



EUROPEAN
SPALLATION
SOURCE



SasView : A Small Angle Scattering Analysis Software Package

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

Grenoble, 3rd April 2017



Science & Technology Facilities Council
ISIS

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

OAK RIDGE
National Laboratory

Analysis Software - Who's Job is it Anyway?

Analysis is where the science is → the USER'S JOB

Scattering is a tool and part of providing the tool should
be analysis tools → the FACILITY'S JOB

Data on disk is useless to EVERYBODY

Analysis Software - Who's Job is it Anyway?

But ... where are the resources?

More pressing tasks for all of us : maintaining & improving instrumentation, bringing in and supporting users, dealing with instrument control and data reduction software ...

Data Analysis is bottom of the heap ...

... need to pool resources.

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 8 active facilities

ORNL, ISIS, NIST, ESS, ILL, TUD/RID, ANSTO and Diamond

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
Bug and Enhancement Ticket System - Trac

Bi-weekly developer calls

Code Camps

1st at NIST April 2013
2nd at ISIS April 2014
3rd at ESS Feb 2015
4th at TU Delft/RID March 2016
5th at ORNL October 2016
6th at ILL/ESRF April 2017

5 Year Roadmap

<http://www.sasview.org>

<http://github.com/SasView>

Development Model

www.sasview.org

Task and bug tracking trac.sasview.org

This screenshot shows the Trac web interface for the SasView project. At the top, there's a navigation bar with links for Wiki, Timeline, Roadmap, Browse Source, View Tickets (which is selected), New Ticket, Search, Admin, and Tags. Below the navigation is a search bar and a link to Available Reports. A message indicates there are 3 Active Tickets by Milestone (247 matches). The main content area displays two tables of tickets. The first table, 'Results (1 - 100 of 247)', lists tickets from #219 to #494. The second table, 'Milestone Admin Tasks (12 matches)', lists tickets from #626 to #700. Both tables include columns for Ticket, Summary, Component, Version, Type, Owner, Status, and Created.

Automated Builds build.sasview.org

This screenshot shows the Jenkins dashboard at jenkins.esss.dk. The top navigation bar includes links for All, Bumps-Builds, Master-Builds, Periodic-builds, Refl1d-Builds, and Release. It also features a search bar and a log in link. The main content area is divided into several sections: 'Build Queue' (empty), 'Build Executor Status' (listing master, build_on_sasviewbuild01, build_on_sasviewbuild02, build_on_sasviewbuild03, build_on_sasviewbuild04, build_on_sasviewbuild05, build_on_sasviewbuild12, sasviewbuild05, sasviewbuild14, sasviewbuild18, and sasviewbuild24, all marked as offline), and a large table of builds. The table columns are S, W, Name, Last Success, Last Failure, and Last Duration. The table lists various builds like bumps_Ubuntu14.04_test, PeriodicUbuntu14.04_test, etc., with their respective success rates and last run times.

Hosted by UT

Hosted by ESS

Current Development Team

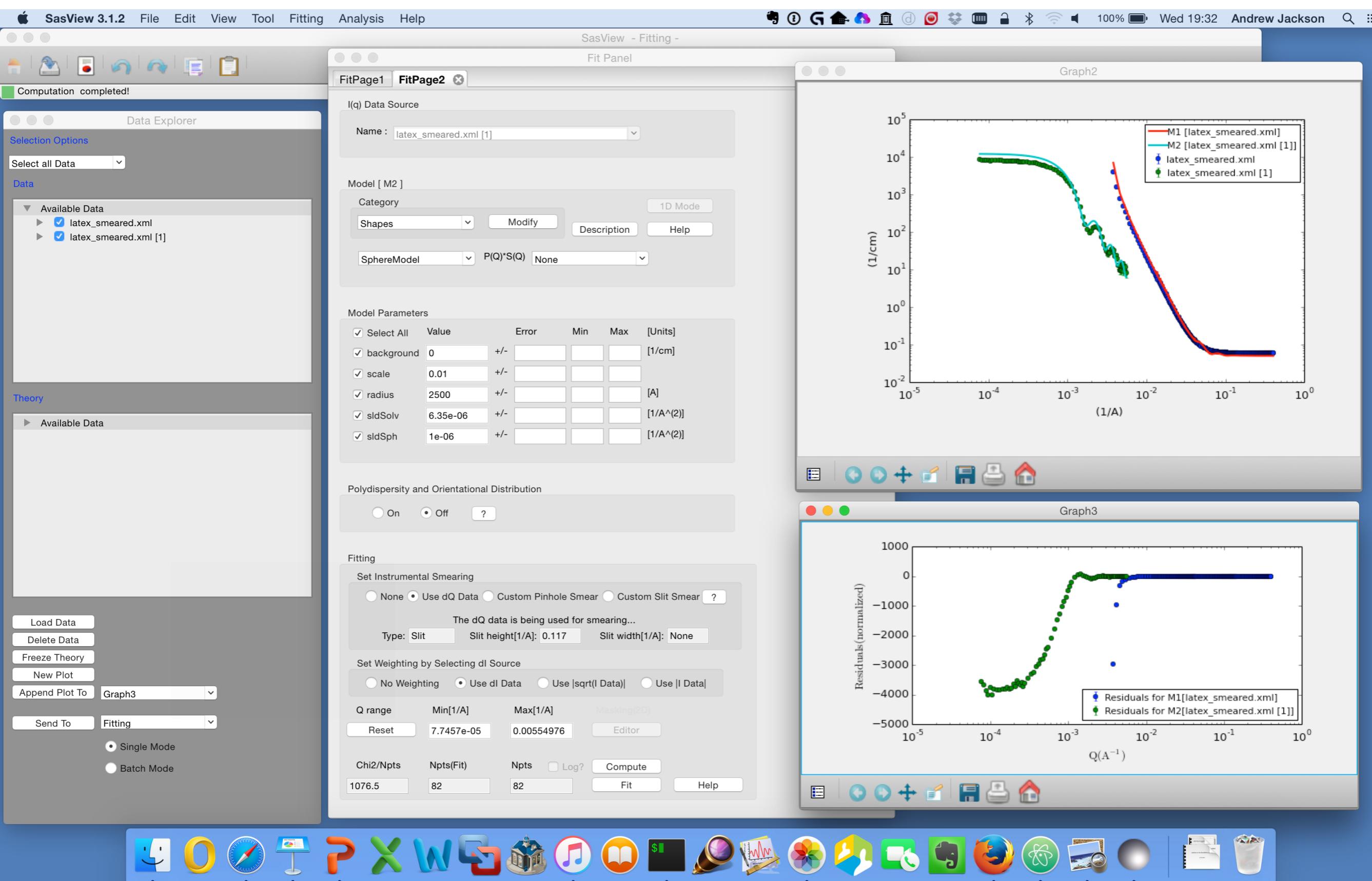
- Paul Butler (NIST)
- Mathieu Doucet (ORNL)
- Andrew Jackson (ESS)
- Steve King (STFC)



- Jurrian Bakker (TUD)
 - Wim Bouwman (TUD)
 - Miguel Gonzales (ILL)
 - Richard Heenan (STFC)
 - Dirk Honecker (ILL)
 - Paul Kienzle (NIST)
 - Jeff Kryzwon (NIST)
 - Ricardo Leal (ORNL)
 - David Mannicke (ANSTO)
 - Andrew Nelson (ANSTO)
 - Torben Nielsen (ESS)
 - Lewis O'Driscoll (STFC)
 - Steve Parnell (TUD)
 - Wojciech Potrzebowski (ESS)
 - Piotr Rozyczko (ESS)
 - Tim Snow (Diamond)
 - Adam Washington (STFC)
-
- and thanks to the many previous contributors, particularly Jae Hie Cho and Alina Gervaise

What Can SasView Do Currently?

1D Analysis



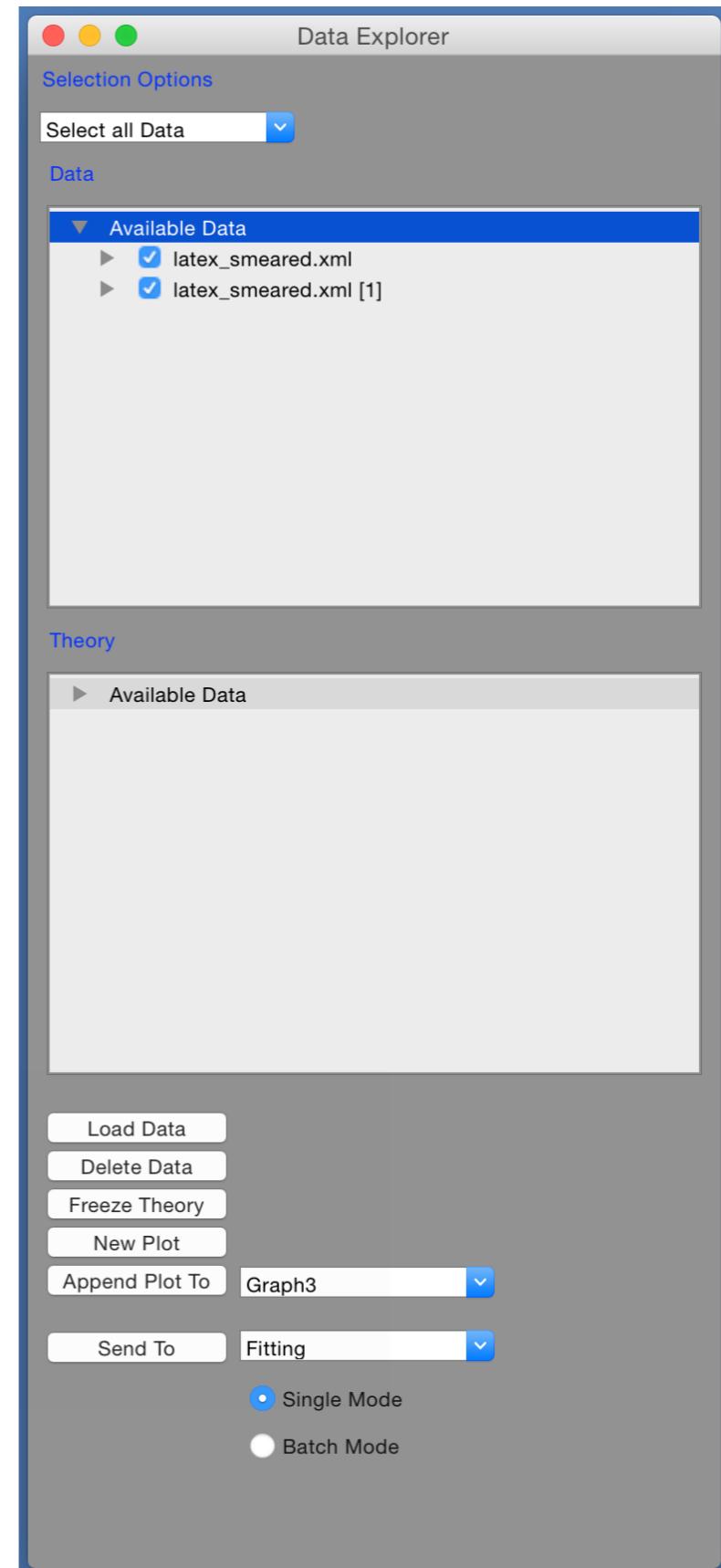
1D Analysis

Load Data ...

Select Data Sets ...

Here we have SANS & USANS from latex spheres

Send to Fitting ...



1D Analysis

Send to fitting ...

Select a model ...



Fit Panel

FitPage1 FitPage2

I(q) Data Source
Name : latex_smeared.xml [1]

Model [M2]
Category: Shapes 1D Mode
SphereModel P(Q)*S(Q) None

Model Parameters

Select All	Value	Error	Min	Max	[Units]
<input checked="" type="checkbox"/>	background	0	+/-		[1/cm]
<input checked="" type="checkbox"/>	scale	0.01	+/-		
<input checked="" type="checkbox"/>	radius	2500	+/-		[Å]
<input checked="" type="checkbox"/>	sldSolv	6.35e-06	+/-		[1/Å ²]
<input checked="" type="checkbox"/>	sldSph	1e-06	+/-		[1/Å 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/Å]: 0.117 Slit width[1/Å]: None

Set Weighting by Selecting dl Source
 No Weighting Use dl Data Use |sqrt(I) Data| Use |I| Data

Q range Min[1/Å] Max[1/Å] Masking(2D)
Reset 7.7457e-05 0.00554976 Editor

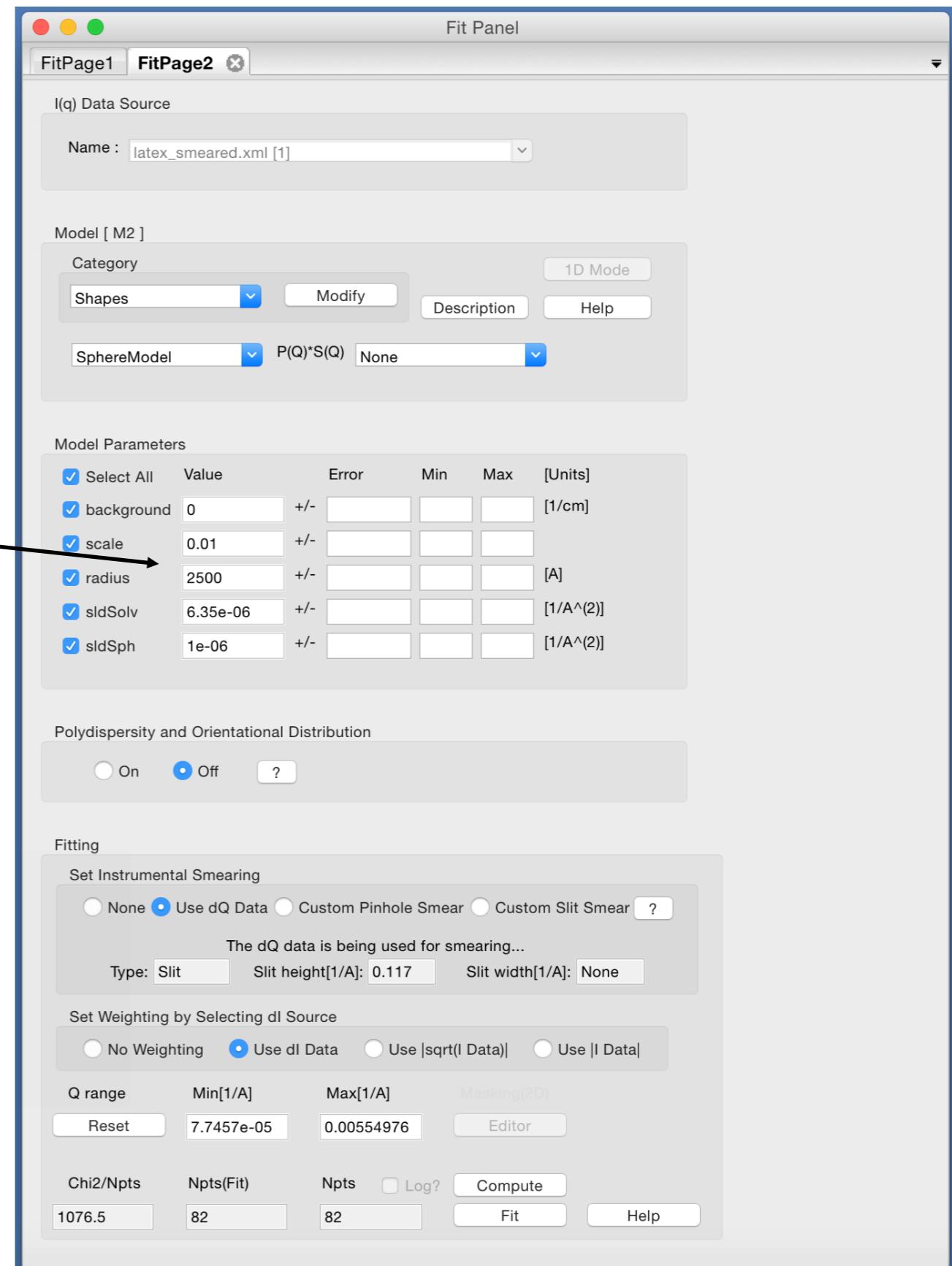
Chi2/Npts Npts(Fit) Npts Log? Compute
1076.5 82 82 Fit Help

1D Analysis

Send to fitting ...

Select a model ...

Set parameters ...



