SasView : A Small Angle Scattering Analysis Software Package

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

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 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
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 in Delft hosted by TU Delft / RID March 2016
5th at ORNL October 2016

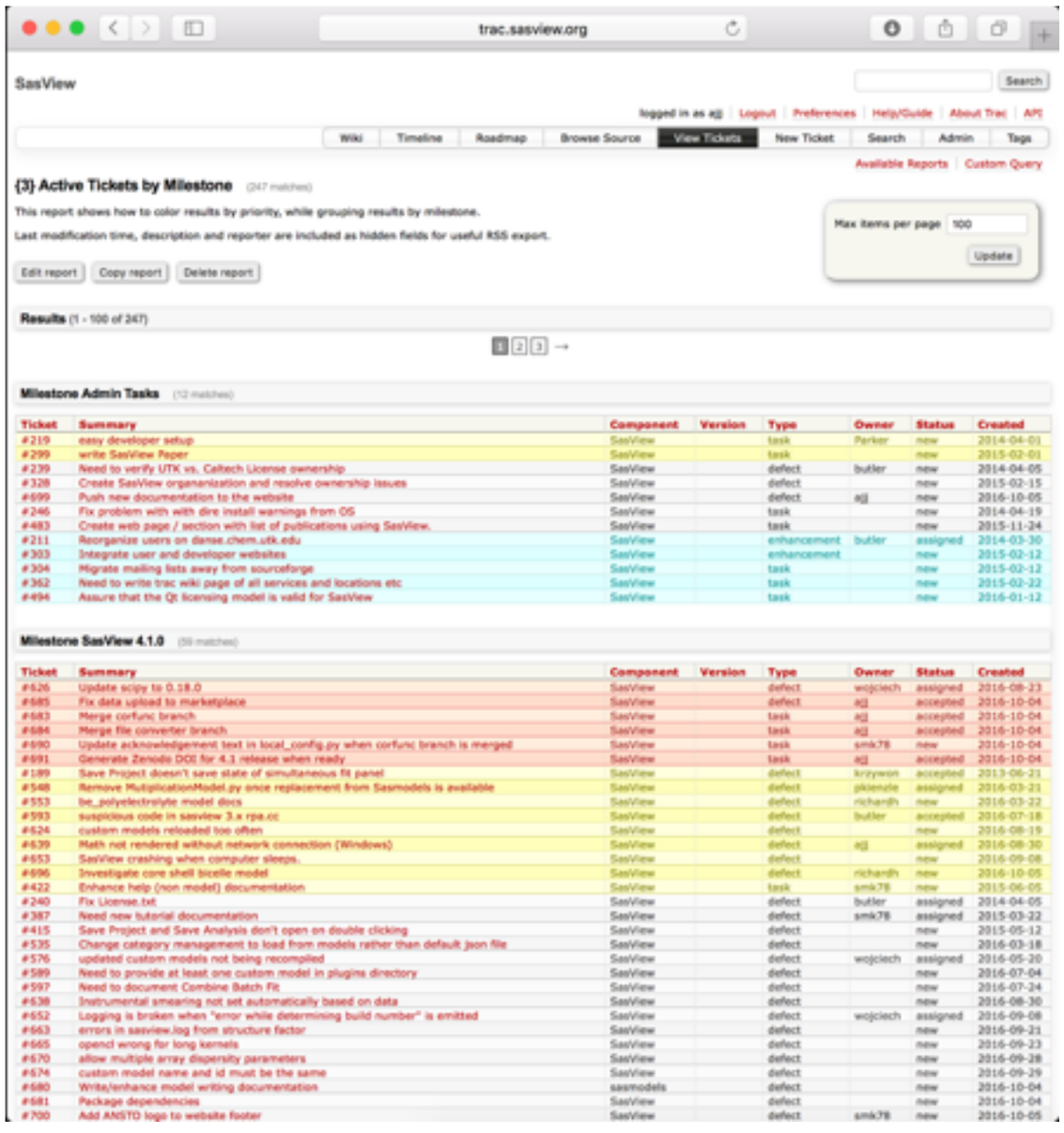
5 Year Roadmap

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

Development Model

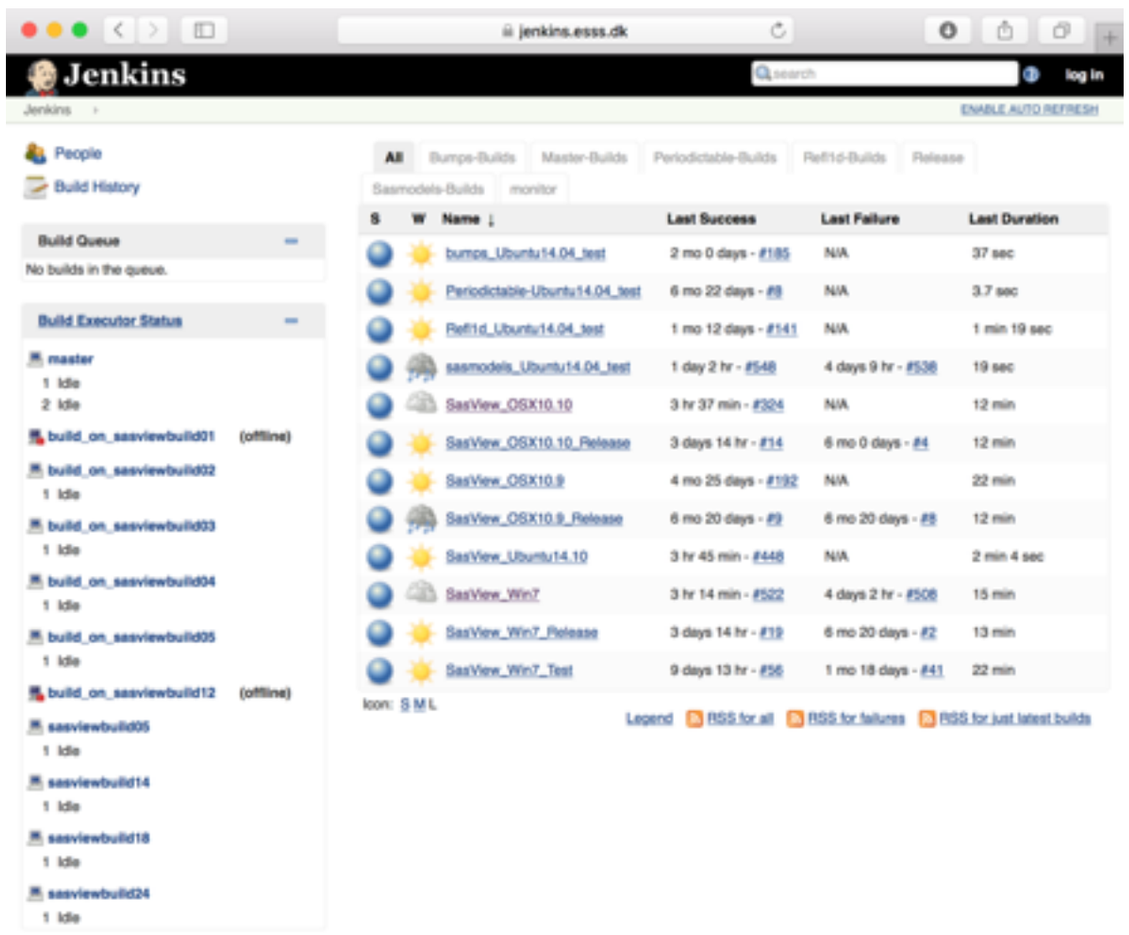
www.sasview.org

Task and bug tracking – trac.sasview.org



Hosted by UT

Automated Builds build.sasview.org



Hosted by ESS

Current Development Team

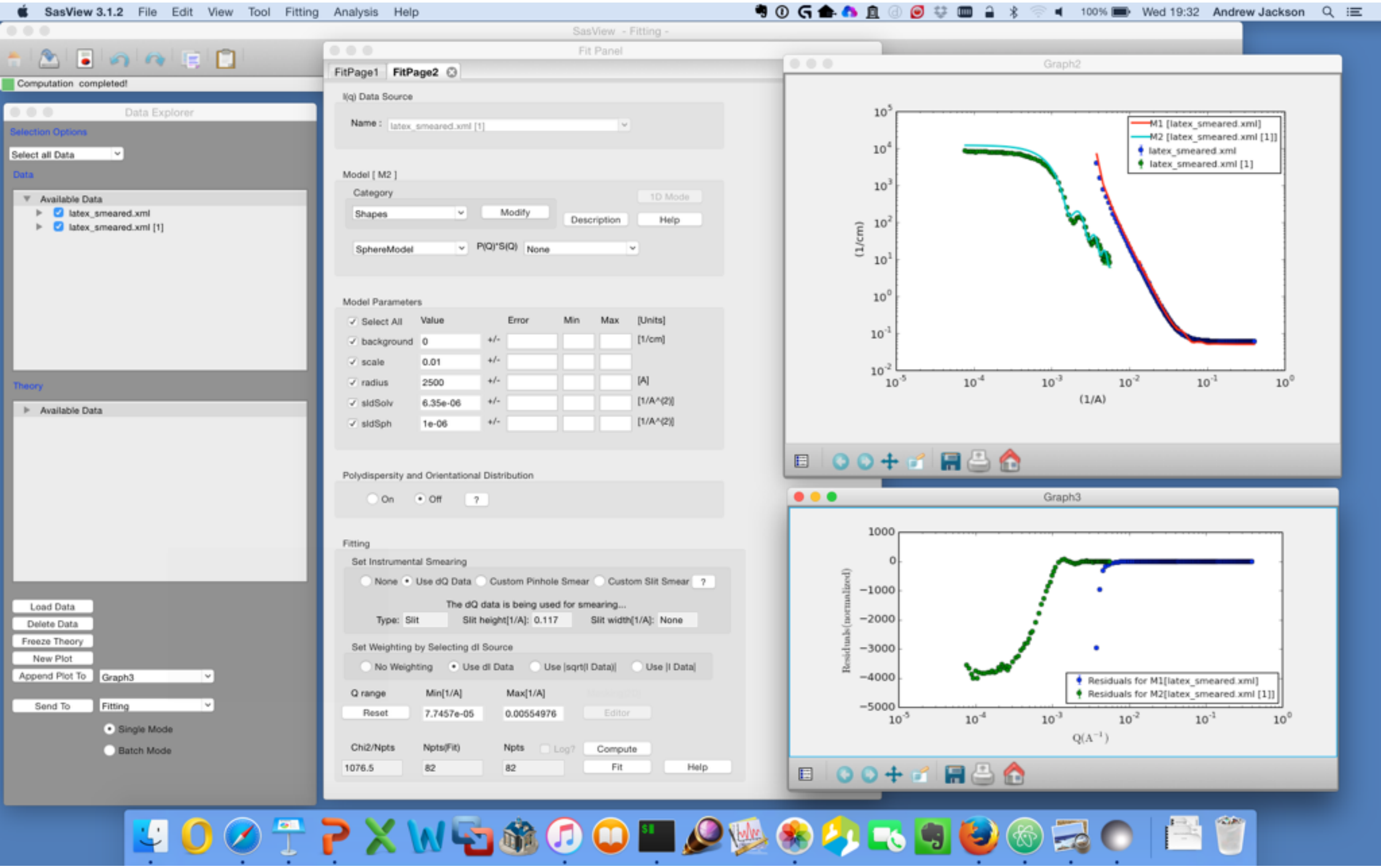
- Paul Butler (NIST)
- Mathieu Doucet (ORNL)
- Andrew Jackson (ESS)
- Steve King (ISIS)

- Jurrian Bakker (TUD)
- Wim Bouwman (TUD)
- Miguel Gonzales (ILL)
- Richard Heenan (ISIS)
- Dirk Honecker (ILL)
- Paul Kienzle (NIST)
- Jeff Kryzwon (NIST)
- Ricardo Leal (ORNL)
- David Mannicke (ANSTO)
- Torben Nielsen (ESS)
- Lewis O'Driscoll (ISIS)
- 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

What Can SasView Do Currently?

1D Analysis


SasView 3.1.2 File Edit View Tool Fitting Analysis Help
100% 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 :
latex_smeared.xml [1]
Model [M2]
Category
Shapes
Modify
1D Mode
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
Editor
Chi2/Npts
Npts(Fit)
Npts
Log?
Compute
1076.5
82
82
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 for M1[latex_smeared.xml]
Residuals for M2[latex_smeared.xml [1]]
Residuals (normalized)
Q(A^-1)

