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SPALLATION
SOURCE



SasView : A Small Angle Scattering Analysis Software Package

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

SINE 2020 WP 10 Meeting, Grenoble, 24th – 25th 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 an analysis tool and part of providing the tool
should be the necessary software → the FACILITY'S JOB

Data sat on disk is useless to EVERYBODY

We need to work together!

Analysis Software - Who's Job is it Anyway?

But ... where are the resources?

More pressing tasks for all of us ...

Facility scientists & staff : maintaining & improving instrumentation, bringing in and supporting users, dealing with instrument control and data reduction software ...

Users : data analysis should be high priority ... But in fact the priority is publication. Users want to get rapidly from data to answer – if it is going to need major investment of time then low priority. Especially for “one-time” and industrial users.

Writing shareable data analysis software 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 two staff 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

Released under BSD 3-clause license

Bug and Enhancement Ticket System

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

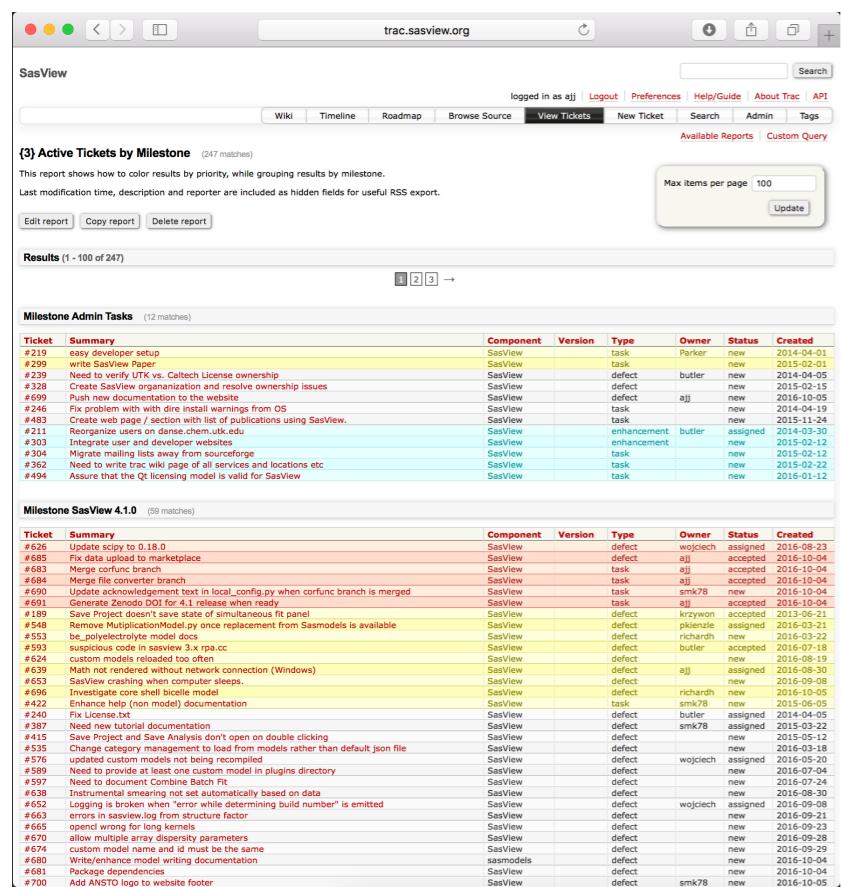
<http://www.sasview.org>

<http://github.com/SasView>

Development Model

www.sasview.org

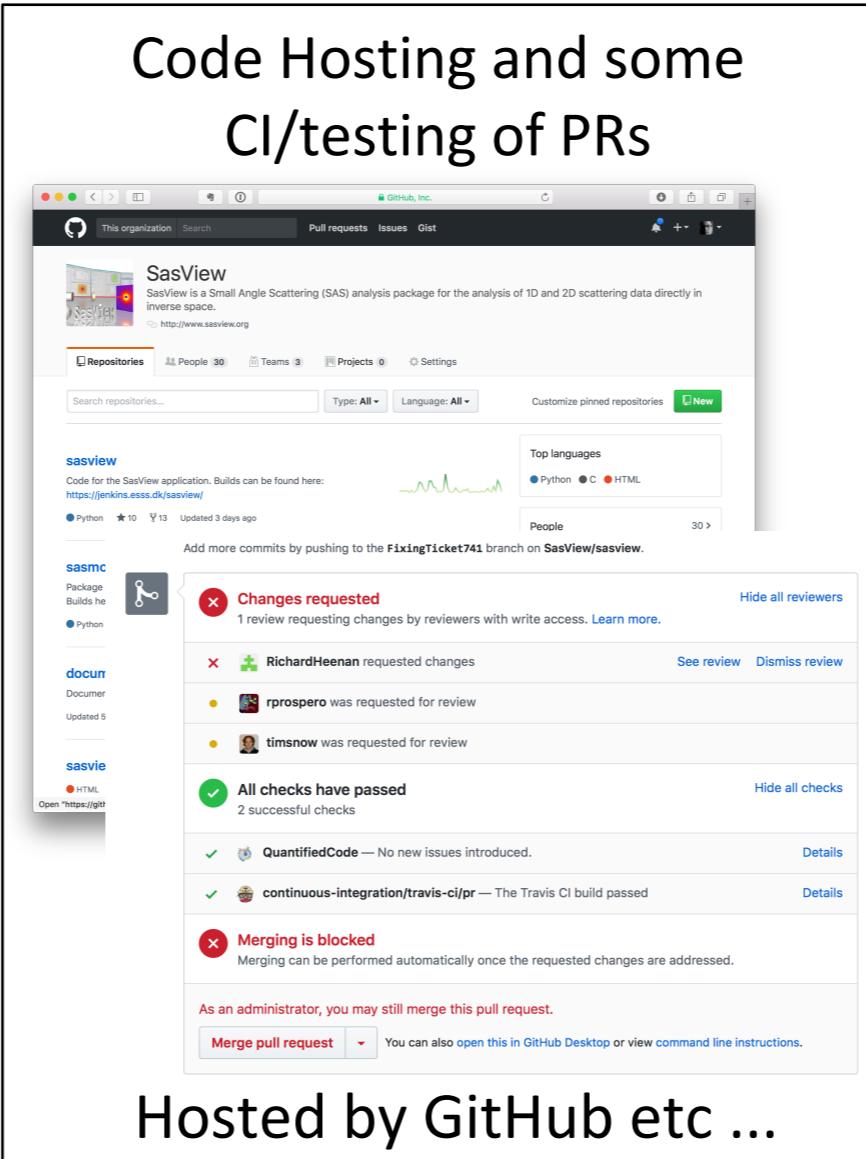
Task and bug tracking.
Developer wiki
trac.sasview.org



This screenshot shows the Trac web interface for SasView. The top navigation bar includes links for Wiki, Timeline, Roadmap, Browse Source, View Tickets (which is selected), New Ticket, Search, Admin, and Tags. A search bar is at the top right. Below the navigation is a section titled '(3) Active Tickets by Milestone' with a count of 247 matches. It includes a dropdown for 'Max items per page' set to 100 and a 'Update' button. Below this is a table of tickets with columns for Ticket, Summary, Component, Version, Type, Owner, Status, and Created. The first ticket listed is #219, 'easy developer setup'. The bottom section shows a table for 'Milestone SasView 4.1.0' with 59 matches, listing similar columns for each ticket.

Hosted by UT

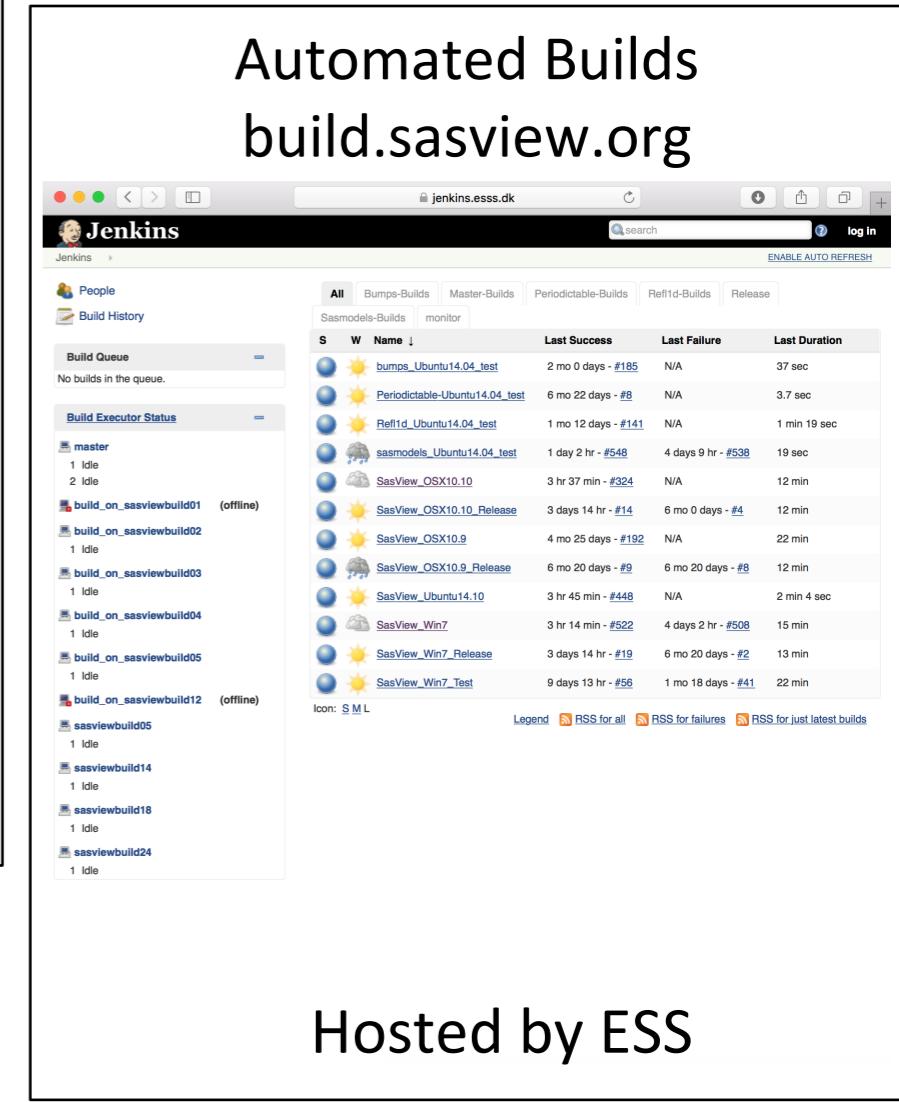
Code Hosting and some
CI/testing of PRs



This screenshot shows the GitHub organization page for SasView. It features a repository overview with sections for SasView, sasmc, docum, and sasvie. The SasView repository has a summary of 1 pull request, 30 people, 3 teams, and 0 projects. Below this is a 'Pull requests' section with one open pull request from 'ajj' to 'smk78' with the title 'FixingTicket741'. The pull request has 1 review requesting changes from 'RichardHeenan'. The code status shows 'All checks have passed'. At the bottom, there's a note about merging being blocked due to changes requested.

Hosted by GitHub etc ...

Automated Builds
build.sasview.org



This screenshot shows the Jenkins dashboard for SasView. It displays a list of build jobs categorized by type: All, Bumps-Builds, Master-Builds, Periodic-builds, RefId-Builds, and Release. The 'All' tab is selected, showing various builds like 'bumps_Ubuntu14.04_test', 'Periodicable-Ubuntu14.04_test', and 'SasView_Win7_Release'. Each job entry includes details such as the last success time, last failure time, and duration. The bottom of the dashboard shows a legend for build status icons: green for success, yellow for warning, and red for failure.

Hosted by ESS

Development Model Communications

The image displays three separate screenshots of communication platforms:

- Twitter (Top Left):** Shows the SasView account (@SasView) profile and a feed of tweets from the Mantid Project (@mantidproject) and SSI - software.ac.uk (@SoftwareSaved). The Mantid tweet discusses a typo fix related to the BBSR licence.
- Slack (Bottom Right):** Shows a screenshot of the SasView Slack workspace. The #general channel is selected, displaying a log message from andyfaff about a logging setup issue. Other users like wpotrzebowski and ricleal are also visible in the conversation.
- Facebook (Bottom Left):** Shows the SasView page (@sasviewanalysis) with a post featuring a large image of the SasView software interface, which displays a 3D scattering pattern from a sample.

Mailing lists
management@sasview.org
help@sasview.org
developers@sasview.org
users@sasview.org

Current Development Team

“Management” Team

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



Code Camp VI hosted by ESRF & ILL – April 4th – 11th 2017

- 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

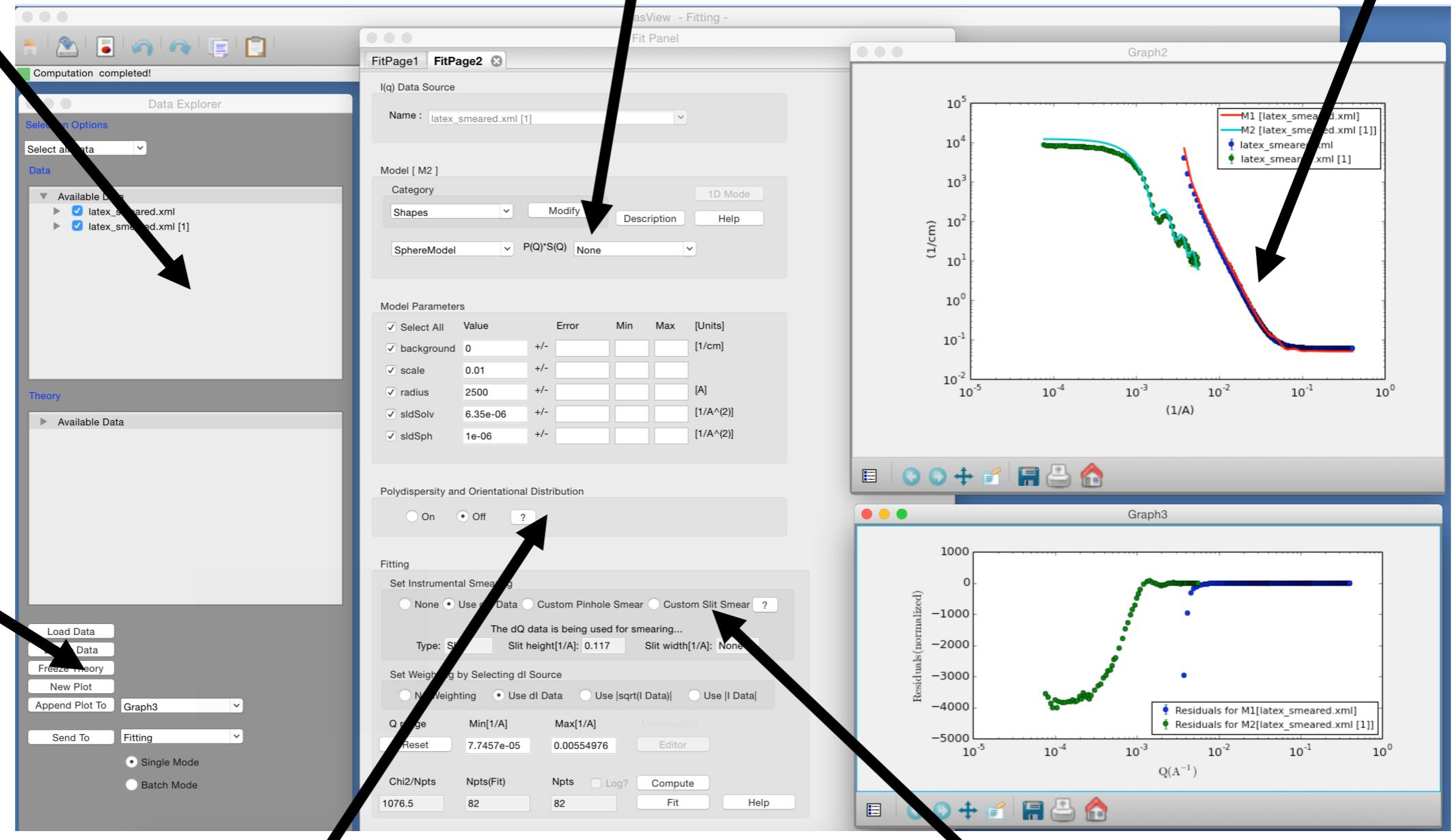
What Can SasView Do?