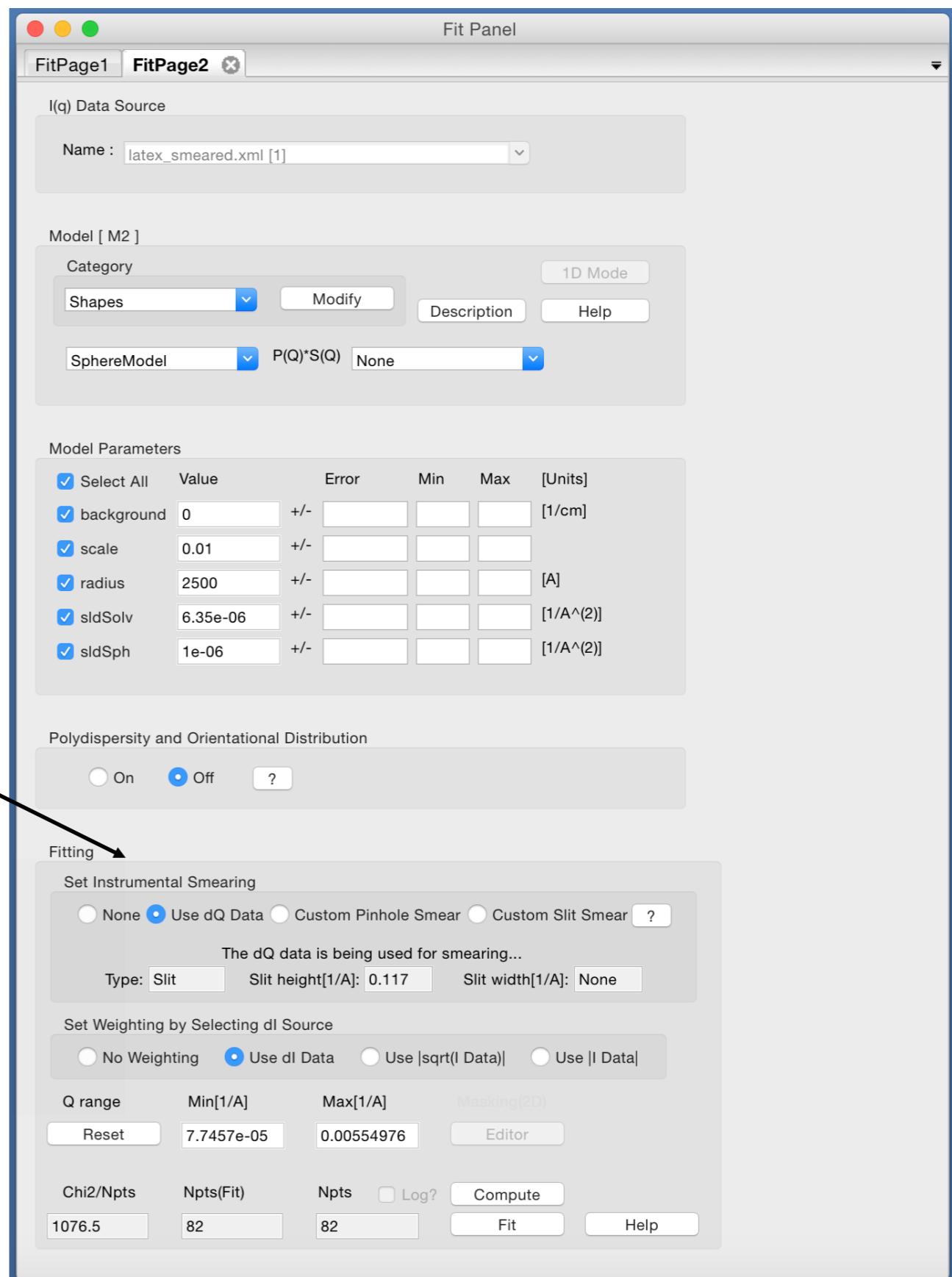
1D Analysis

Send to fitting ...

Select a model ...

Set parameters ...

Use resolution ...



1D Analysis

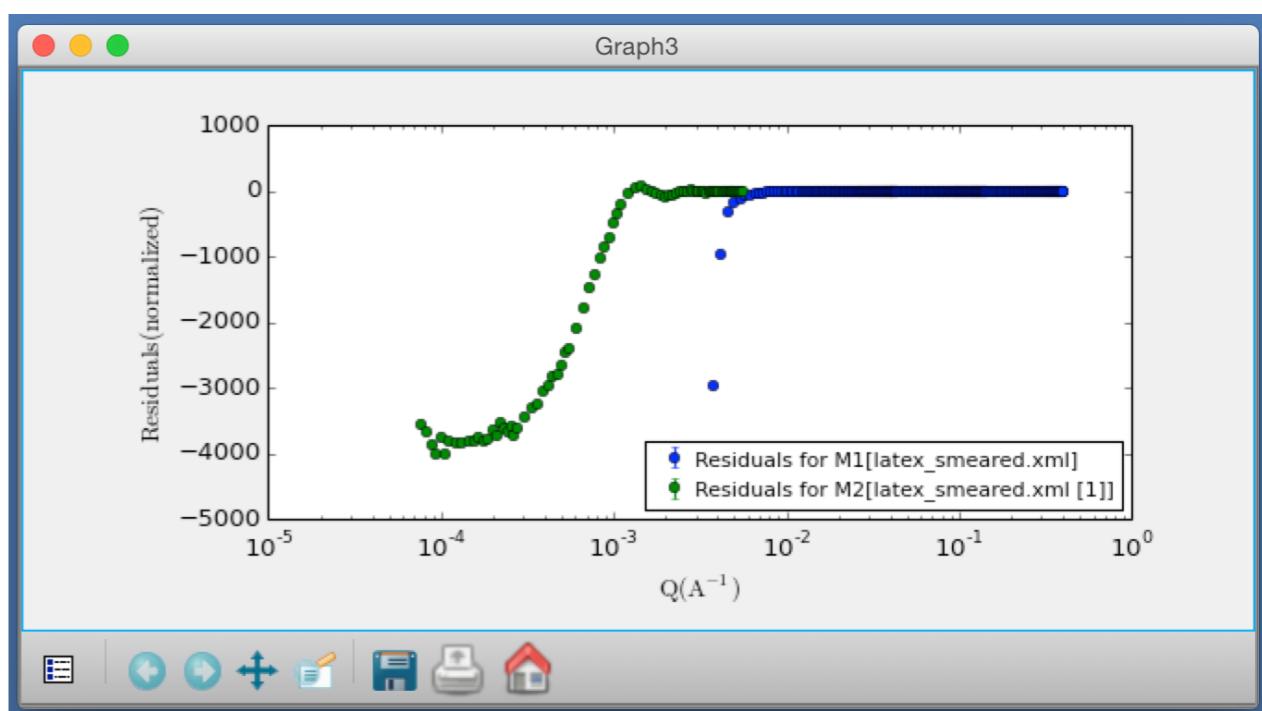
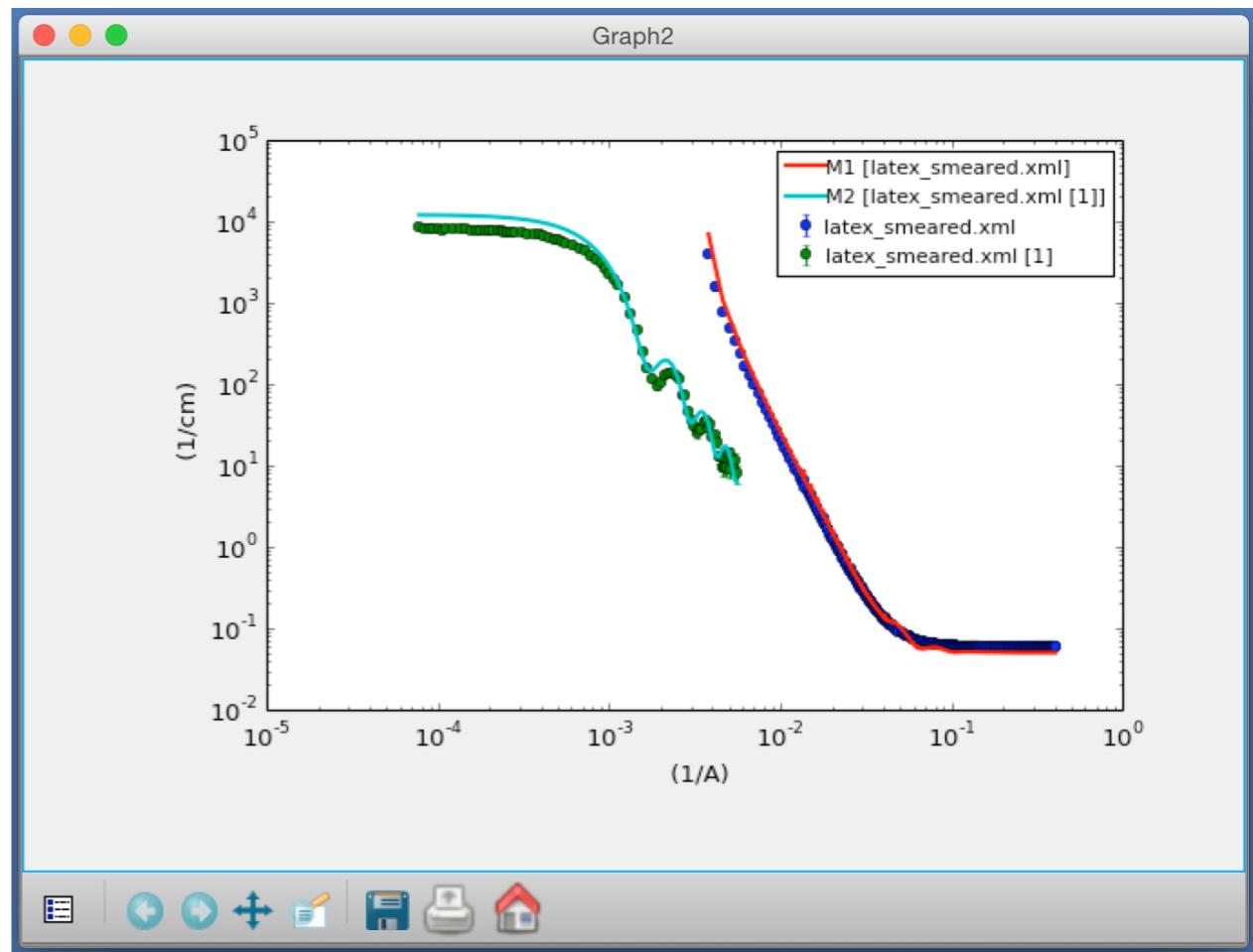
Send to fitting ...

Select a model ...

Set parameters ...

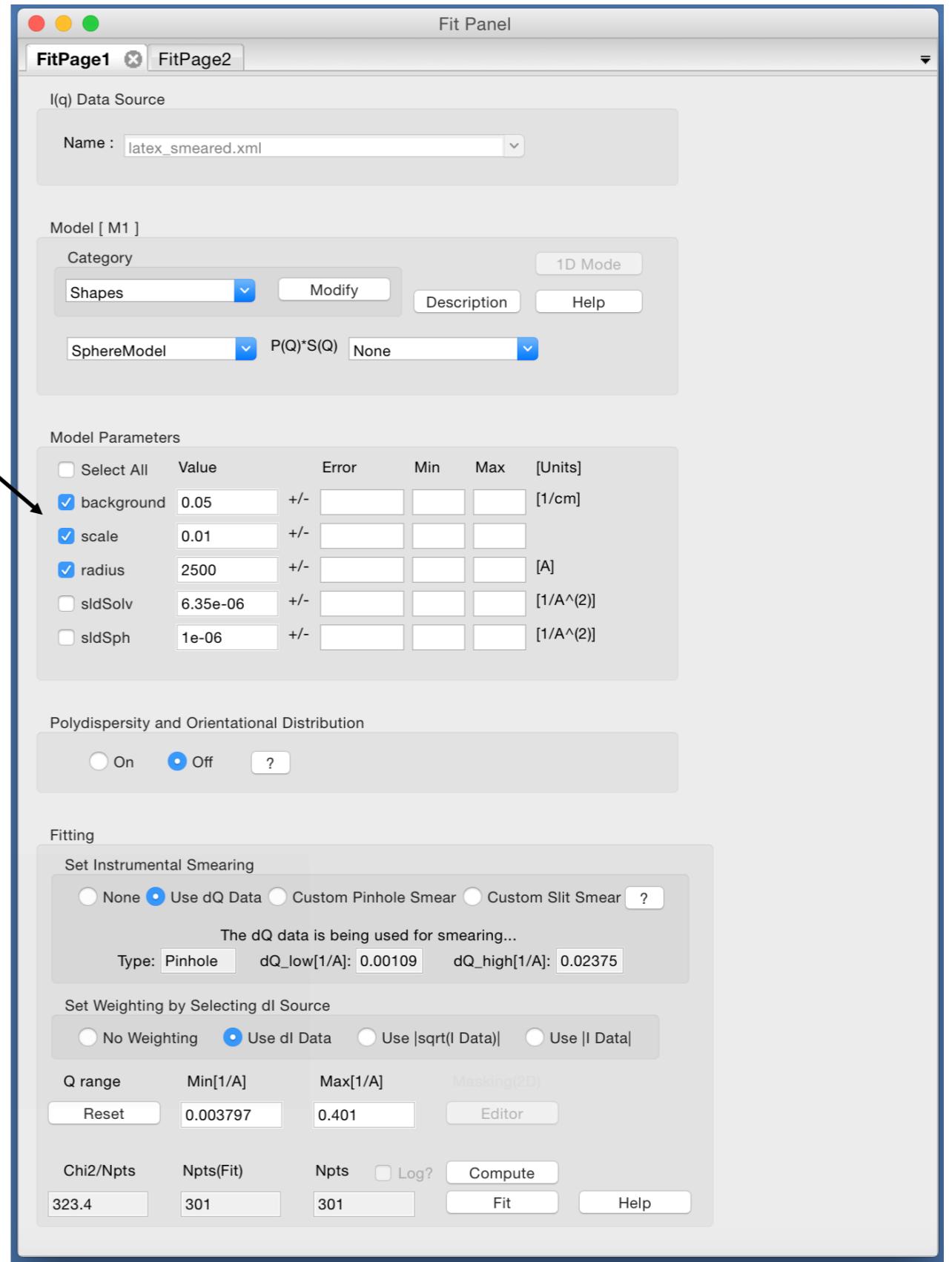
Use resolution ...

How does it look?



1D Analysis

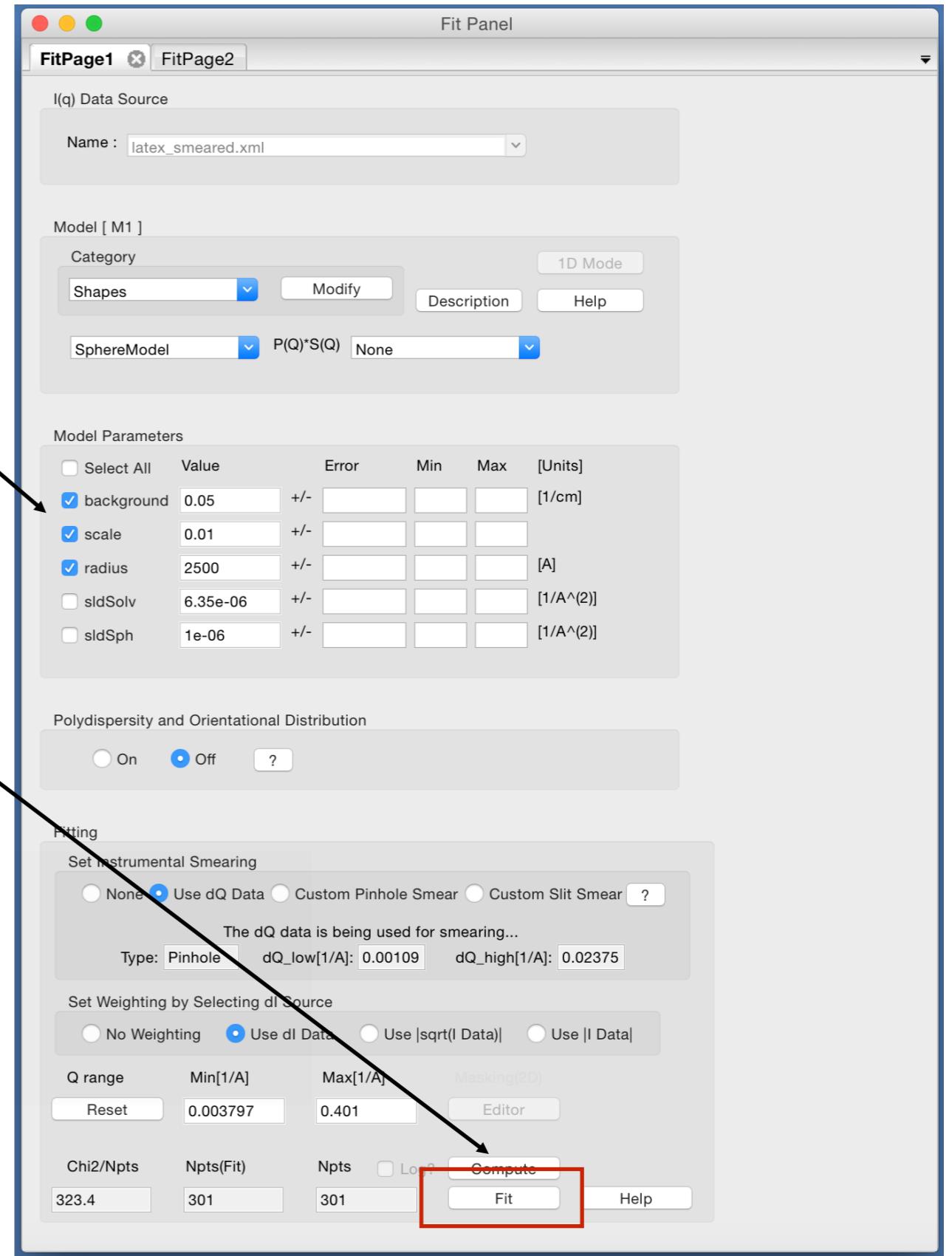
Choose which parameters to fit ...



