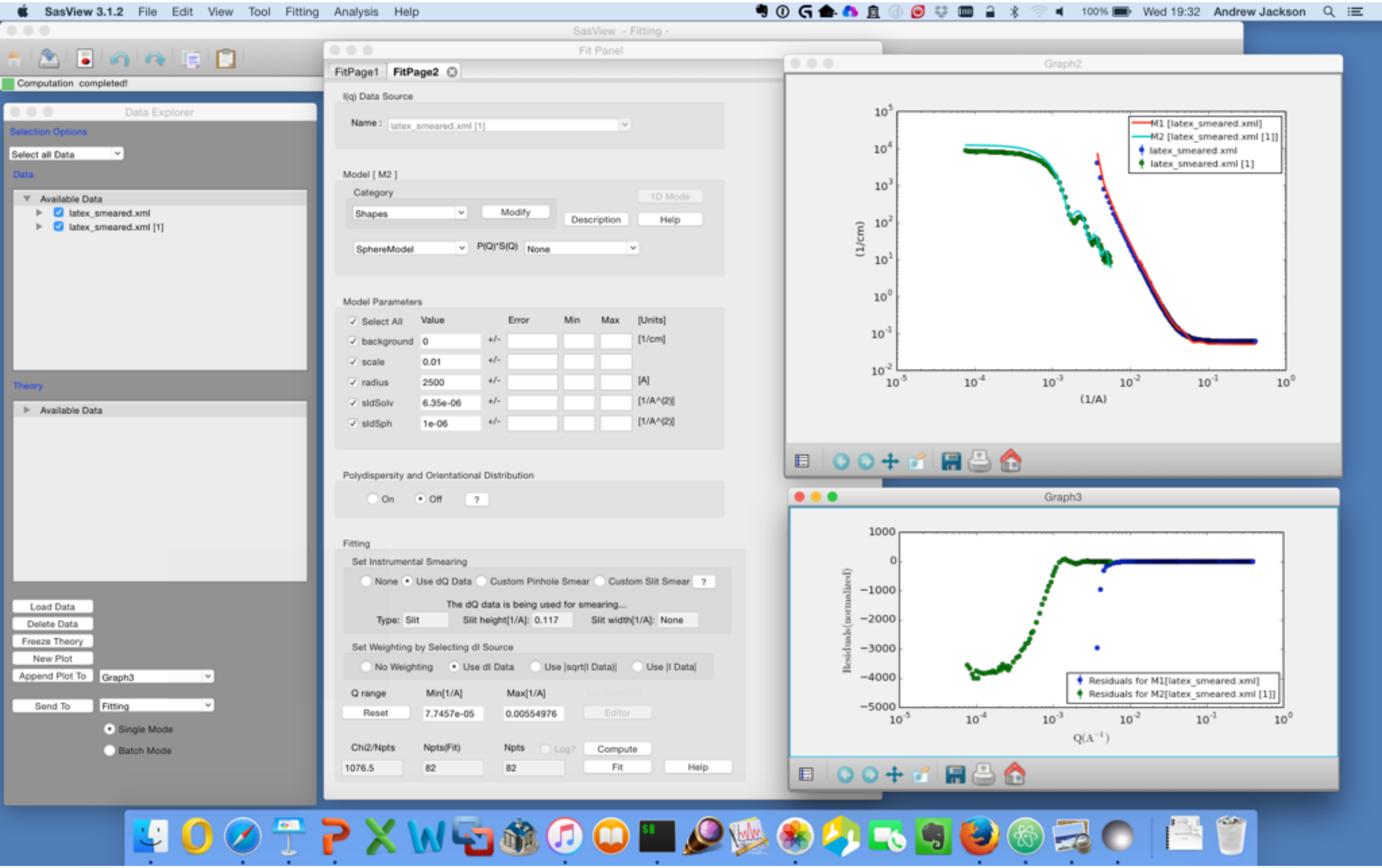
- Large number of 1D scattering models
- 2D analysis for oriented objects
- Batch mode
- Magnetic contrast with polarisation analysis
- Lots of extra tools



www.sasview.org



1D Analysis



SasView 3.1.2 File Edit View Tool Fitting Analysis Help
Wed 19:32 Andrew Jackson
SasView - Fitting -
Computation completed!
Data Explorer
Selection Options
Select all Data
Data
Available Data
latex_smeared.xml
latex_smeared.xml [1]
Theory
Available Data
Load Data
Delete Data
Freeze Theory
New Plot
Append Plot To
Graph3
Send To
Fitting
Single Mode
Batch Mode
Fit Panel
FitPage1
FitPage2
I(q) Data Source
Name :
Model [M2]
Category
Shapes
Modify
Description
Help
SphereModel
P(Q)*S(Q)
None
Model Parameters
Select All
Value
Error
Min
Max
[Units]
background 0 [1/cm]
scale 0.01
radius 2500 [A]
sldSolv 6.35e-06 [1/A^(2)]
sldSph 1e-06 [1/A^(2)]
Polydispersity and Orientational Distribution
On Off ?
Fitting
Set Instrumental Smearing
None Use dQ Data Custom Pinhole Smear Custom Slit Smear ?
The dQ data is being used for smearing...
Type: Slit Slit height[1/A]: 0.117 Slit width[1/A]: None
Set Weighting by Selecting dI Source
No Weighting Use dI Data Use |sqrt(I Data)| Use |I Data|
Q range Min[1/A] Max[1/A]
Reset 7.7457e-05 0.00554976
Chi2/Npts Npts(Fit) Npts
1076.5 82 82
Compute
Fit
Help
Graph2
M1 [latex_smeared.xml]
M2 [latex_smeared.xml [1]]
latex_smeared.xml
latex_smeared.xml [1]
(1/cm)
(1/A)
Graph3
Residuals(normalized)
Residuals for M1[latex_smeared.xml]
Residuals for M2[latex_smeared.xml [1]]
Q(A^-1)

1D Analysis

Load Data …

Select Data Sets …

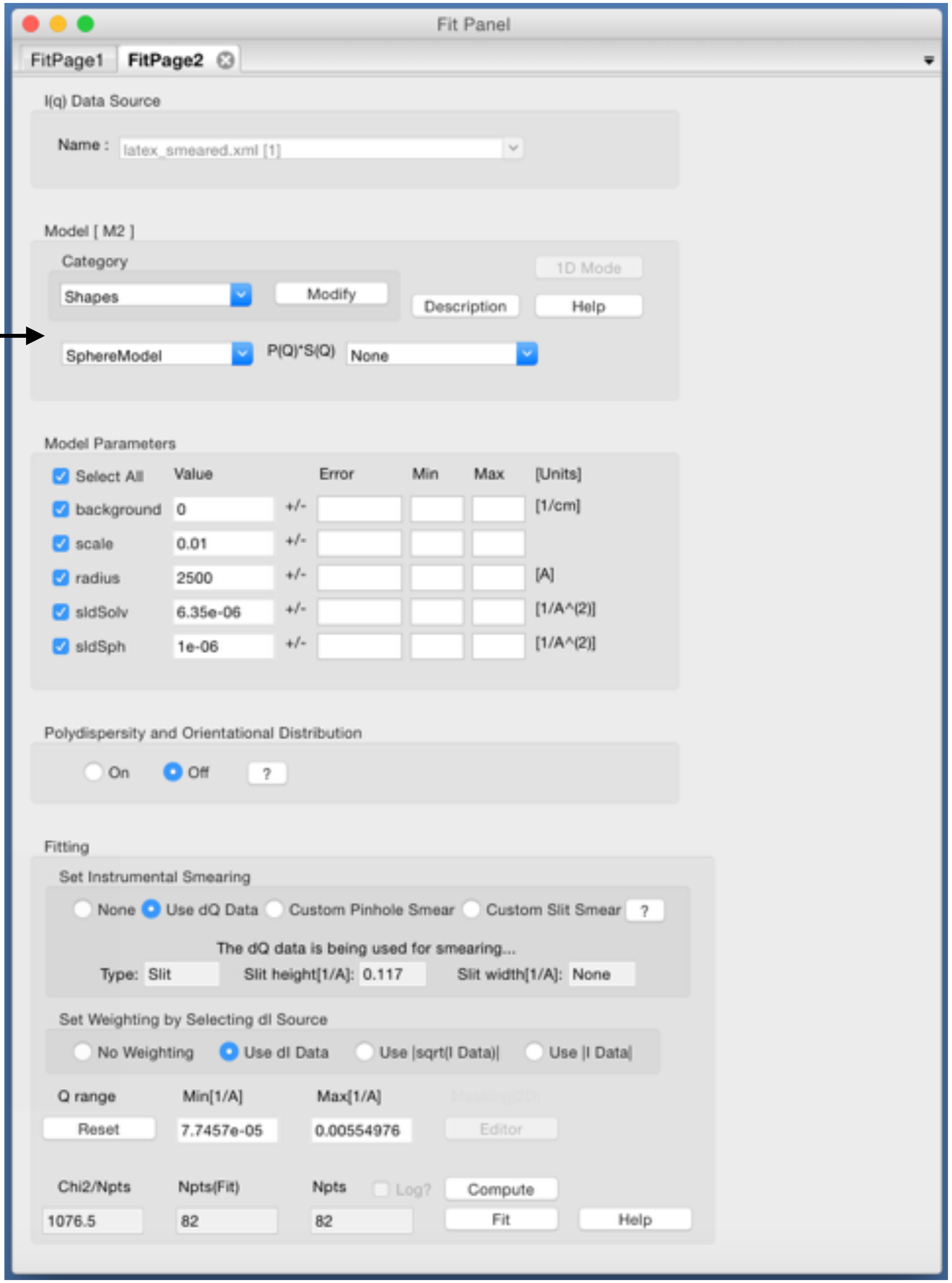
Here we have SANS & USANS from latex spheres