1D Analysis

Load Data …

Select Data Sets …

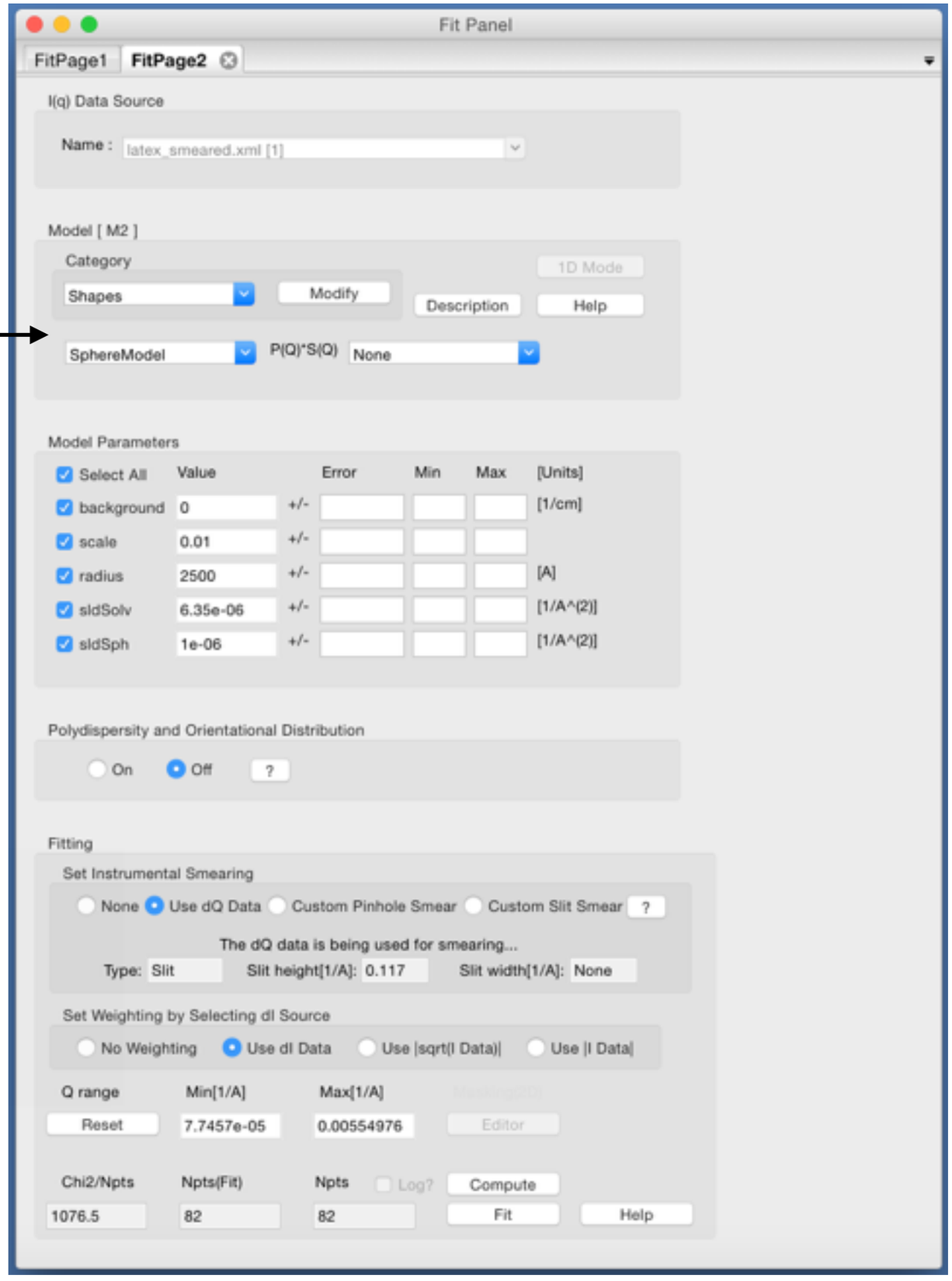
Here we have SANS & USANS from latex spheres