1D Analysis

Choose which parameters to fit ...

... and press the Fit button!



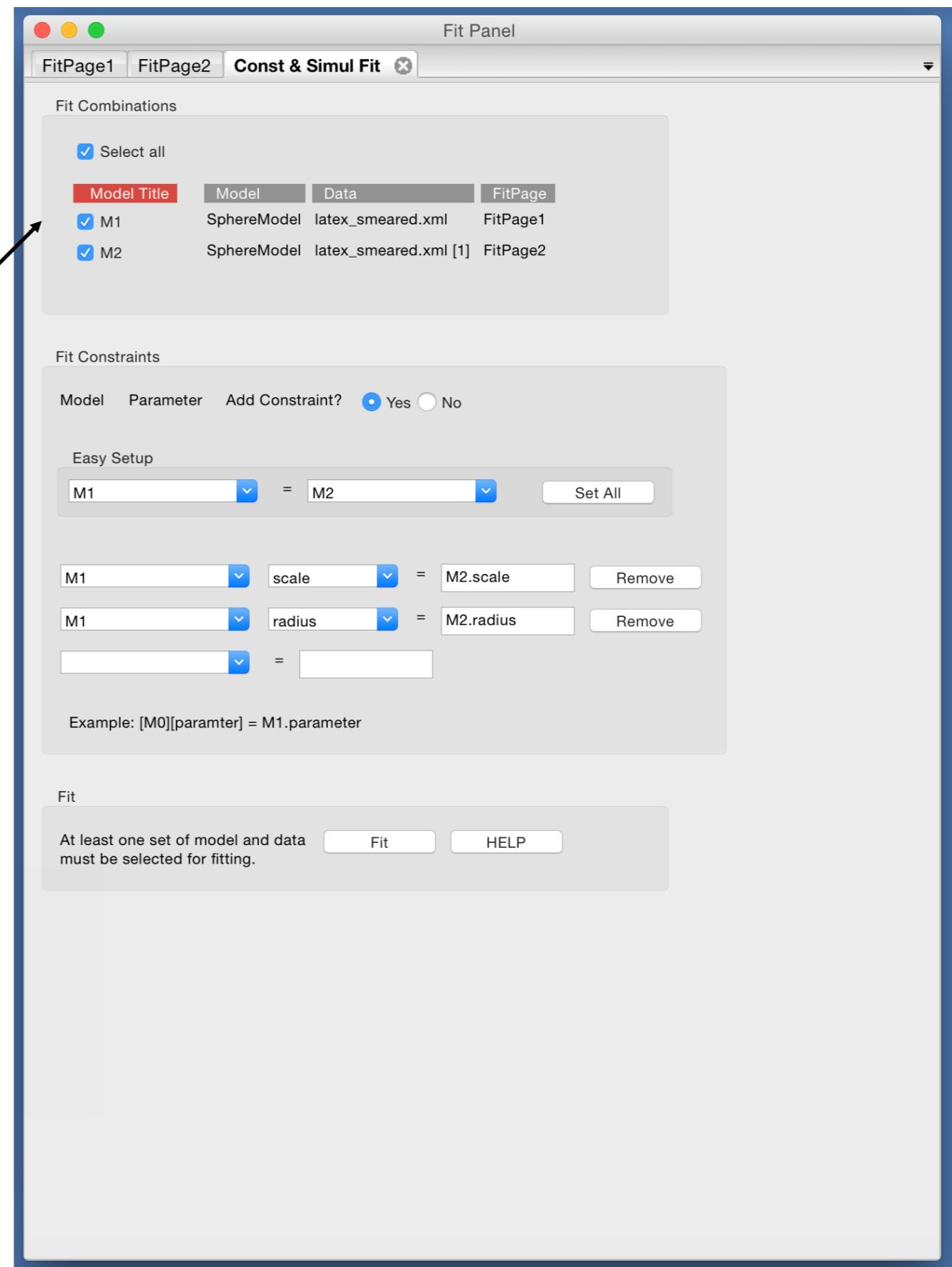
Constraints / Simultaneous Fit

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

Constraints / Simultaneous Fit

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

Set up a simultaneous fit ...

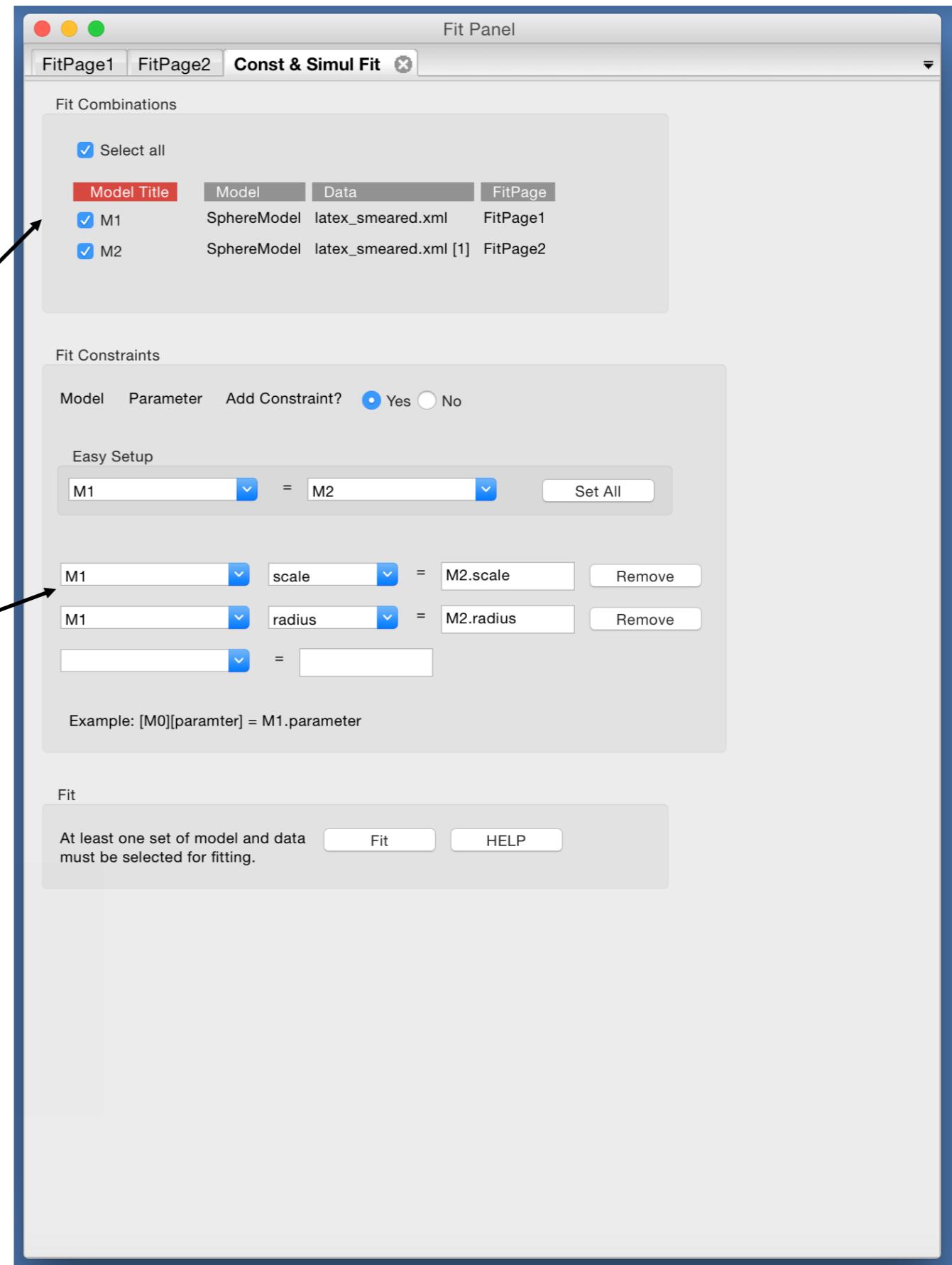


Constraints / Simultaneous Fit

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

Set up a simultaneous fit ...

... with constraints



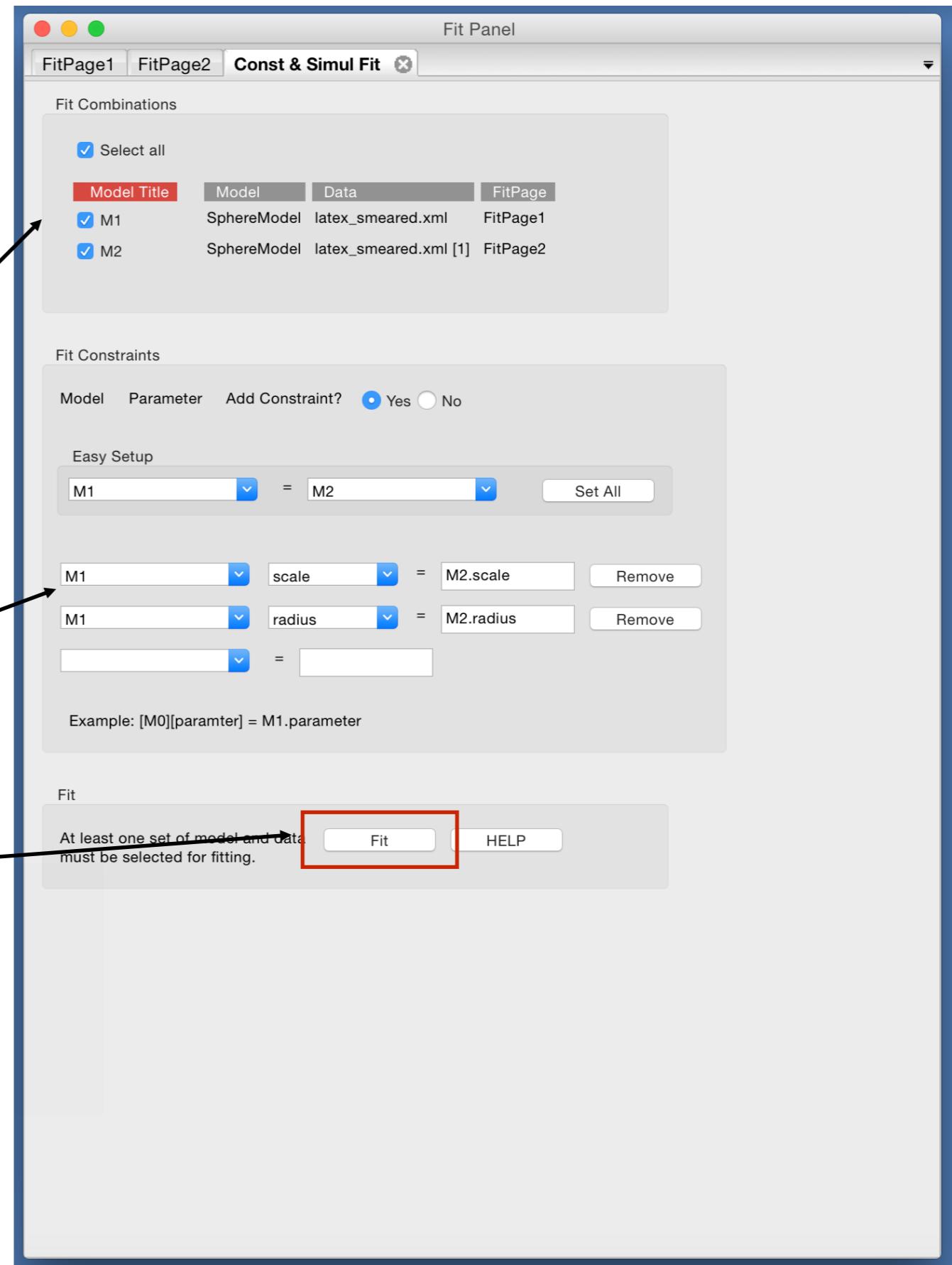
Constraints / Simultaneous Fit

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

Fit Panel

FitPage1 FitPage2 Const & Simul Fit

I(q) Data Source
Name : latex_smeared.xml [1]

Model [M2]
Category: Shapes Modify Description Help
SphereModel P(Q)*S(Q) None

Model Parameters
 Select All Value Error Min Max [Units]
 background 2.6088 +/- 0.48857 [1/cm]
 scale 0.0075699 +/- 6.9289e-06 [A]
 radius 2324 +/- 0.32602 [A]
 sldSolv 6.35e-06 +/- [1/A^2]
 sldSph 1e-06 +/- [1/A^2]

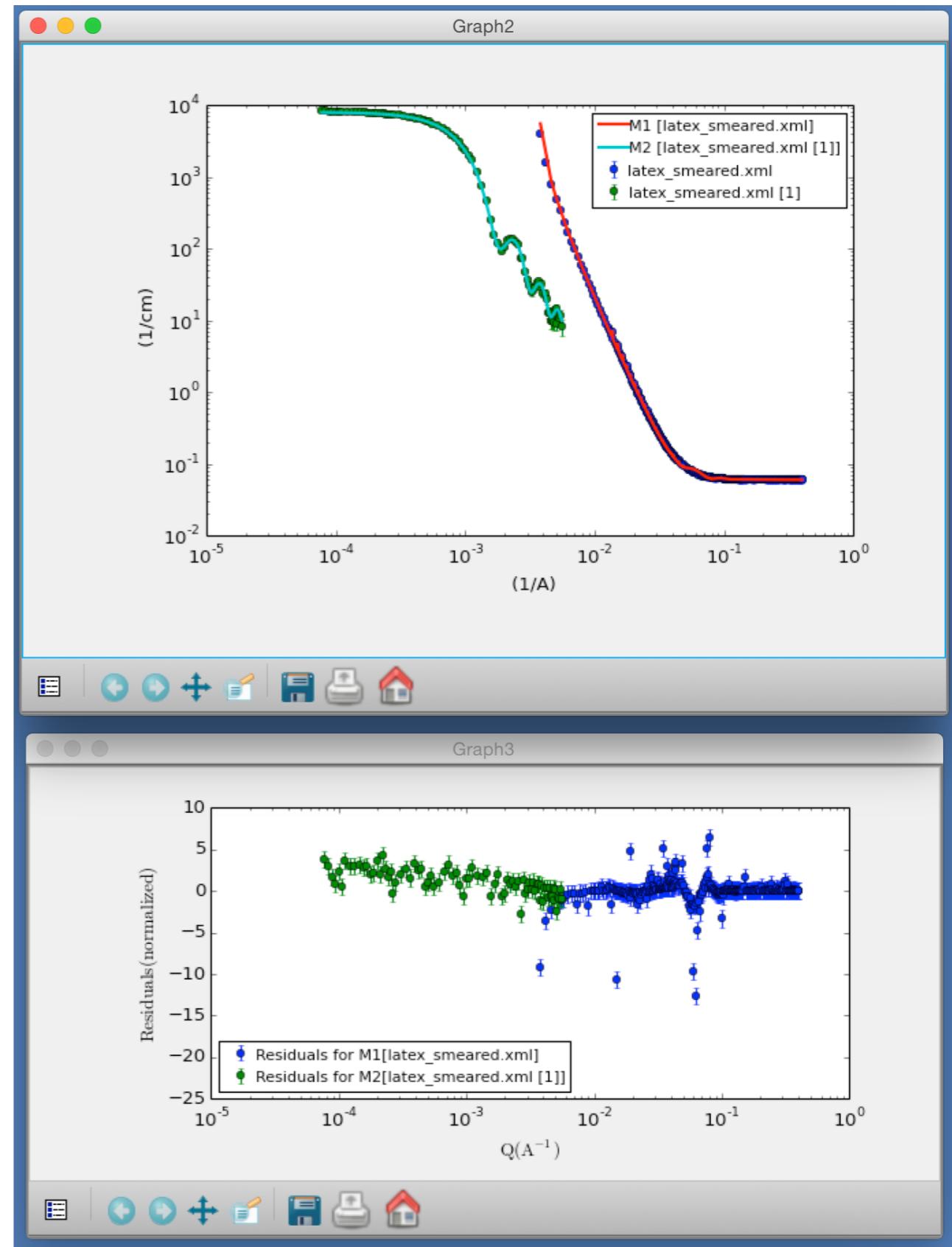
Polydispersity and Orientational Distribution
 On Off ?