Send to Fitting …

1D Analysis

Send to fitting …

Select a model …



1D Analysis

Send to fitting …

Select a model …

Set parameters …

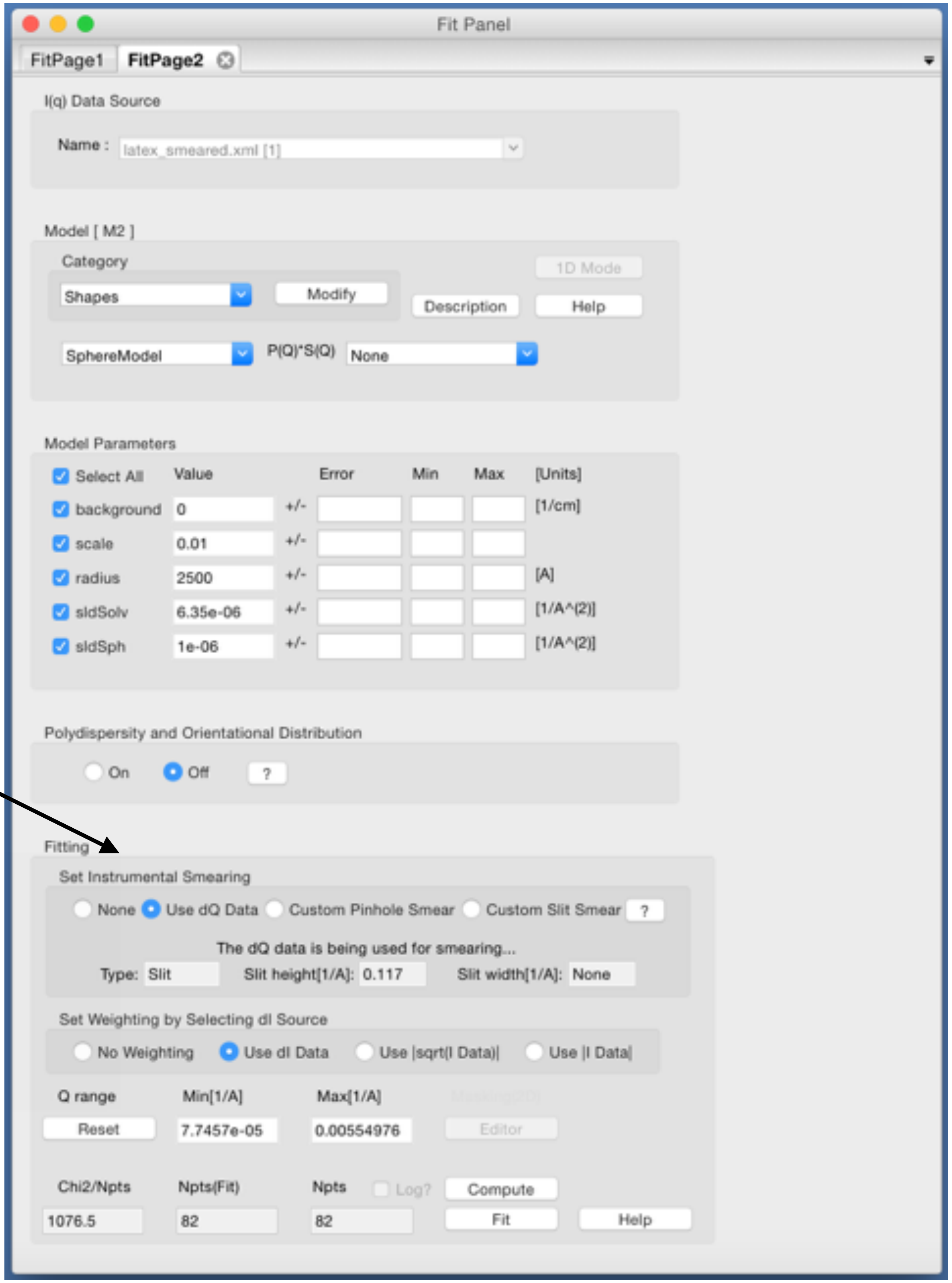
1D Analysis

Send to fitting …

Select a model …

Set parameters …

Use resolution …



1D Analysis

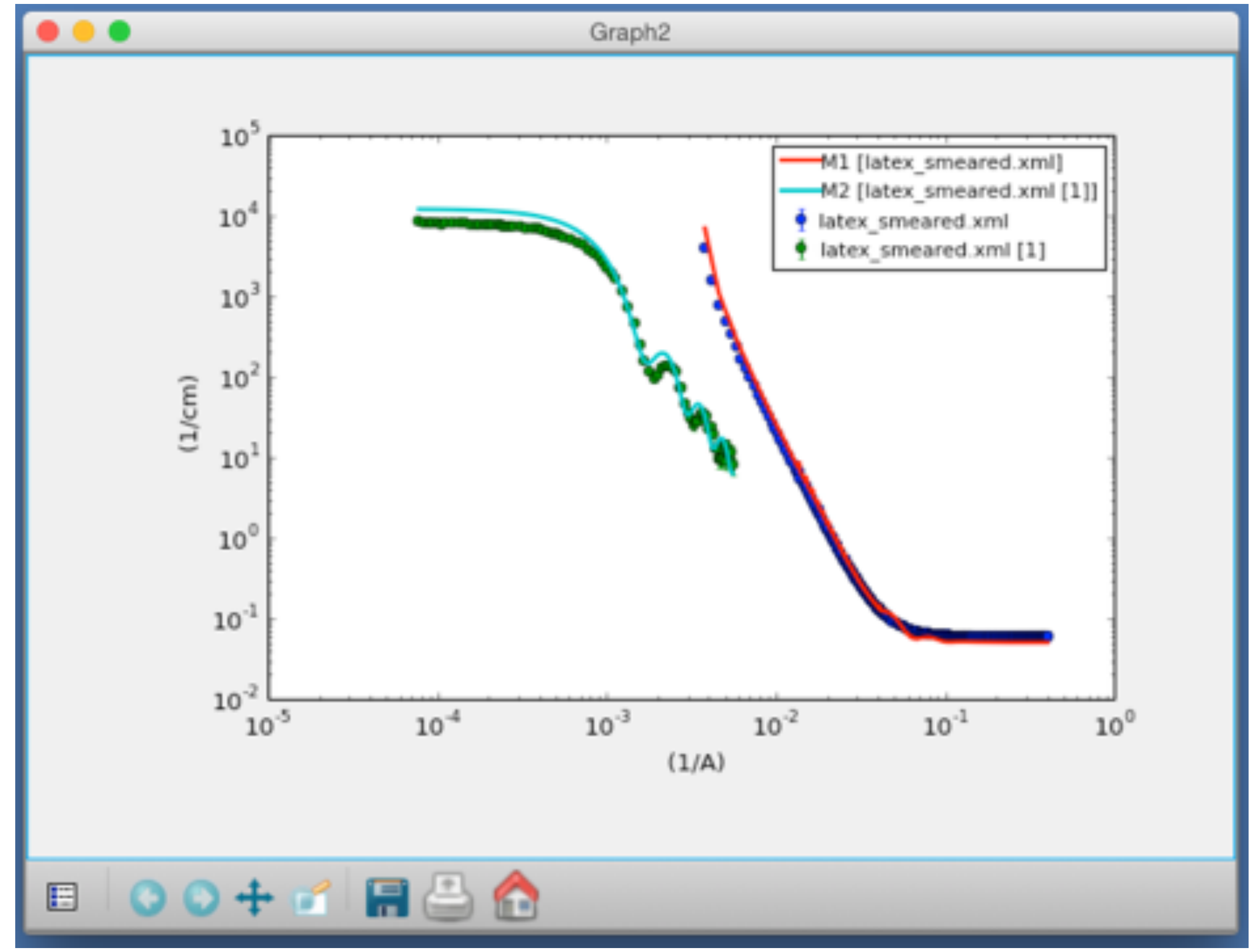
Send to fitting …