1D Analysis

Data management
Common data formats supported, including NXcansas & *cansas1D*

Wide choice of built-in models (> 70)
 $P(Q)$, $S(Q)$ & $P(Q)*S(Q)$

Simultaneous fitting

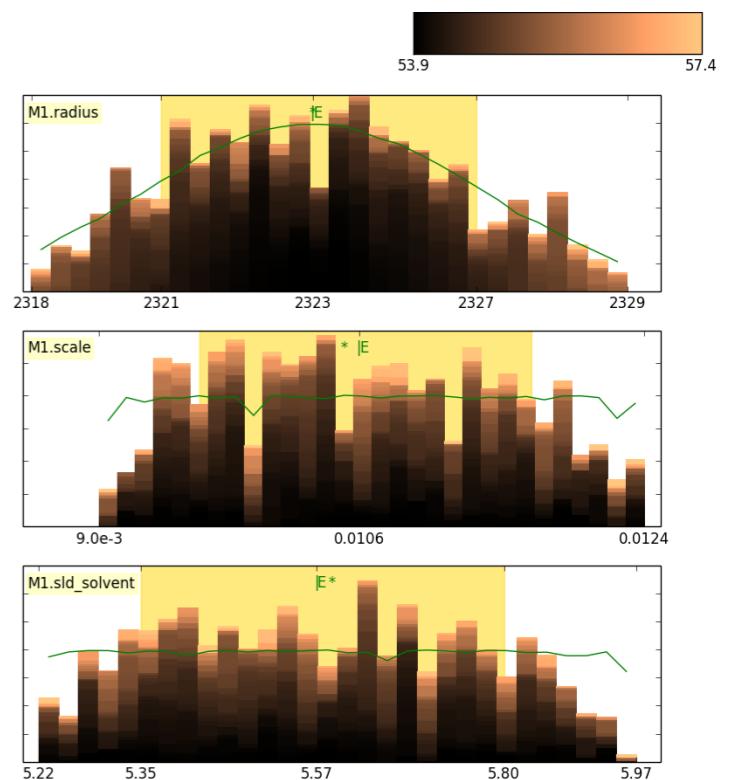
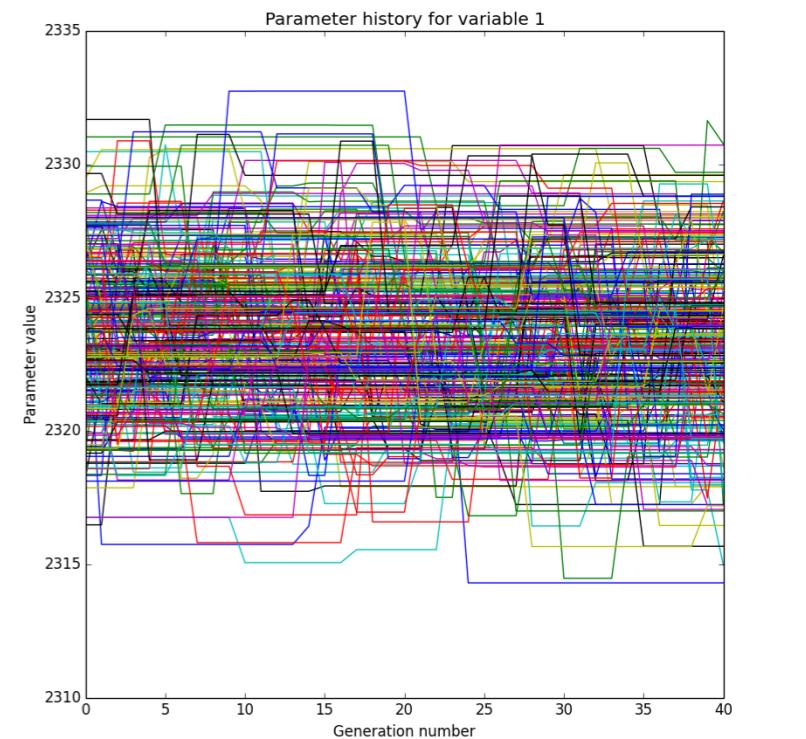
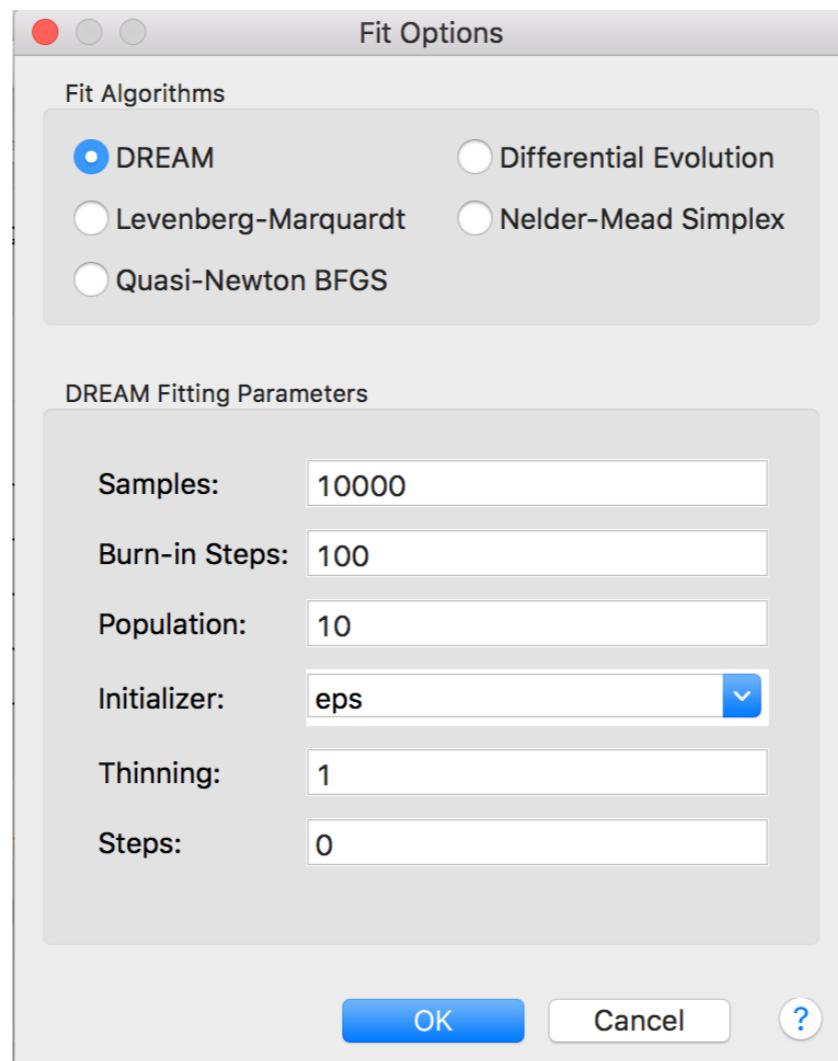
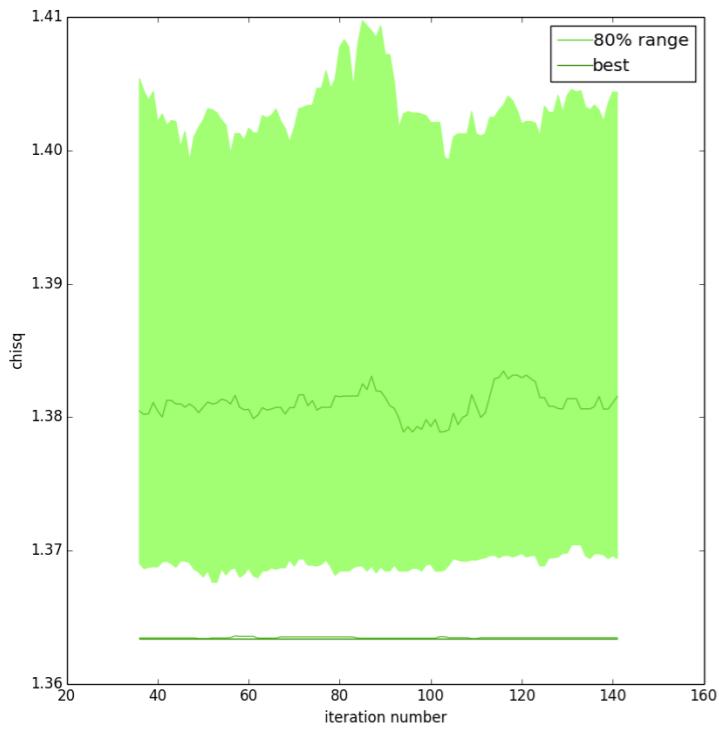
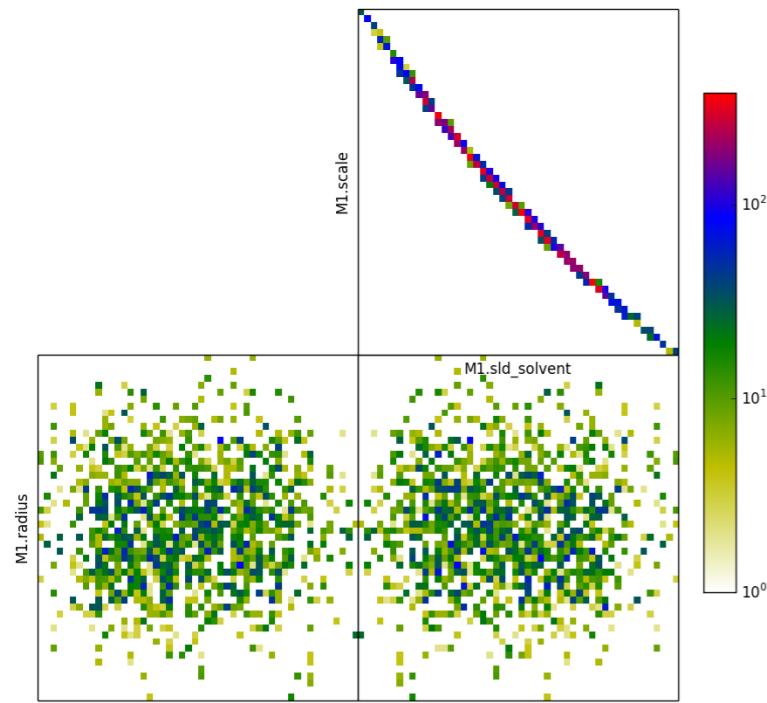


Analysis
Tool Choice
&
Plotting

Generic parameter polydispersity
Choice of distribution and distribution parameters

Resolution smearing (pinhole and slit)
Automatically from data or provide parameters

Fitting Algorithms



Uses bumps package from P. Kienzle

Invariant Calculation

Invariant

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

Name:

Total Q Range (1/ \AA): Min : Max :

Outputs

Volume Fraction +/-
Specific Surface +/- [1/ \AA]

Invariant Total [Q^*] +/- [1/(cm \cdot \AA^3)]

Customized Inputs

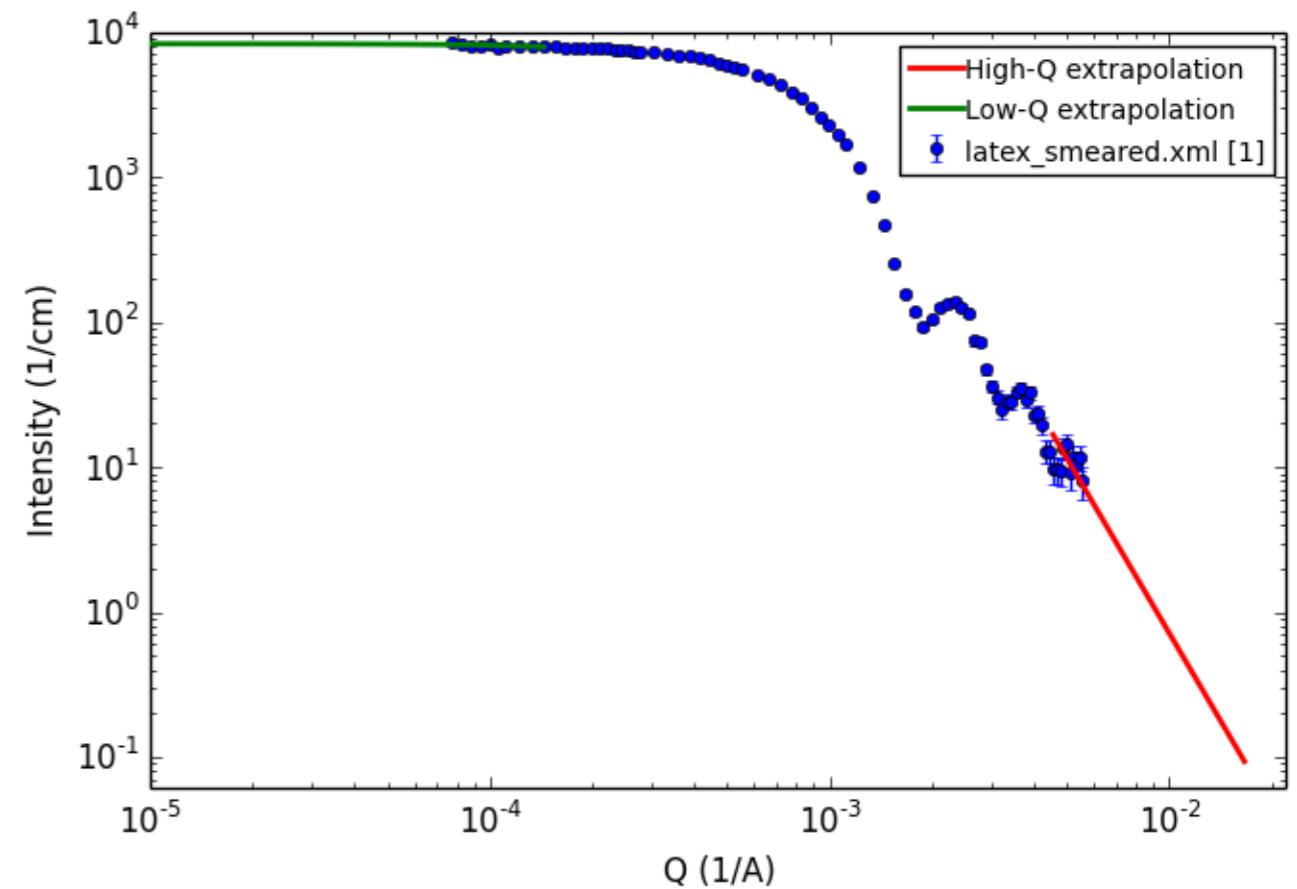
Background: [1/cm] Scale:
Contrast: [1/ Porod Constant: [1/(cm \cdot \AA^4)] (optional)

Extrapolation

Extrapolation Min: Max:
Maximum Q Range [1/ \AA]:

Low Q High Q

Enable Extrapolate Low Q Enable Extrapolate high-Q
Npts Npts
 Guinier Power Law
 Power Law Fix Fit
Power



Invariant Details

Invariant Chart

Q* from Low-Q	<input type="text" value="0.638%"/>
Q* from Data	<input type="text"/> 93.1%
Q* from High-Q	<input type="text" value="6.24%"/>

Numerical Values

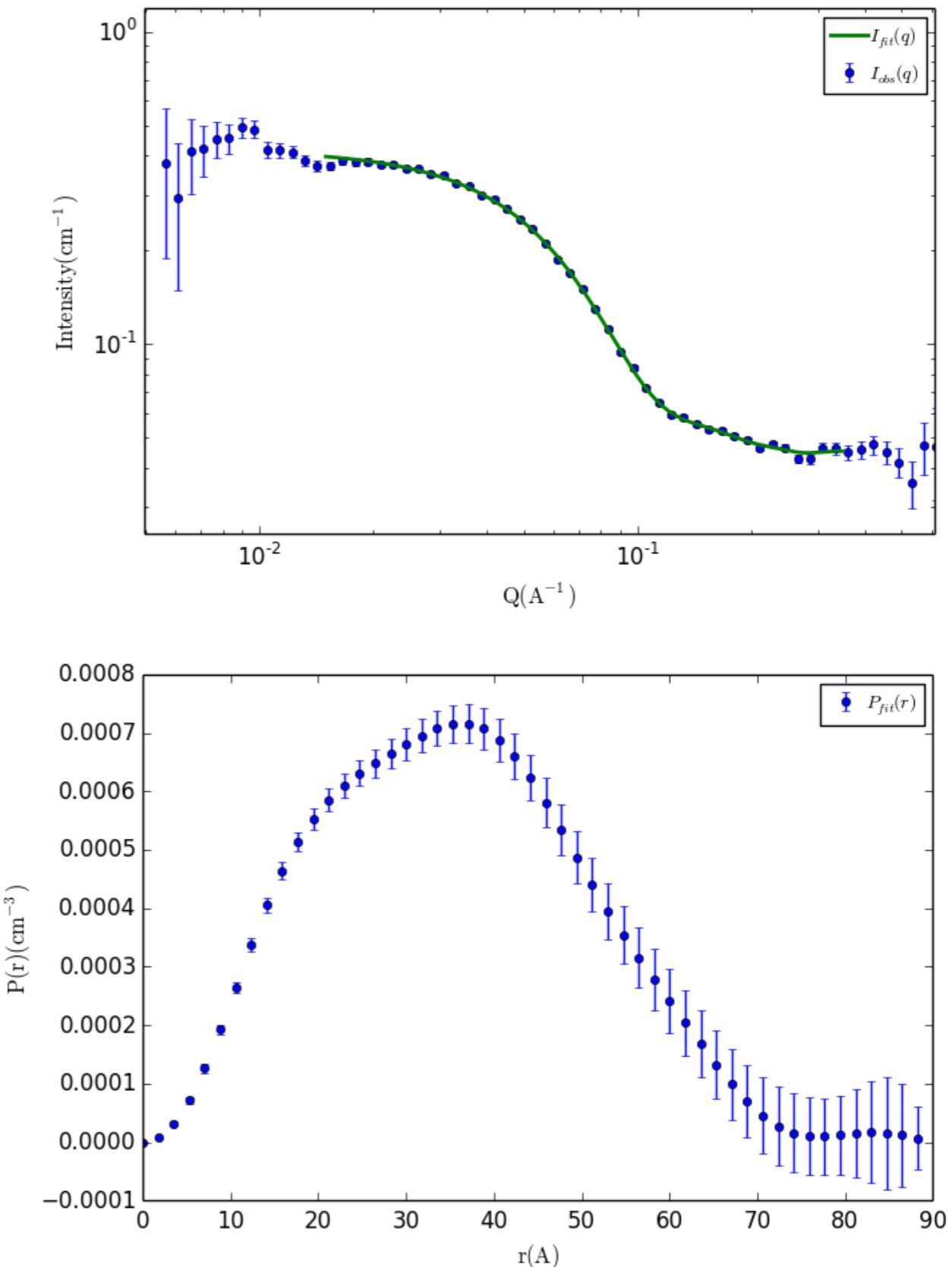
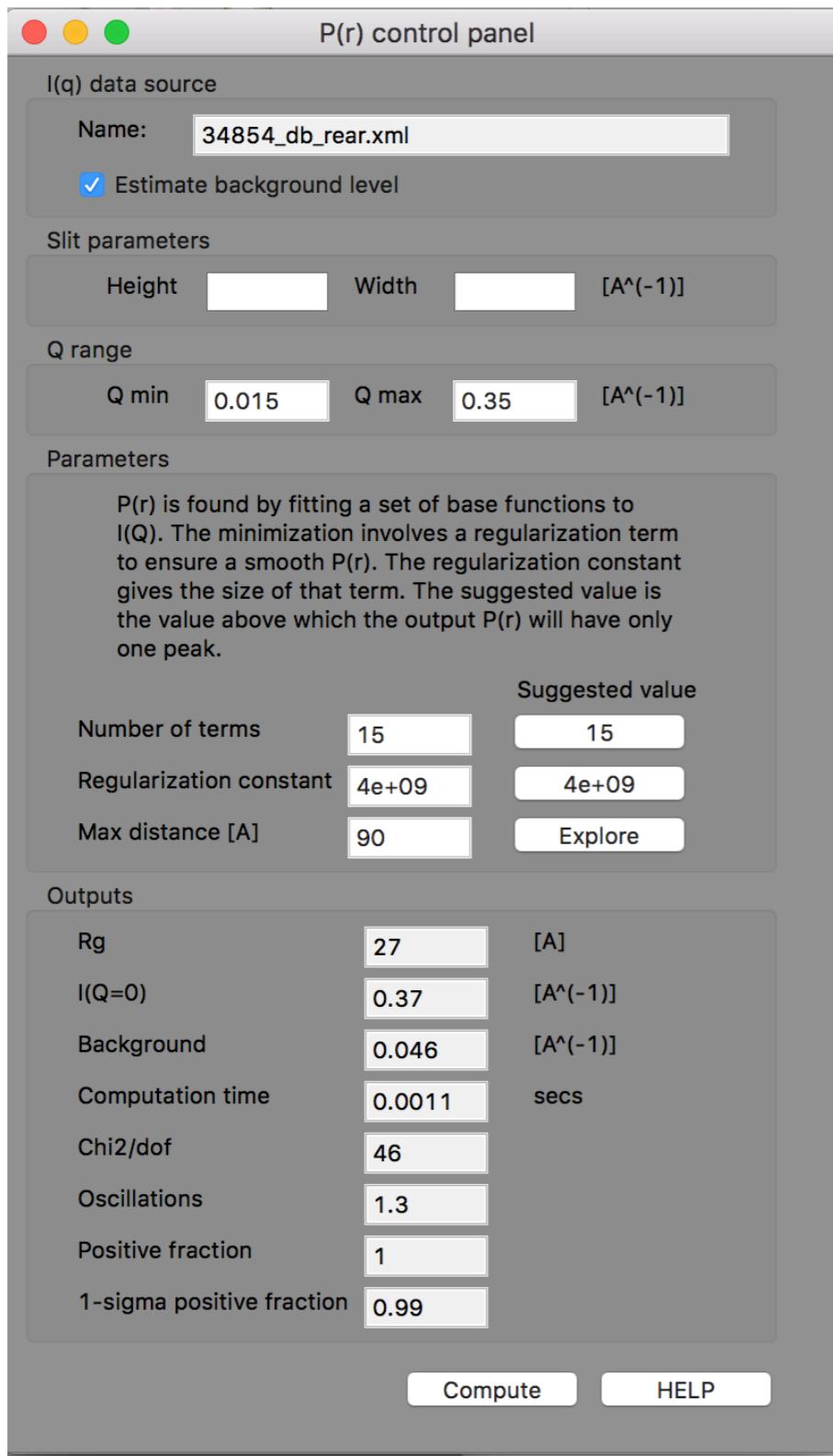
Q* from Low-Q	<input type="text" value="2.84e-06"/> +/- <input type="text" value="1.11e-09"/> [1/(cm * \AA^3)]
Q* from Data	<input type="text" value="0.000415"/> +/- <input type="text" value="1.18e-06"/> [1/(cm * \AA^3)]
Q* from High-Q	<input type="text" value="2.78e-05"/> +/- <input type="text" value="7.3e-06"/> [1/(cm * \AA^3)]