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

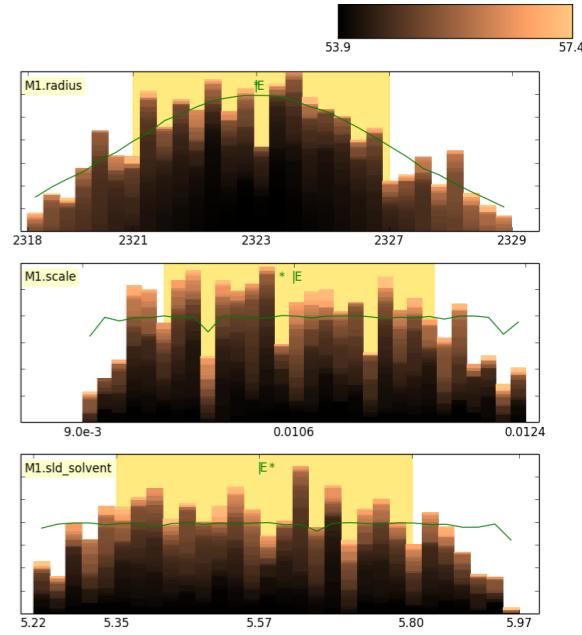
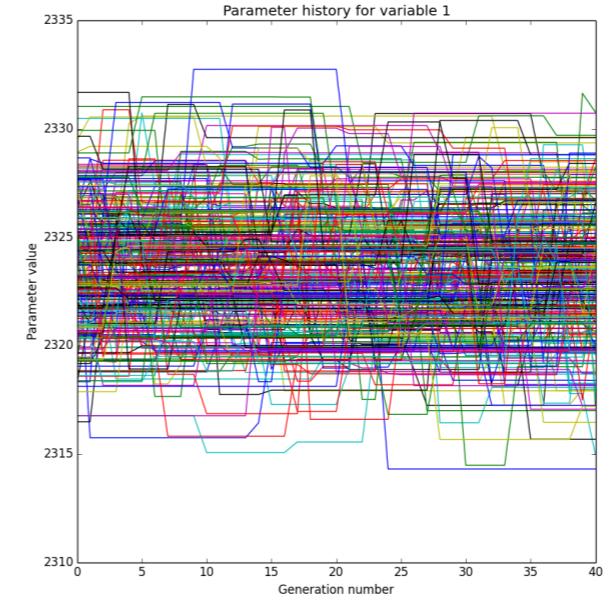
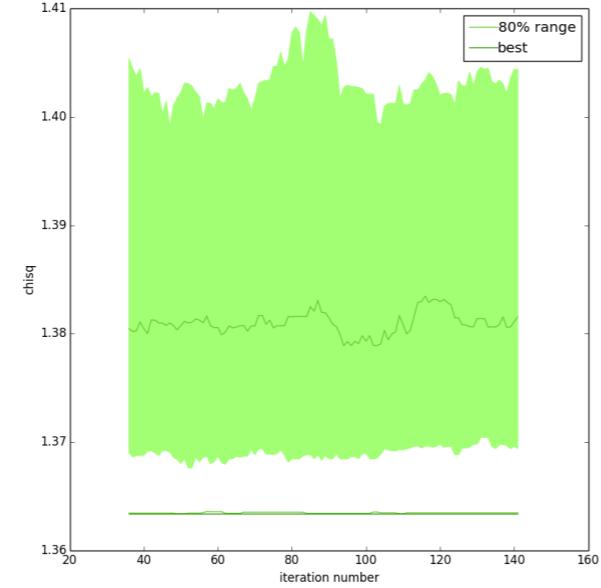
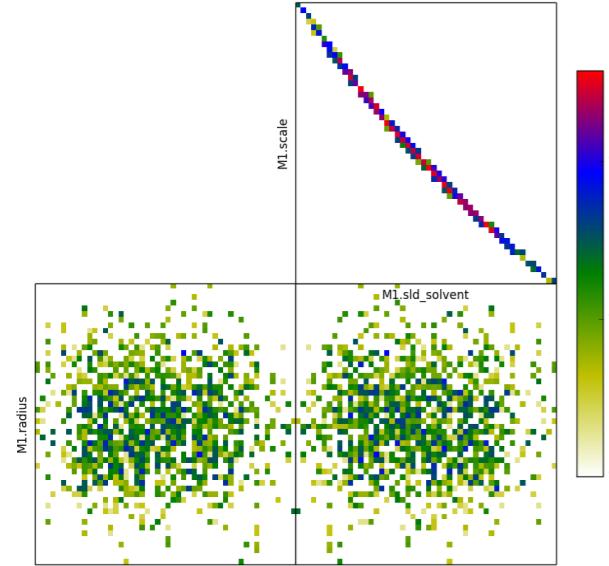
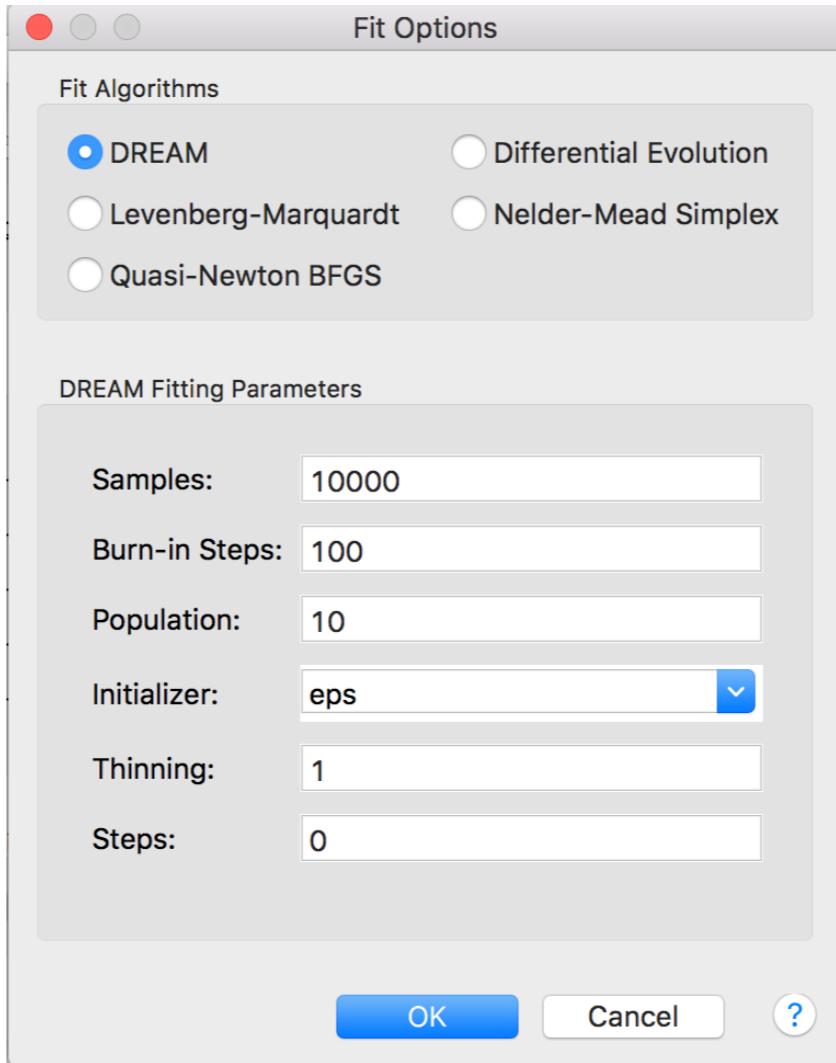
Set Weighting by Selecting dl Source
 No Weighting Use dl Data Use |sqrt(I) Data| Use |I| Data|

Q range Min[1/A] Max[1/A] Masking(2D)
 Reset 7.7457e-05 0.00554976 Editor

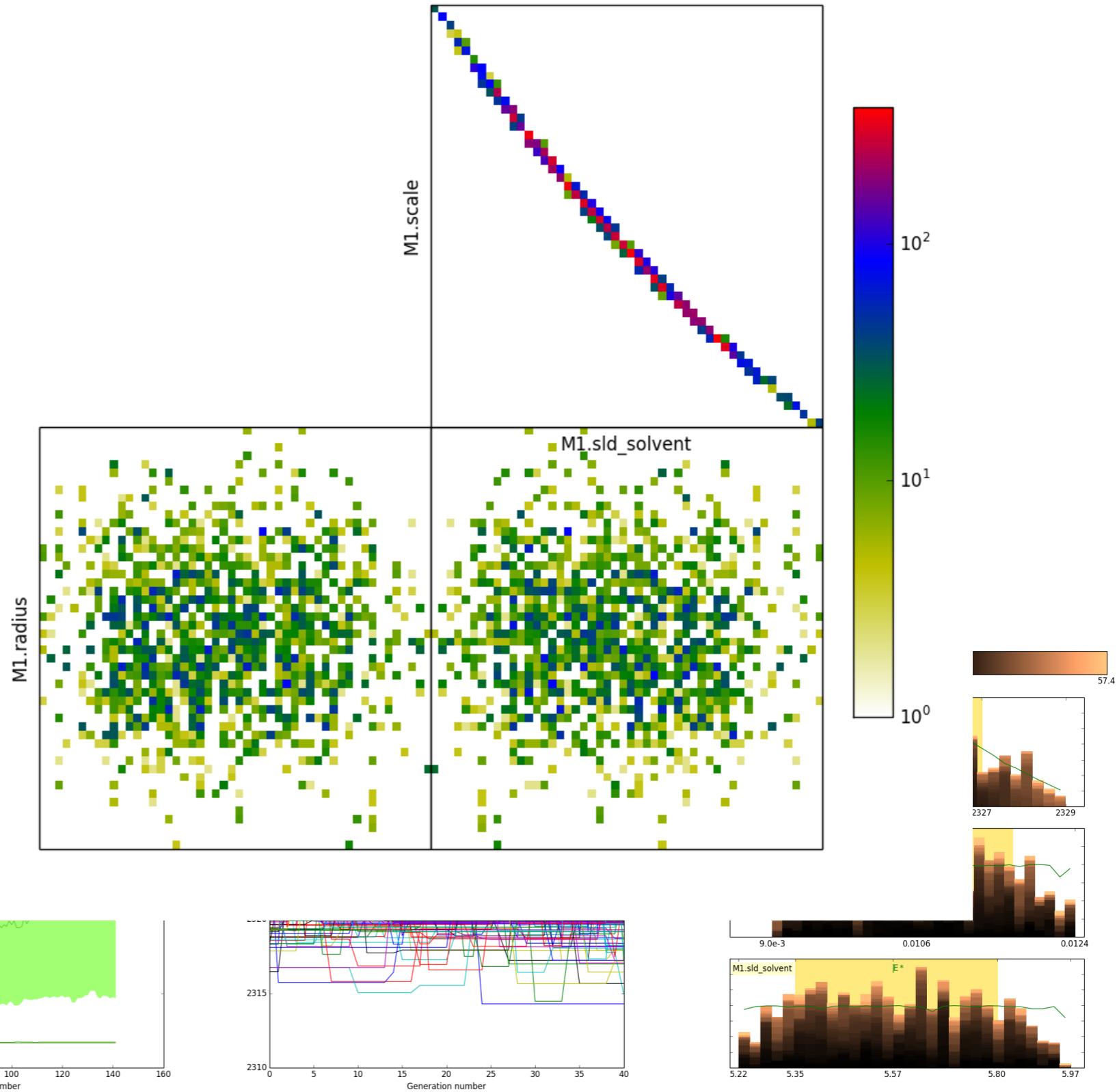
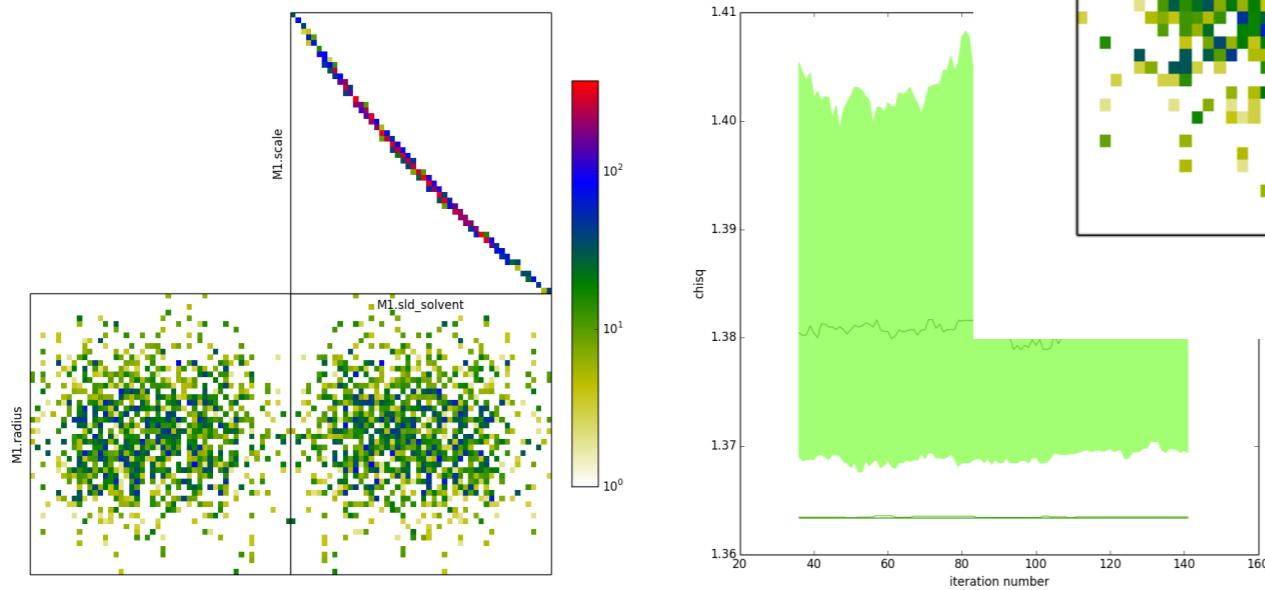
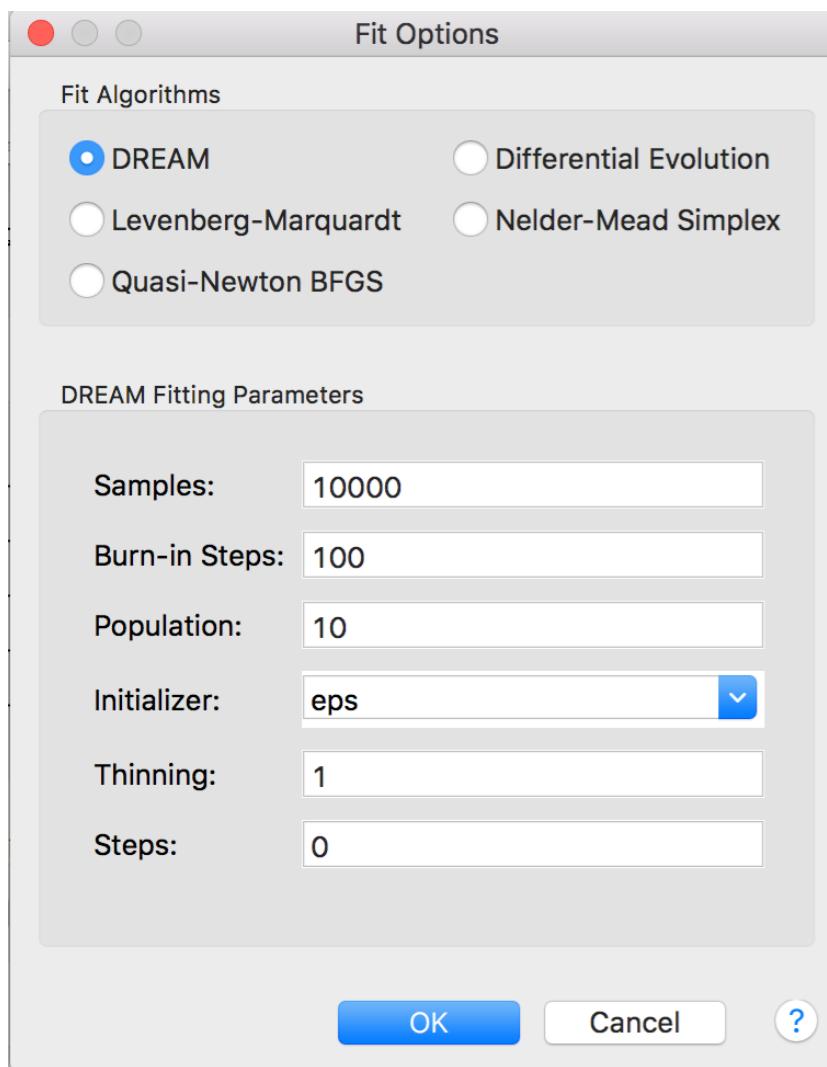
Chi2/Npts Npts(Fit) Npts Log? Compute
 3.5962 82 82 Fit Help