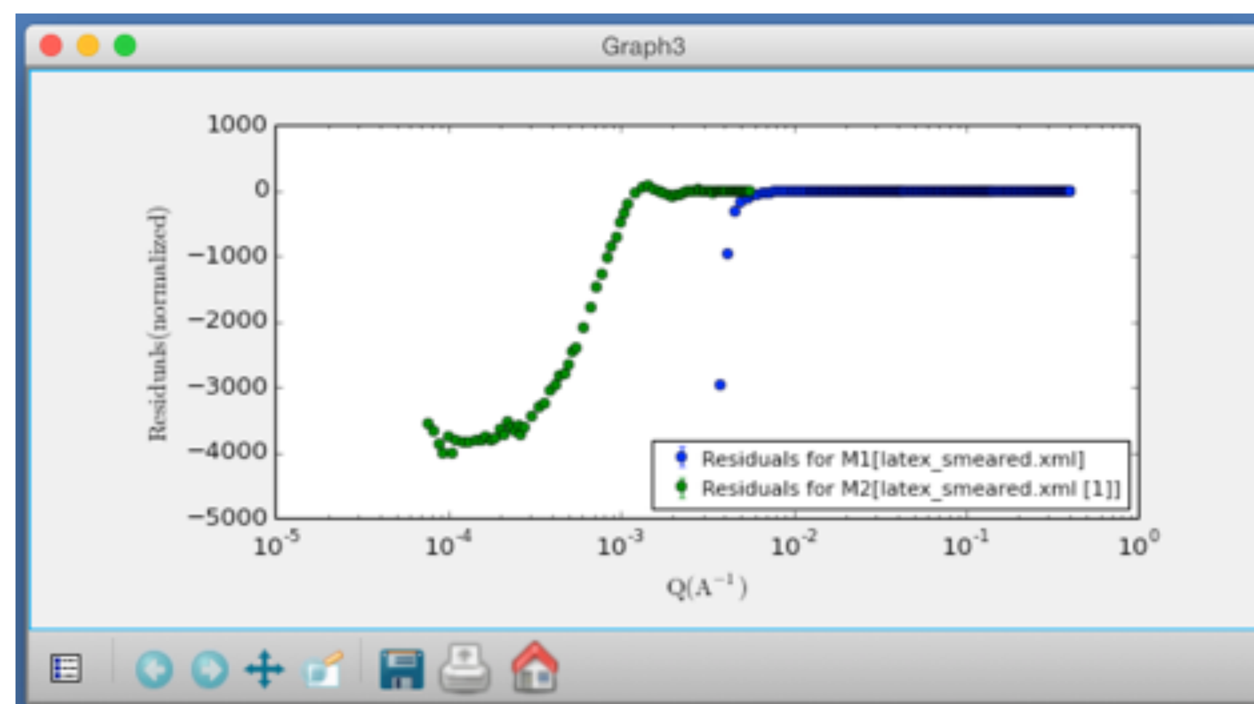
Select a model …

Set parameters …

Use resolution …

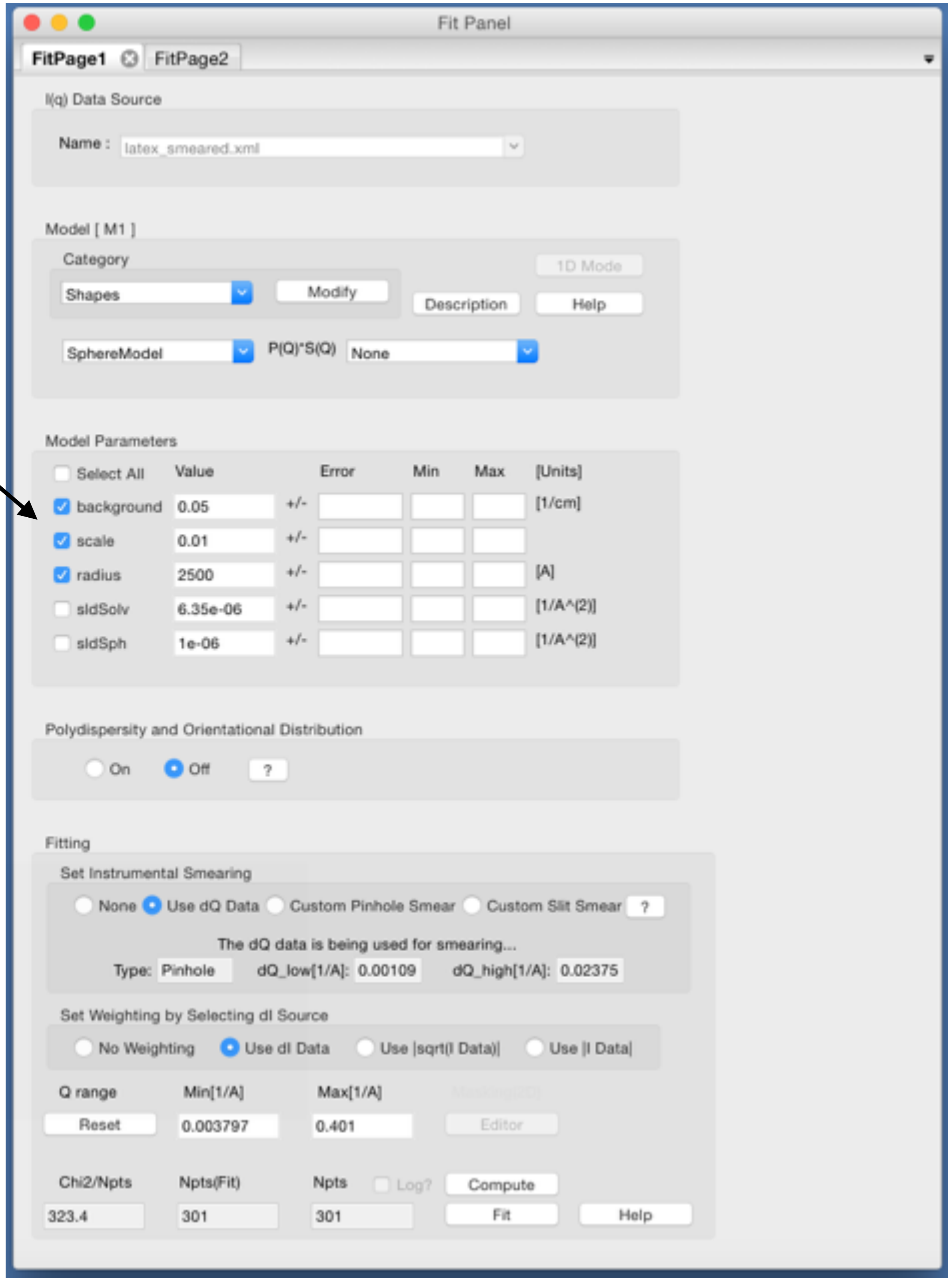
How does it look?





1D Analysis

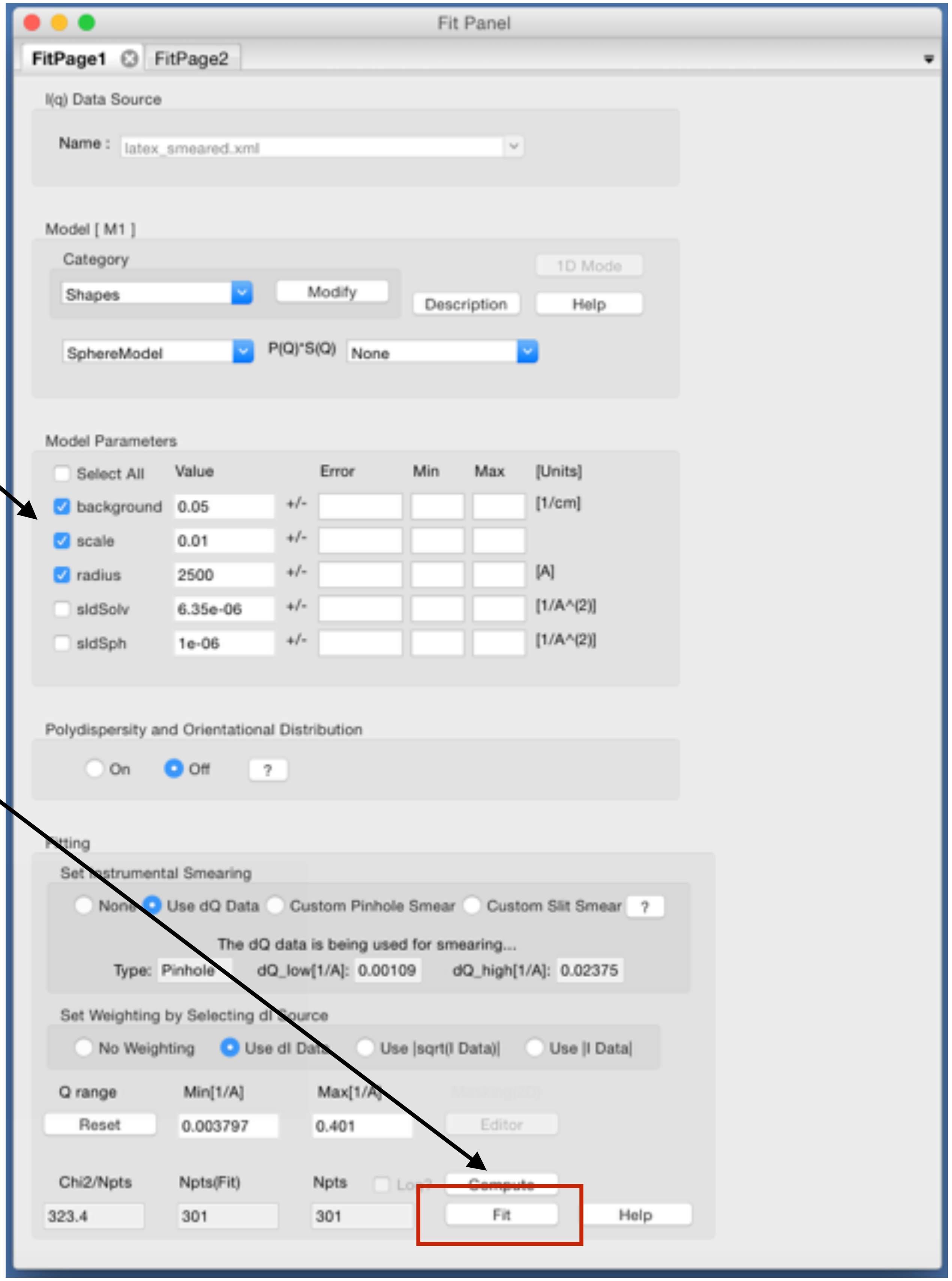
Choose which parameters to fit …



1D Analysis

Choose which parameters to fit …

… and press the Fit button!