Send to Fitting …

1D Analysis

Send to fitting …

Select a model …

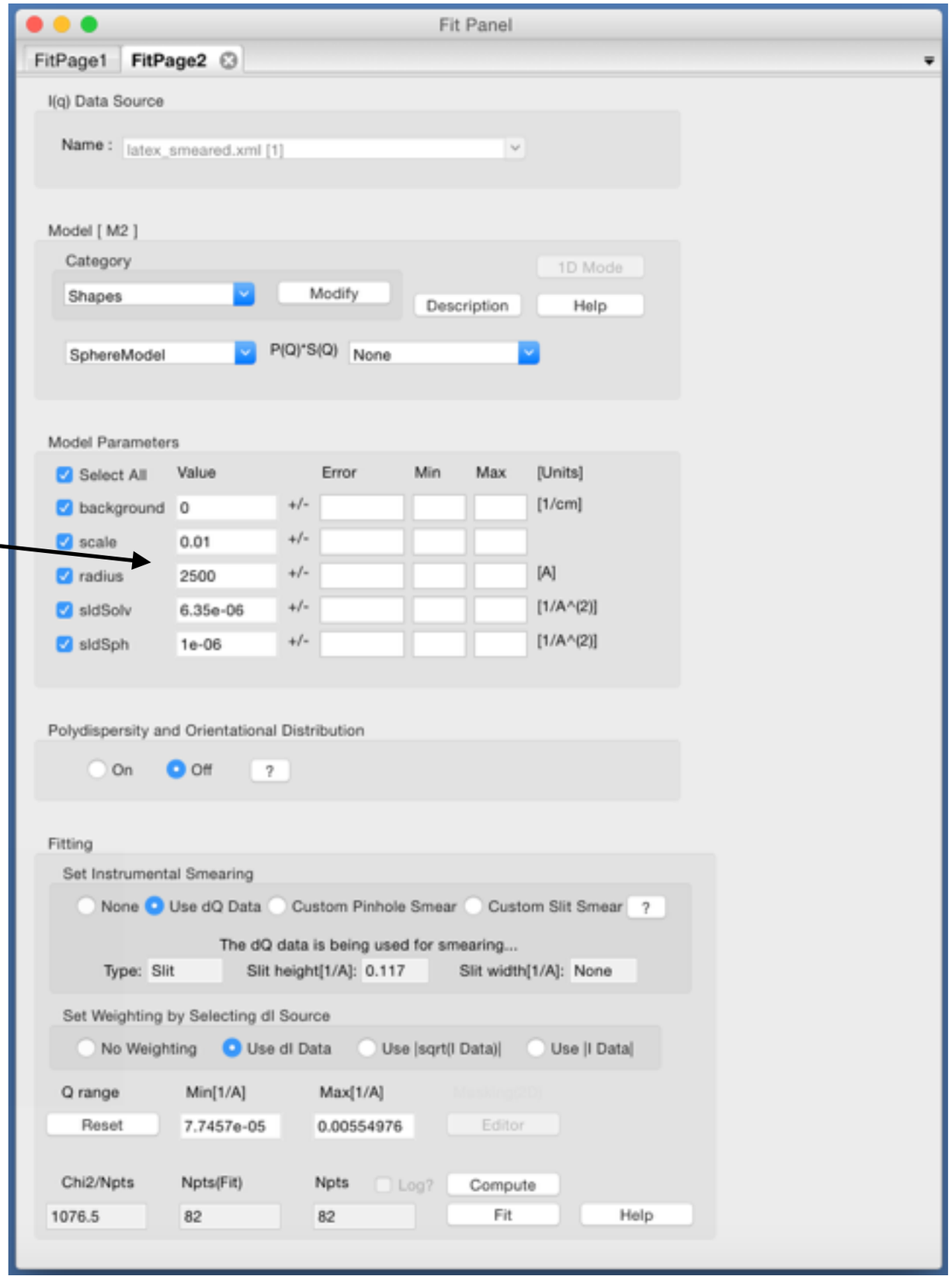


1D Analysis

Send to fitting …

Select a model …

Set parameters …



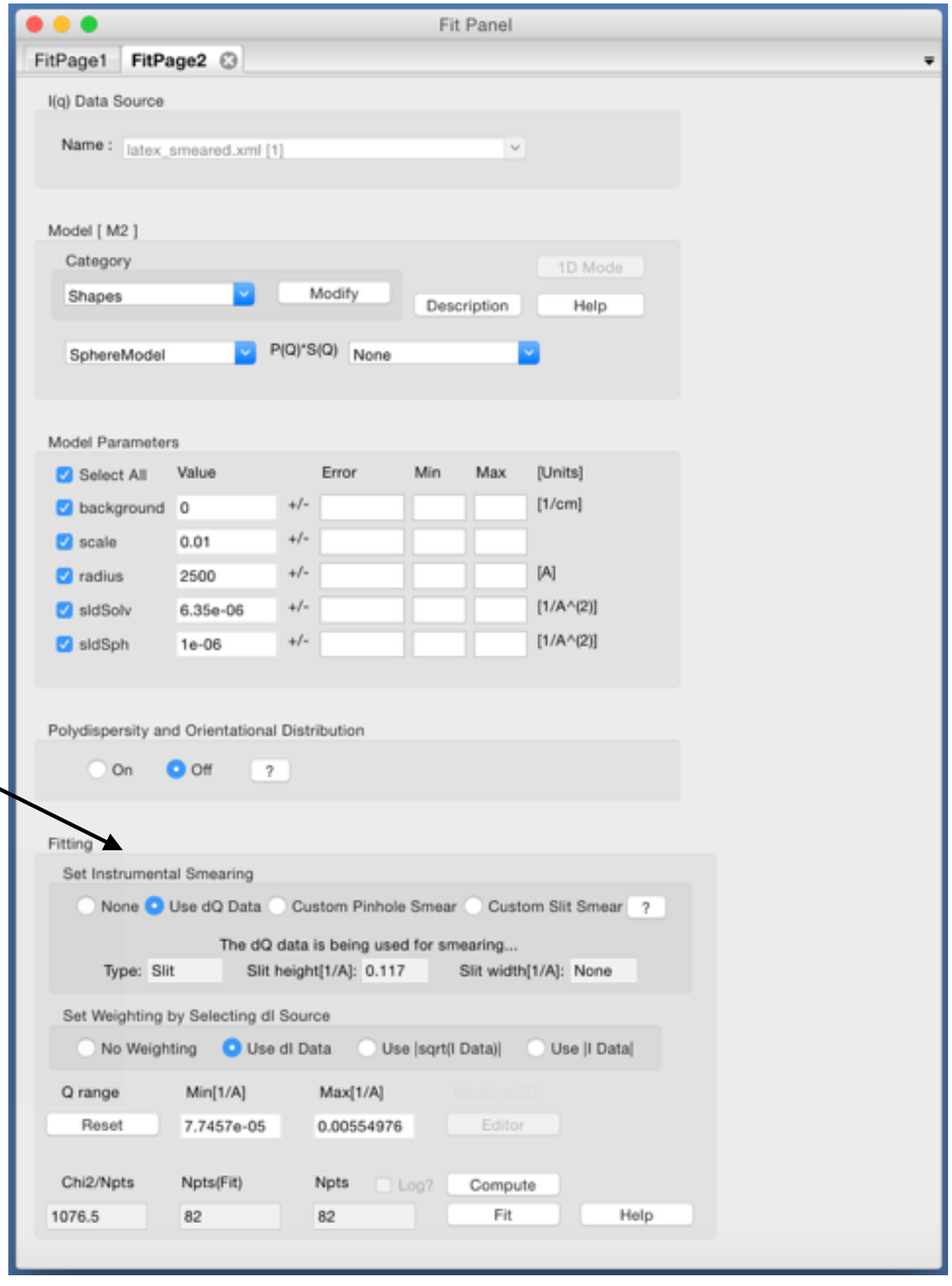
1D Analysis

Send to fitting …

Select a model …

Set parameters …

Use resolution …



1D Analysis

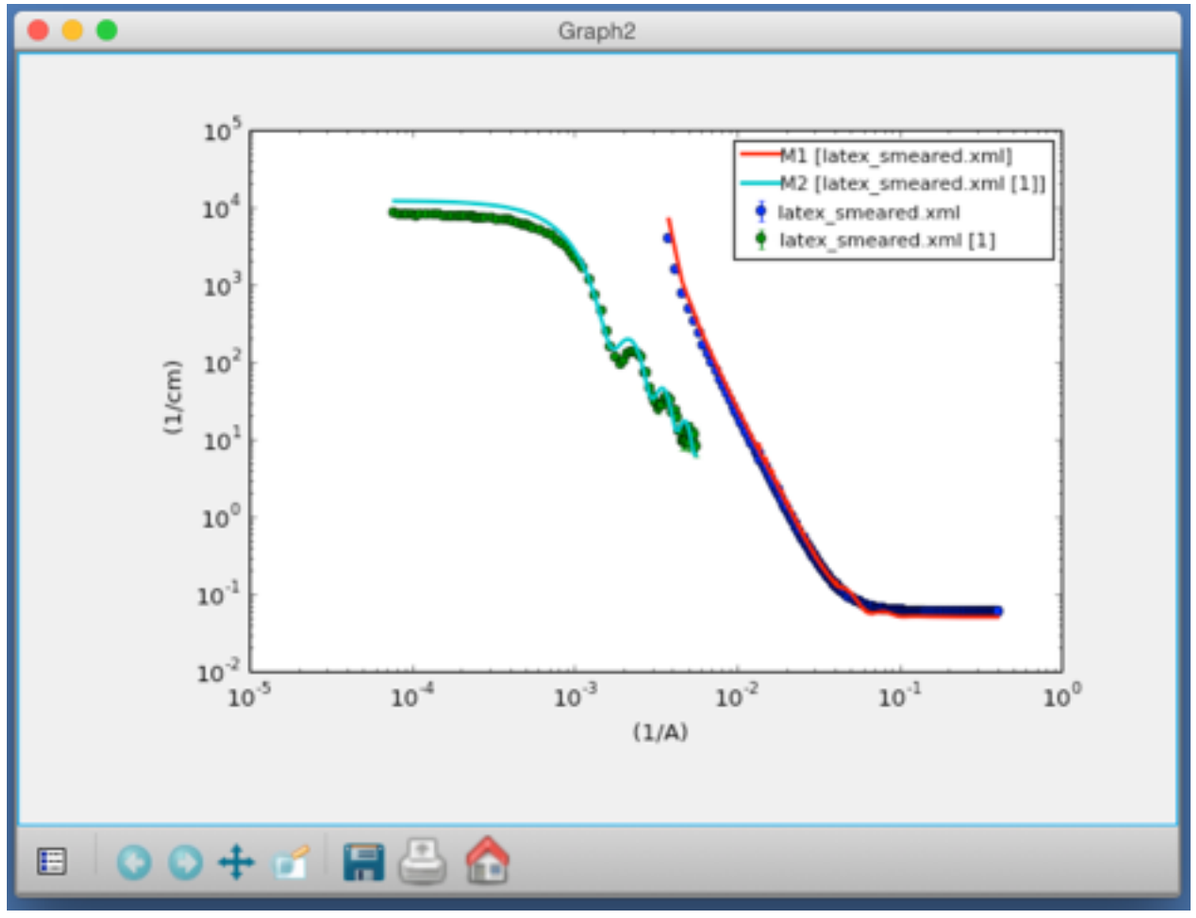
Send to fitting …

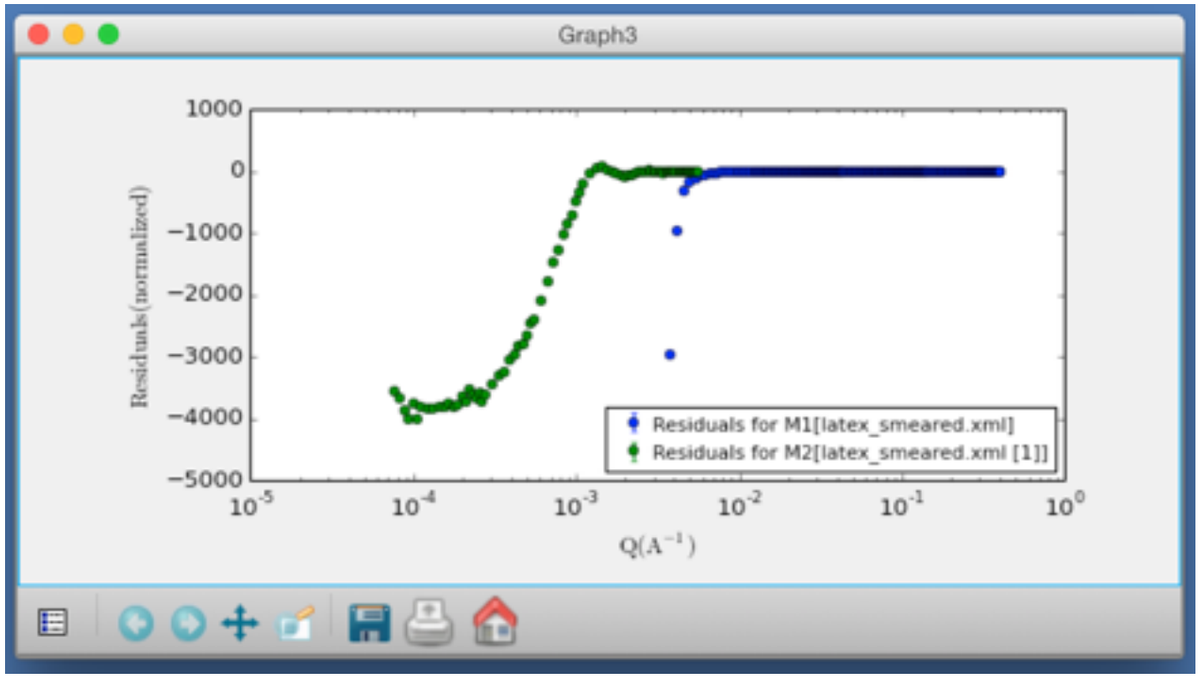
Select a model …

Set parameters …

Use resolution …

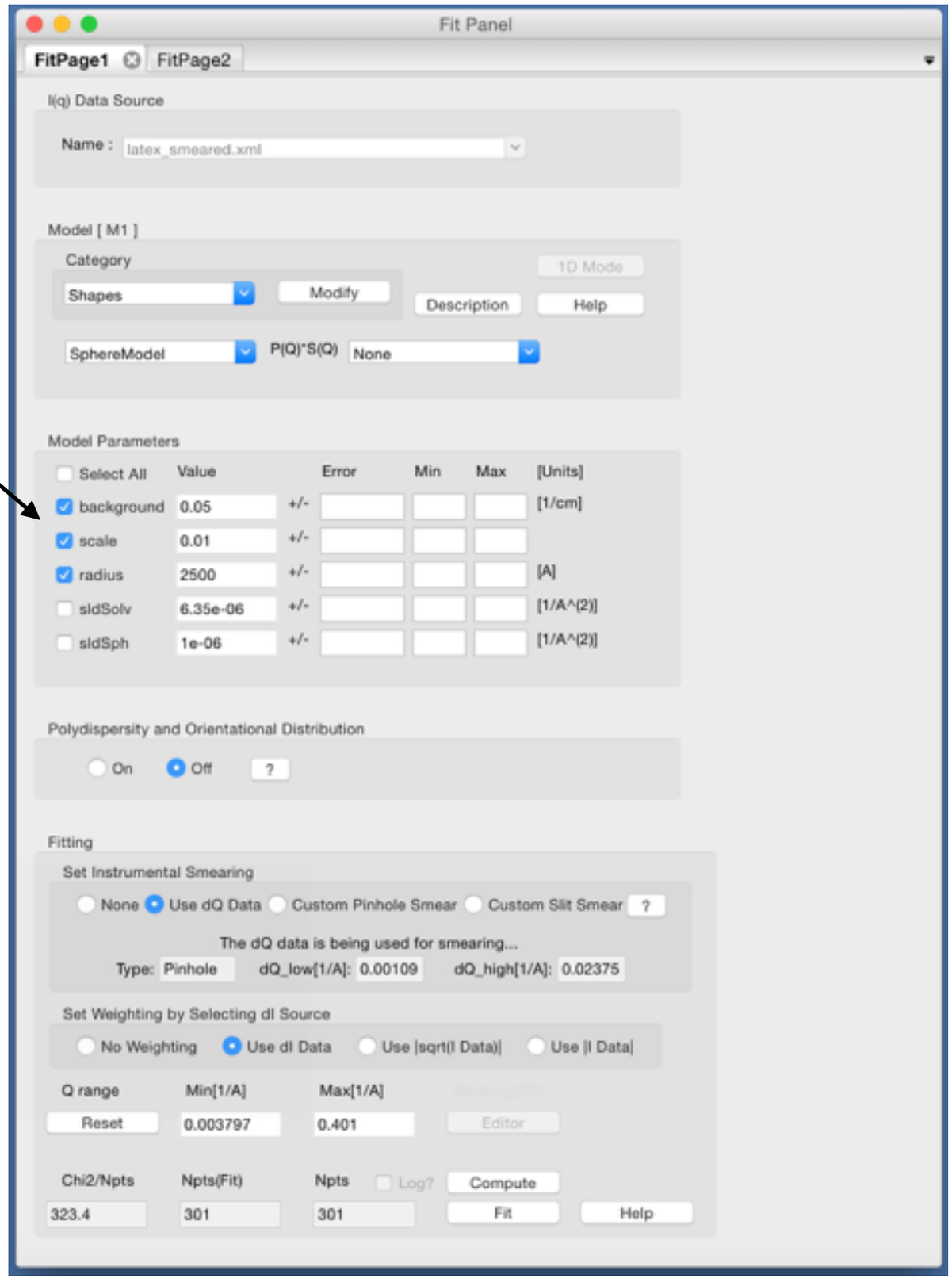
How does it look?





1D Analysis

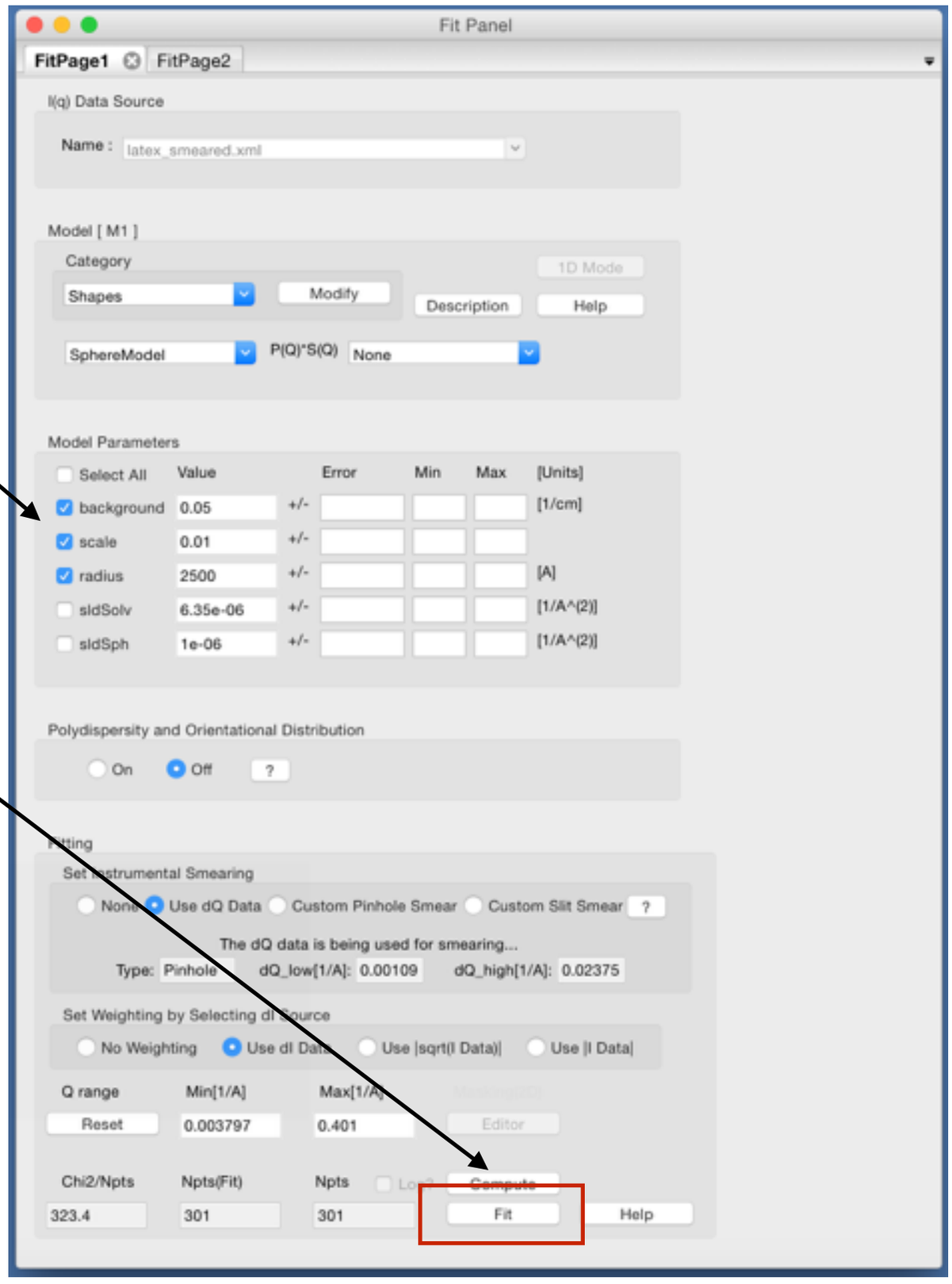
Choose which parameters to fit …



1D Analysis

Choose which parameters to fit …

… and press the Fit button!



Constraints / Simultaneous Fit

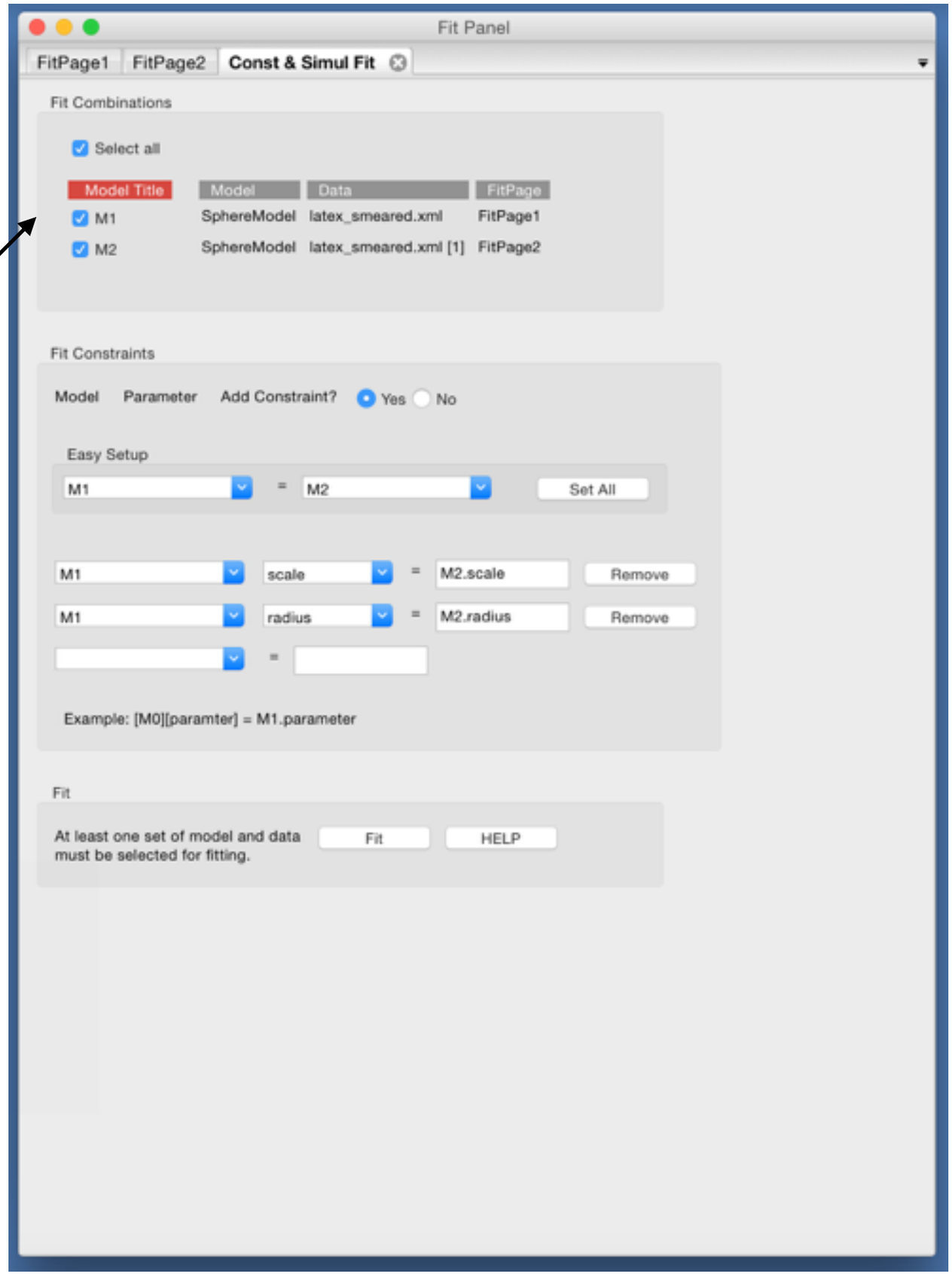
But wait! We have two data sets of the same sample :