Warning

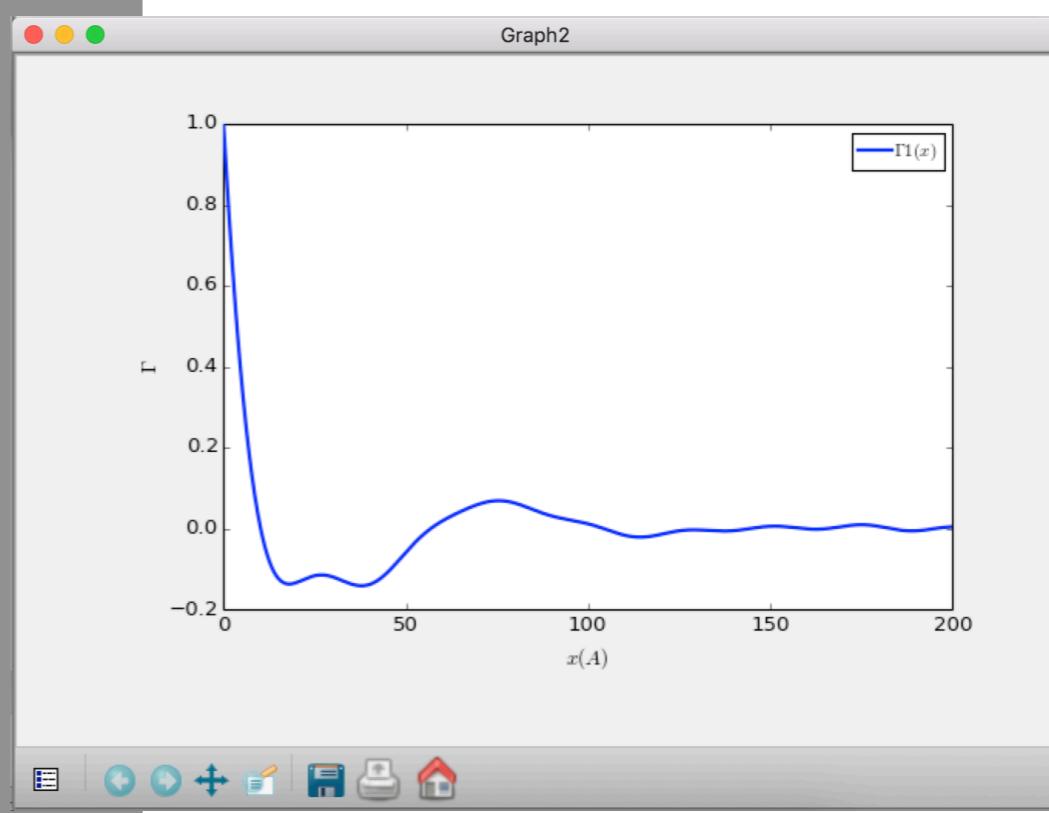
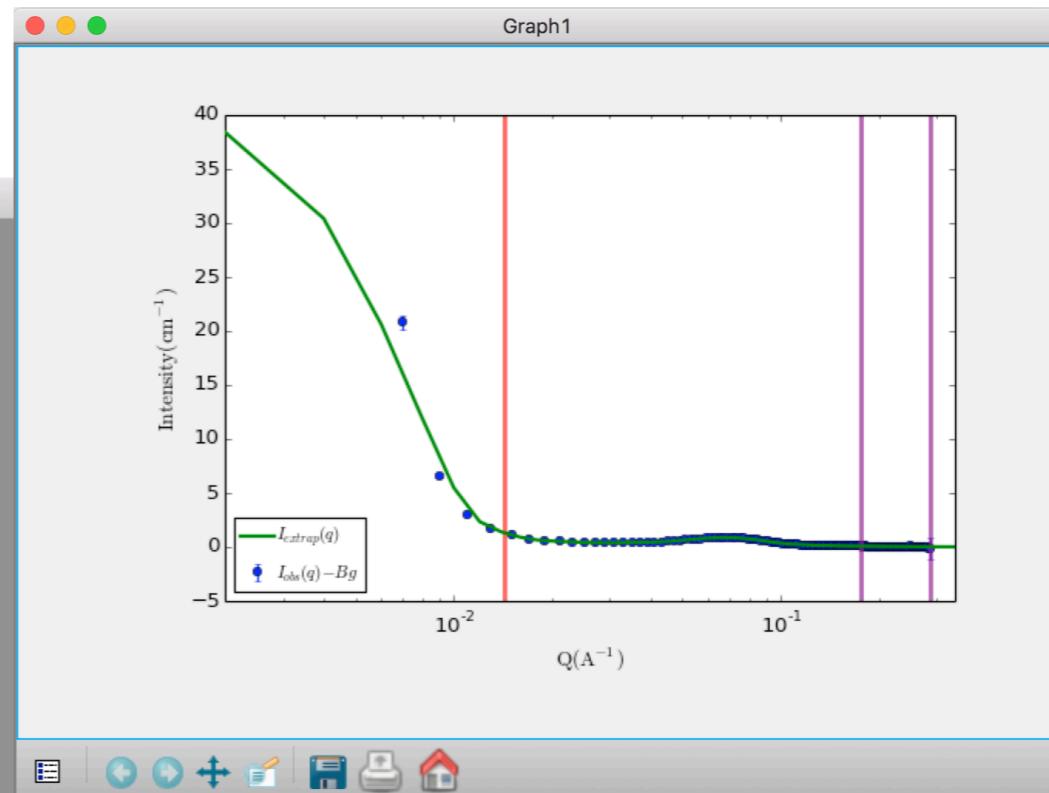
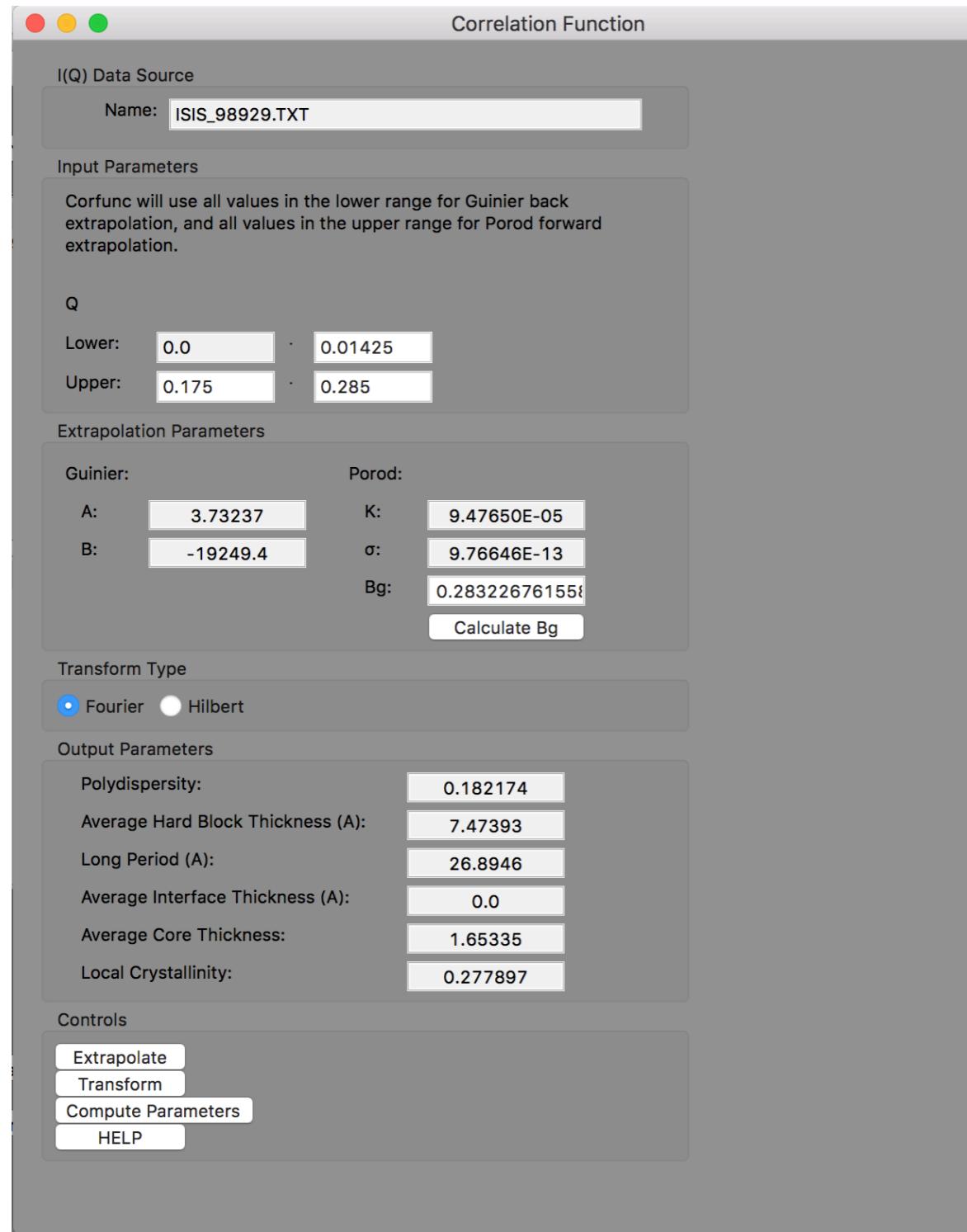
Extrapolated contribution at High Q is higher than 5% of the invariant.
The sum of all extrapolated contributions is higher than 5% of the invariant.
The calculations are likely to be unreliable!

Ok

P(r) Inversion



Correlation Function Analysis (new!)



SESANS Analysis

Fit panel - Active Fitting Optimizer: Levenberg-Marquardt

FitPage1

I(q) Data Source
Name : sphere2micron.ses

Model [M1]
Category
Sphere Modify Description Help
sphere P(Q)*S(Q) None

Model Parameters

Parameter	Value	Error	Min	Max	[Units]
<input checked="" type="checkbox"/> scale	0.005323	+/- 5.2808e-0	0	inf	
<input type="checkbox"/> background	0	+/-	-inf	inf	1/cm
<input type="checkbox"/> sld	1	+/-	-inf	inf	1e-6/Ang^2
<input type="checkbox"/> sld_solvent	6	+/-	-inf	inf	1e-6/Ang^2
<input checked="" type="checkbox"/> radius	10383	+/- 114.45	0	inf	Ang

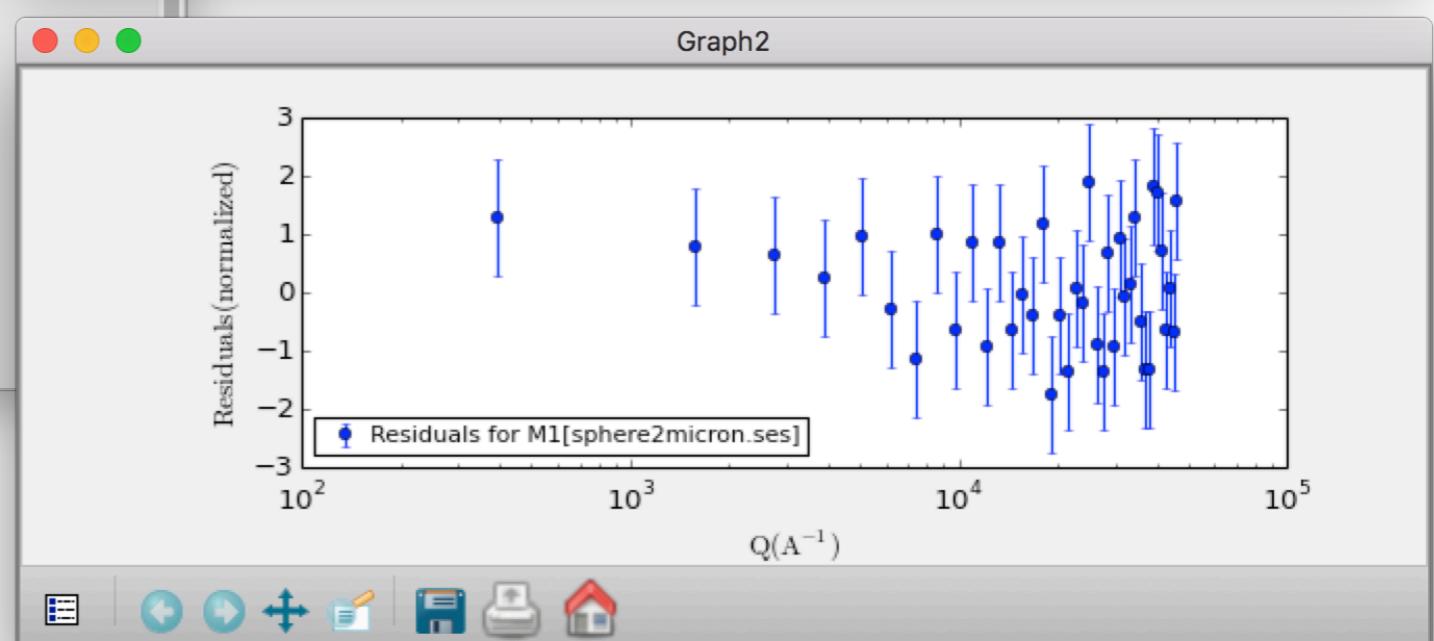
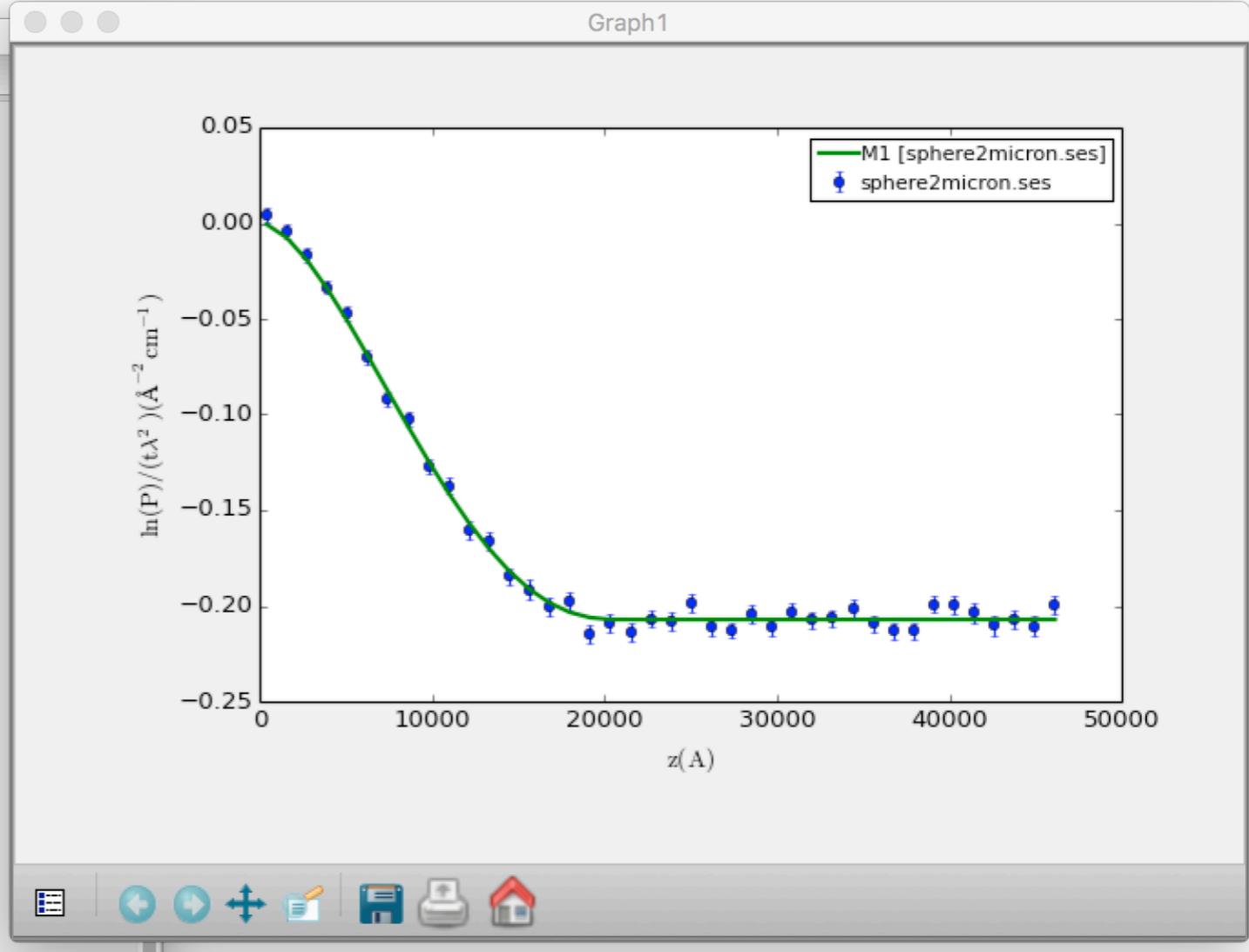
Polydispersity and Orientational Distribution
 On Off ?