Constraints / Simultaneous Fit

But wait! We have two data sets of the same sample : SANS + USANS …

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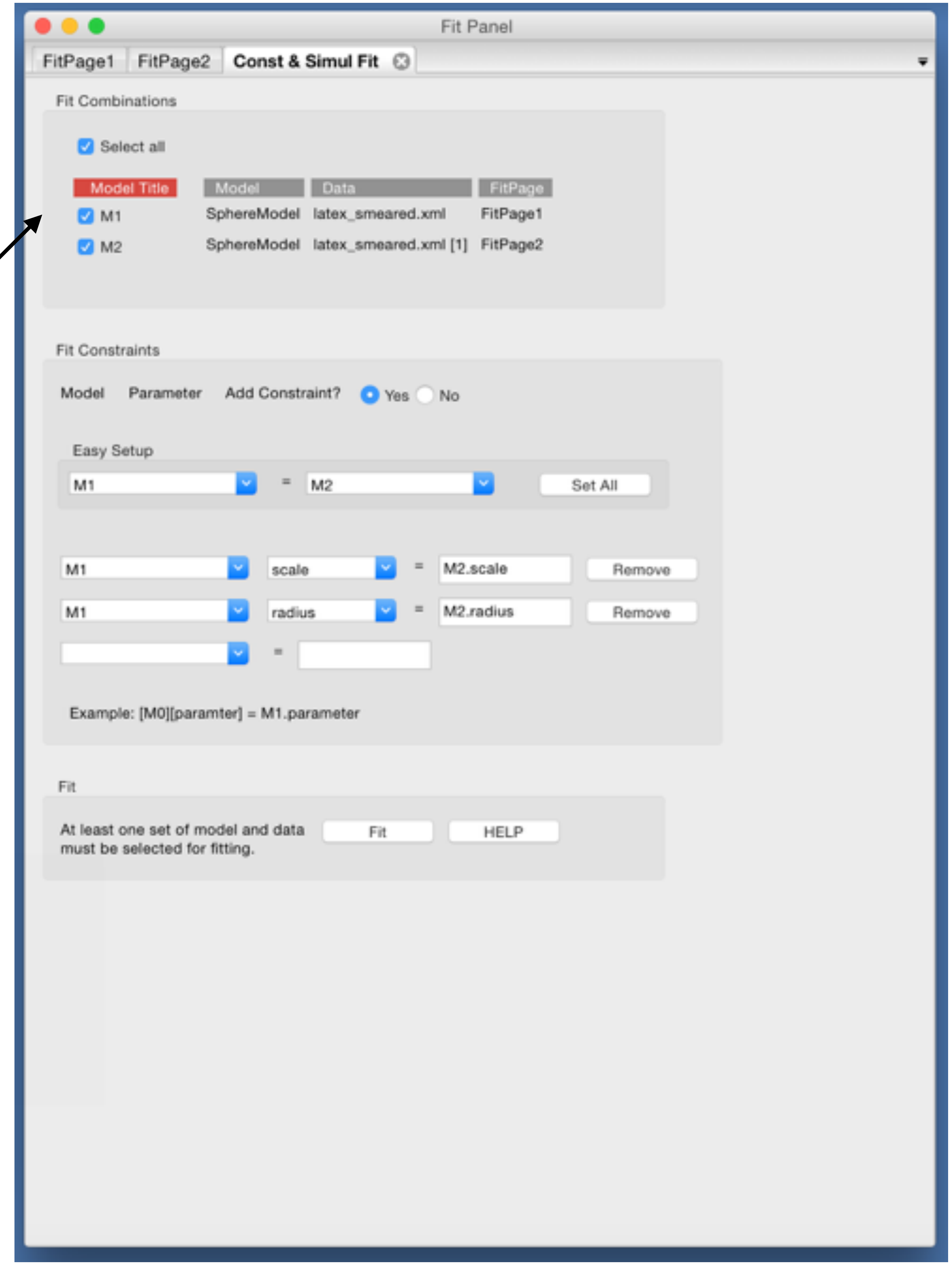
Set up a simultaneous fit …