SANS + USANS …

Constraints / Simultaneous Fit

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

Set up a simultaneous fit …

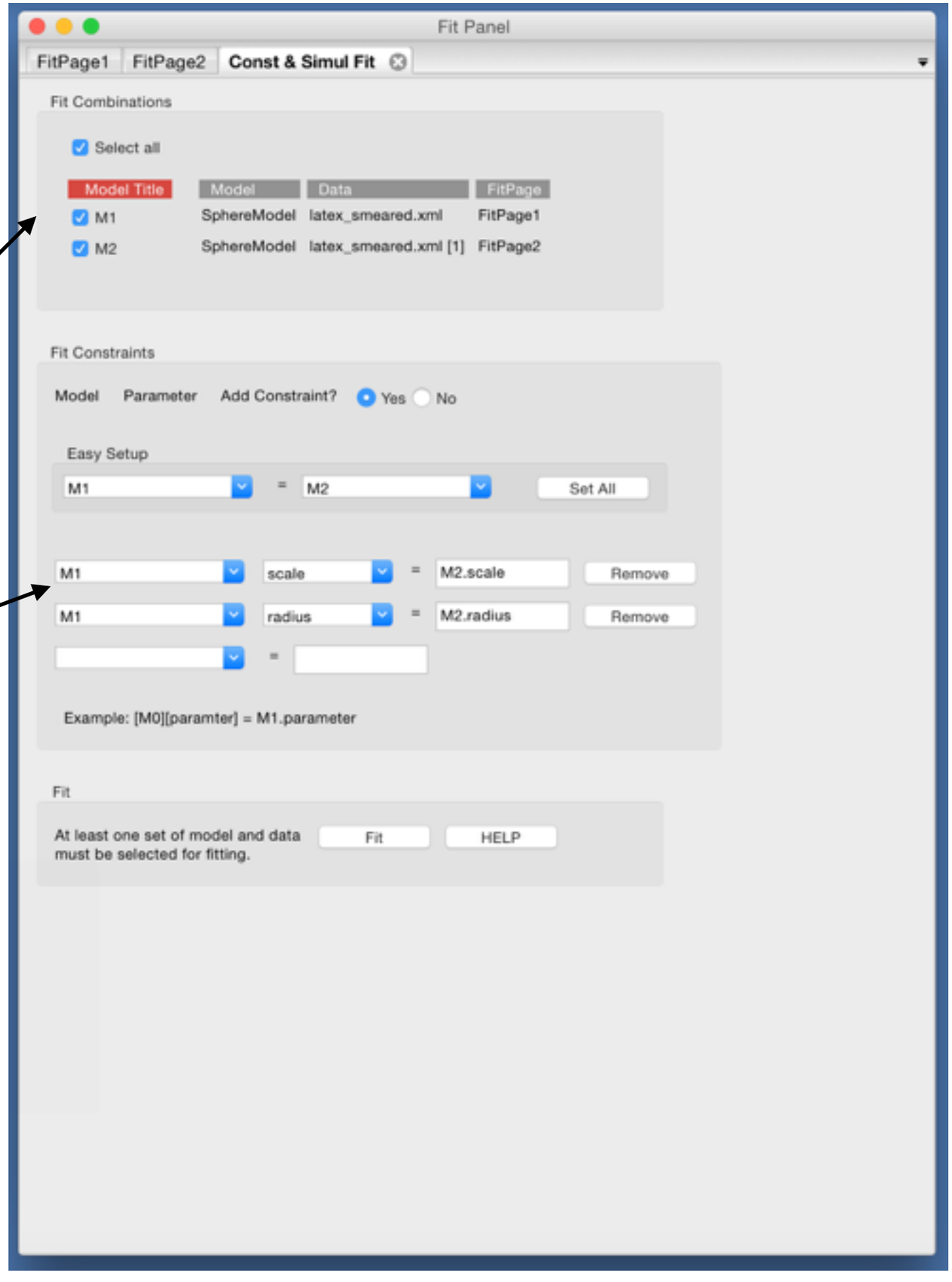


Constraints / Simultaneous Fit

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

Set up a simultaneous fit …

… with constraints



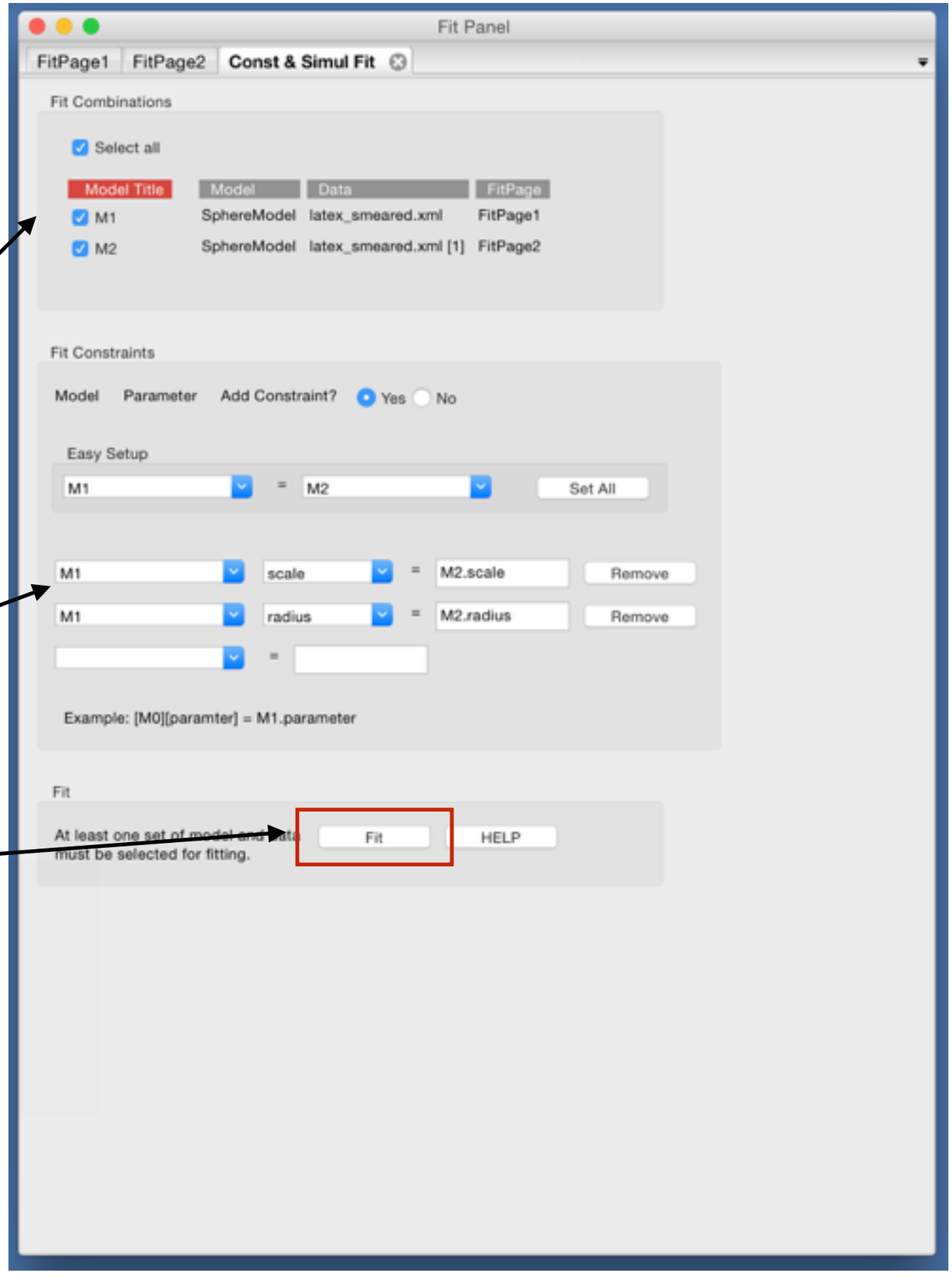
Constraints / Simultaneous Fit

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

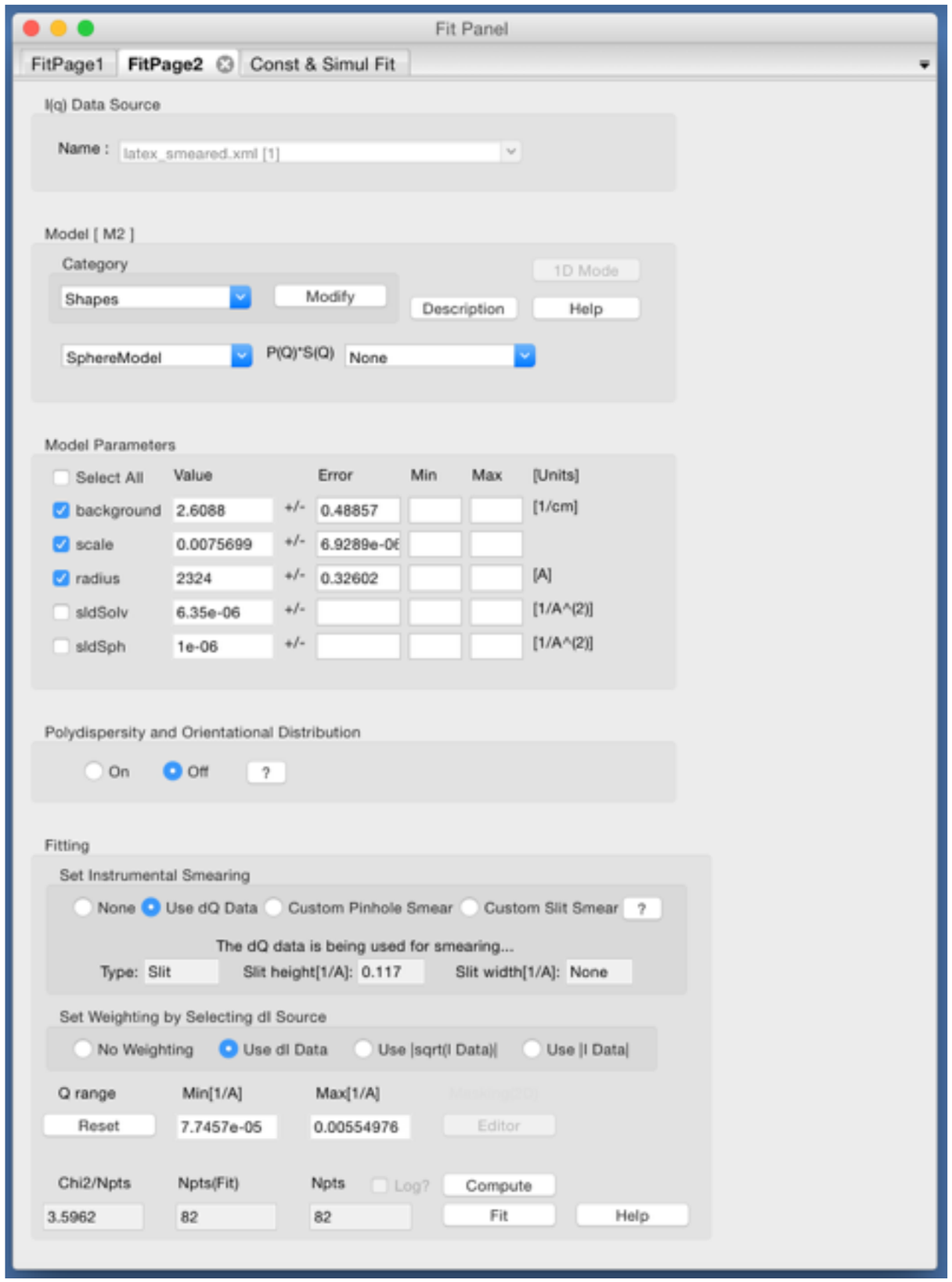
Set up a simultaneous fit …

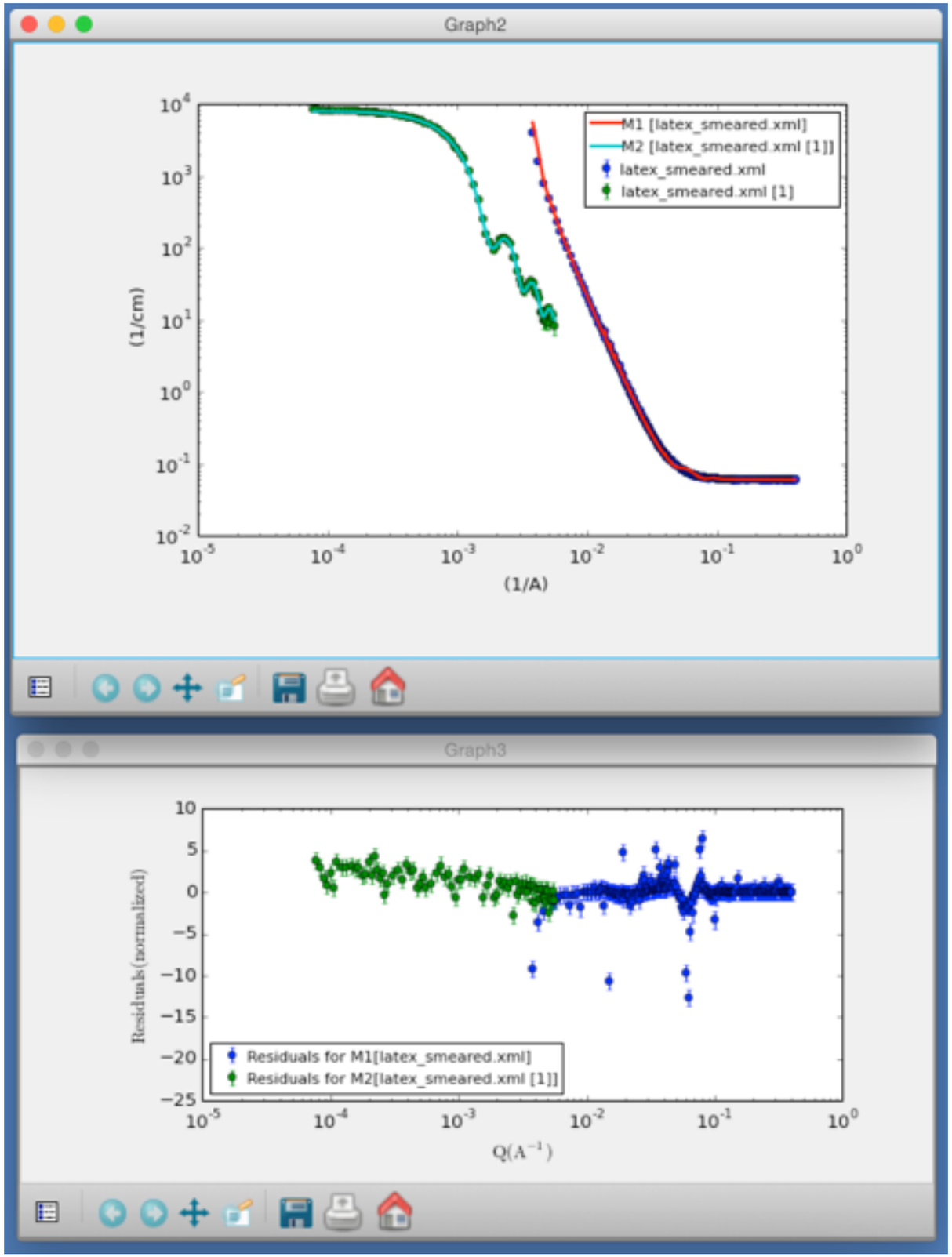
… with constraints

Now press the Fit button!