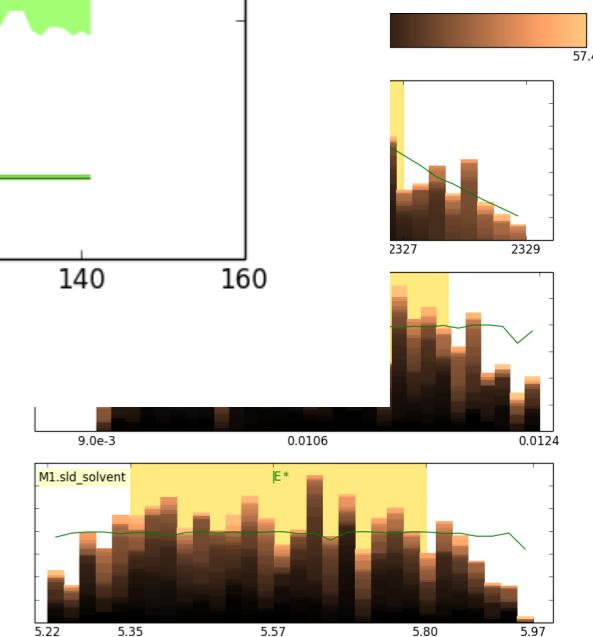
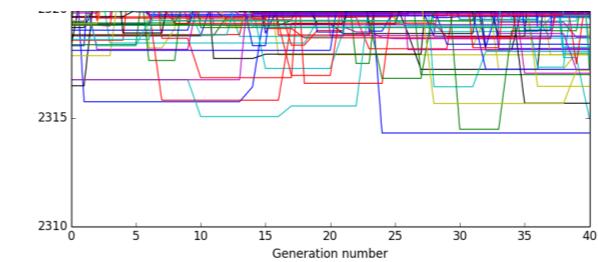
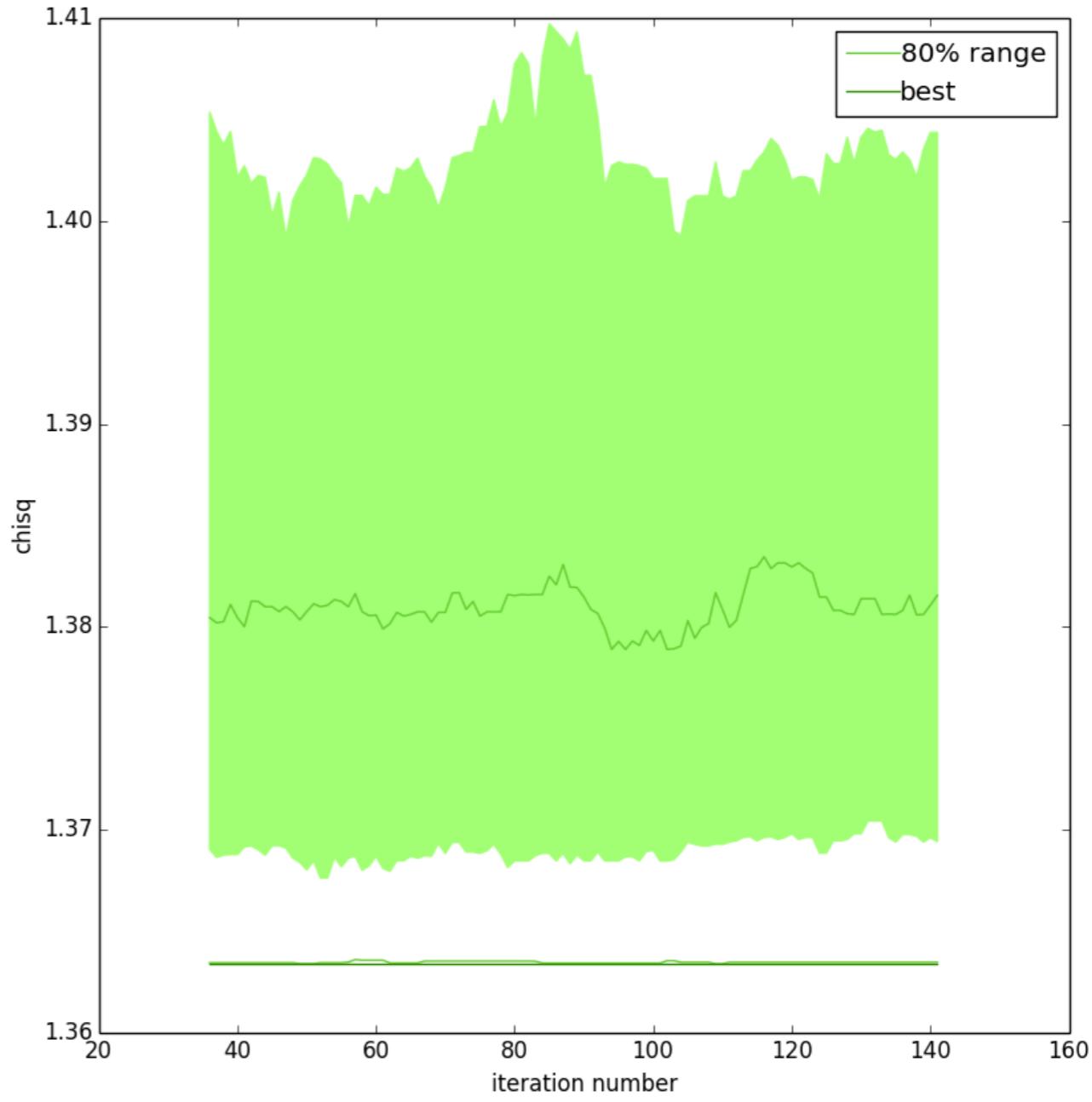
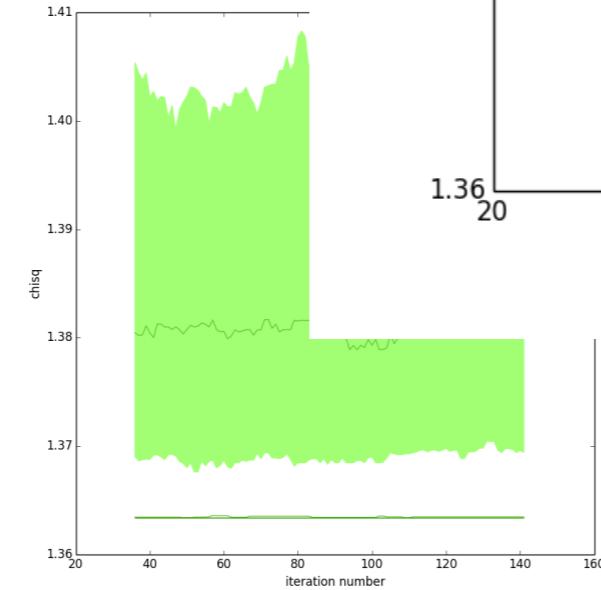
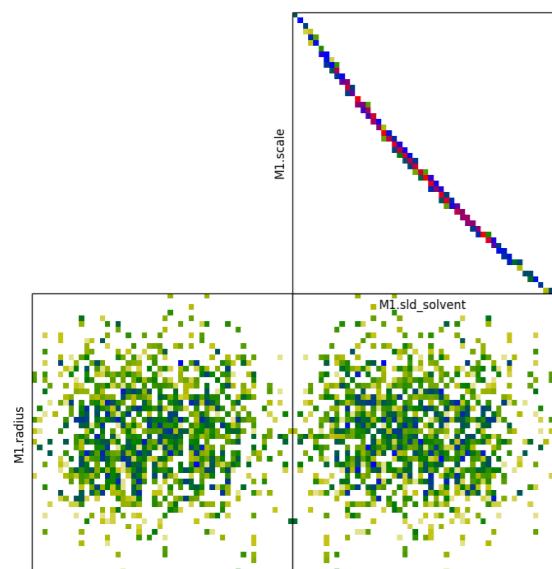
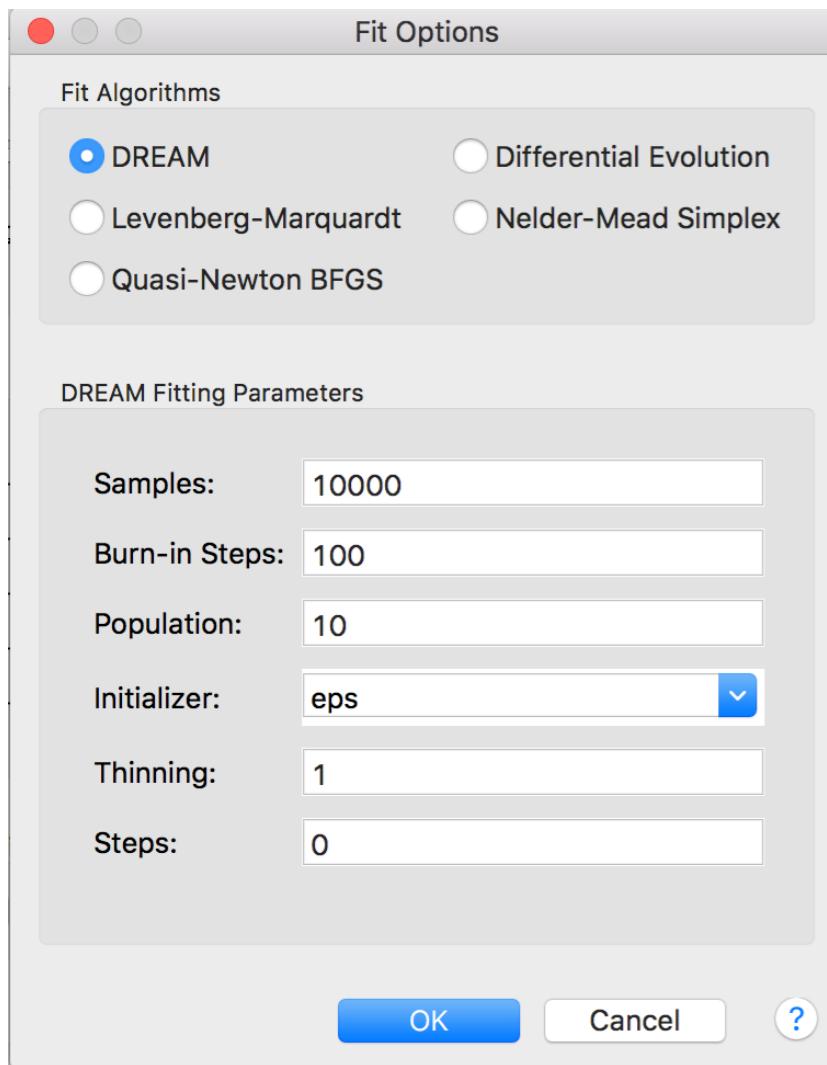
Fitting Algorithms



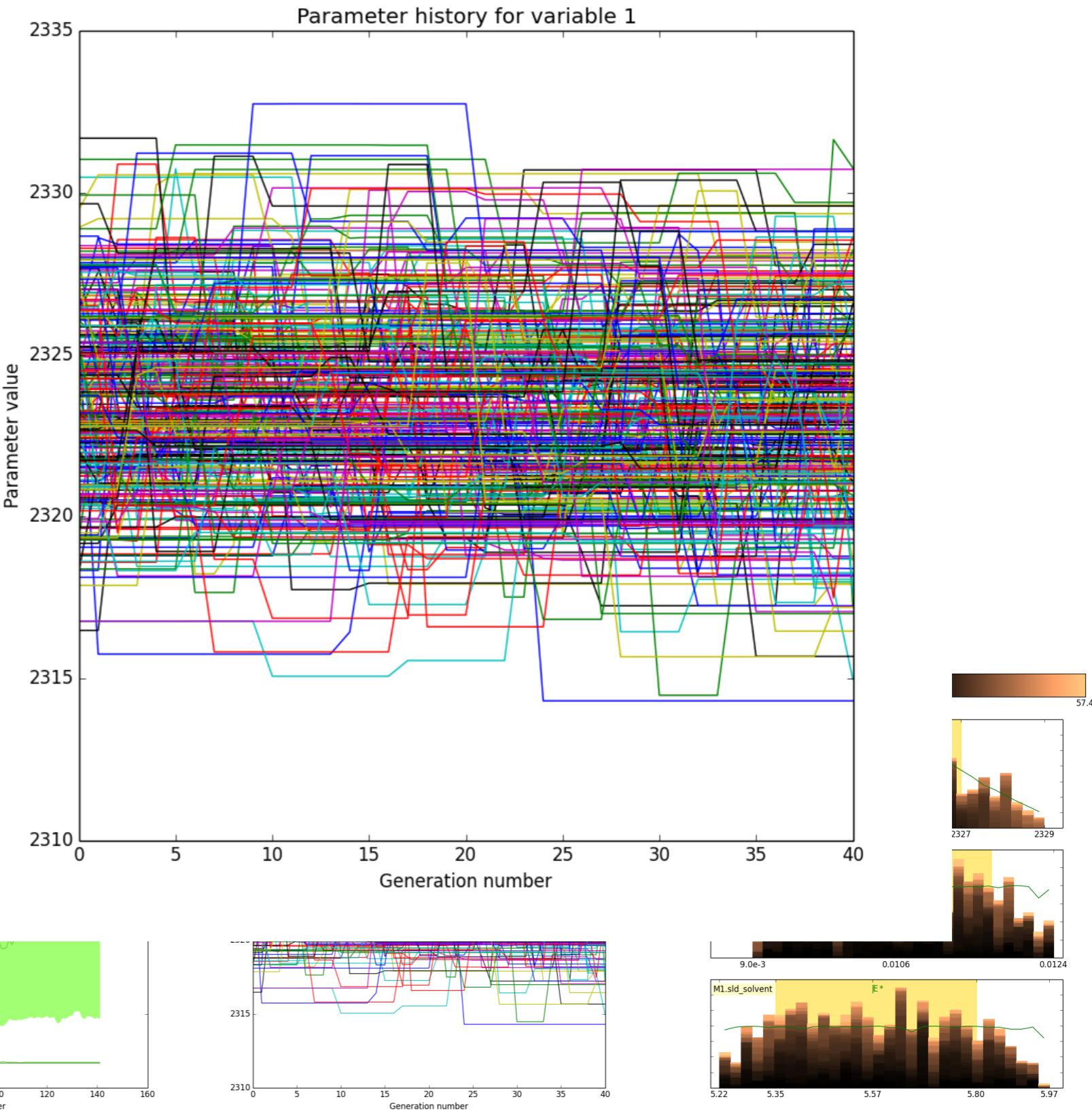
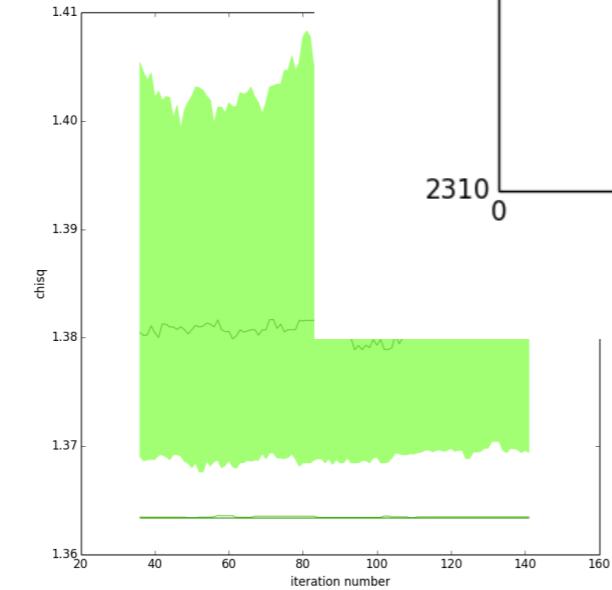
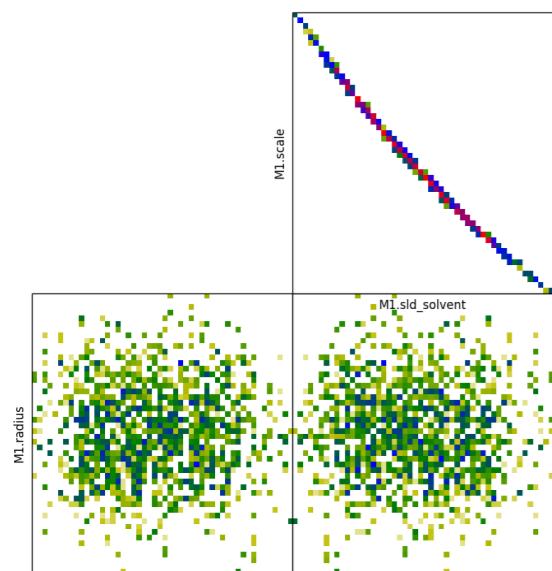
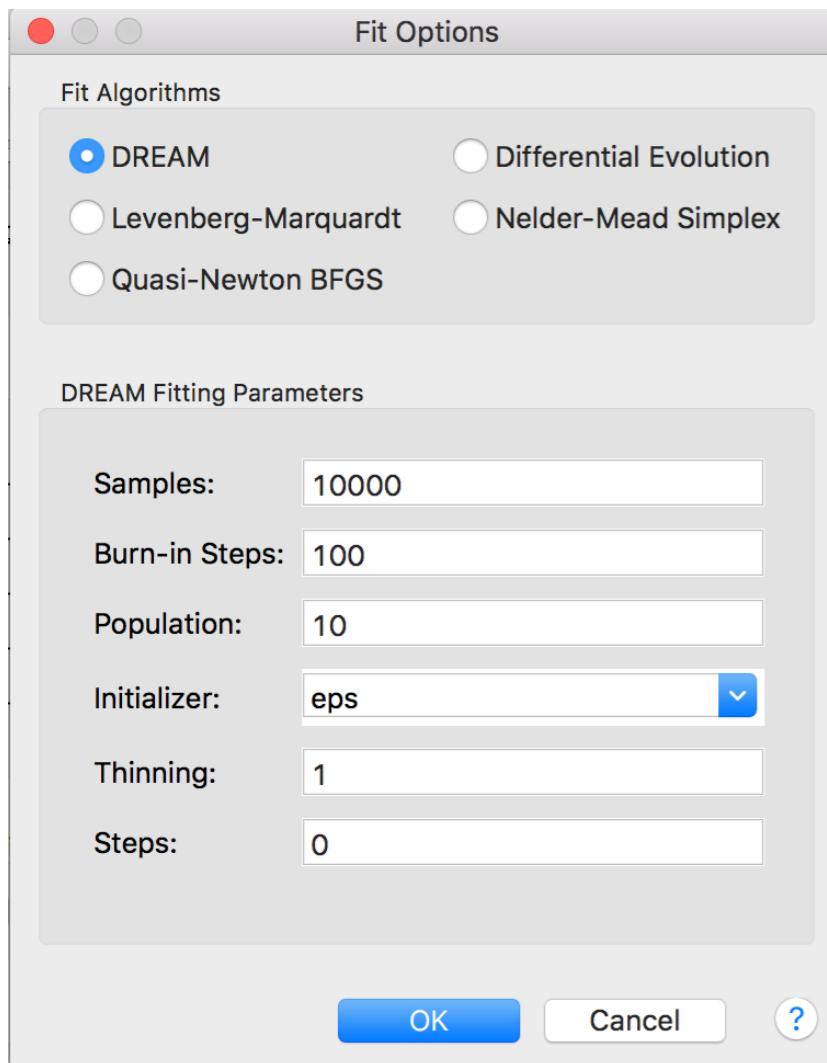
Fitting Algorithms