Fitting

Set Instrumental Smearing
 None Use dQ Data Custom Pinhole Smear Custom Slit Smear ?
 The dQ data is being used for smearing...
 Type: Pinhole 19.578 dQ[%]: 2304.9

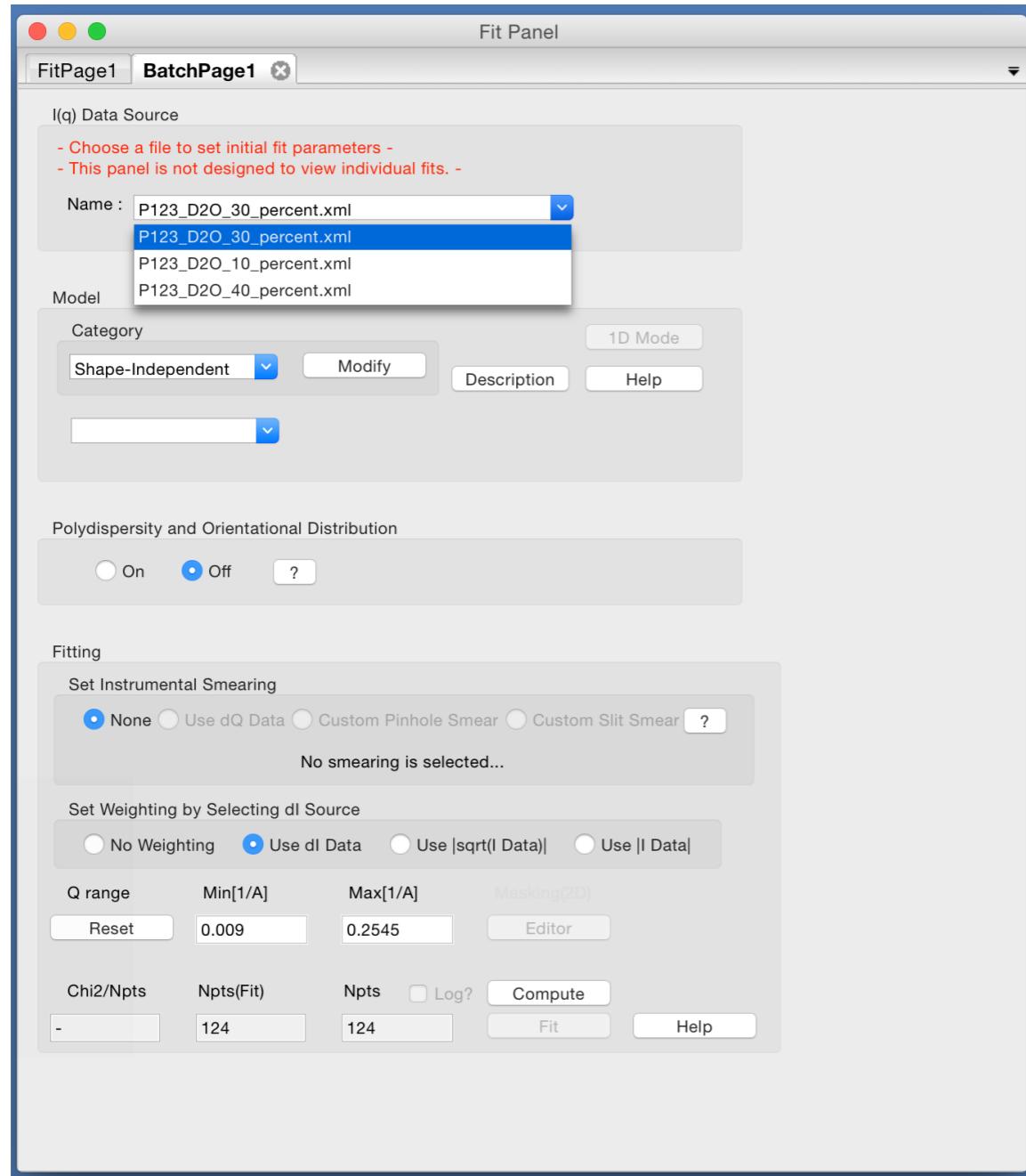
Set Weighting by Selecting dl Source
 No Weighting Use dl Data Use |sqrt(I) Data| Use ||I Data|

Automatic Hankel Transform of SANS models

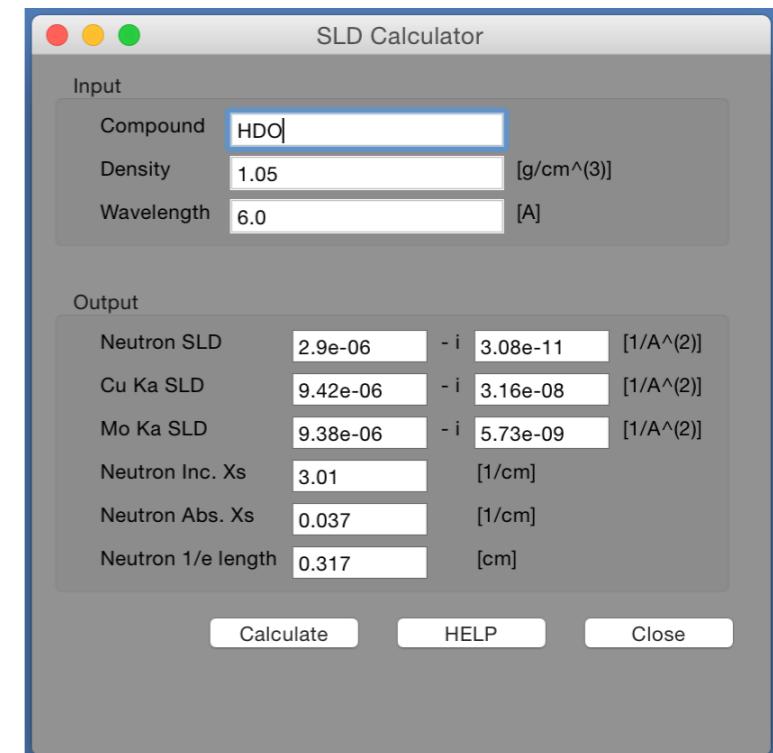


Other Features

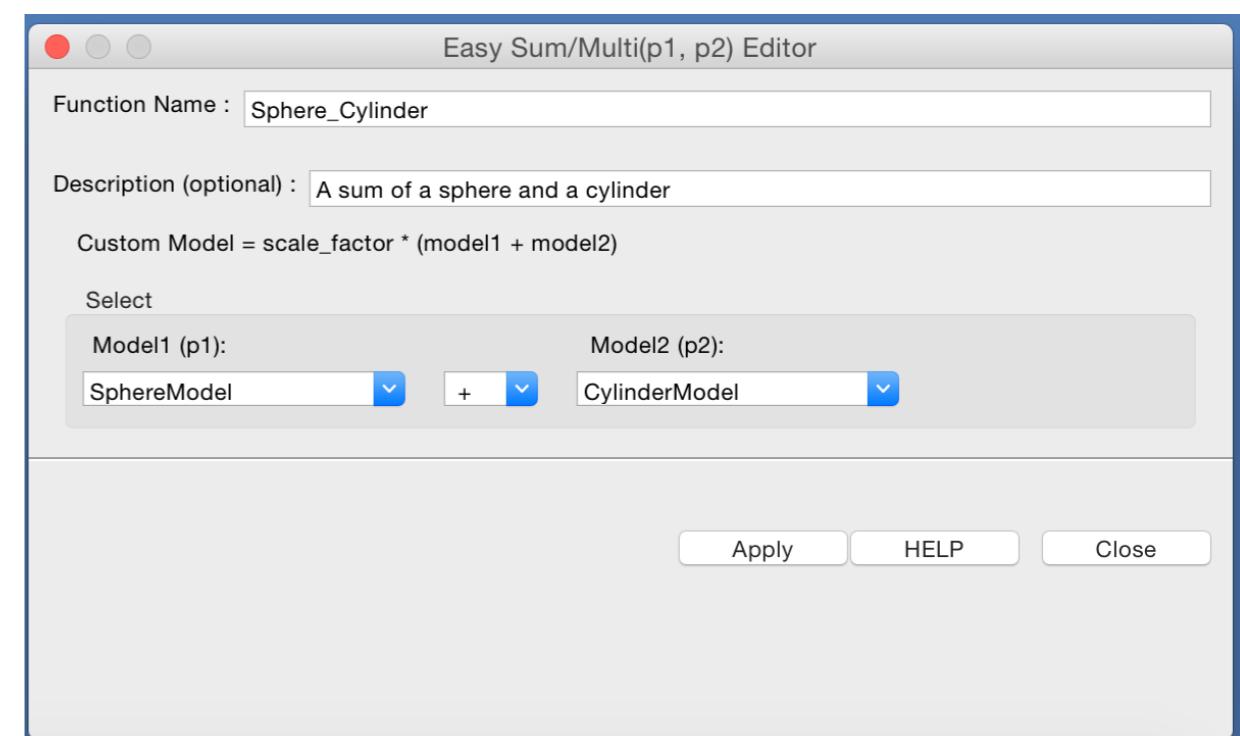
Batch fitting ...



SLD Calculator ...



Sum & Multiplication of Models ...



2D Modelling

Oriented systems & Magnetic Scattering

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

www.rsc.org/softmatter

PAPER

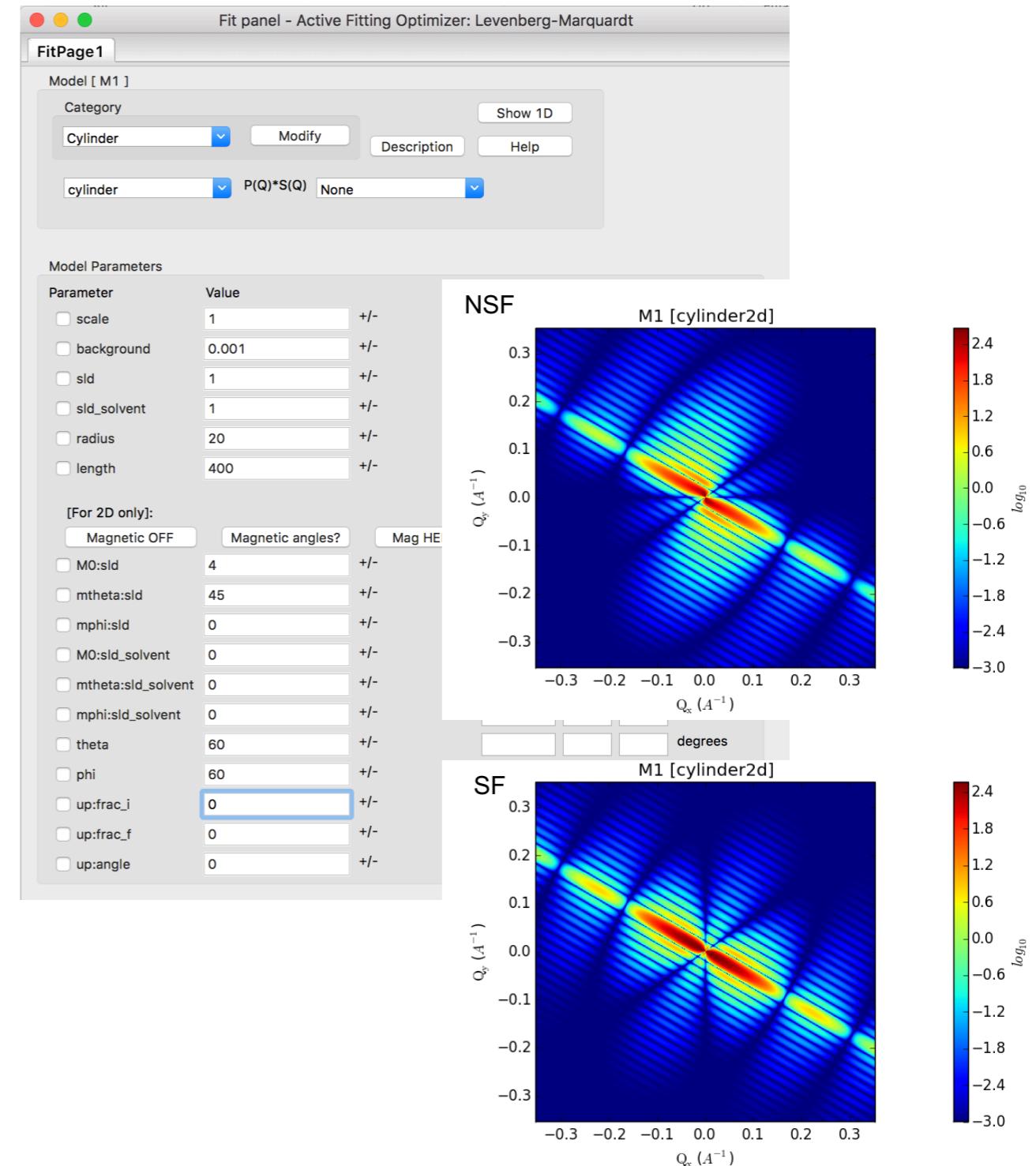
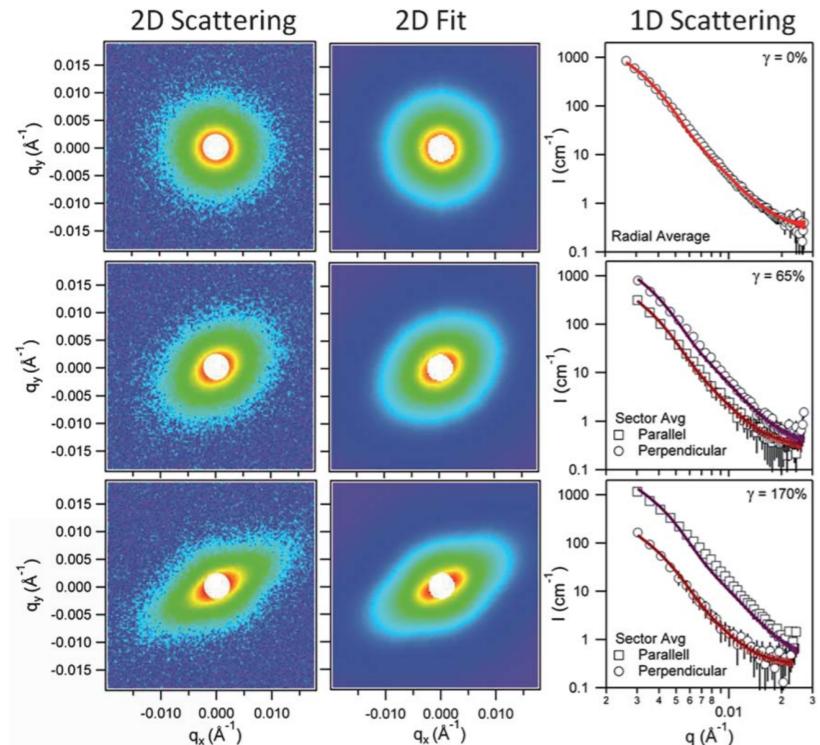
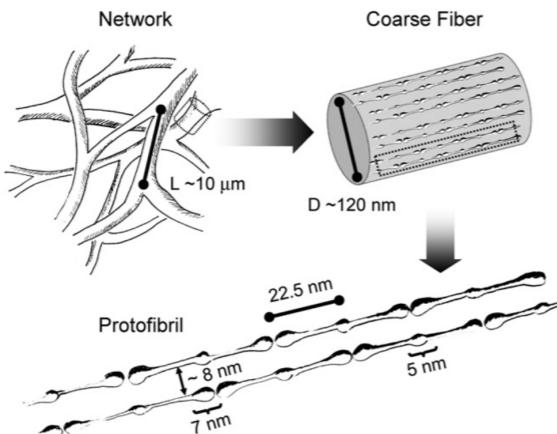
In situ neutron scattering study of structural transitions in fibrin networks under shear deformation

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 when using C
- 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 Marketplace

Users can share their models with the community

Documentation & example output

Models can be tested and included in future releases of sasmodels & SasView

The screenshot shows a web browser window for the SasView Marketplace at marketplace.sasview.org. The page has a dark header with the title "SasView Marketplace", a search bar, and a "Submit" button. A "Log In" link is in the top right. To the right of the main content area, there's a sidebar titled "Categories:" with links to various model types: Structure Factor, Shape-Independent, Other, Cylinder, Ellipsoid, Lamellae, Paracrystal, Sphere, and All Models. The main content area features a "Welcome to the SasView Marketplace!" heading, instructions for contributing Python models, information about uploading SasView text files, and a disclaimer about model contributions.

Welcome to the SasView Marketplace!

The Marketplace allows members of the SAS Community to contribute plug-in fitting models for the popular [SasView](#) data analysis program for all to use. (Please note: these plug-in models require SasView version 4.0 or later).

Contributed models should be written in Python (compatibility with python 2.7.x is currently required) or, if computational speed is an issue, in a combination of Python and C. You only need to upload the .py/.c source code files to the Marketplace!

Instructions on how to code a new plug-in model are available [here](#). It may also be helpful to examine the library models in the \sasmodels-data\models sub-folder of your SasView installation directory.

You also have the option to upload a SasView text file of the scattering function data computed by your model. If you do this a graph of the scattering function will appear under the Marketplace entry for your model.

Disclaimer: Models are expected to be contributed to the Marketplace in good faith and with the best intentions, and come without any warranty as to their correctness and suitability for purpose. Neither the author of the model or the SasView Development Team will be held liable for any loss or damage arising from conclusions drawn from the use of a model contributed to the Marketplace. This includes models that are marked as 'verified' by the SasView Development Team.

<http://marketplace.sasview.org>

SasView 4.1 is Out!

www.sasview.org

Official Releases available for Windows and Mac



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 ...

UI Refactoring (“SasView 5.0”)

Move to QT - current and well supported toolkit
Complete separation of GUI and calculation code
Provision of CLI & updated Python API

Sasmodes Enhancements

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

Constraints refactor

Multi-GPU support

Interface with SasFit models



Documentation

Tutorials
Manual

And much more!