Constraints / Simultaneous Fit





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

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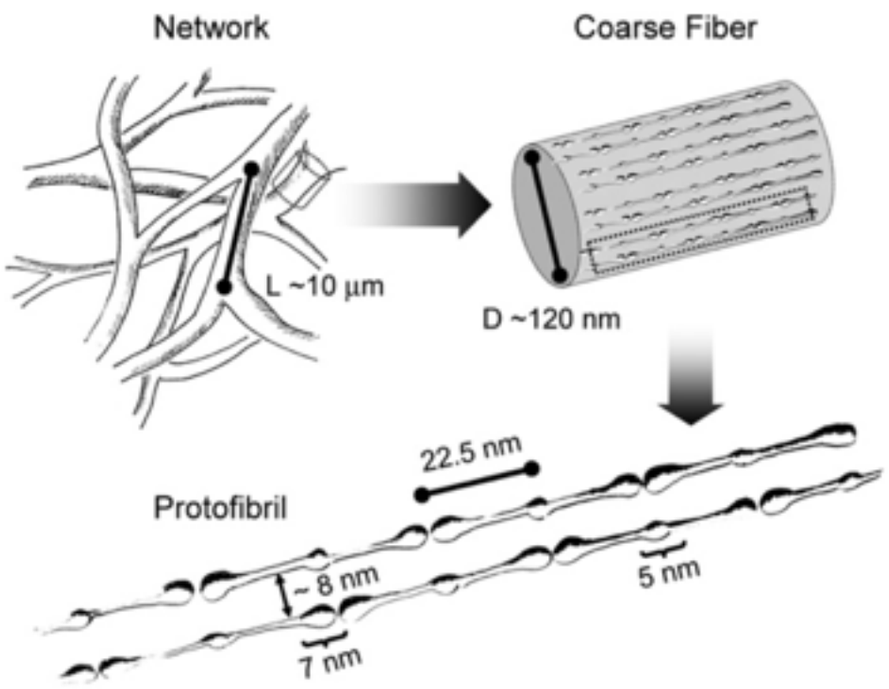
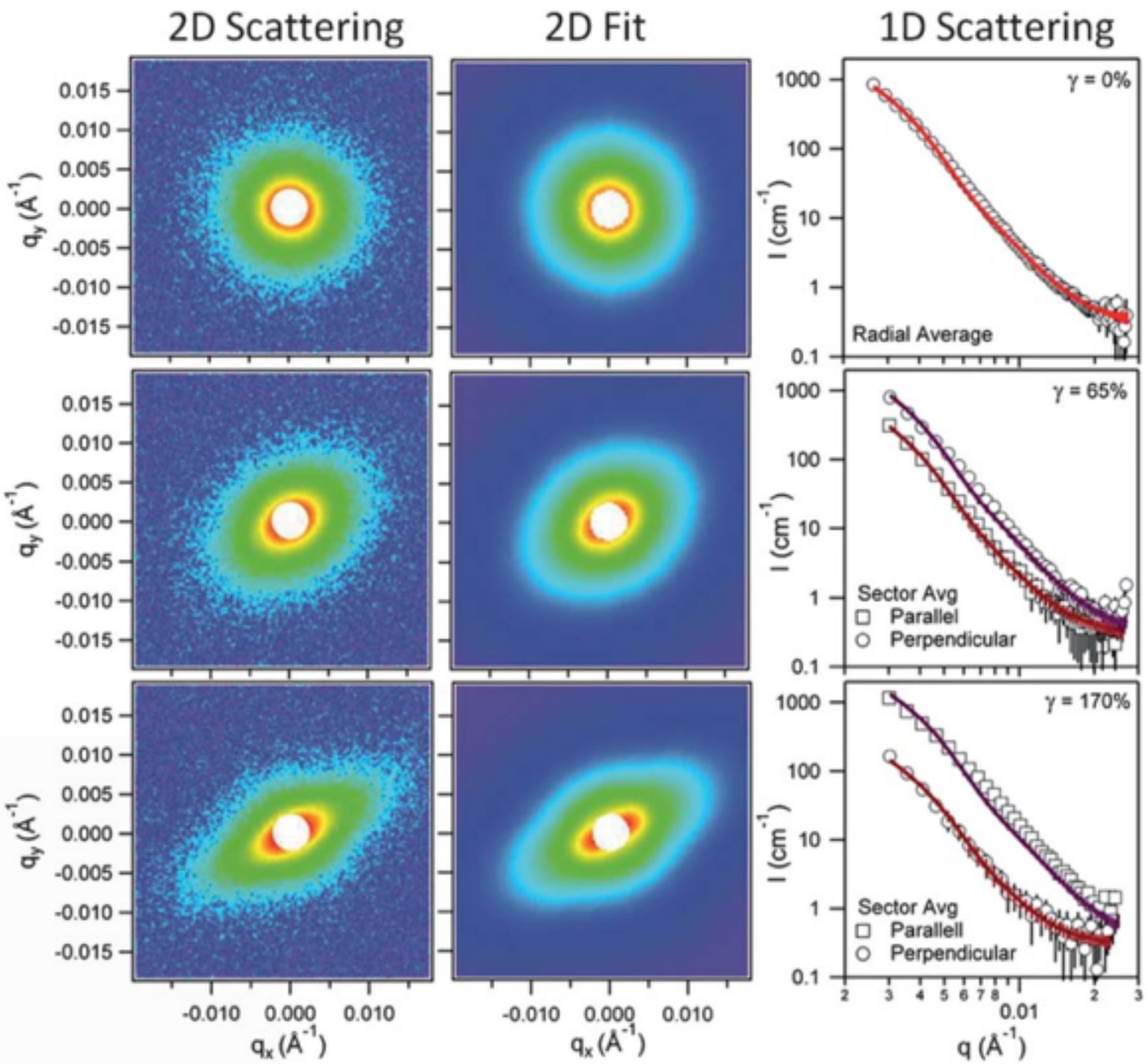
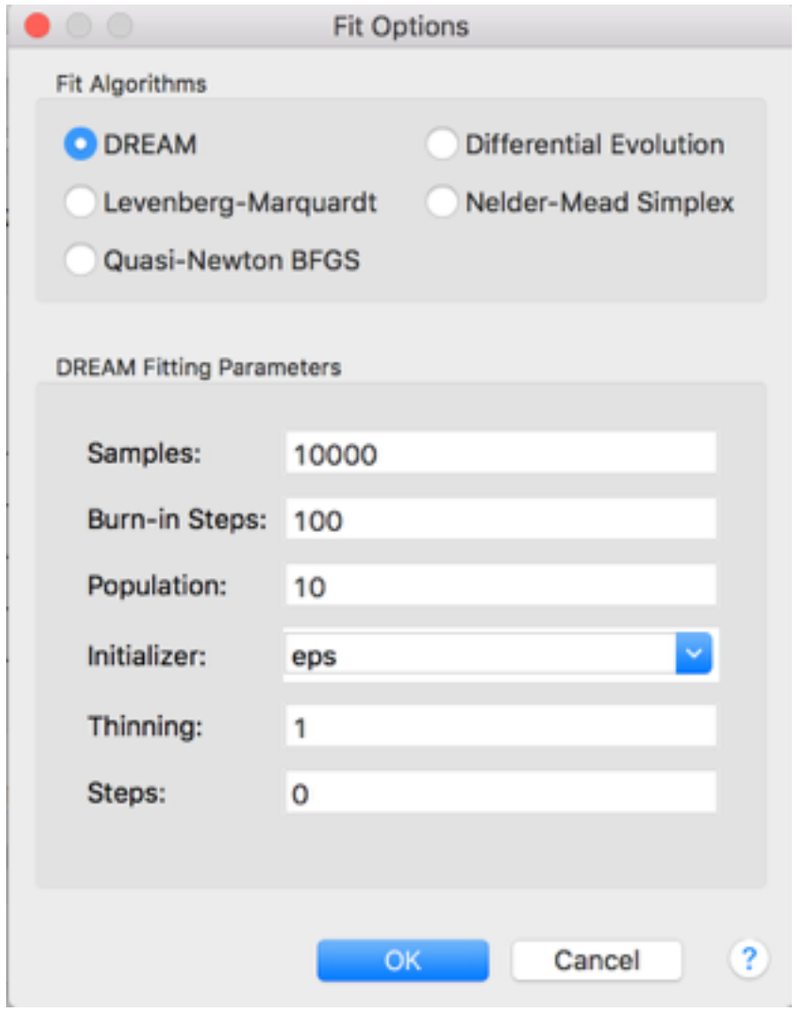
DOI: 10.1039/c1sm06176c

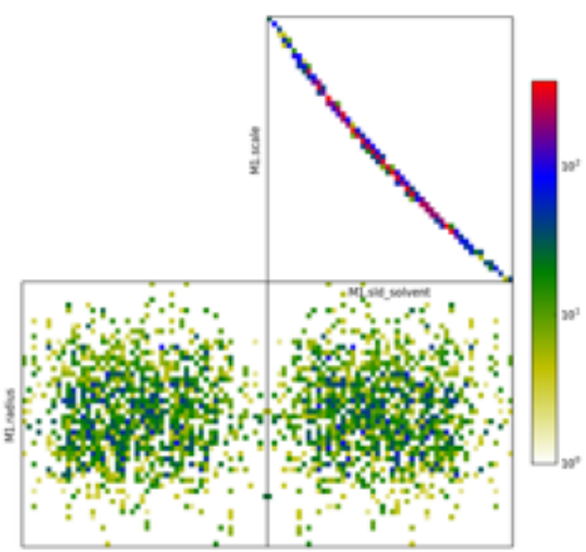
Small angle neutron scattering (SANS) is used to decipher the origin of the strain h
biopolymer networks by directly measuring the structural response of a fibrin gel to
deformation. A special Couette shear cell is used to systematically probe the structu
a fibrin clot over strain values in the range of $\gamma = 1$–170%. The SANS results indic
hardening response of coarse fibrin gels occurs in two distinct regions having differ
mechanical signatures that are separated by an intermediate strain softening regime
($\gamma < 10\%$) there is a measurable increase in the shear modulus upon the application
there are no significant changes to the clot structure. At higher strain values ($\gamma > 30\%$
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.