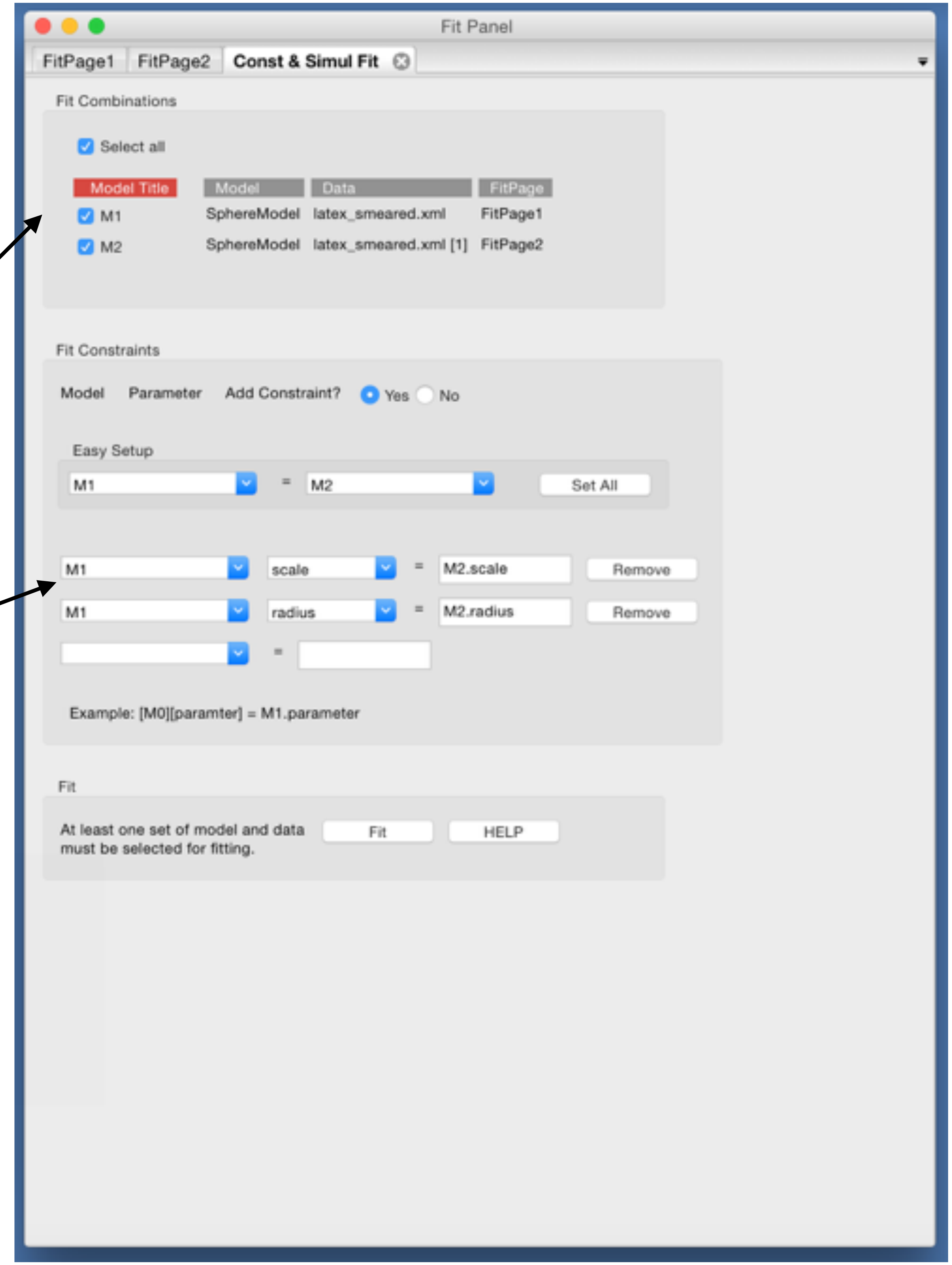


Constraints / Simultaneous Fit

But wait! We have two data sets of the same sample : SANS + USANS …

Set up a simultaneous fit …

… with constraints



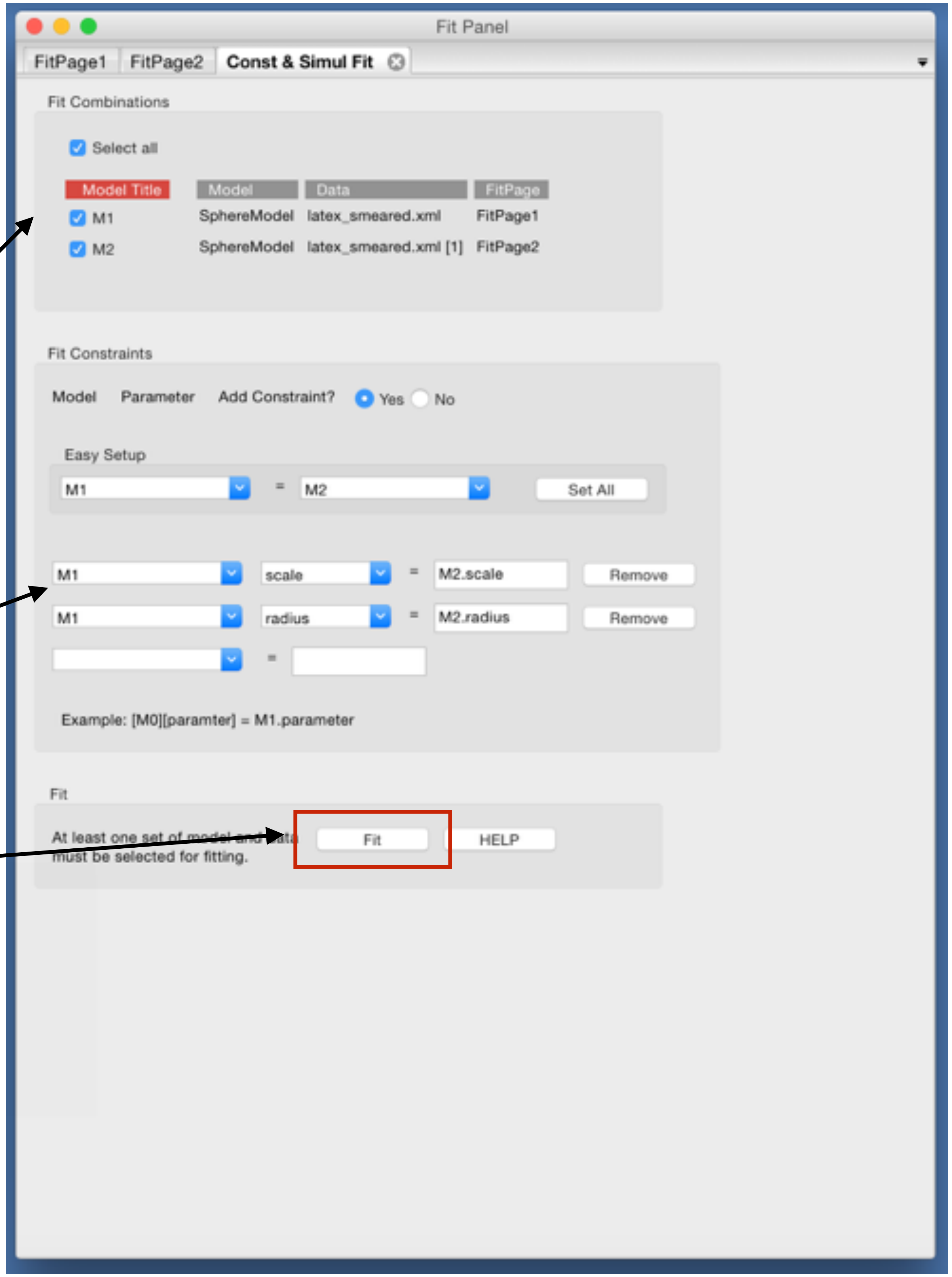
Constraints / Simultaneous Fit