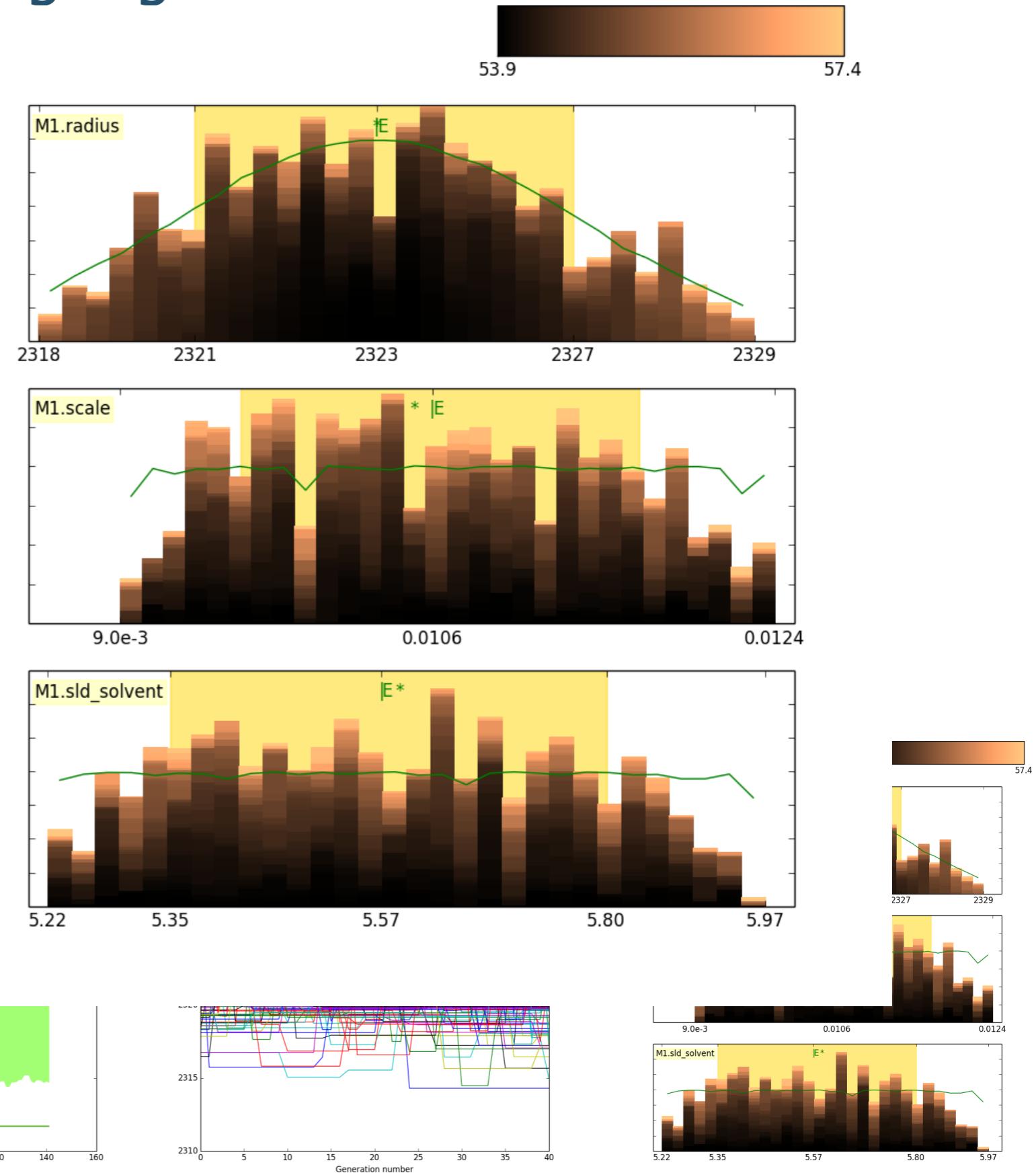
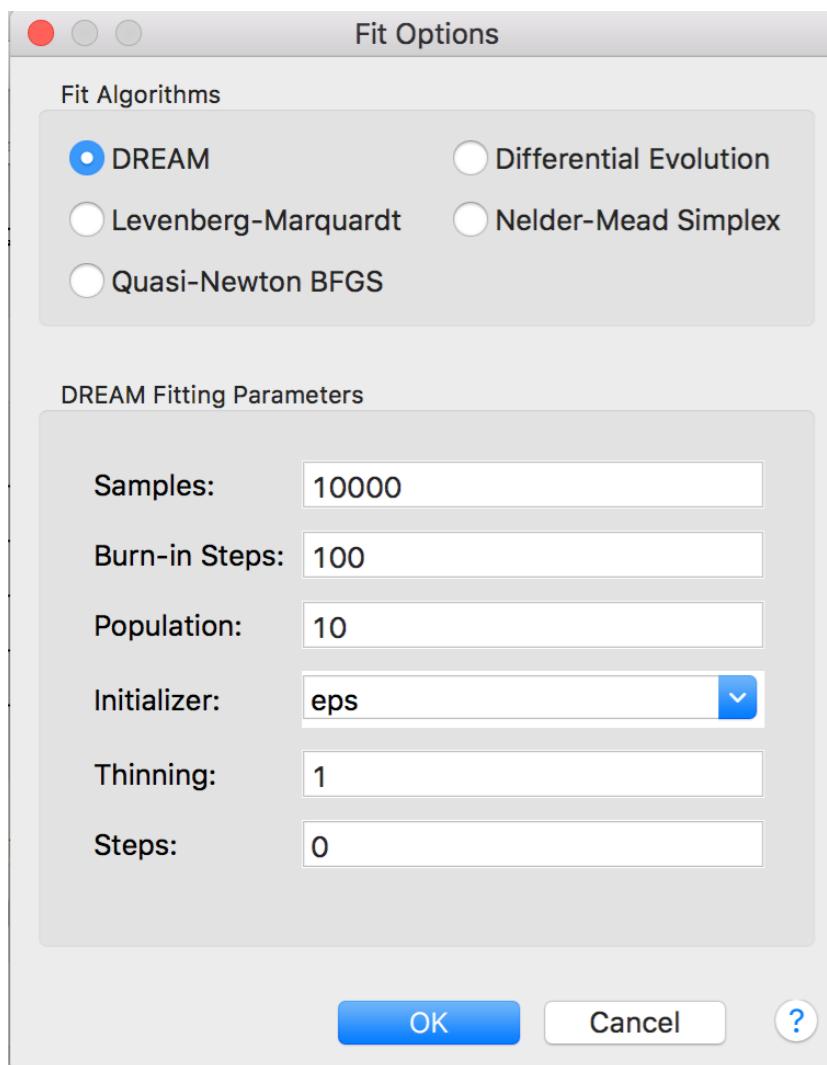
Fitting Algorithms



Fitting Algorithms



Fitting Algorithms



Invariant Calculation

Invariant

I(q) Data Source
For more information, click on Details button.

Name: **latex_smeared.xml [1]**

Total Q Range (1/ \AA): Min : **7.7457e-05** Max : **0.00554976**

Outputs

Volume Fraction **2.26e-13** +/- **1.67e-18**
Specific Surface **[1/ \AA]**

Invariant Total [Q^*] **0.000445** +/- **7.4e-06** **[1/(cm * \AA^3)]**

Customized Inputs

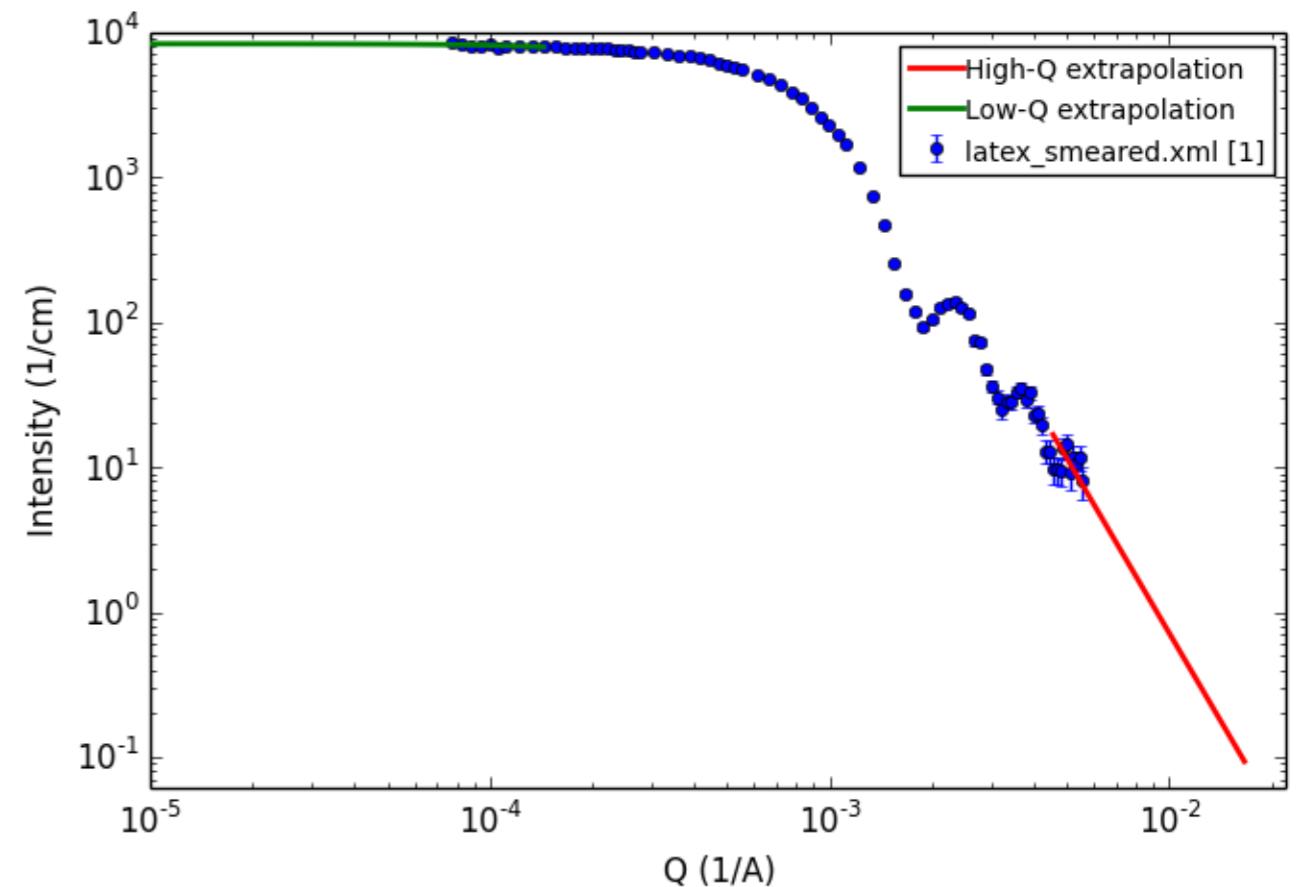
Background: **0.0** [1/cm] Scale: **1.0**
Contrast: **1.0** [1/ Porod Constant: **[1/(cm * \AA^4)]** (optional)

Extrapolation

Extrapolation Min: **1e-05** Max: **10**
Maximum Q Range [1/ \AA]:

Low Q High Q

Enable Extrapolate Low Q Enable Extrapolate high-Q
Npts **10** Npts **10**
 Guinier Power Law
 Power Law Fix Fit
Power **4.0** Power **4**