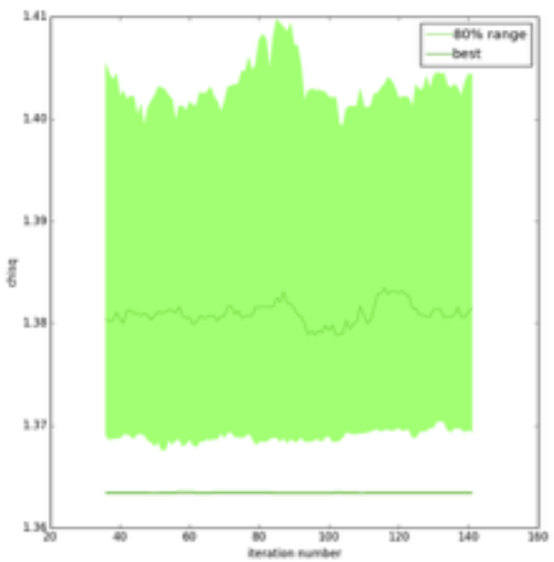


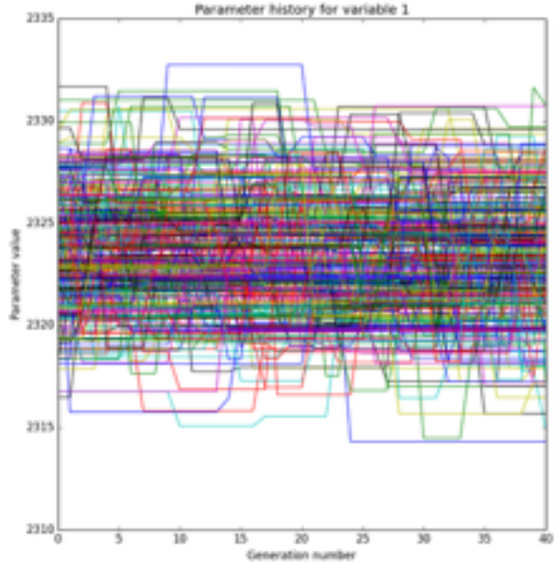


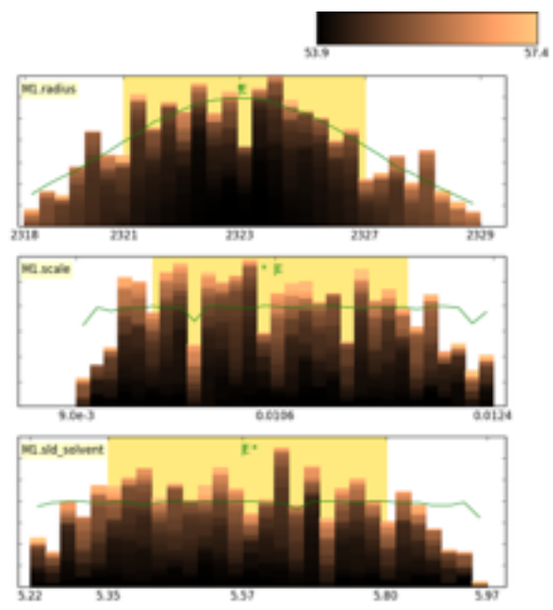
Fitting Algorithms



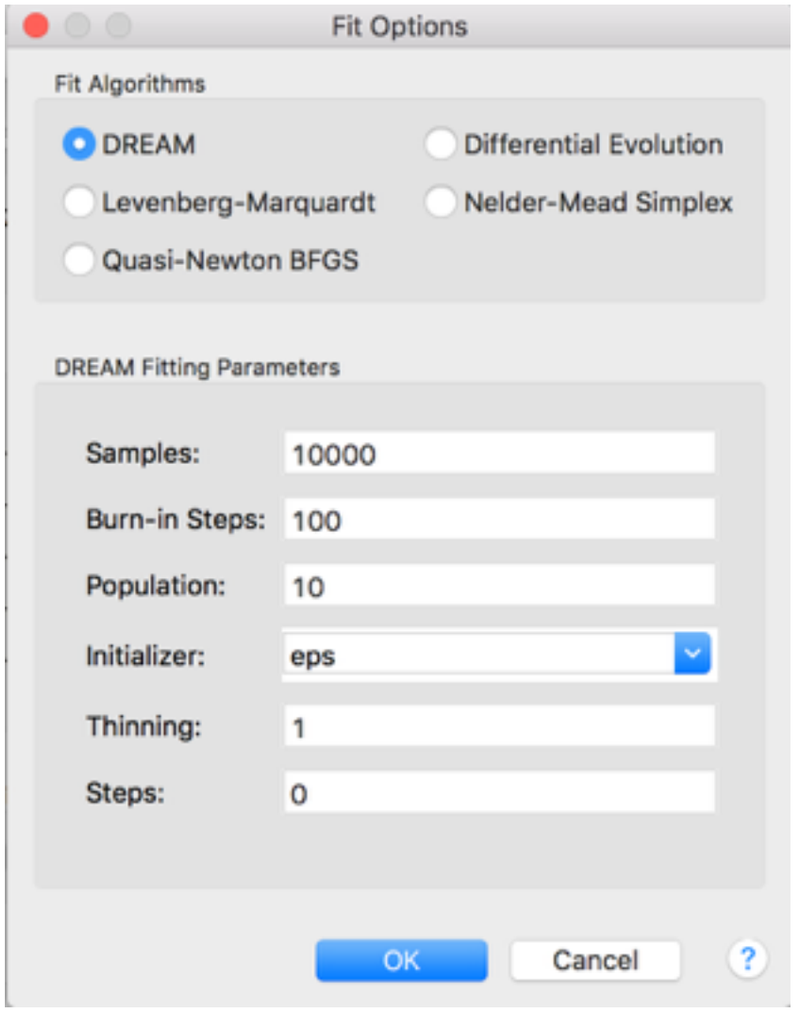


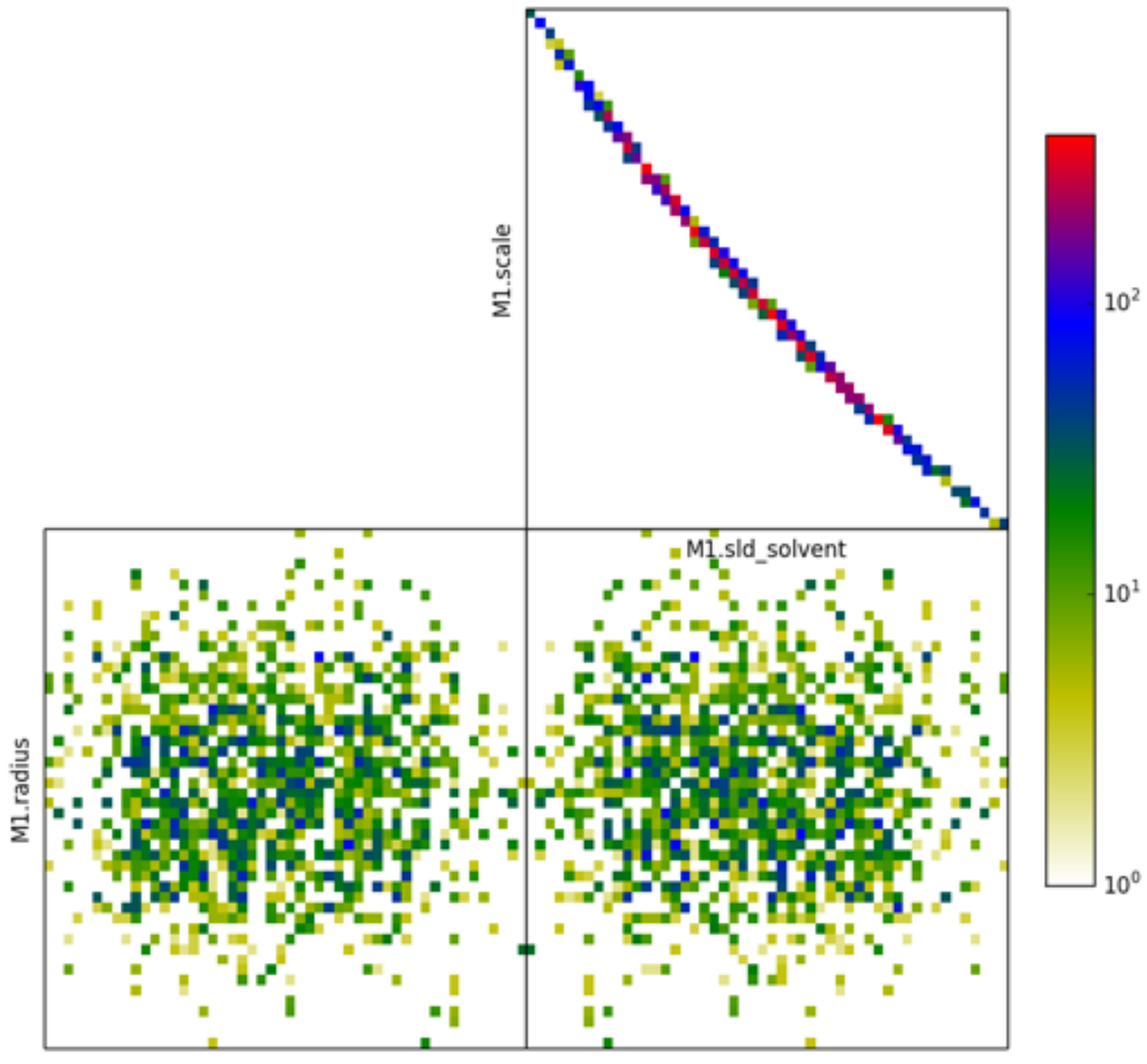


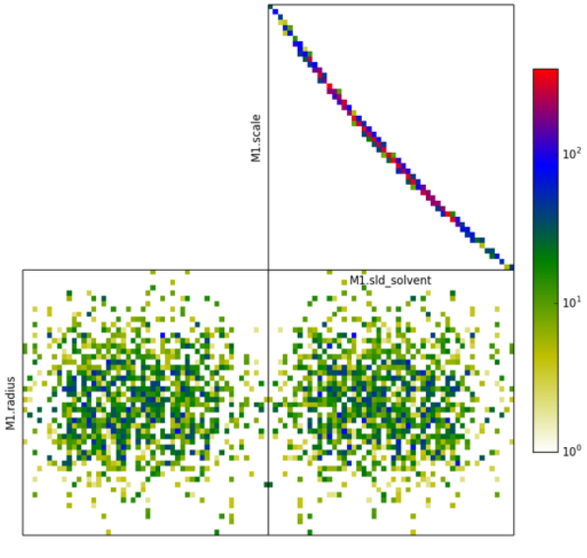


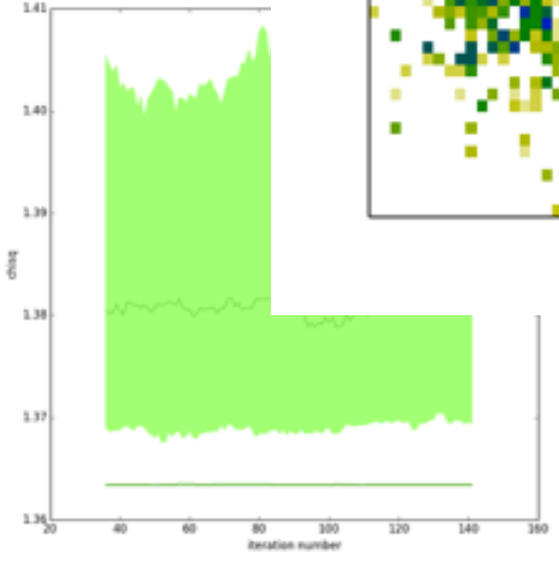


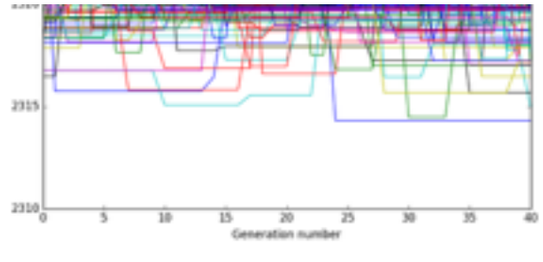
Fitting Algorithms