But wait! We have two data sets of the same sample : SANS + USANS …

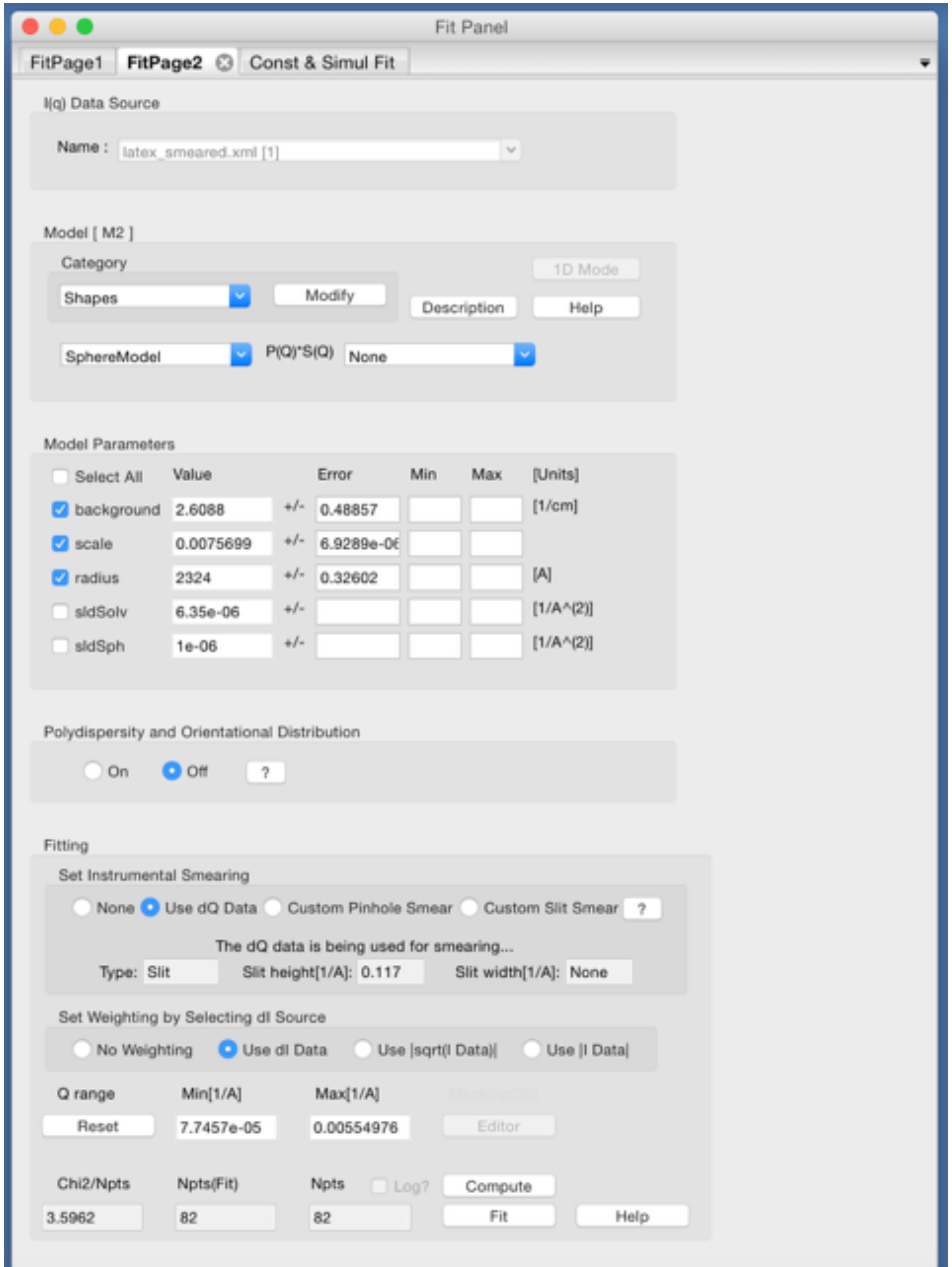
Set up a simultaneous fit …

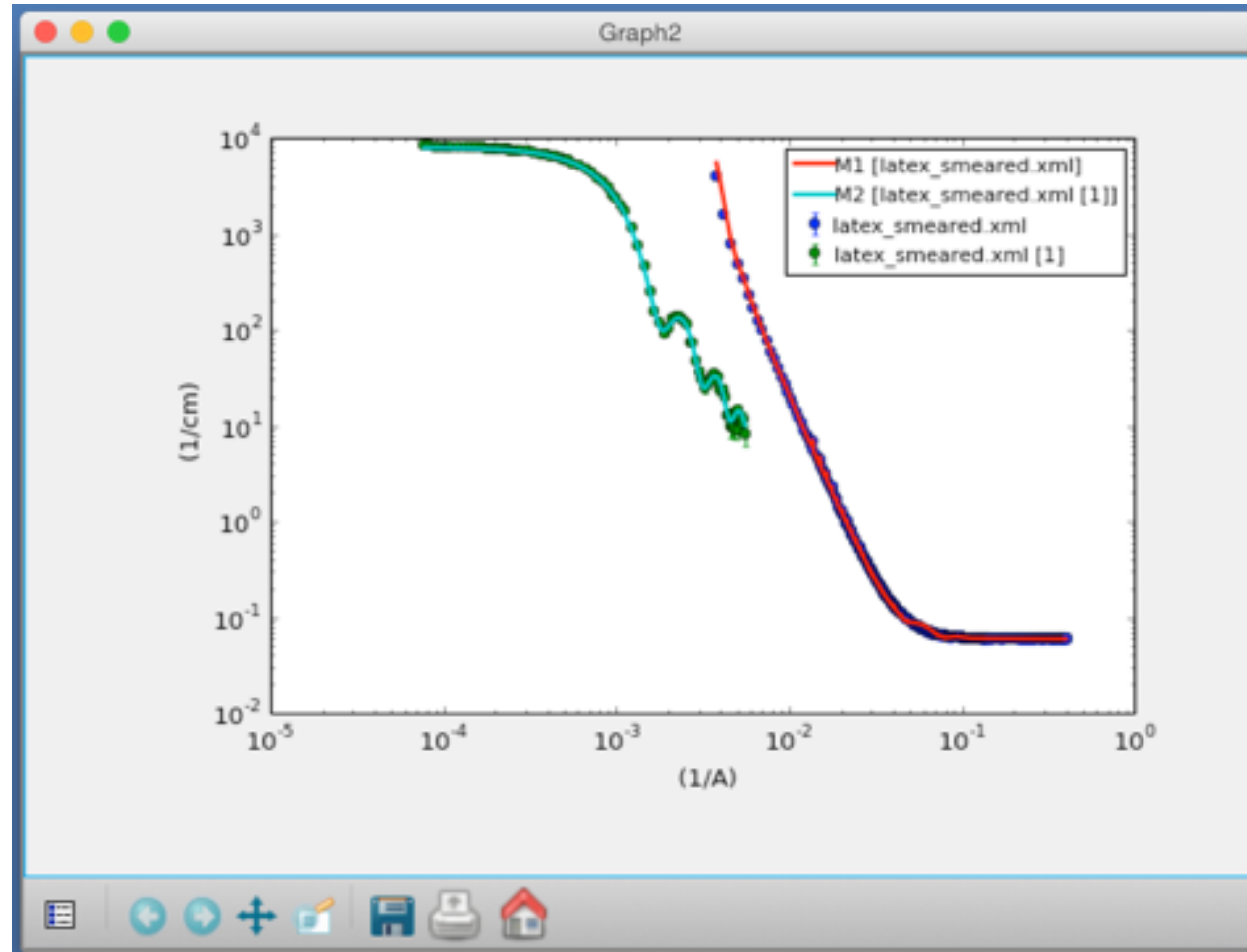
… with constraints

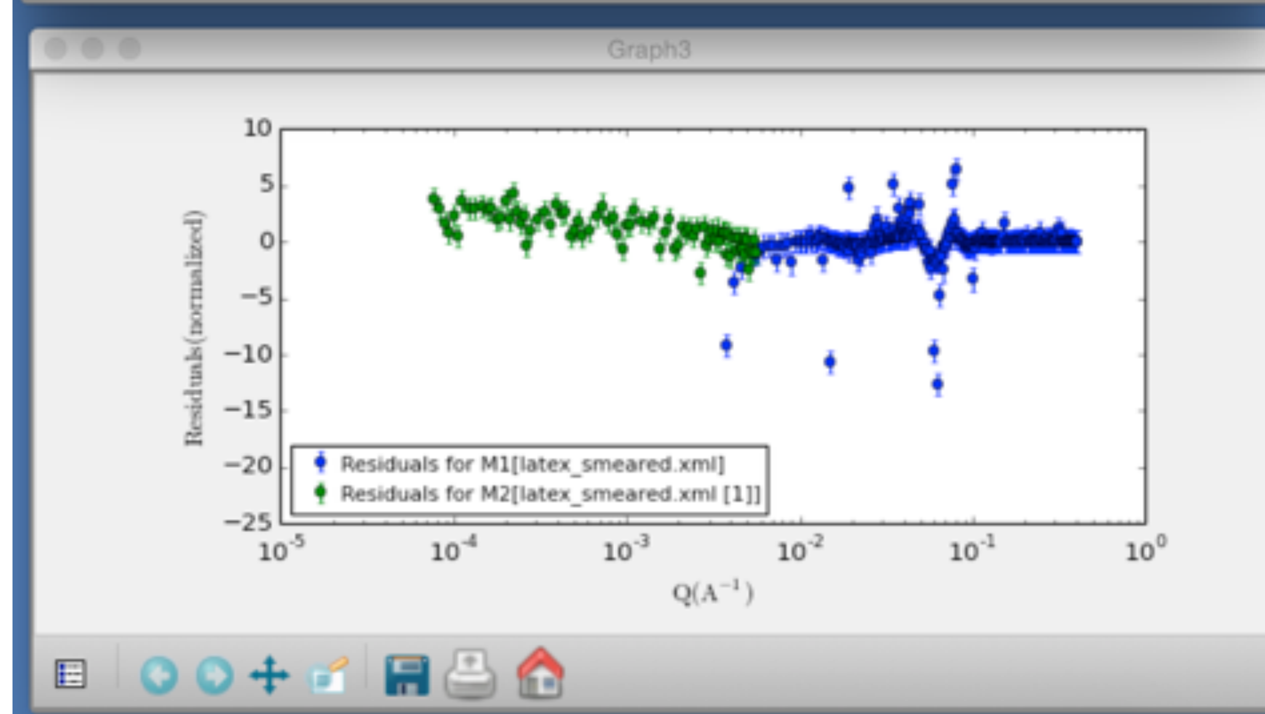
Now press the Fit button!