See Roadmap and Tickets

Questions?



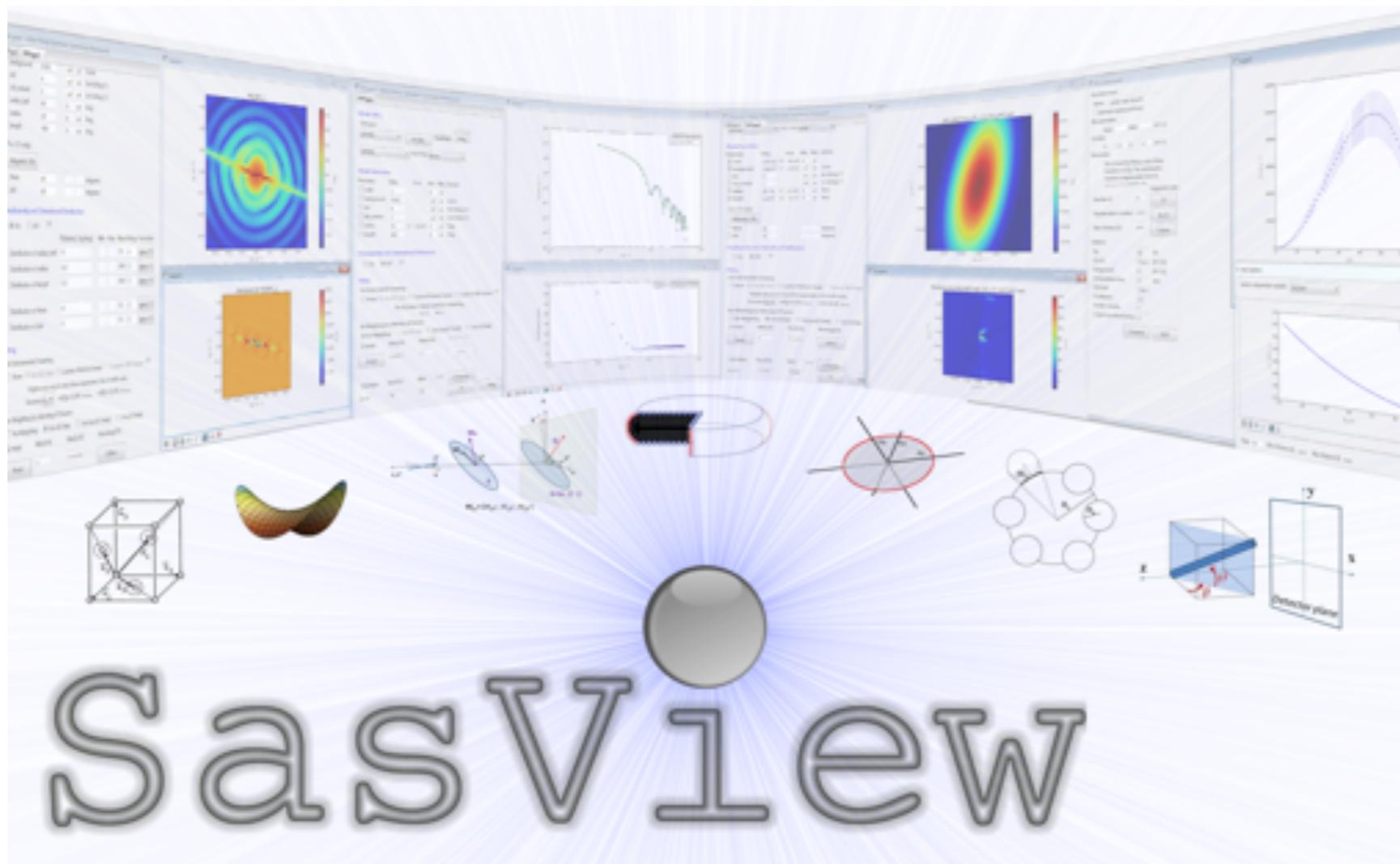
EUROPEAN
SPALLATION
SOURCE



Science & Technology Facilities Council
ISIS



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



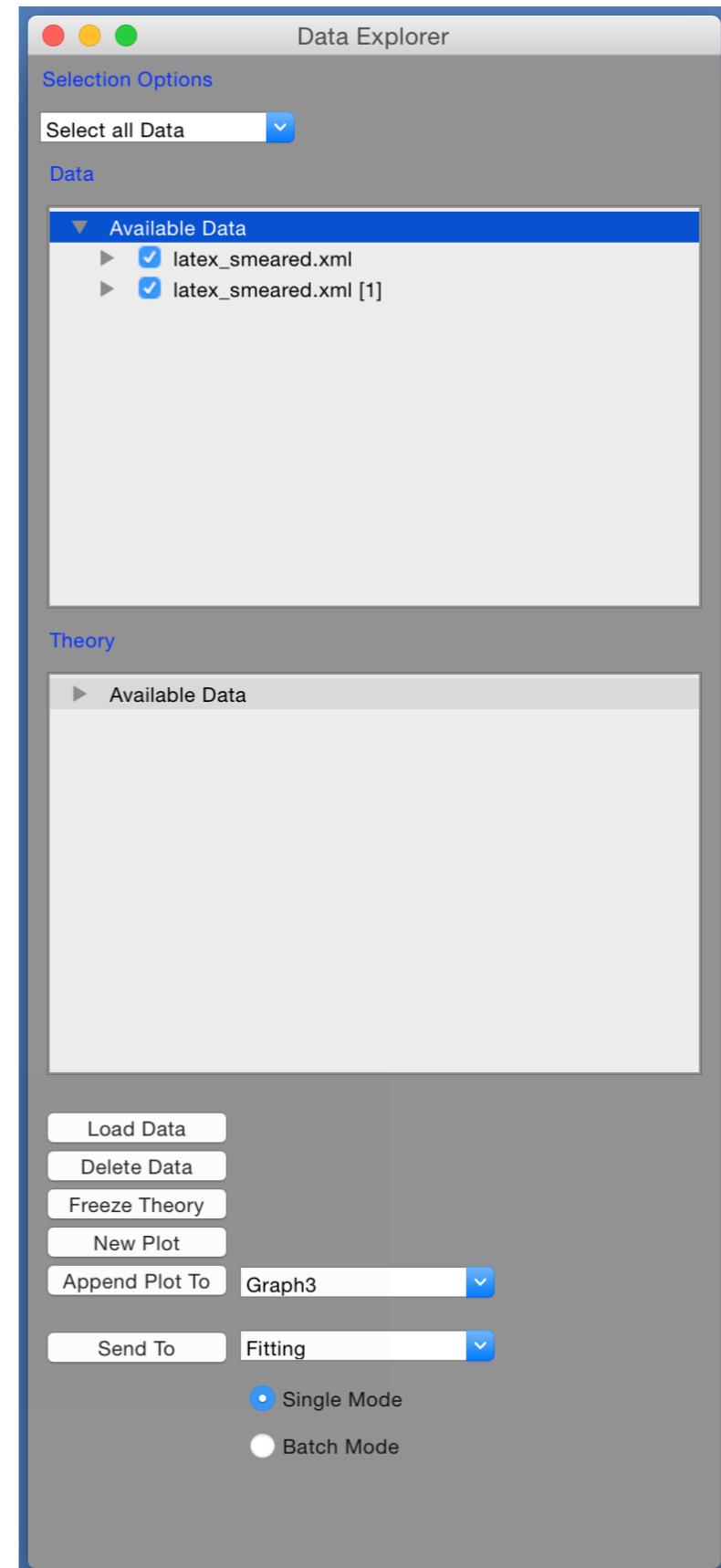
1D Analysis

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 Modify Description Help

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

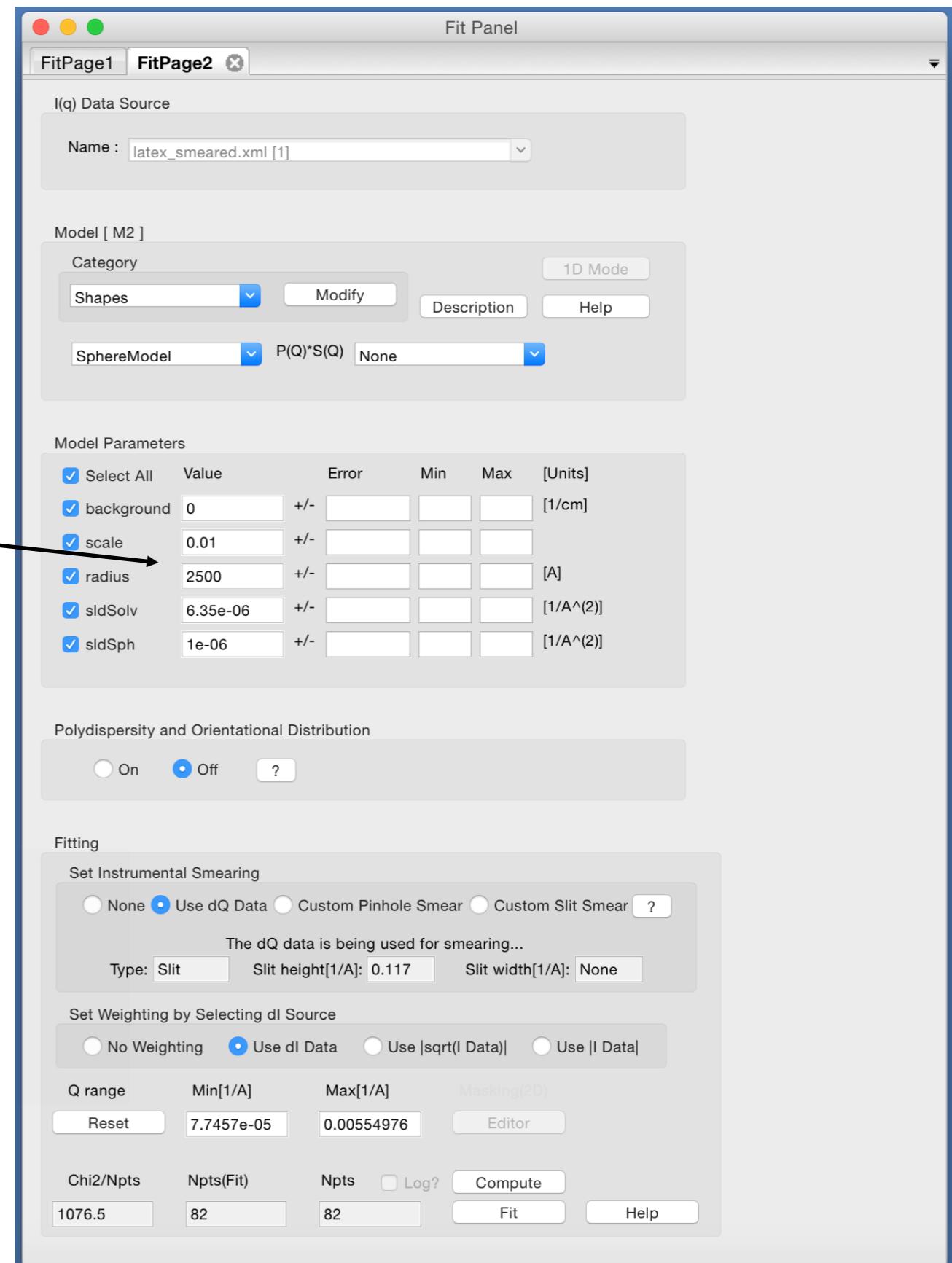
1076.5 82 82 Fit Help

1D Analysis

Send to fitting ...

Select a model ...

Set parameters ...



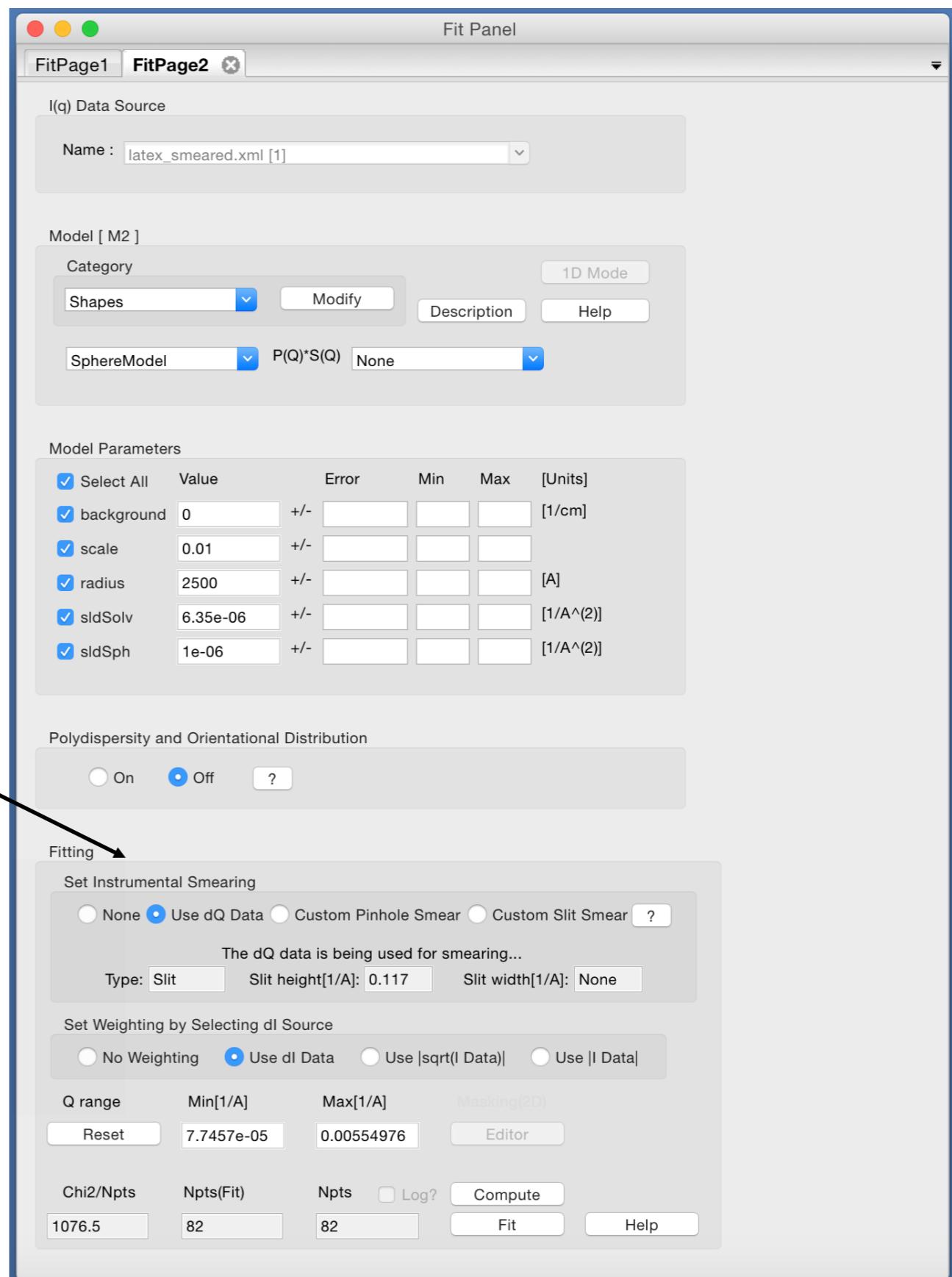
1D Analysis

Send to fitting ...

Select a model ...

Set parameters ...

Use resolution ...