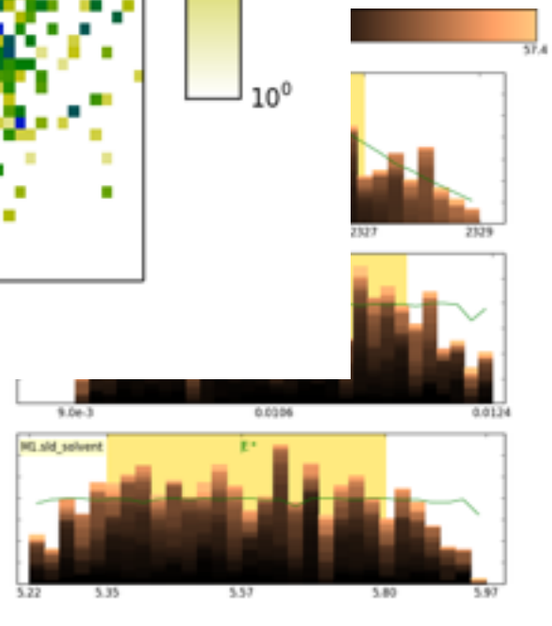




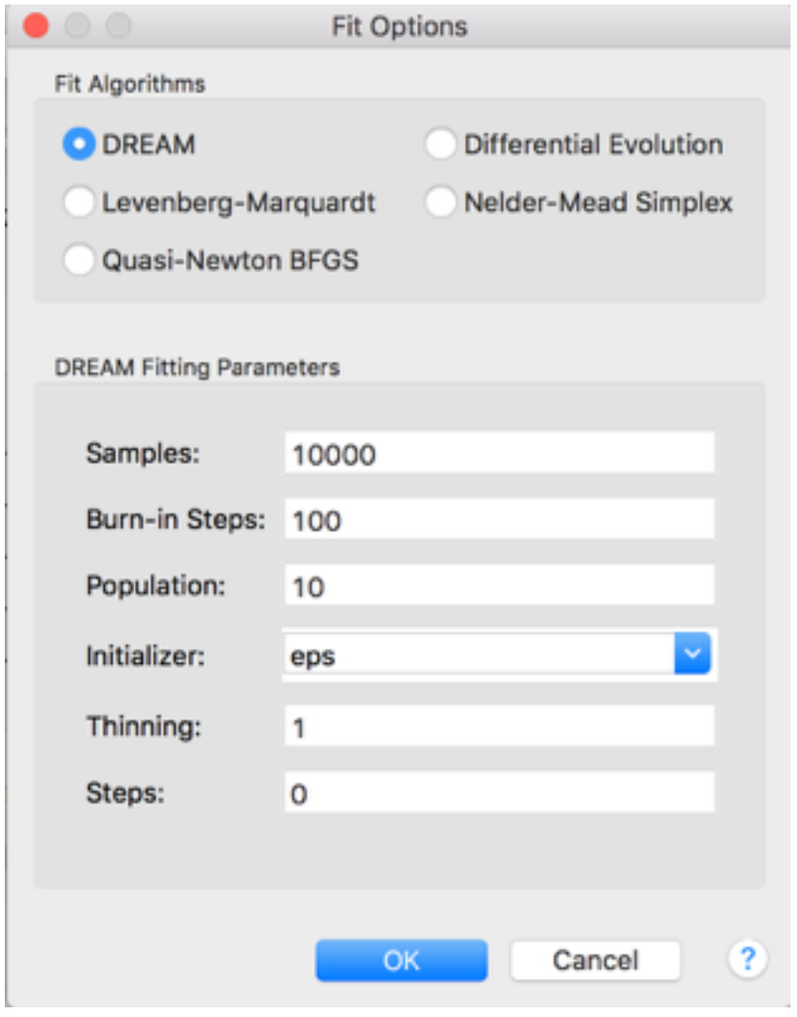


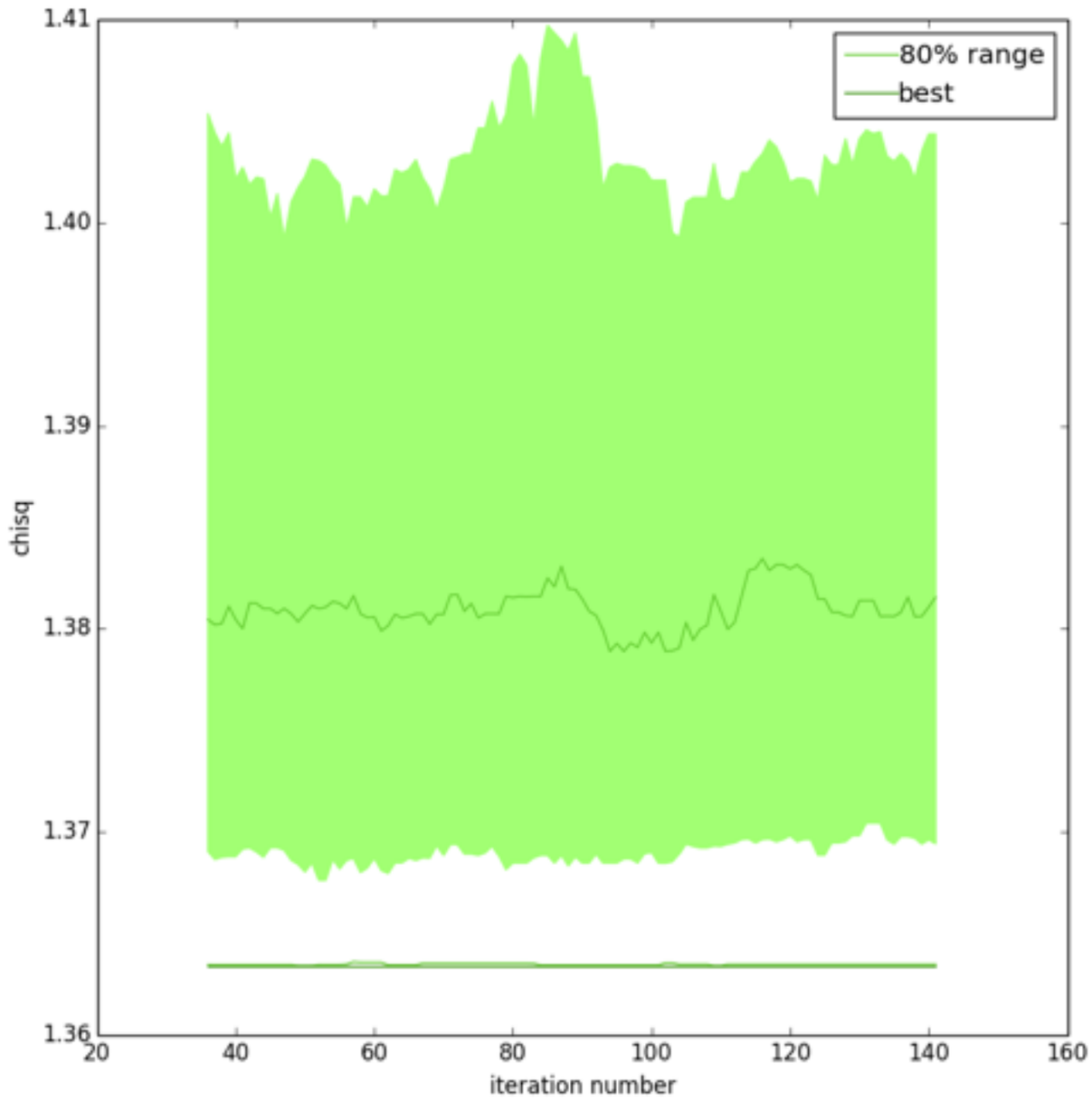


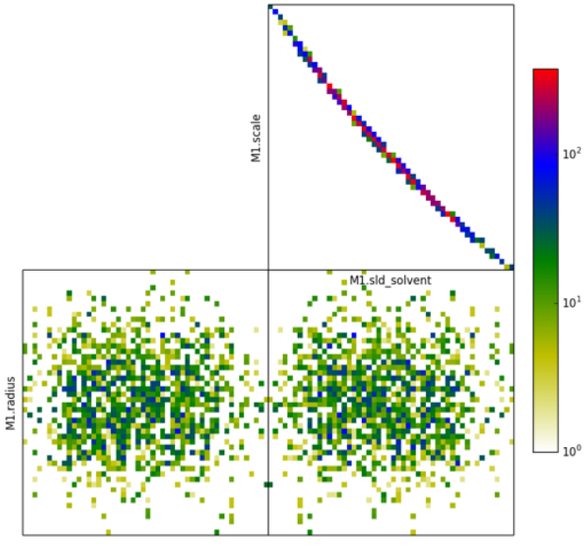


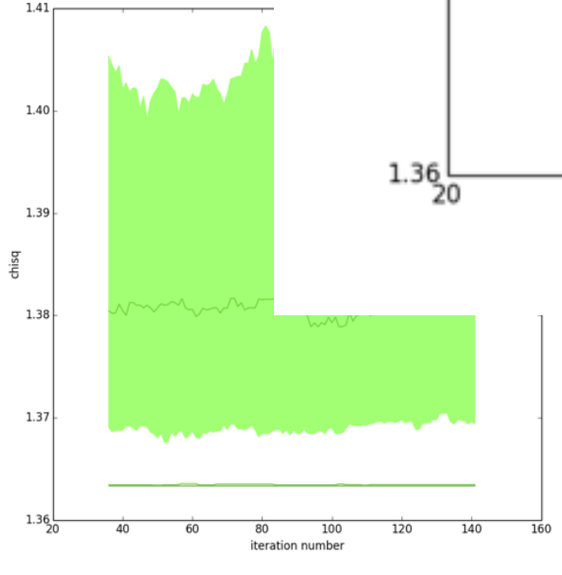


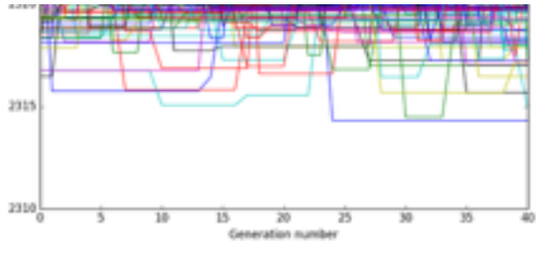
Fitting Algorithms

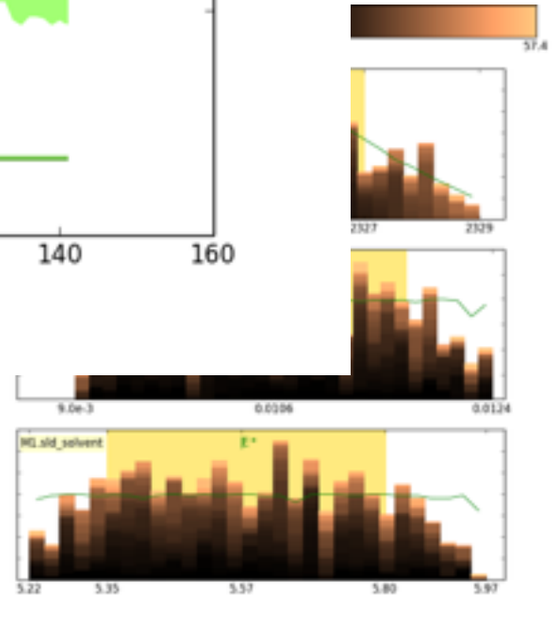












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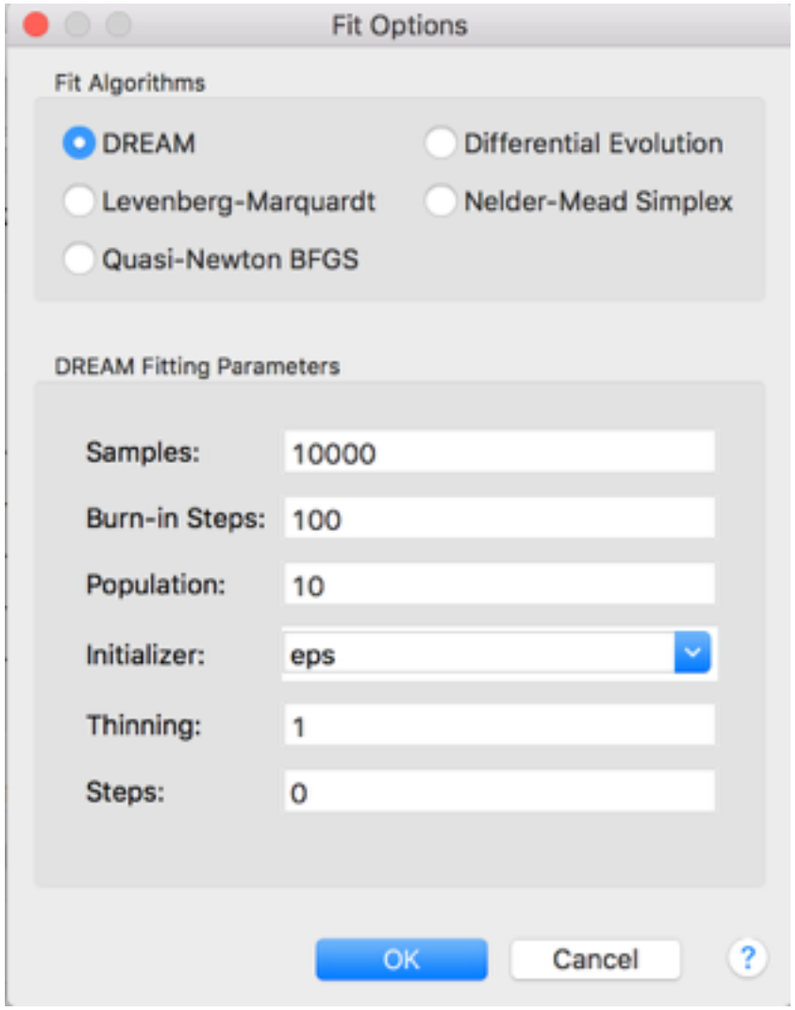