Constraints / Simultaneous Fit







2D Modelling

Cite this: *Soft Matter*, 2011, **7**, 9992

www.rsc.org/softmatter

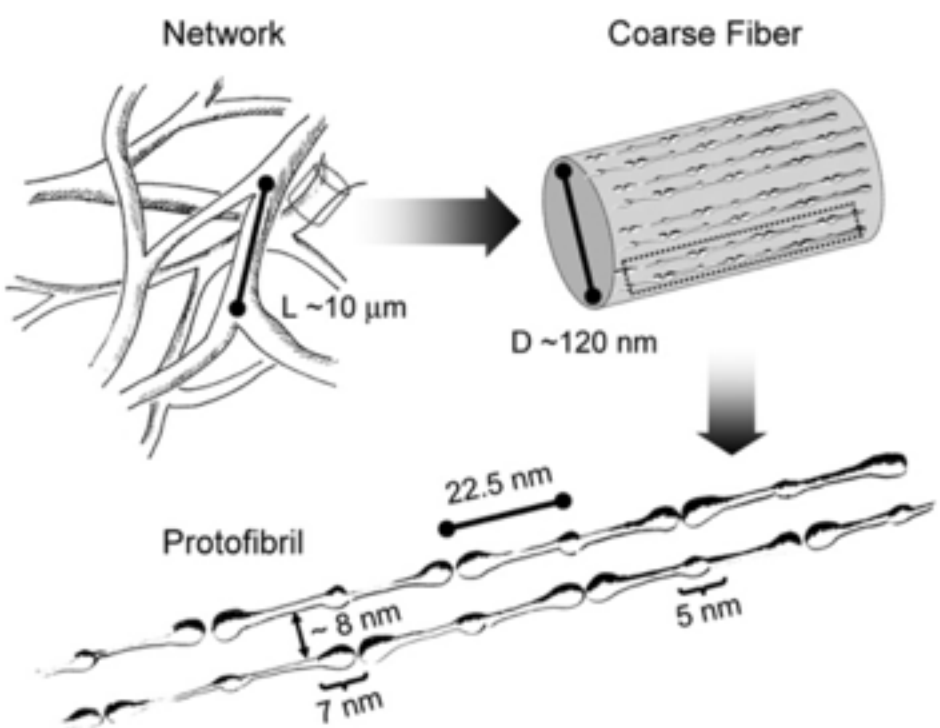
PAPER

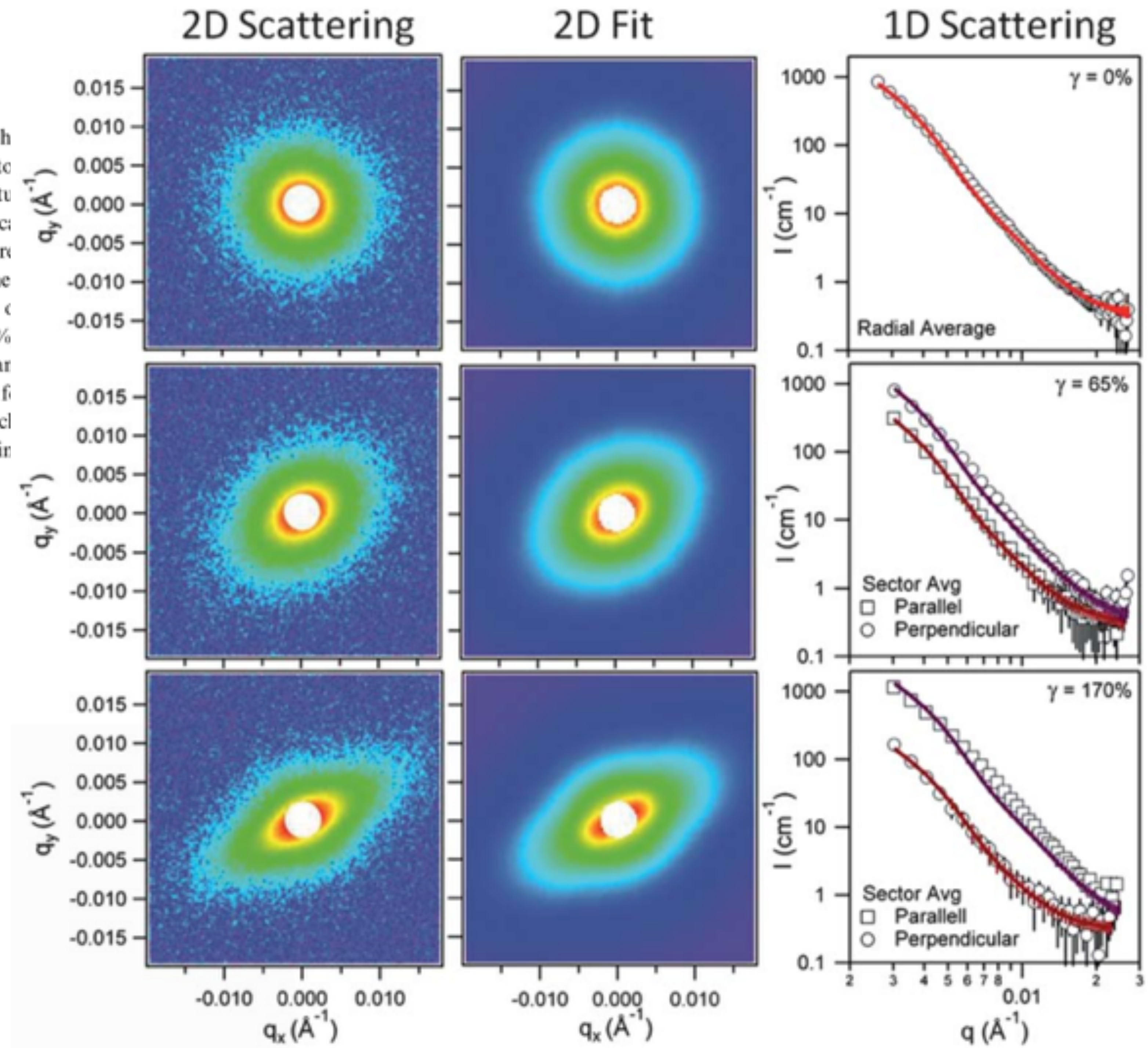
In situ neutron scattering study of structural transitions in fibrin networks under shear deformation

Katie M. Weigandt,[a] Lionel Porcar[bc] and Danilo C. Pozzo*[a]

Received 23rd June 2011, Accepted 5th August 2011
DOI: 10.1039/c1sm06176c

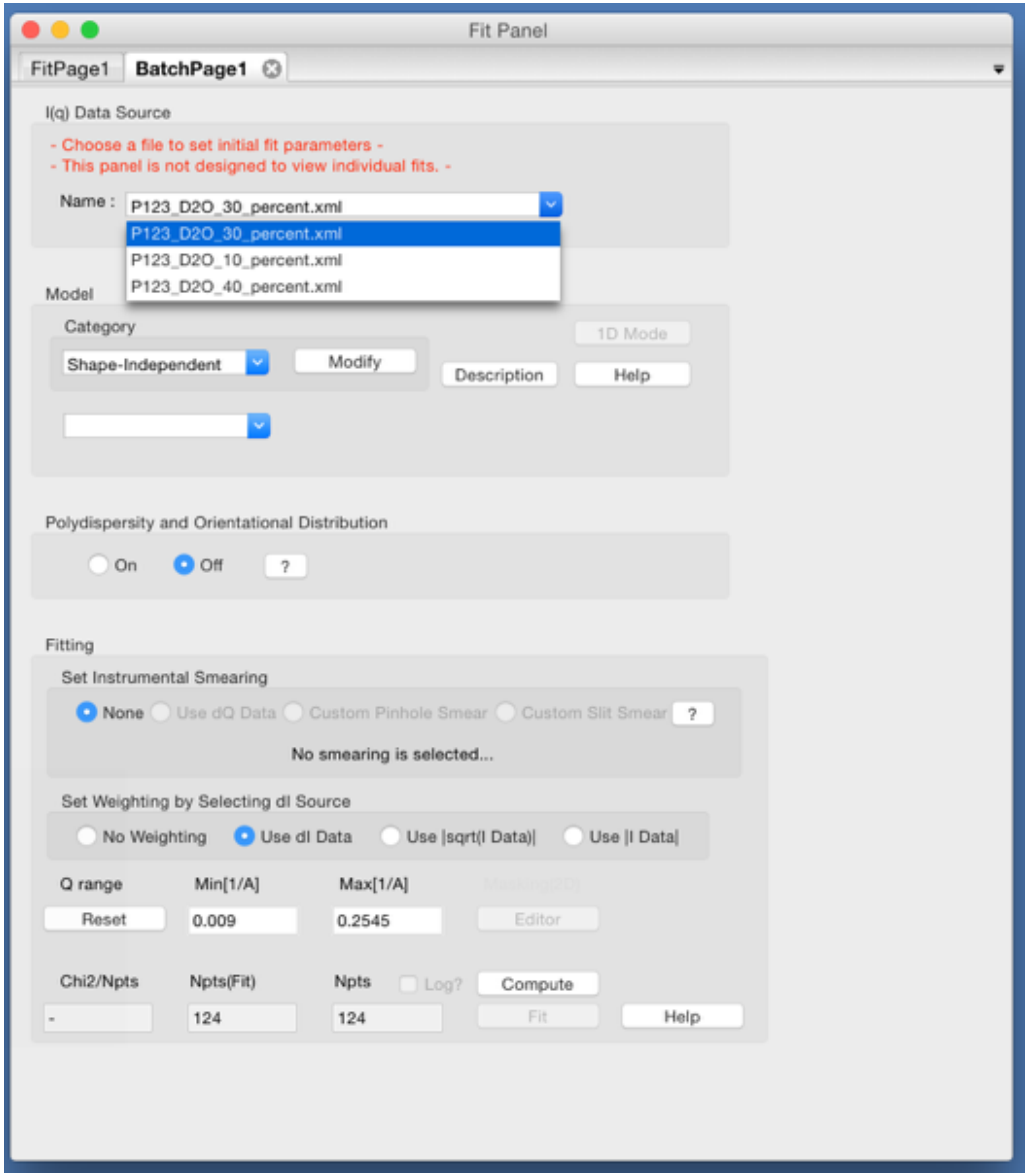
Small angle neutron scattering (SANS) is used to decipher the origin of the strain h
biopolymer networks by directly measuring the structural response of a fibrin gel tc
deformation. A special Couette shear cell is used to systematically probe the structu
a fibrin clot over strain values in the range of γ = 1–170%. The SANS results indic
hardening response of coarse fibrin gels occurs in two distinct regions having differe
mechanical signatures that are separated by an intermediate strain softening regime
(γ < 10%) there is a measurable increase in the shear modulus upon the application c
there are no significant changes to the clot structure. At higher strain values (γ > 30%
hardening regime is directly correlated to significant fiber alignment. The mean diar
determined directly from two-dimensional fits to the anisotropic scattering data is f
monotonically in the high-strain regime. The results suggest that the non-linear mecl
of fibrin clots are the result of a reduction of lateral entropic fluctuations at low strain
between bending and stretching at higher strain values.