1D Analysis

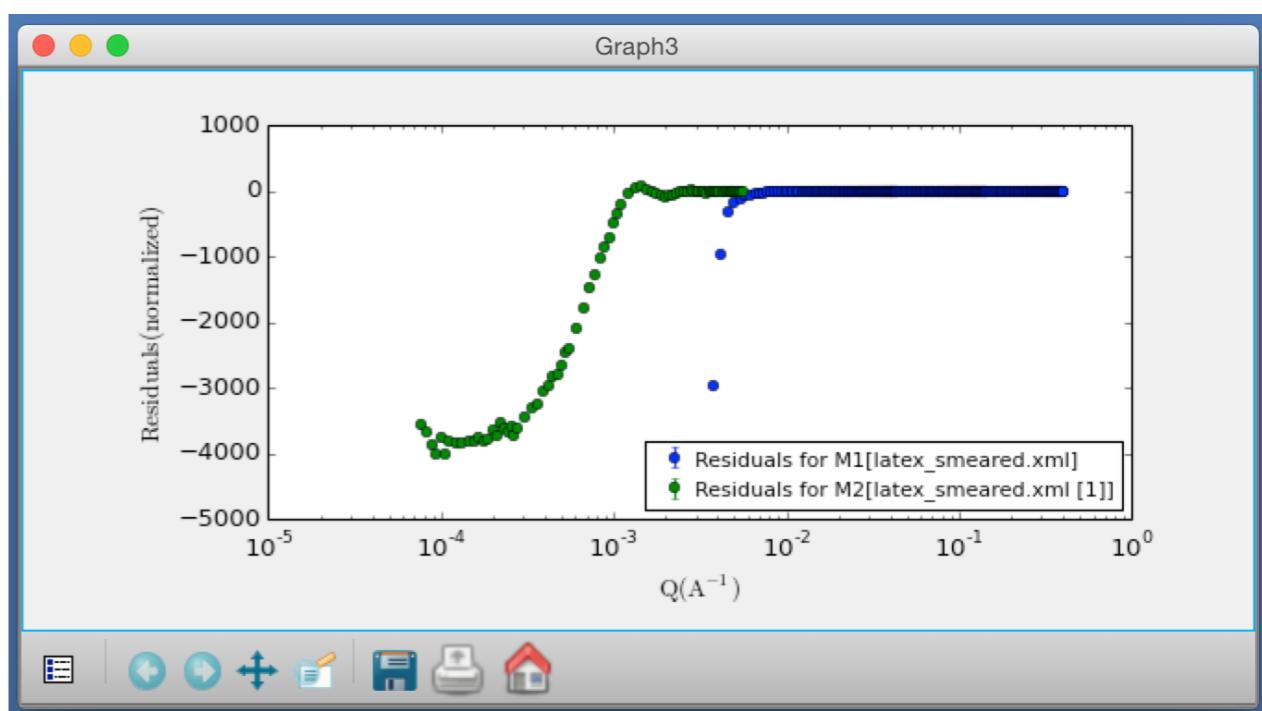
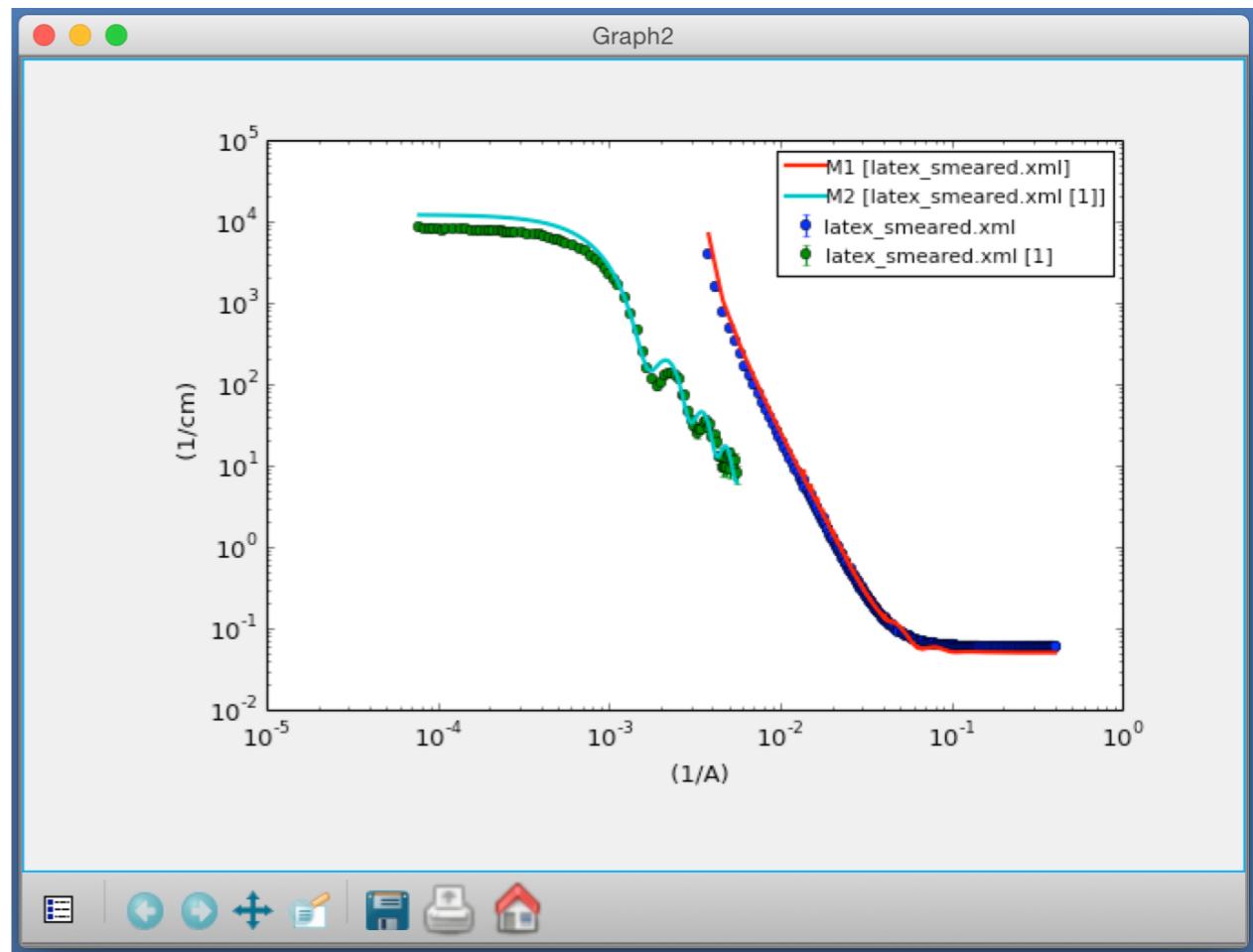
Send to fitting ...

Select a model ...

Set parameters ...

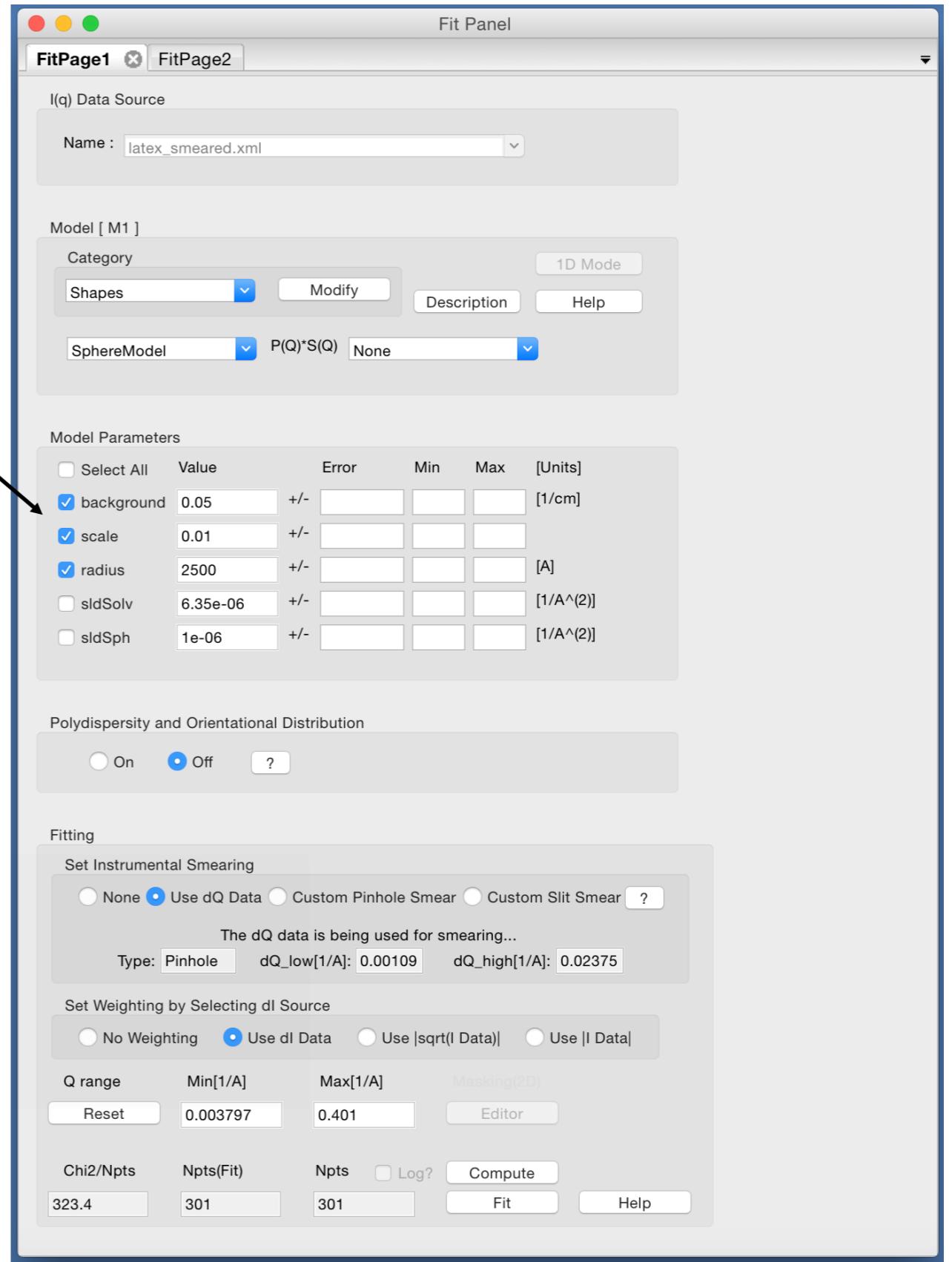
Use resolution ...

How does it look?



1D Analysis

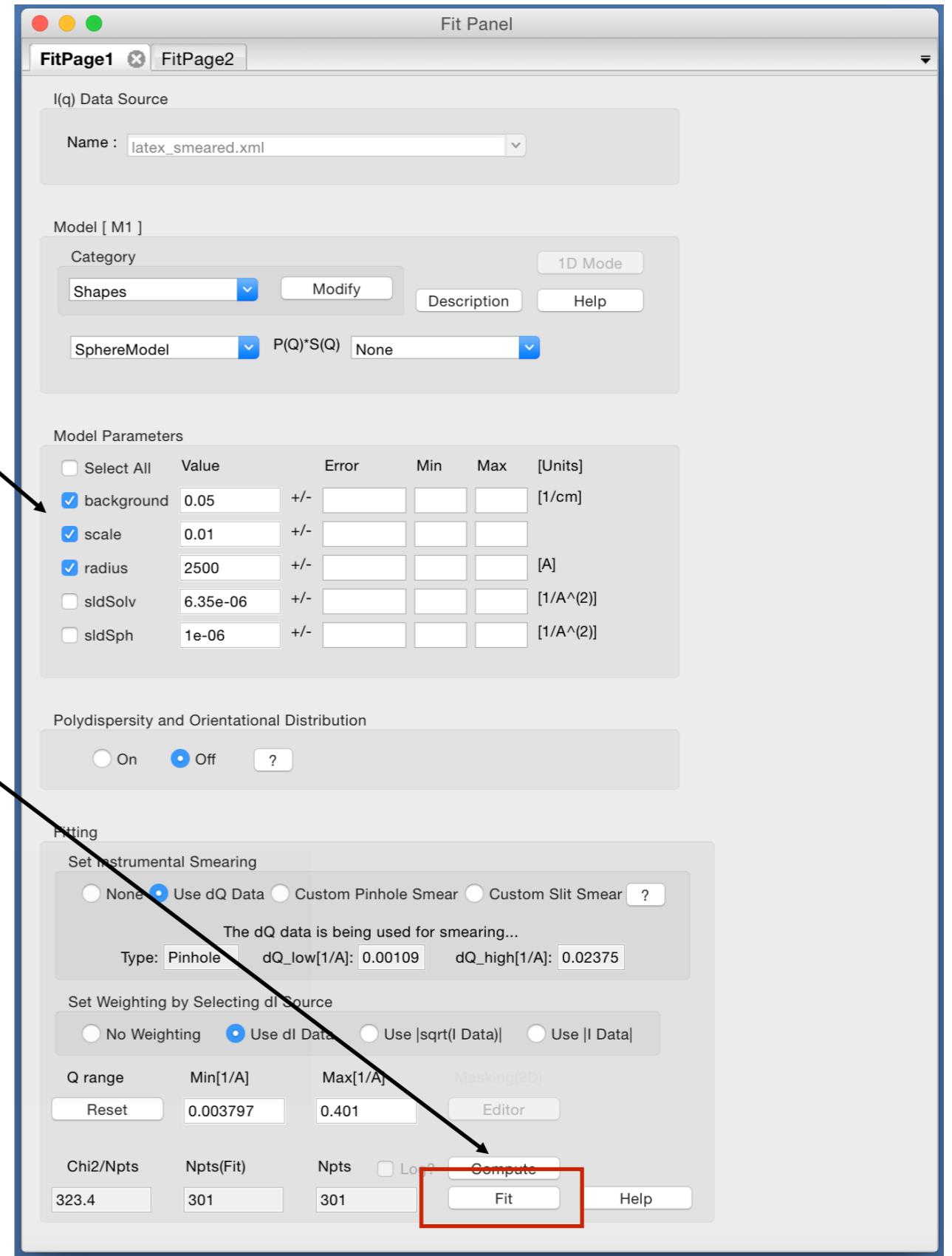
Choose which parameters to fit ...



1D Analysis

Choose which parameters to fit ...

... and press the Fit button!



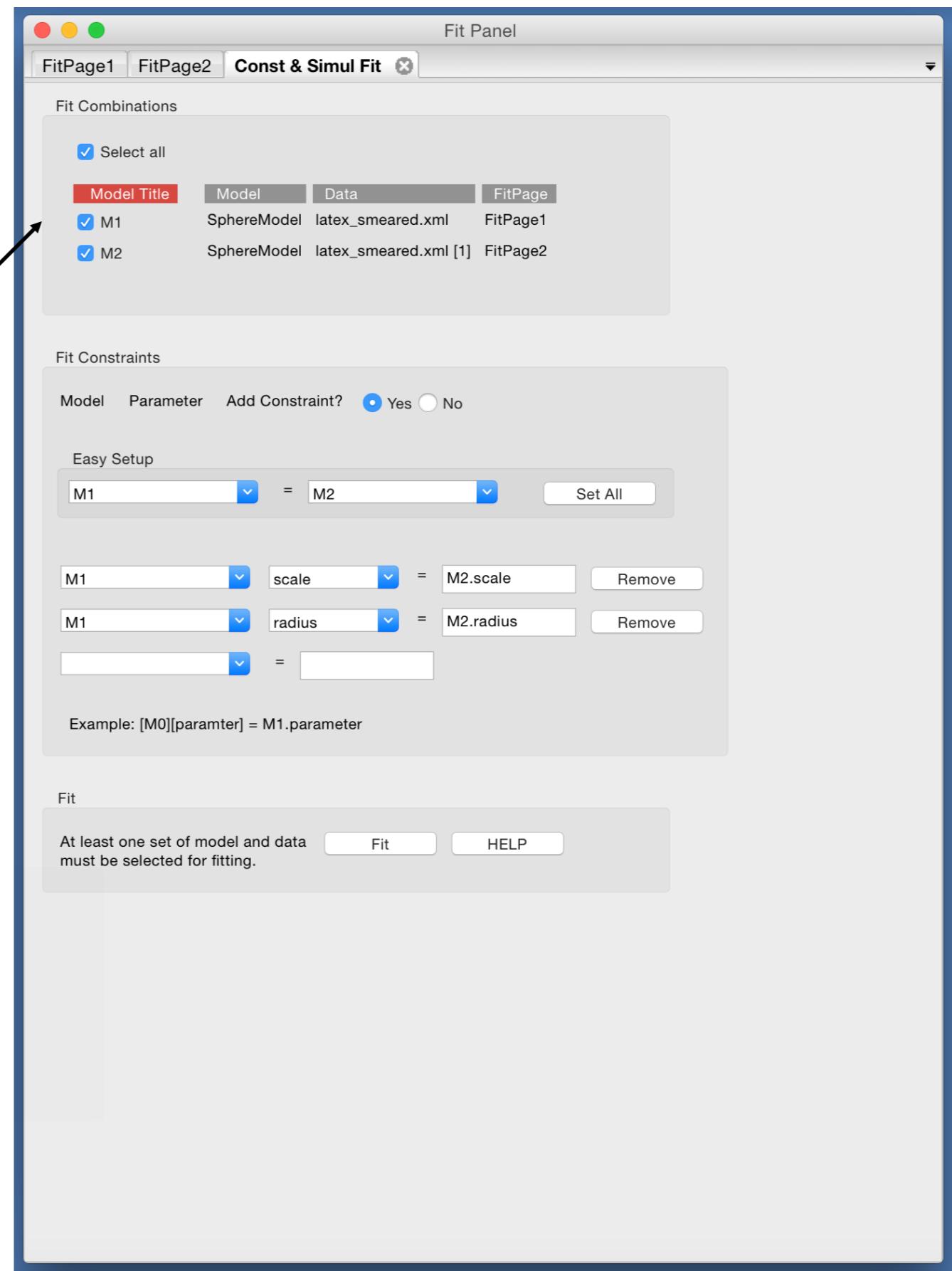
Constraints / Simultaneous Fit

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 ...

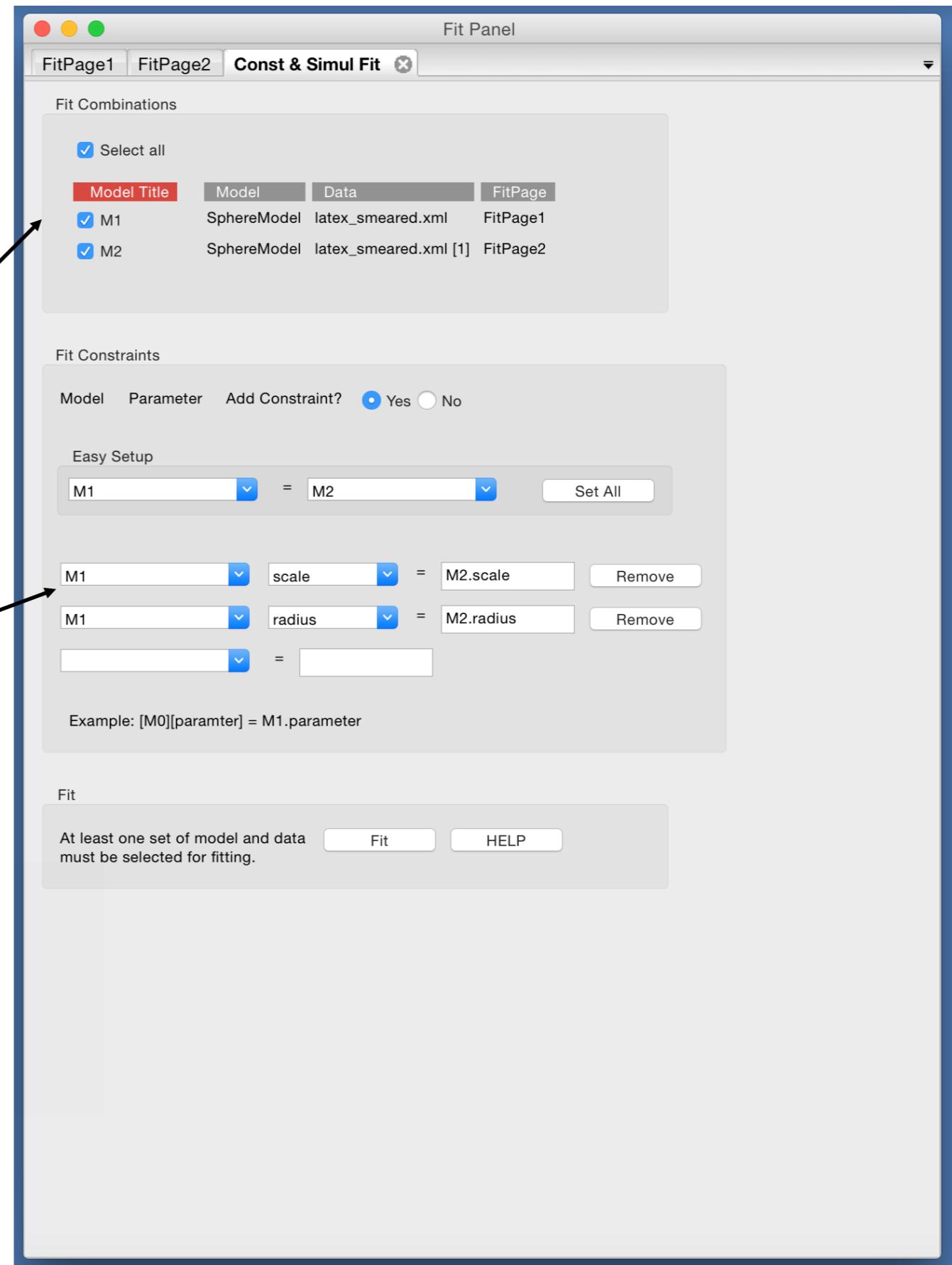


Constraints / Simultaneous Fit

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

Set up a simultaneous fit ...