Invariant Details

Invariant Chart

Q* from Low-Q	0.638%
Q* from Data	93.1%
Q* from High-Q	6.24%

Numerical Values

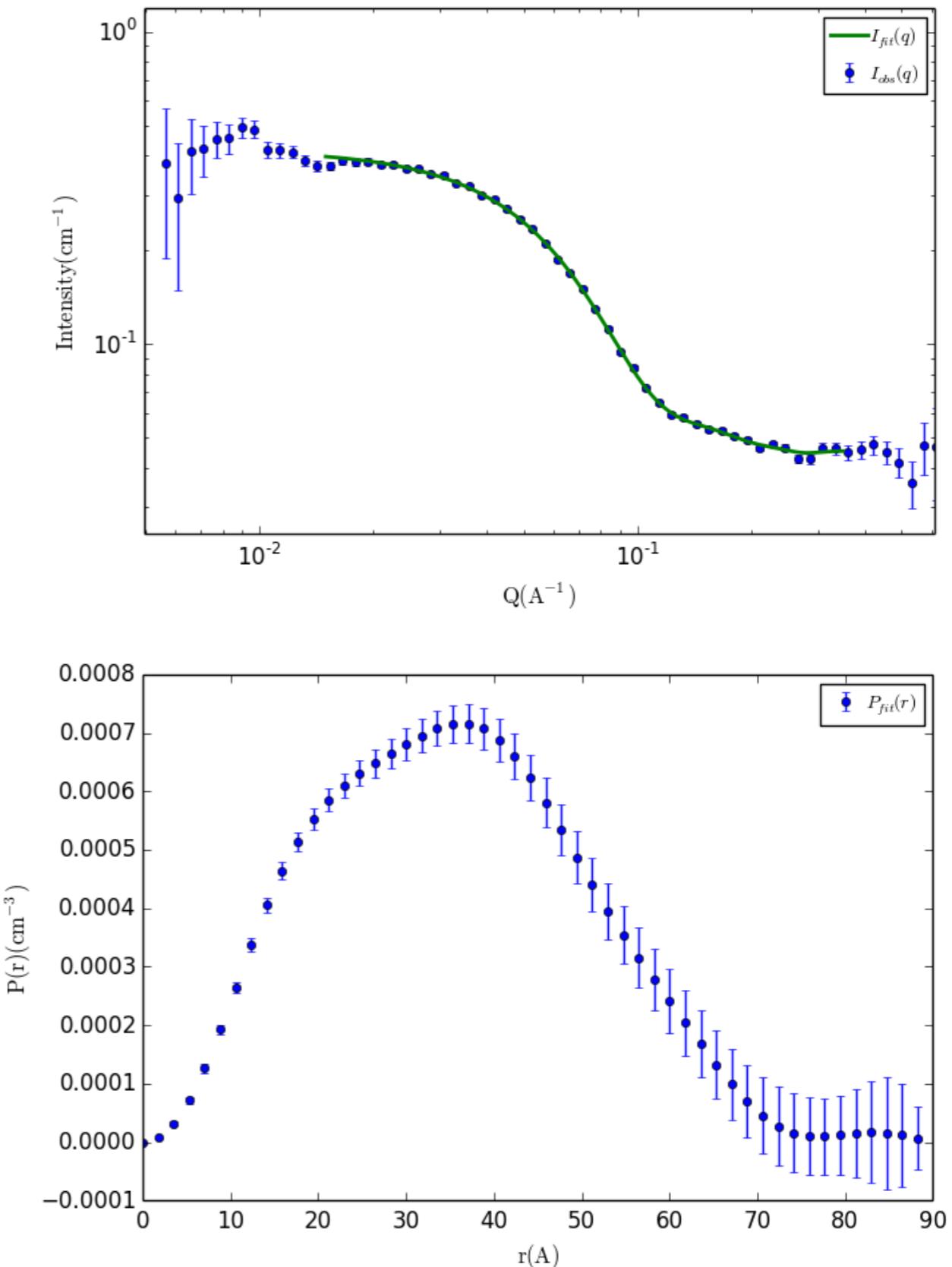
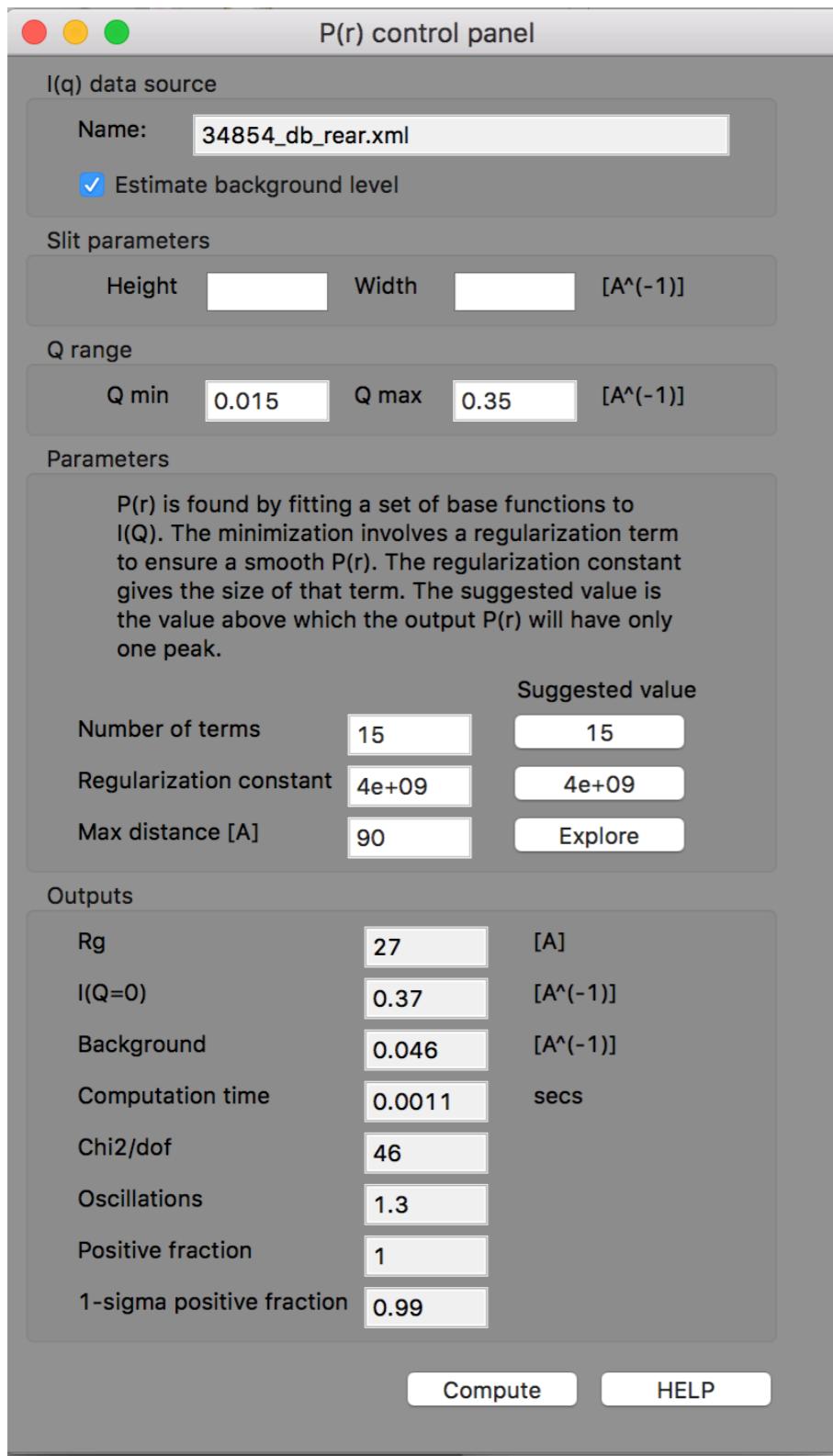
Q* from Low-Q	2.84e-06 +/- 1.11e-09 [1/(cm * \AA^3)]
Q* from Data	0.000415 +/- 1.18e-06 [1/(cm * \AA^3)]
Q* from High-Q	2.78e-05 +/- 7.3e-06 [1/(cm * \AA^3)]

Warning

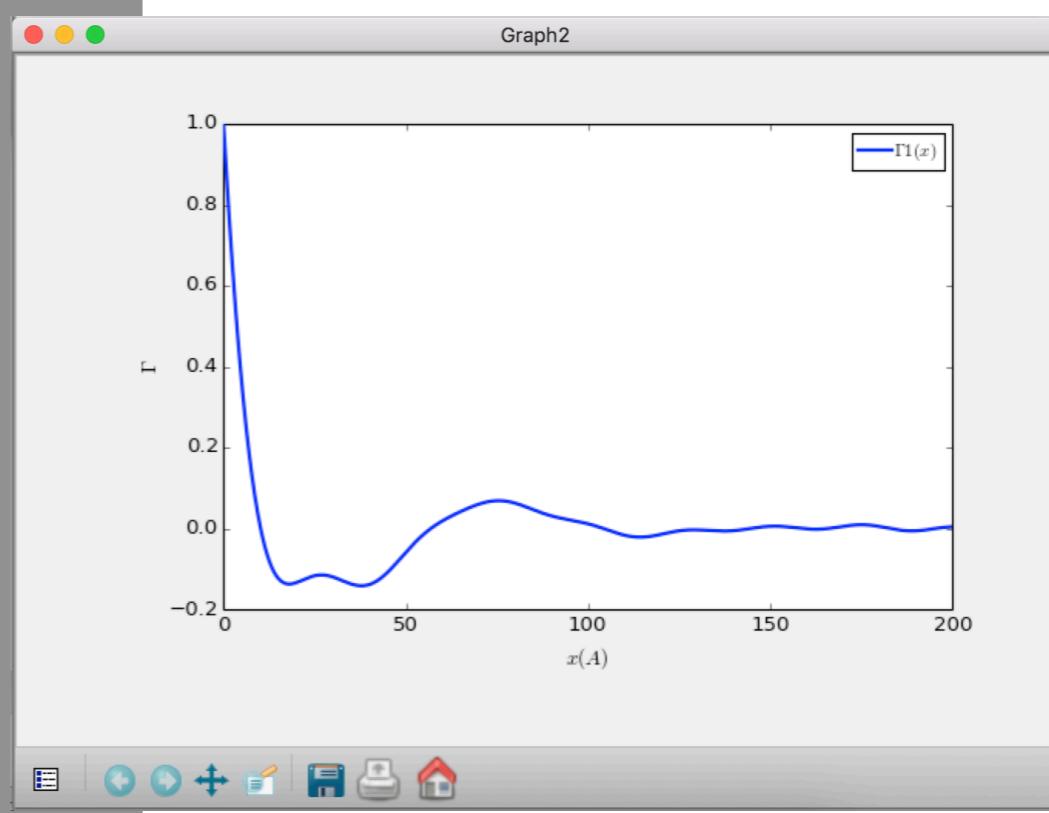
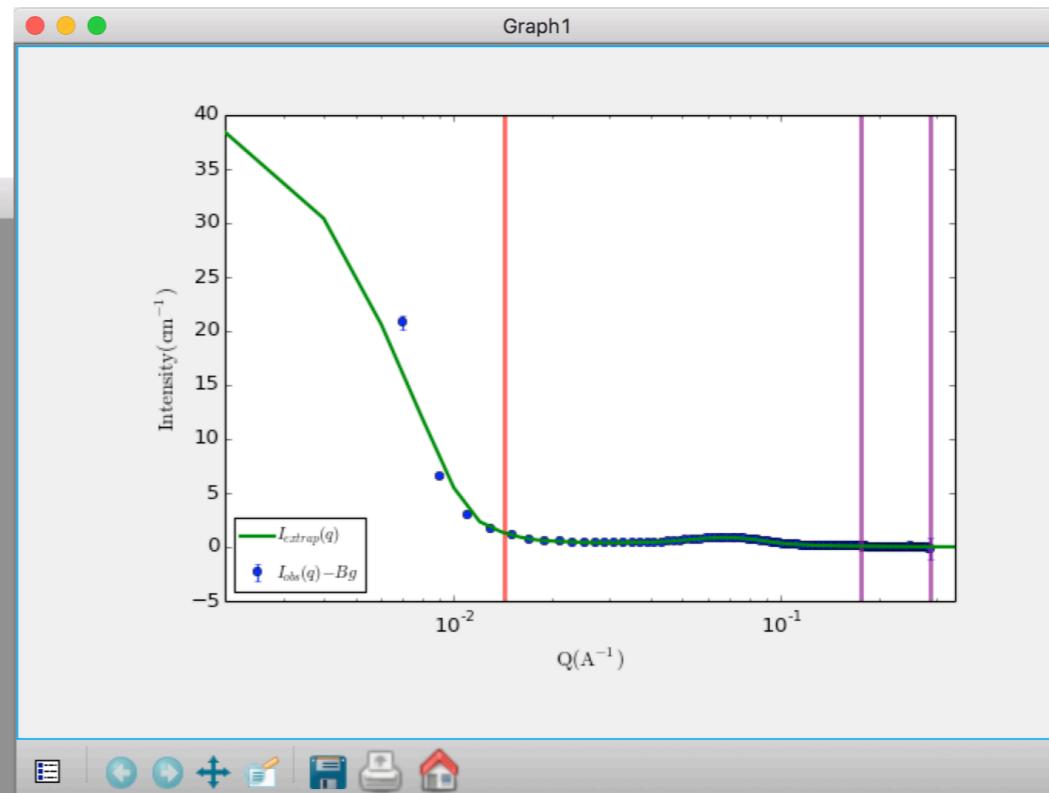
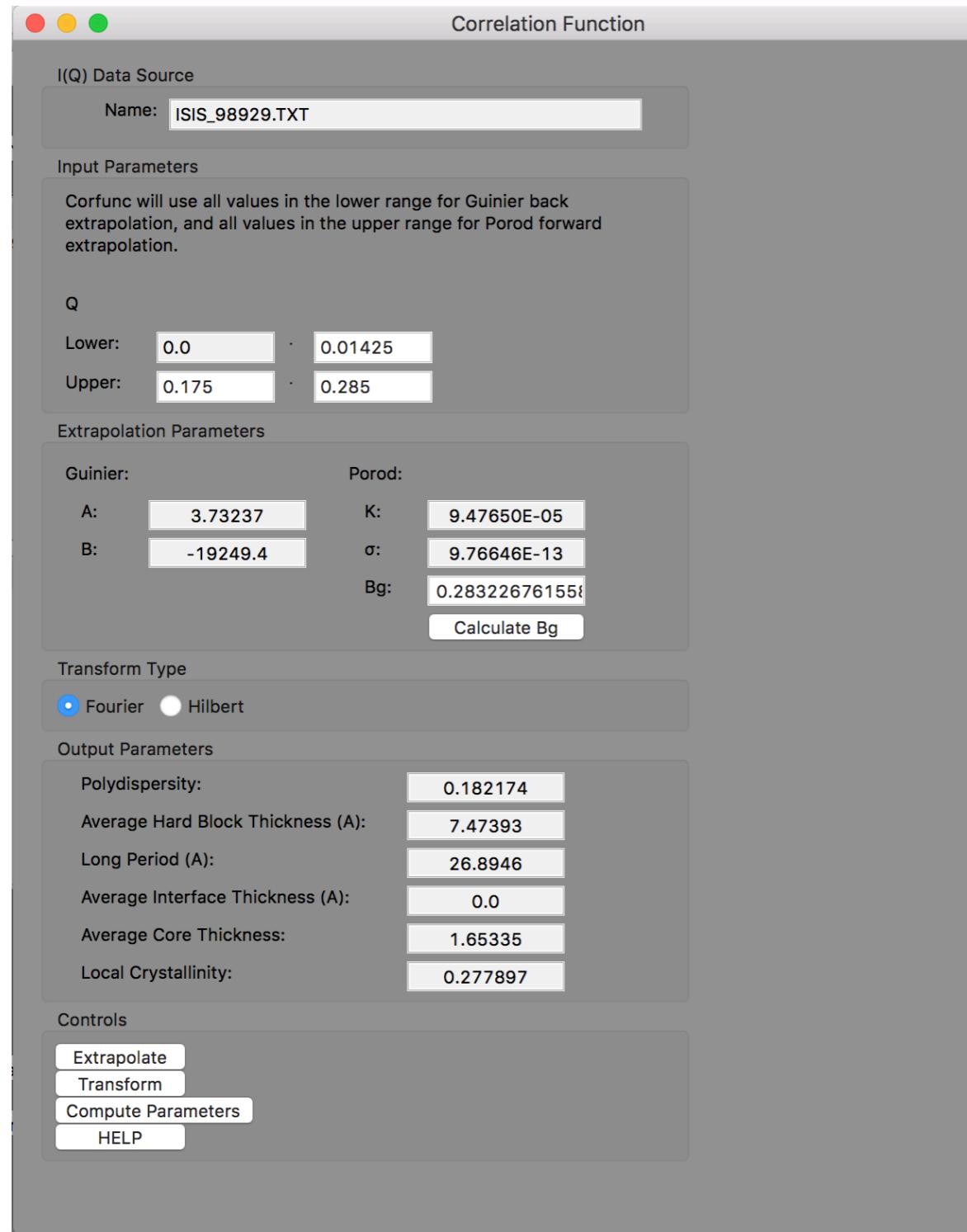
Extrapolated contribution at High Q is higher than 5% of the invariant.
The sum of all extrapolated contributions is higher than 5% of the invariant.
The calculations are likely to be unreliable!

Ok

P(r) Inversion

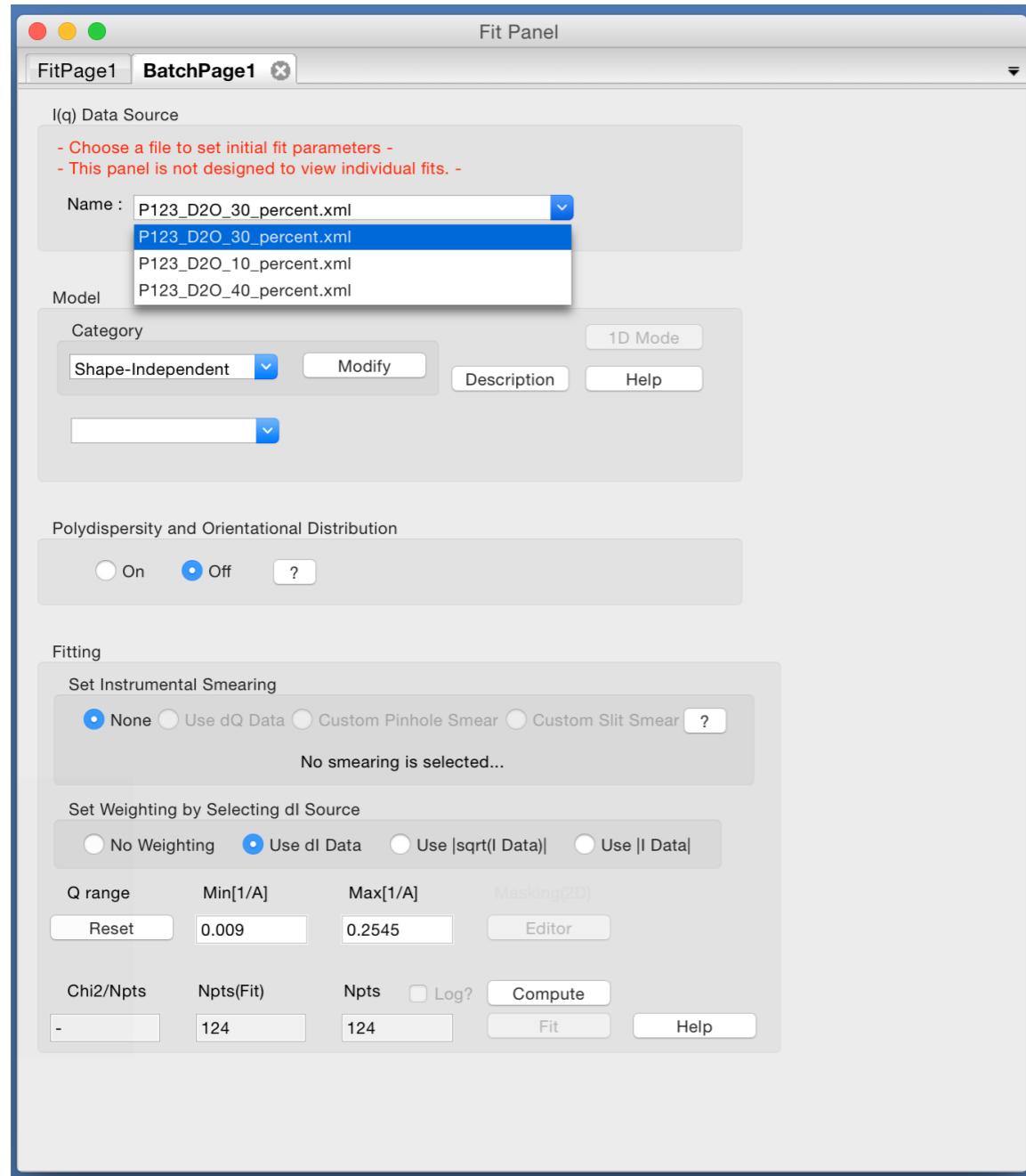


Correlation Function Analysis (new!)