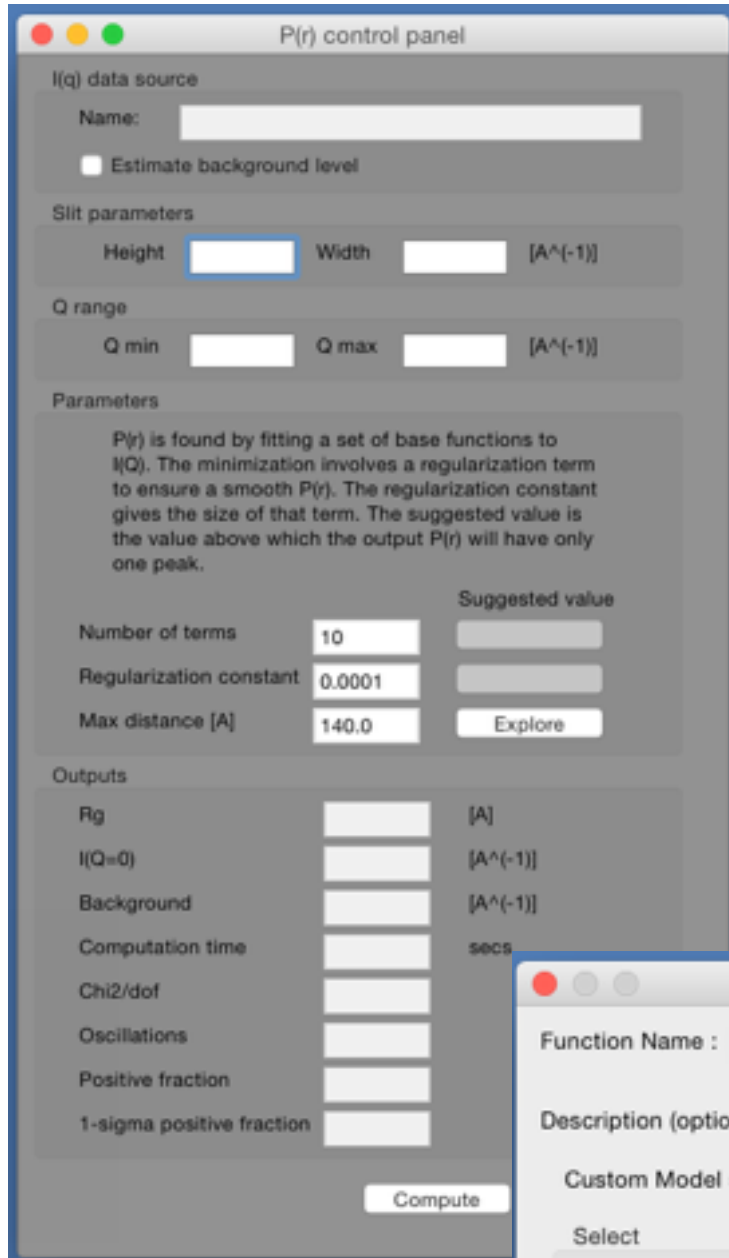
Other Features

Batch fitting …

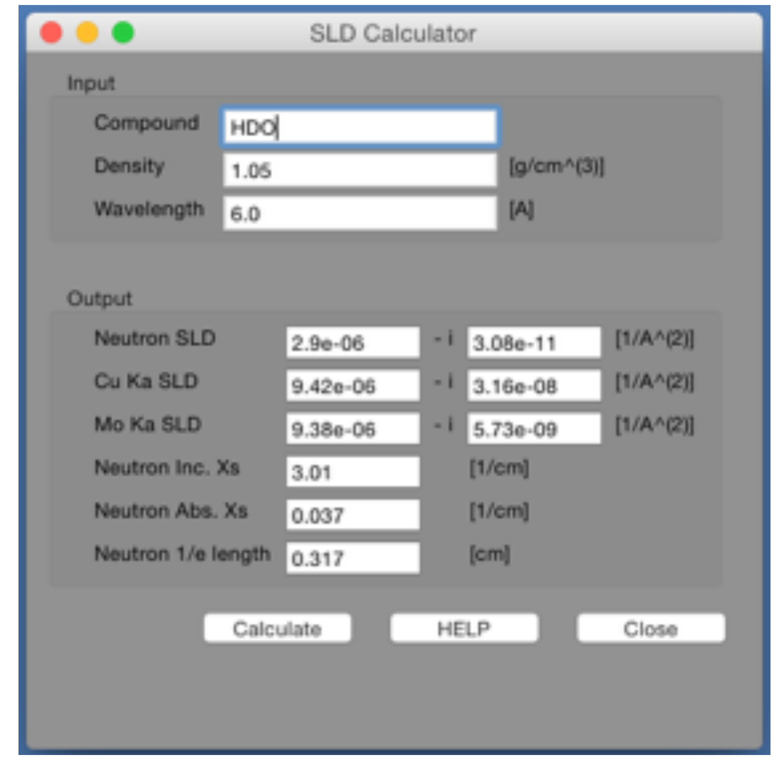


Other Features

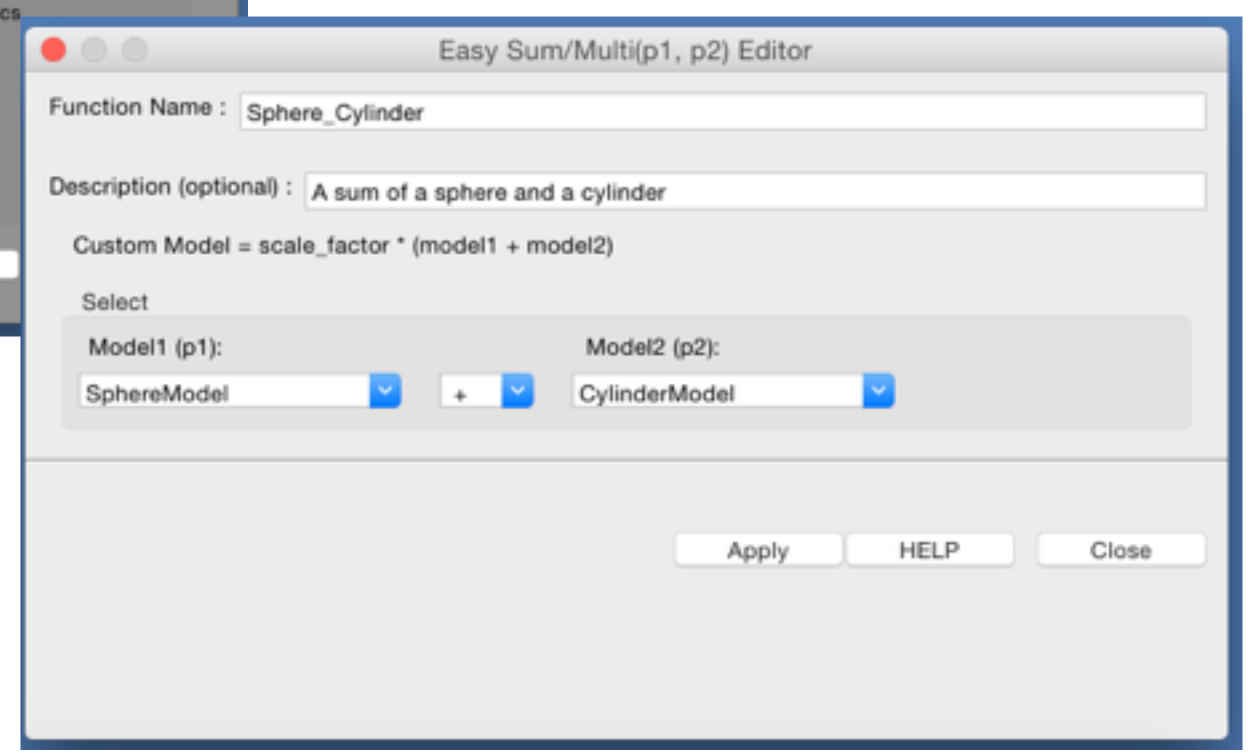
P(r) Inversion …



SLD Calculator …



Sum & Multiplication of Models …



SasView Development

A little history …

Where did SasView come from?

DANSE project output

~ 8.5% of funds were for SANS

Kickoff meeting August 2006

Heritage: NIST IGOR macros

Continuity …

NIST Supported initial transition from NSF funding

Expansion ...

NIST Supported initial transition from NSF funding

Now 7 active facilities
ORNL, ISIS, NIST, ESS, ILL, TUD/RID, ANSTO

SINE2020 Funding at ESS
First major investment since DANSE
http://sine2020.eu

Development Model

Open, Collaborative, Community Development

Code is open source and publicly hosted at Github

Bi-weekly developer calls

Code Camps

1st at NIST April 2013
2nd at ISIS April 2014
3rd at ESS Feb 2015
4th in Delft hosted by TU Delft / RID March 2016

5 Year Roadmap

http://www.sasview.org http://github.com/SasView

The Future … is Now!

SESANS

- Automatic transform of SANS model to P(z)
- Example scripts for fitting SESANS data
- Simultaneous fitting of SANS & SESANS
- Integration of SESANS fitting into GUI

Models

- New models
- New model package (sasmodels)
  - separation of models from GUI
  - simpler addition of models by users
  - speed! GPU and parallel processing

Documentation

- Enhanced, updated documentation for models

Current Development Team

- Paul Butler (NIST)
- Mathieu Doucet (ORNL)
- Steve King (ISIS)
- Andrew Jackson (ESS)

- Jurrian Bakker (TUD)
- Wim Bouwman (TUD)
- Miguel Gonzales (ILL)
- Richard Heenan (ISIS)
- Paul Kienzle (NIST)
- Jeff Kryzwon (NIST)
- Ricardo Leal (ORNL)
- David Manicke (ANSTO)
- Torben Nielsen (ESS)
- Steve Parnell (TUD)
- Wojciech Potrzebowski (ESS)
- Piotr Rozyczko (ESS)
- Adam Washington (Sheffield)

- and thanks to the many previous contributors, particularly Jae Hie Cho and Alina Gervaise

Questions?