... with constraints



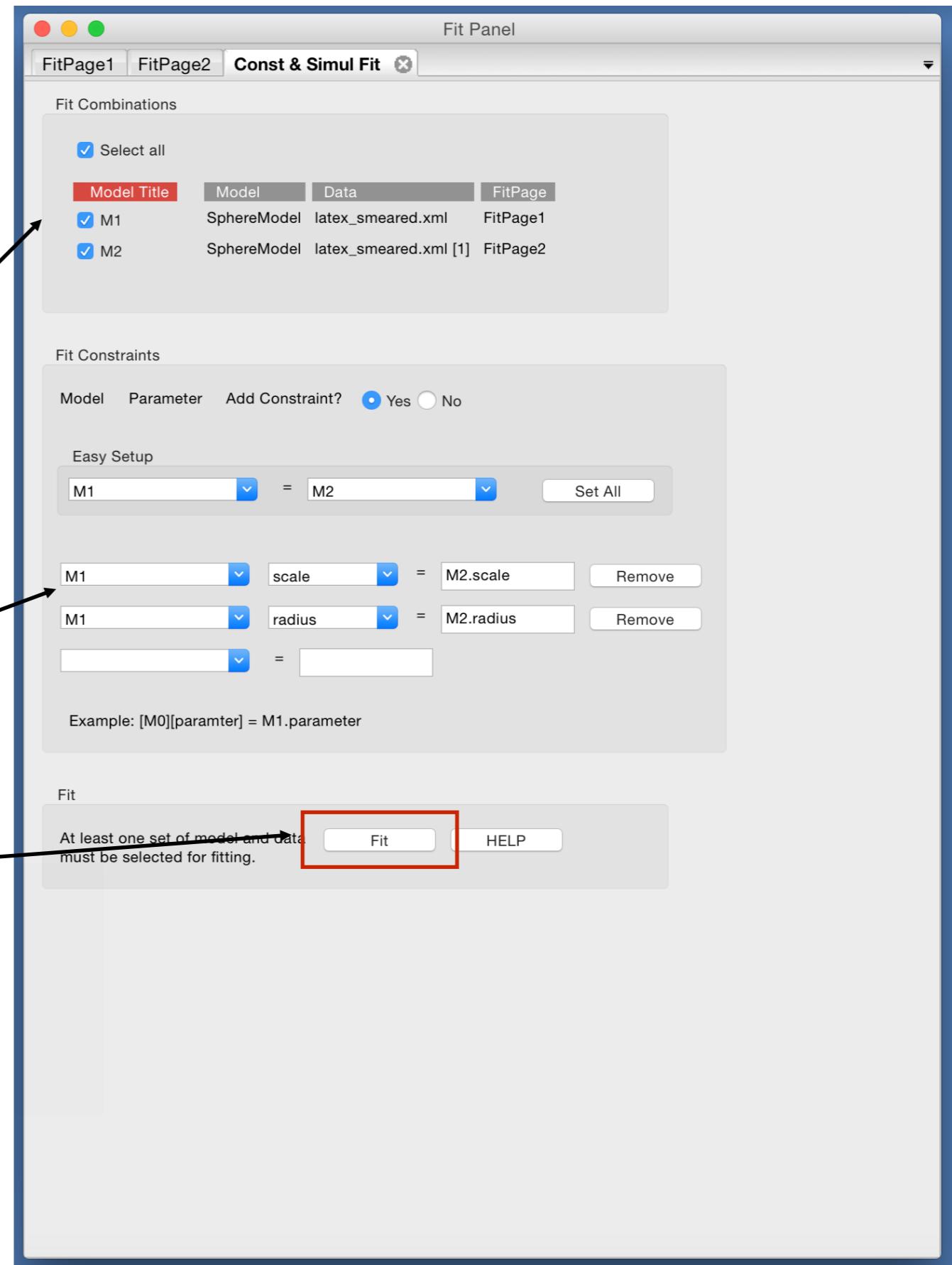
Constraints / Simultaneous Fit

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]

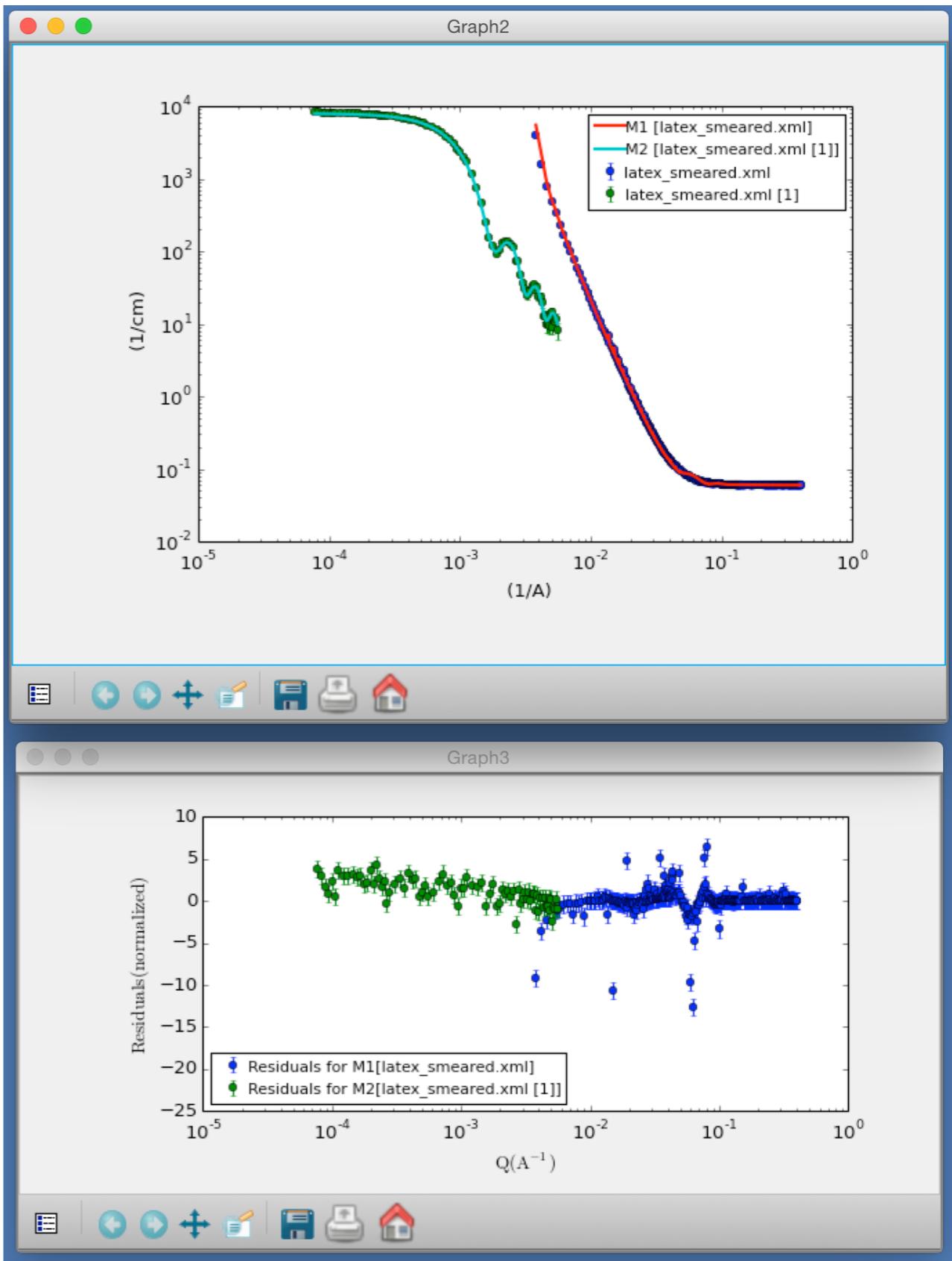
Polydispersity and Orientational Distribution
 On Off ?

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

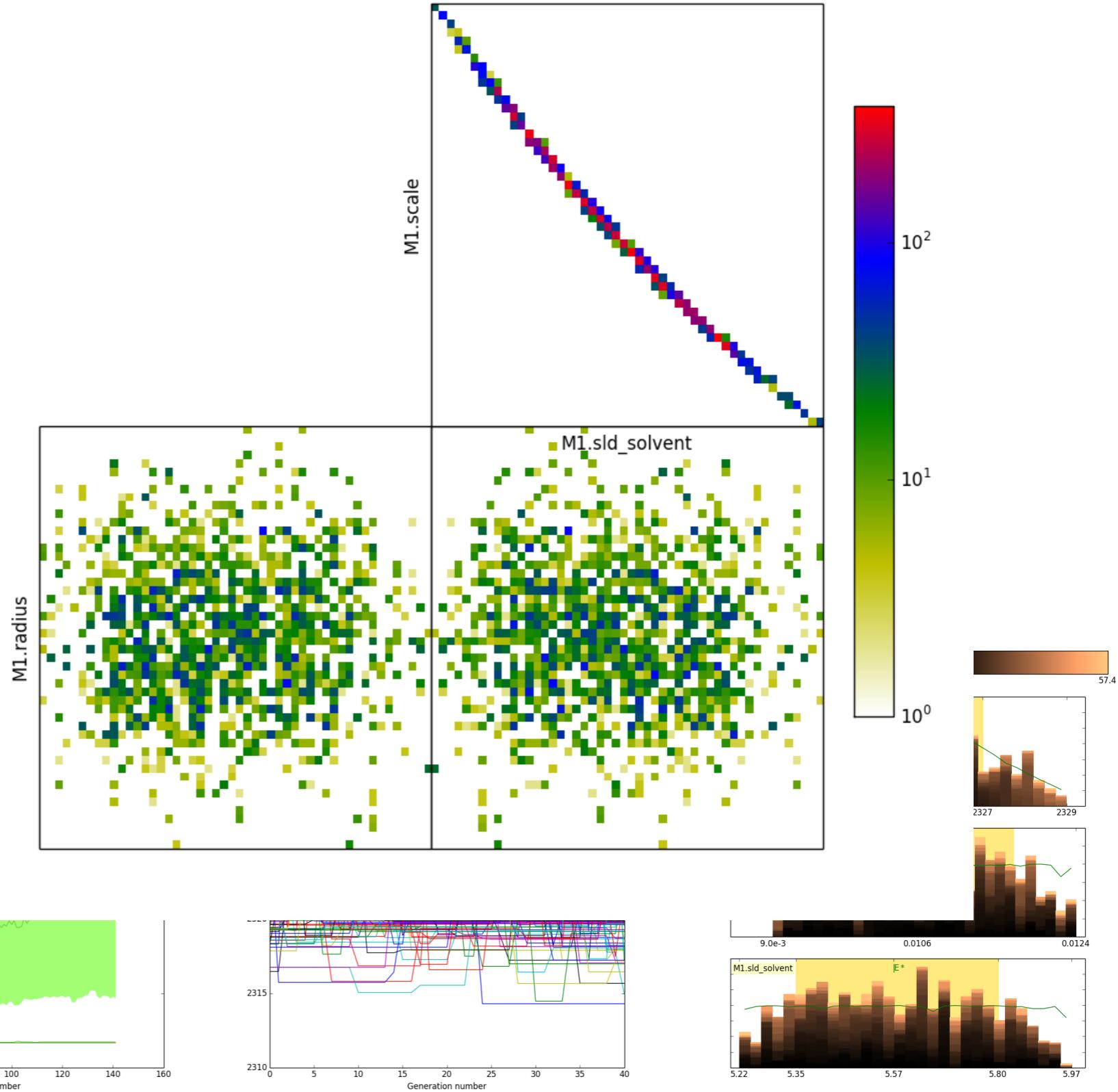
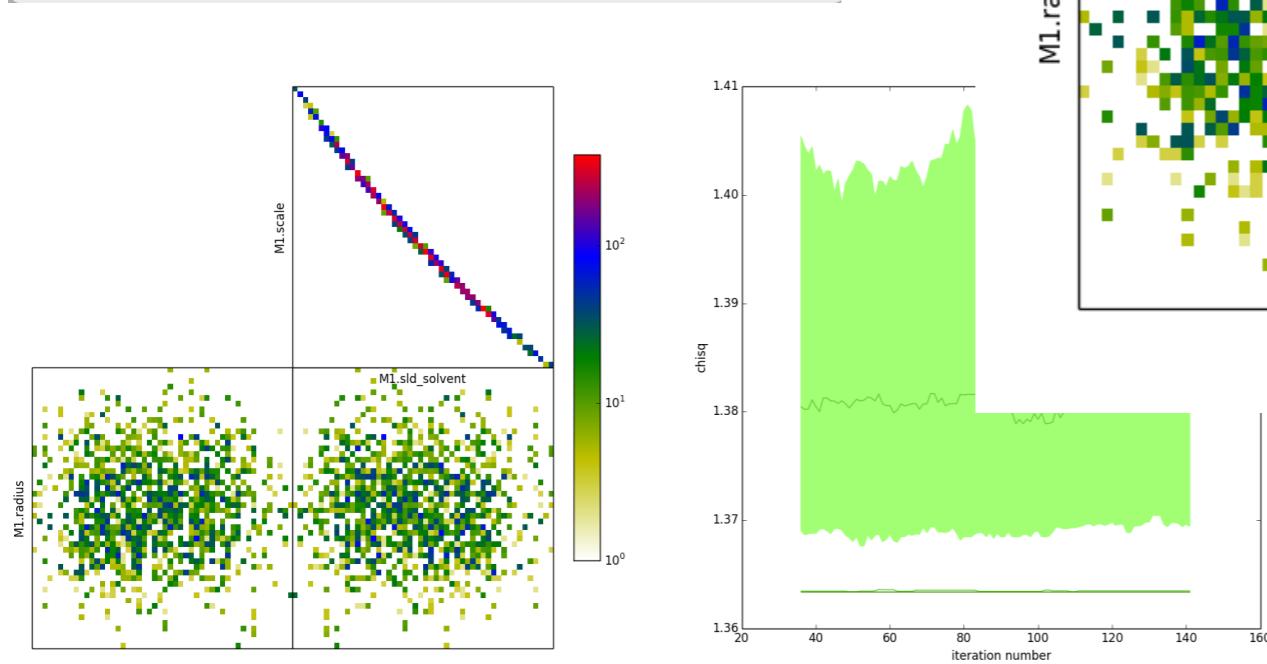
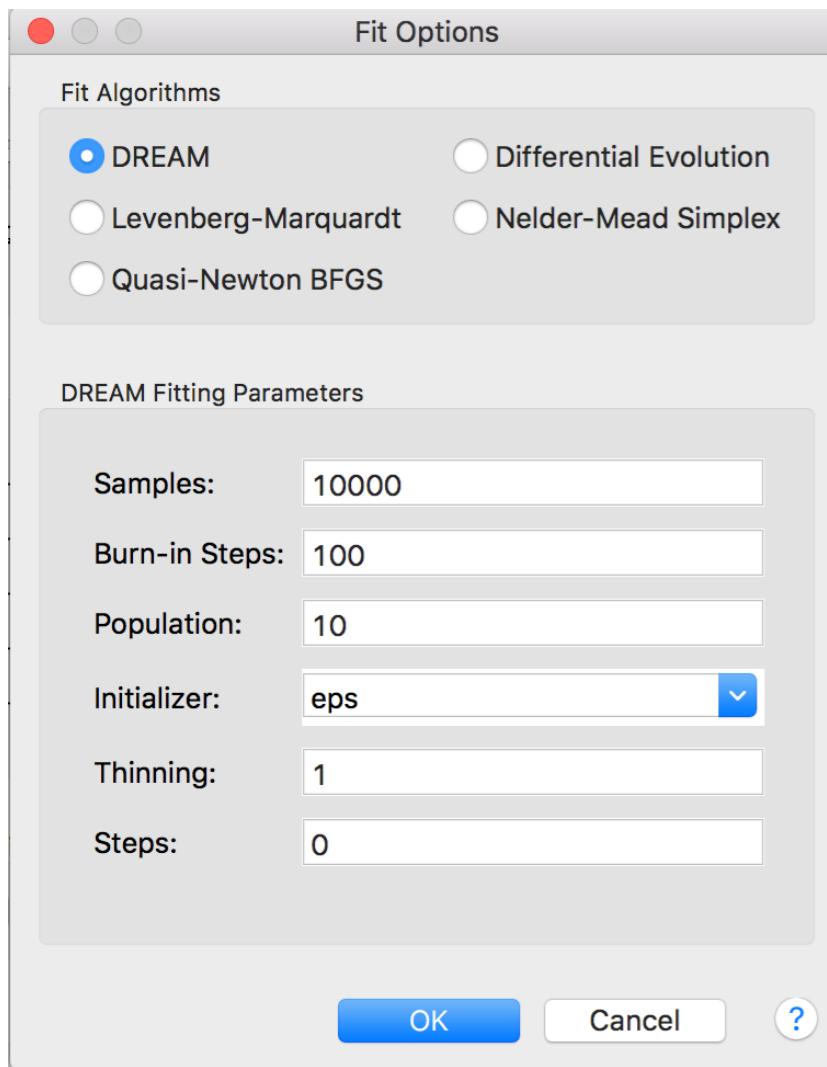
Set Weighting by Selecting dl Source
 No Weighting Use dl Data Use |sqrt(I) Data| Use |I| Data|