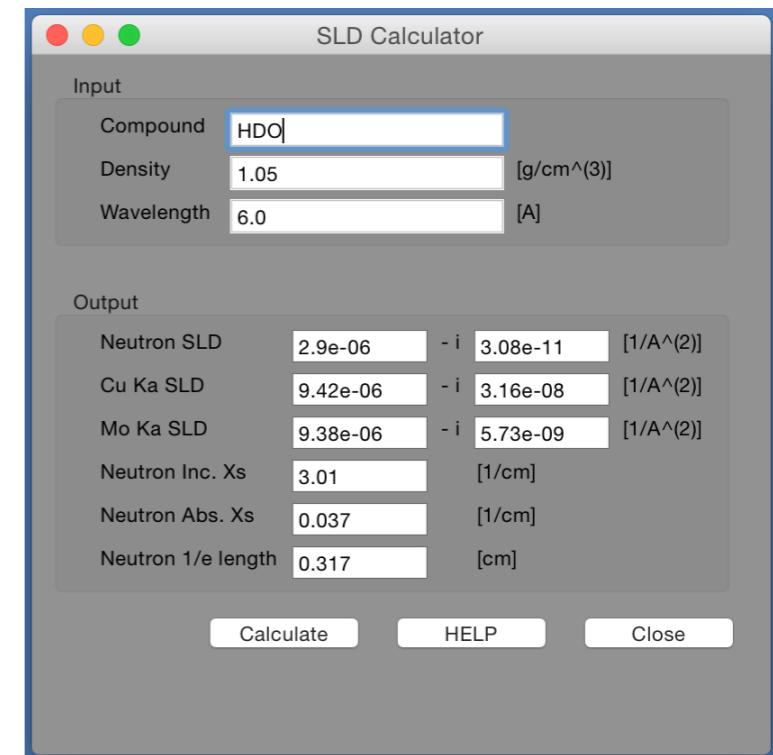


Other Features

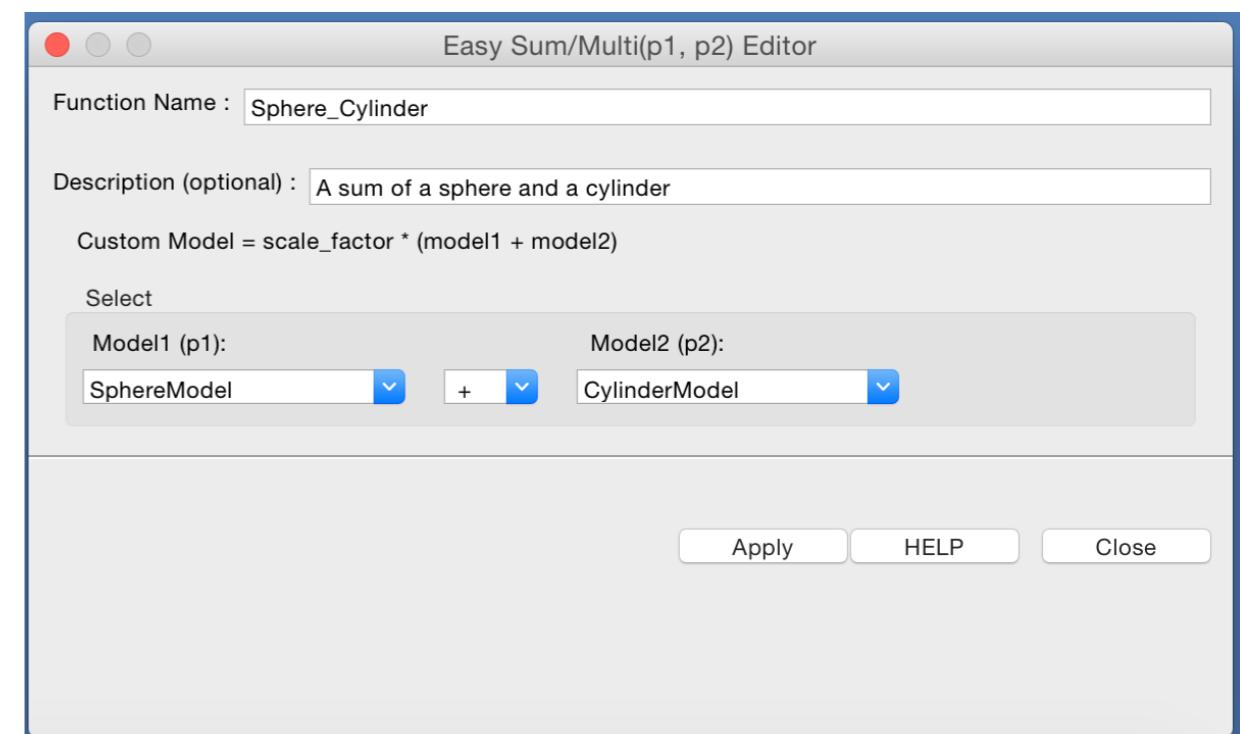
Batch fitting ...



SLD Calculator ...



Sum & Multiplication of Models ...



2D Modelling

Oriented systems & Magnetic Scattering

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

www.rsc.org/softmatter

PAPER

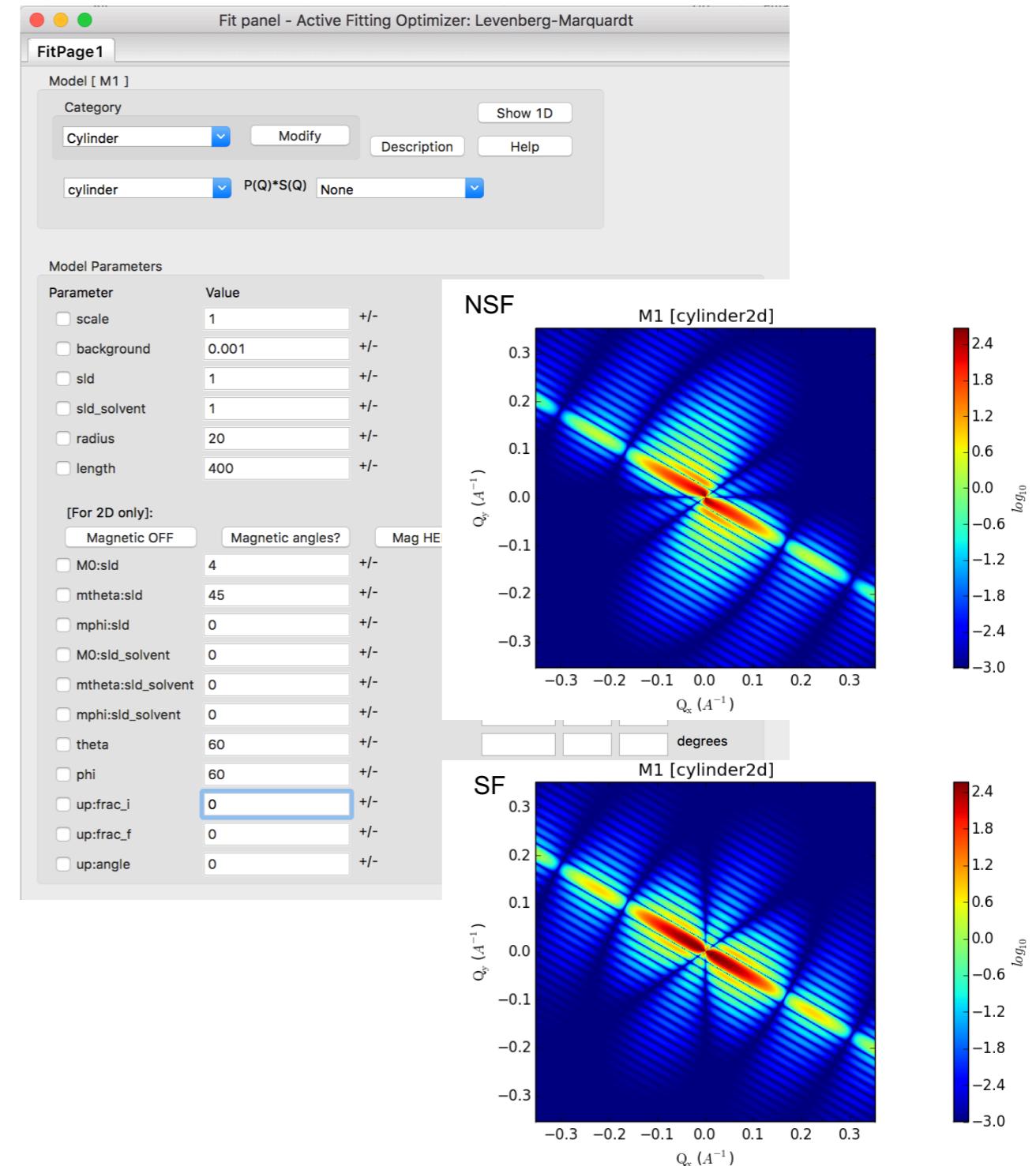
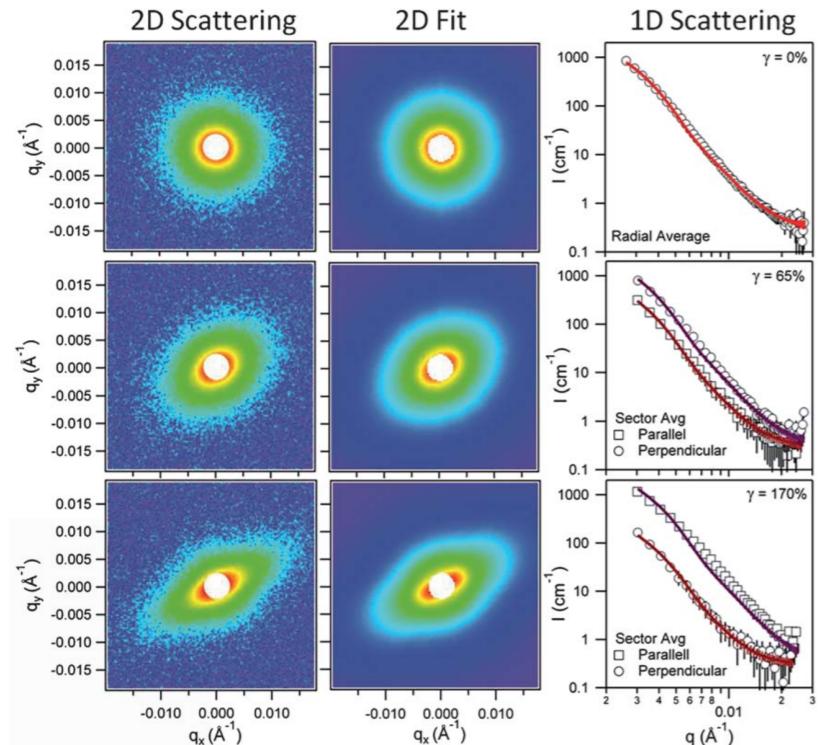
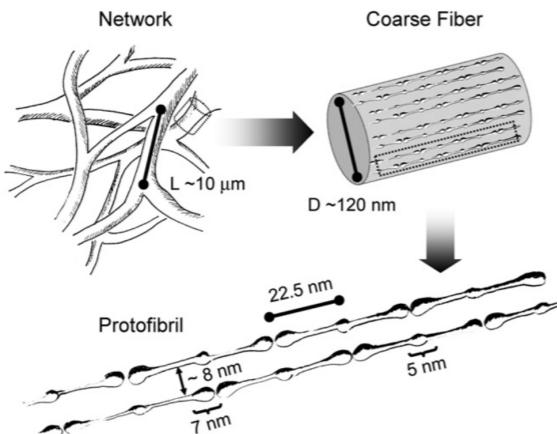
In situ neutron scattering study of structural transitions in fibrin networks under shear deformation

Katie M. Weigandt,^a Lionel Porcar^{b,c} 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 biopolymer networks by directly measuring the structural response to deformation. A special Couette shear cell is used to systematically deform a fibrin clot over strain values in the range of $\gamma = 1\text{--}170\%$. The hardening response of coarse fibrin gels occurs in two distinct mechanical signatures that are separated by an intermediate regime ($\gamma < 10\%$): there is a measurable increase in the shear modulus and there are no significant changes to the clot structure. At higher strain regimes, the hardening response is directly correlated to significant fiber alignment. These results are determined directly from two-dimensional fits to the anisotropy of the scattering signal. The results suggest that the structural transitions of fibrin clots are monotonic in the high-strain regime. The results suggest that the structural transitions of fibrin clots are the result of a reduction of lateral entropic freedom between bending and stretching at higher strain values.



Creating Models

Old Way

- Write a model in python and drop it in plugin folder
 - Easy but no polydispersity available
- Write a model in C and incorporate into SasView
 - Difficult and need to recompile whole programme

New Way

- Models distributed in separate package (sasmodels)
 - separation of models from GUI
 - simpler addition of models by users
 - speed! GPU and parallel processing
- All models work the same
- Write in python and/or C and drop in plugin folder

Creating Models

Pure Python

```
r"""
This model calculates a simple power law with a flat background.
```

Definition

```
.. math::
```

$$I(q) = \text{scale} \cdot q^{-\text{power}} + \text{background}$$

Note the minus sign in front of the exponent. The exponent *power* should therefore be entered as a **positive** number for fitting.

Also note that unlike many other models, *scale* in this model is NOT explicitly related to a volume fraction. Be careful if combining this model with other models.

References

```
None.
```

```
"""
```

```
from numpy import inf, errstate
name = "power_law"
title = "Simple power law with a flat background"

description = """
    Evaluates the function
     $I(q) = \text{scale} \cdot q^{-\text{power}} + \text{background}$ 
    NB: enter power as a positive number!
"""

category = "shape-independent"
```

- Documentation
- Description
- Parameters
- Calculation
- Tests

```
#             ["name", "units", default, [lower, upper], "type", "description"]
parameters = [{"power": "", 4.0, [-inf, inf], "", "Power law exponent"}]

# NB: Scale and Background are implicit parameters on every model
def Iq(q, power):
    # pylint: disable=missing-docstring
    with errstate(divide='ignore'):
        result = q**-power
    return result

Iq.vectorized = True # Iq accepts an array of q values

demo = dict(scale=1.0, power=4.0, background=0.0)

tests = [
    [{"scale": 1.0, "power": 4.0, "background": 0.0,
      [0.0106939, 0.469418], [7.64644e+07, 20.5949]},
```

SasView 4.1 is Out!

www.sasview.org

Models

New models

New model package (sasmmodels)

Separation of models from GUI

Simpler addition of models by users

Speed! GPU and parallel processing

Correlation Function Analysis

CCP13 corfunc algorithm

Documentation

Enhanced, updated documentation for models

SESANS

Automatic transform of SANS model to $P(z)$

Plotting and fitting of SESANS data from GUI

Example scripts for fitting SESANS data

Simultaneous fitting of SANS & SESANS

Future ...

GUI Refactoring

Move to QT - current and well supported toolkit
Complete separation of GUI and calculation code
Non-desktop UIs

Sasmodels Enhancements NSF

Return $F(q)$ from models
Beta approximation
Coherent sums

Constraints refactor
Multi-GPU support
Interface for SasFit models

Documentation

Tutorials
Manual

Future ...

And much more!

See Roadmap and Tickets

**Contributions Needed
All skill sets welcome**

NSF

Models

Testing

Core development

Documentation

Admin and Infrastructure

SasView code camp (<http://trac.sasview.org/wiki/CodeCampVI>)

Start on Tuesday **4th April at 9:00 at room MD-1-21** (ESRF)

Introduction for new contributors: 4th April at 13:00 (possibly at SB401)

Roadmap discussion: Friday **7th April at 15:30** (PSCM common room SB213?)

Until afternoon of Tuesday 11th April

Questions?