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

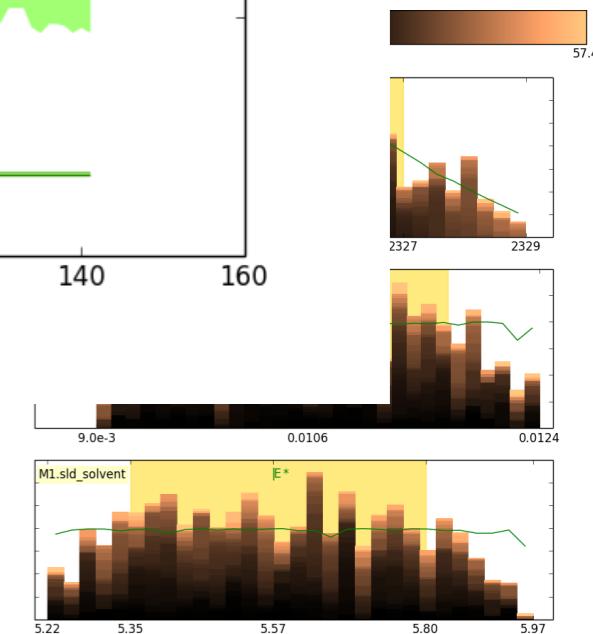
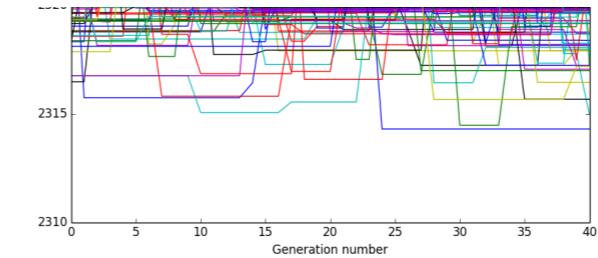
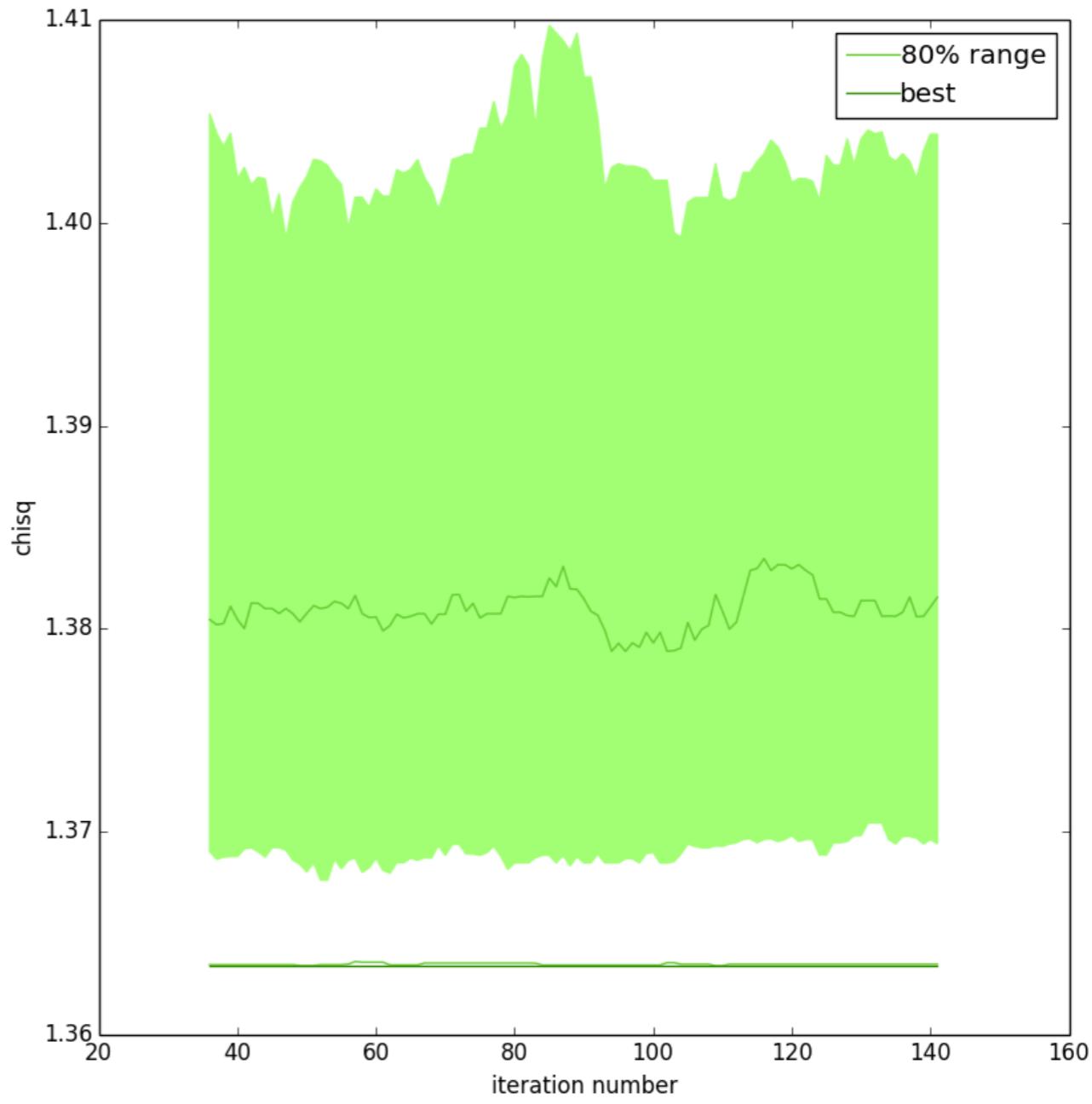
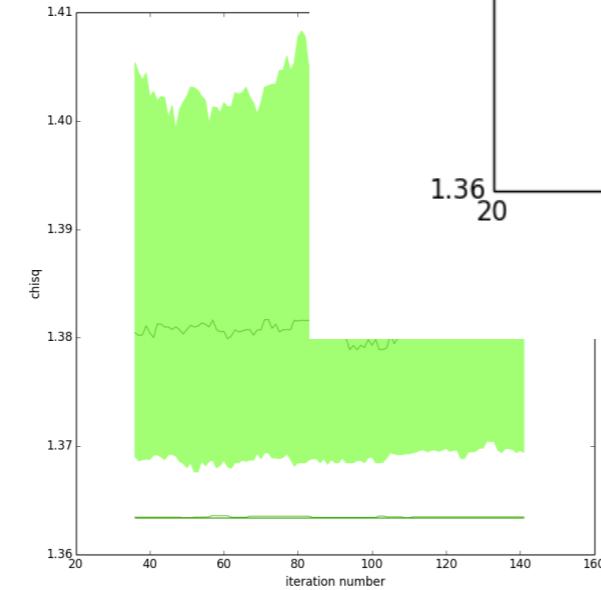
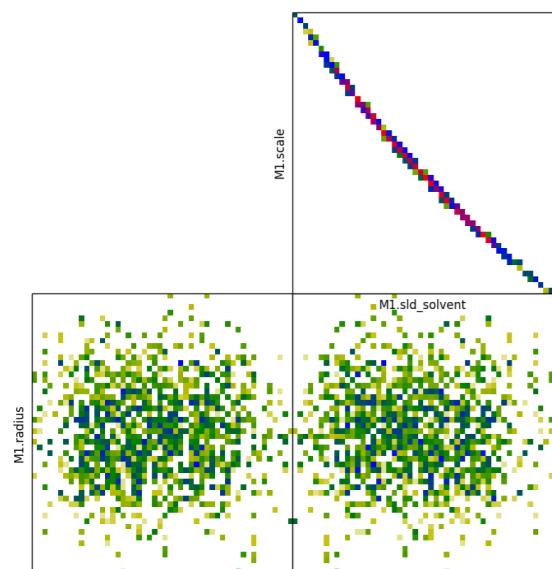
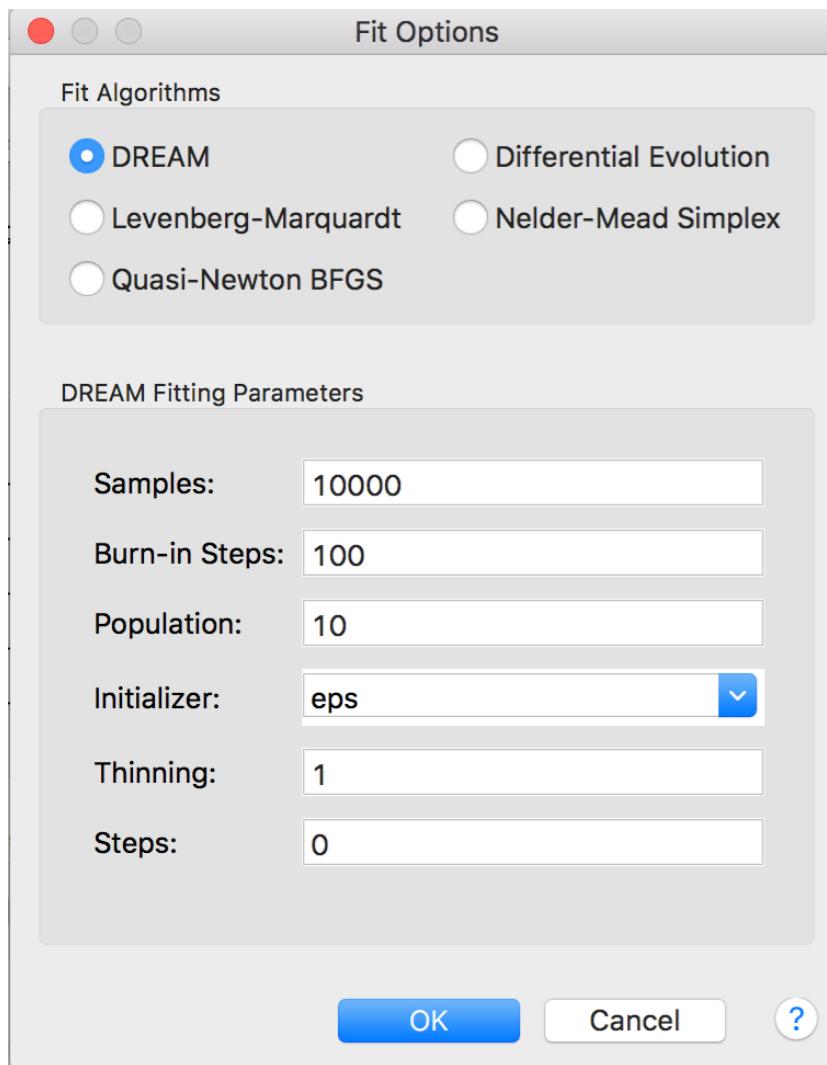
Chi2/Npts Npts(Fit) Npts Log? Compute
 3.5962 82 82 Fit Help



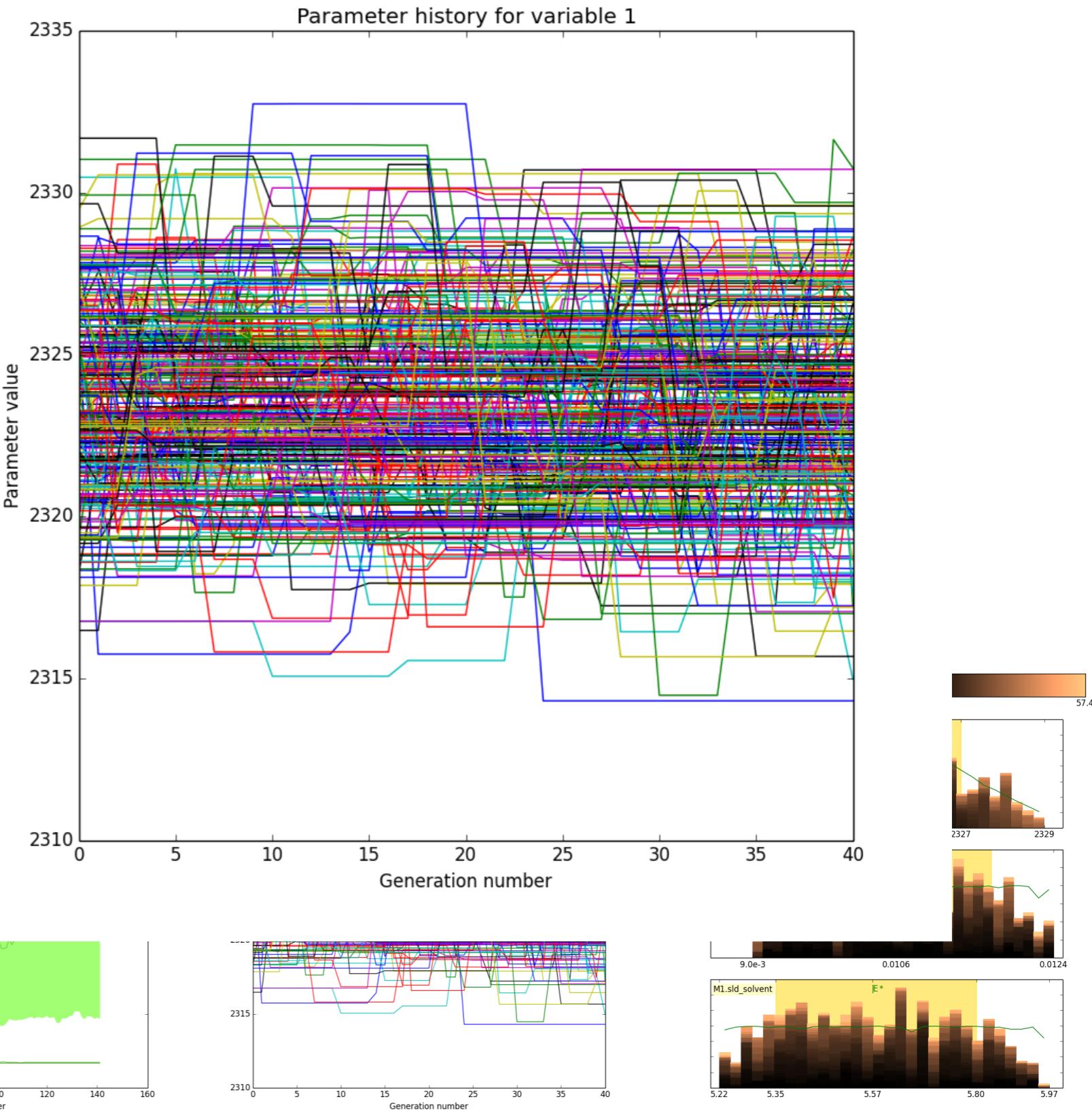
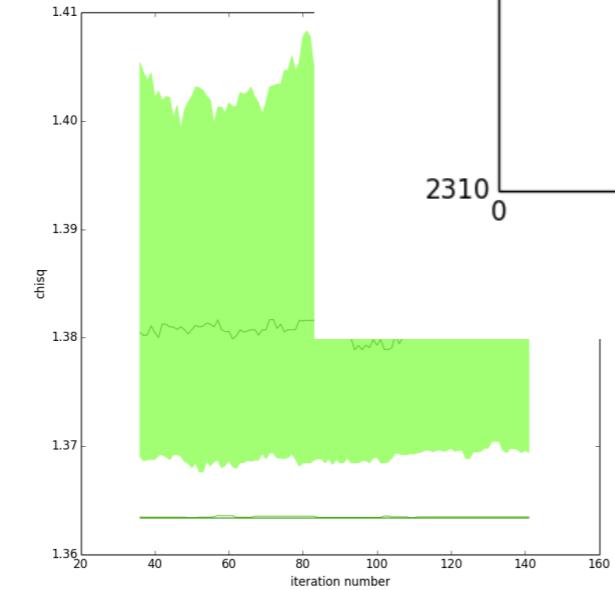
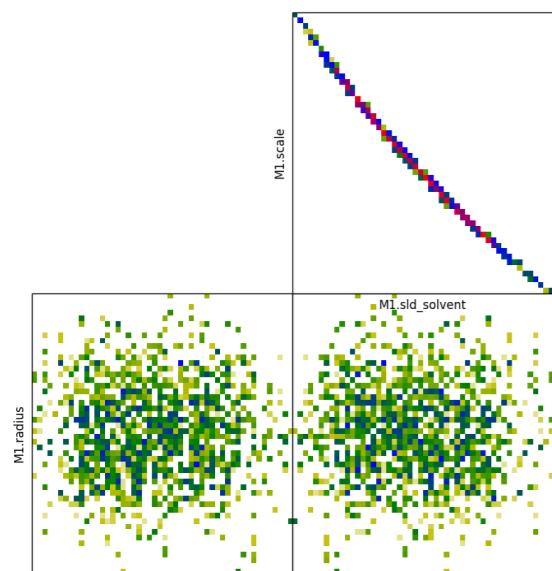
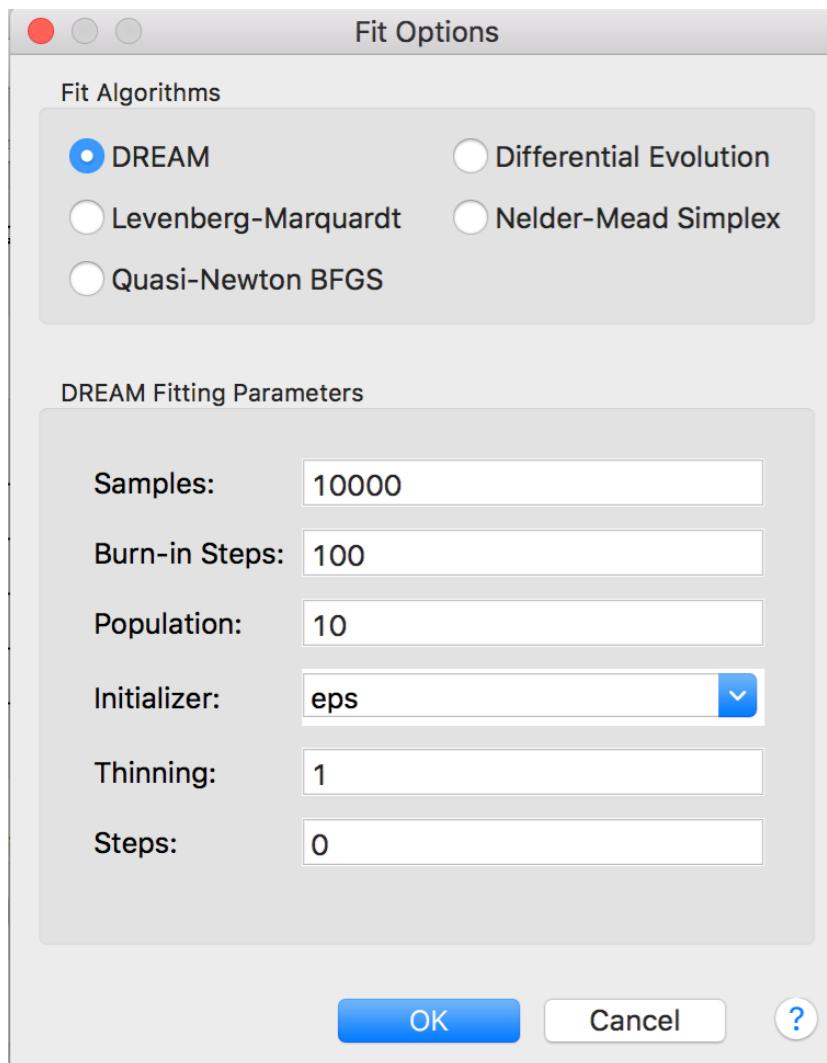
Fitting Algorithms



Fitting Algorithms



Fitting Algorithms



Fitting Algorithms