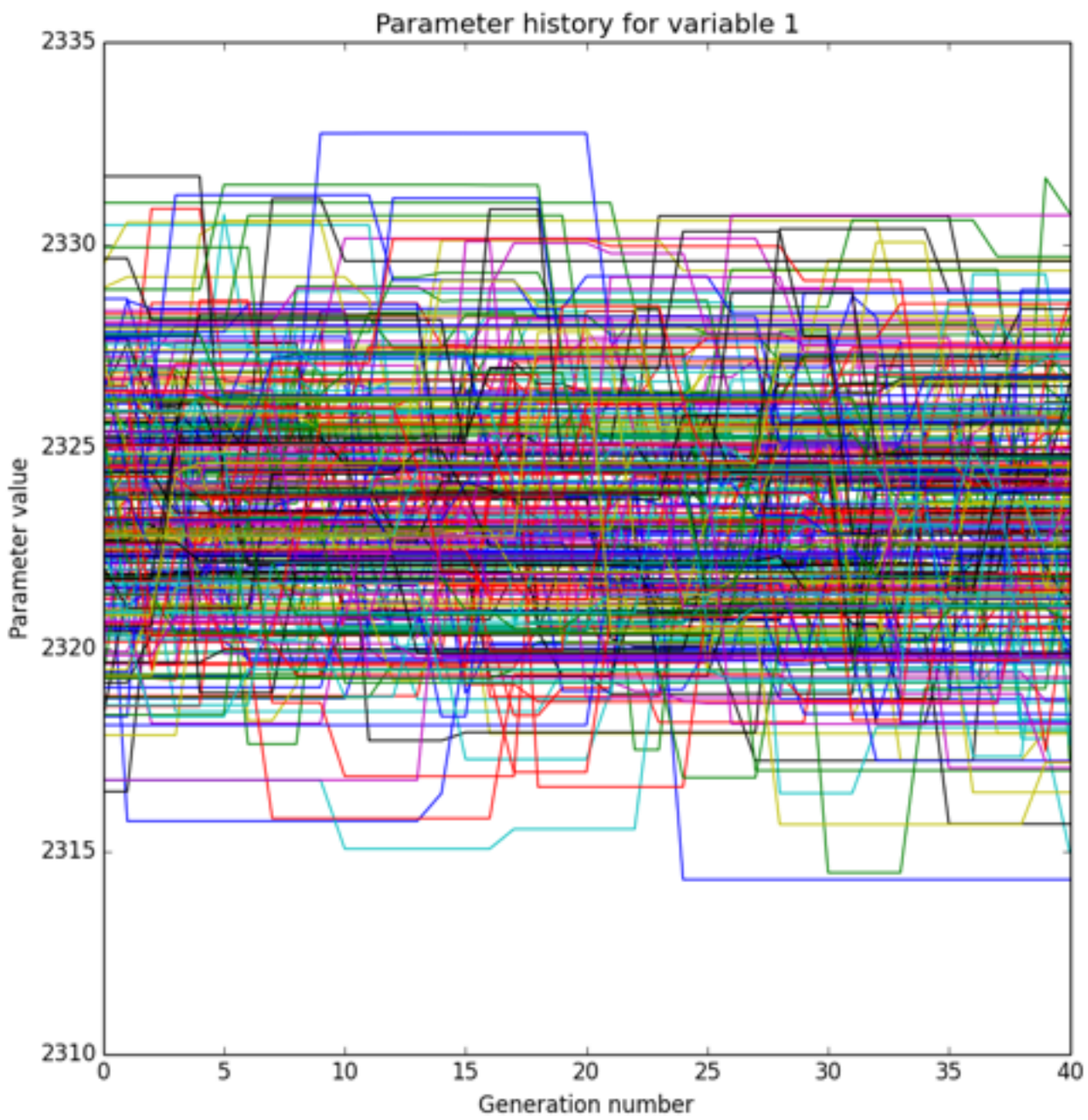

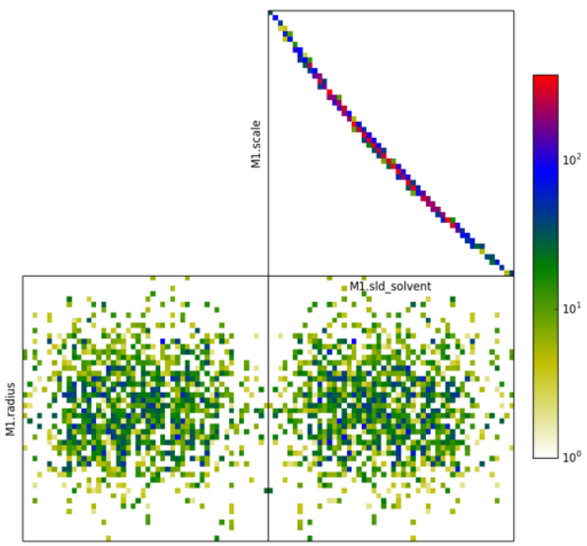

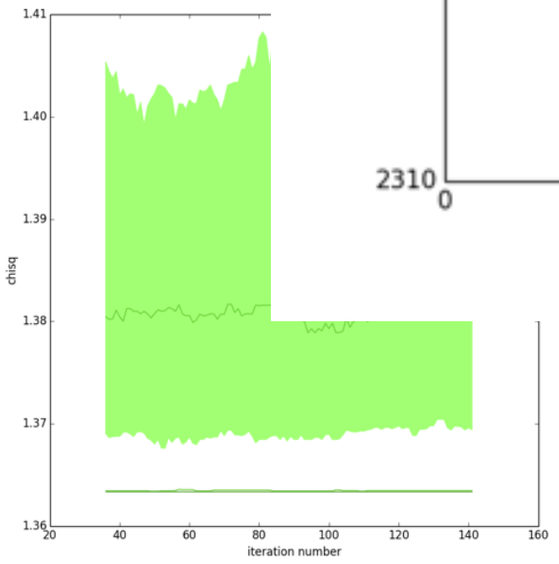

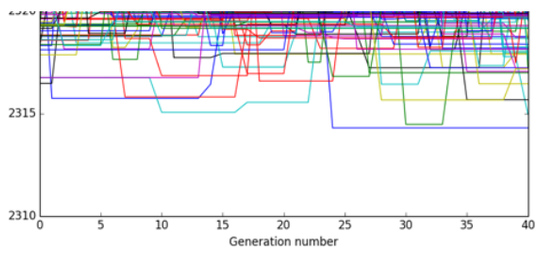

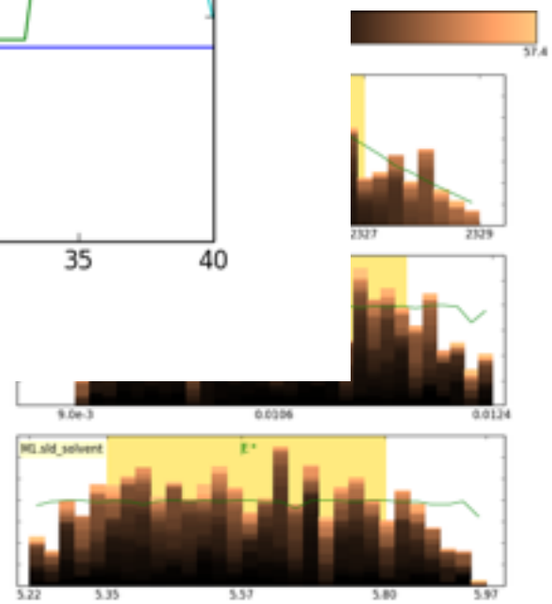

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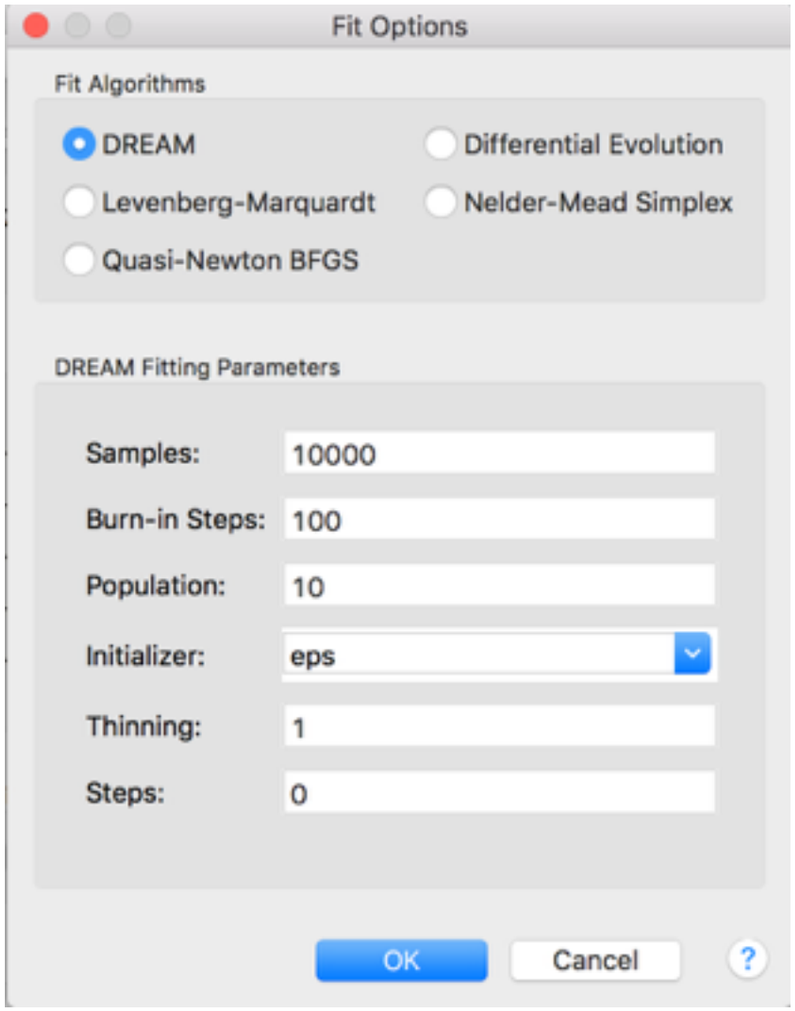
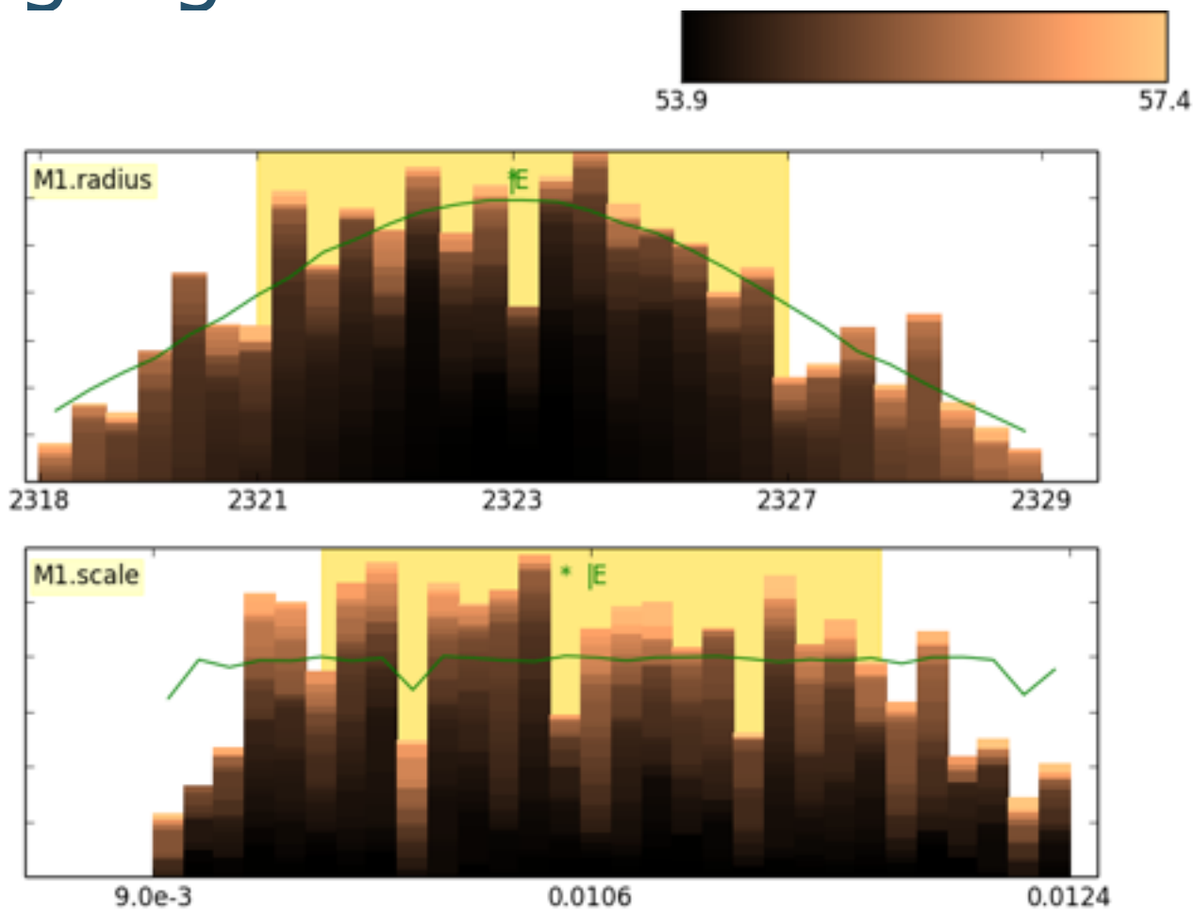
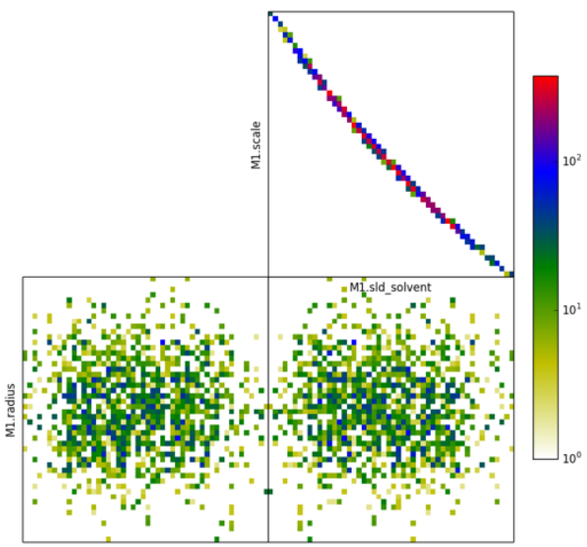
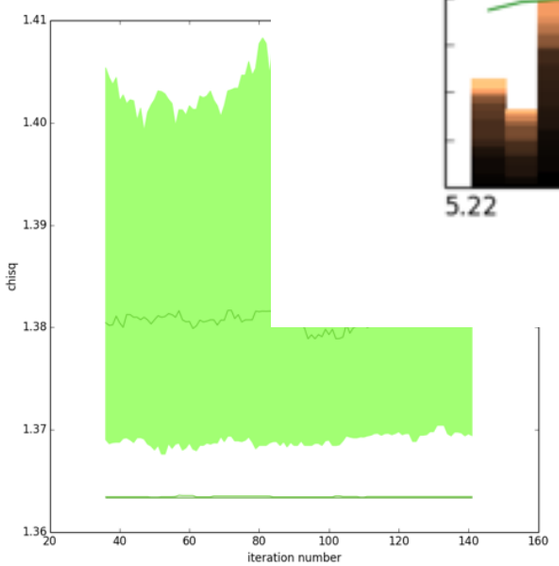
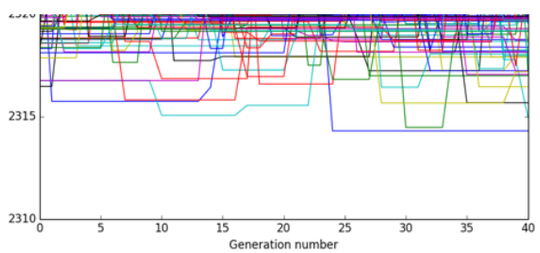
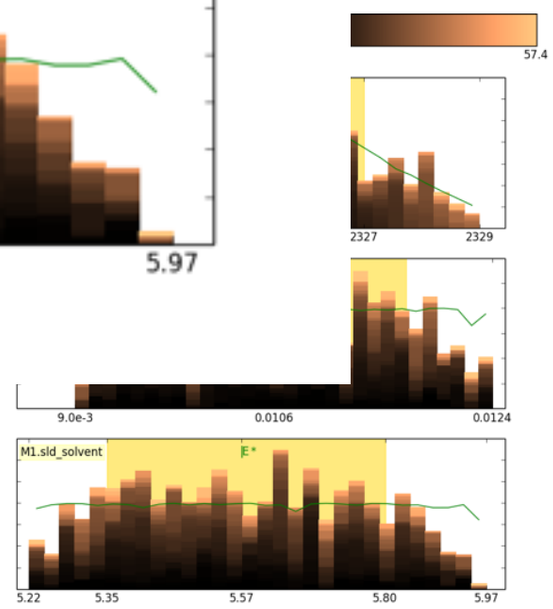






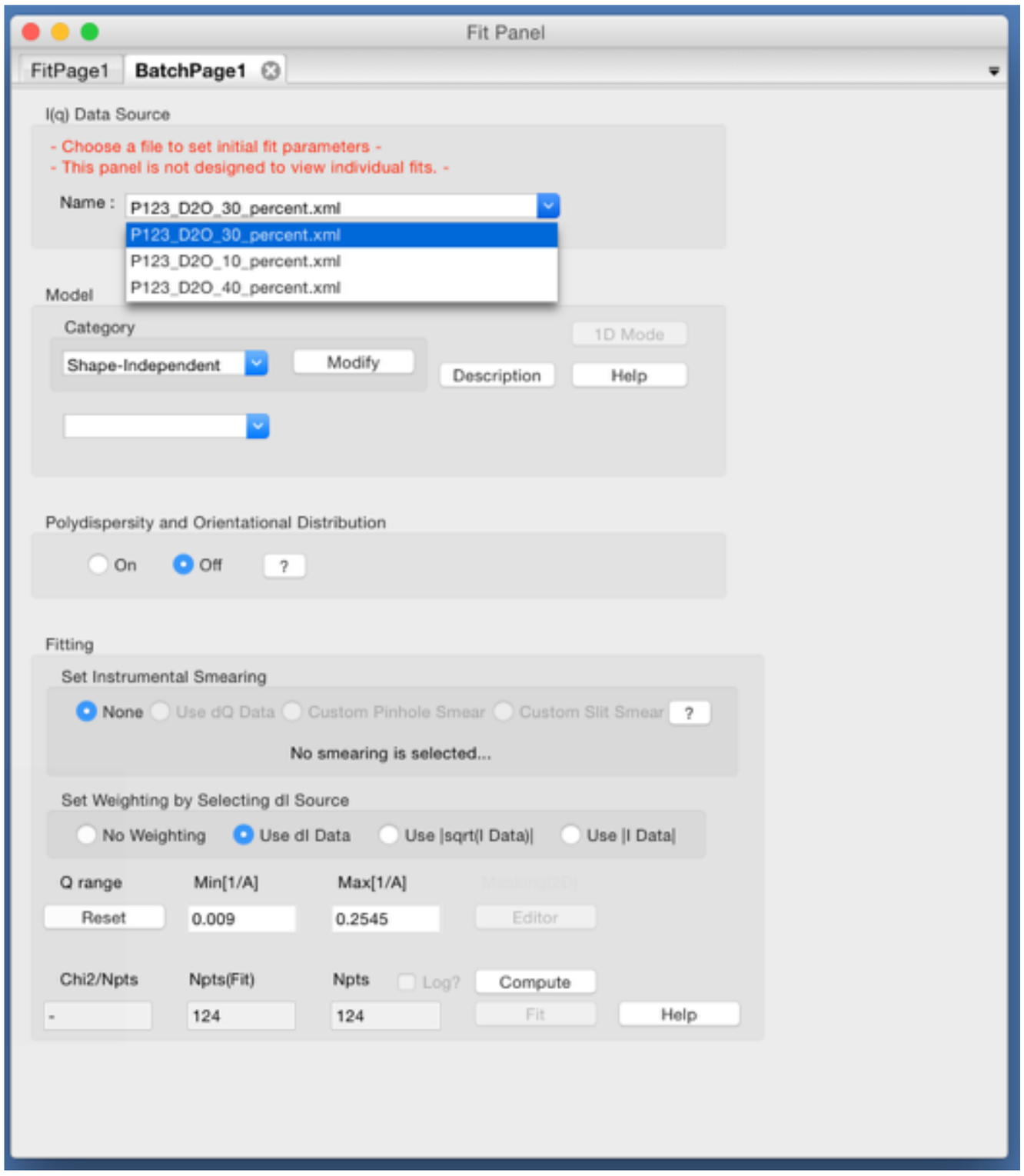






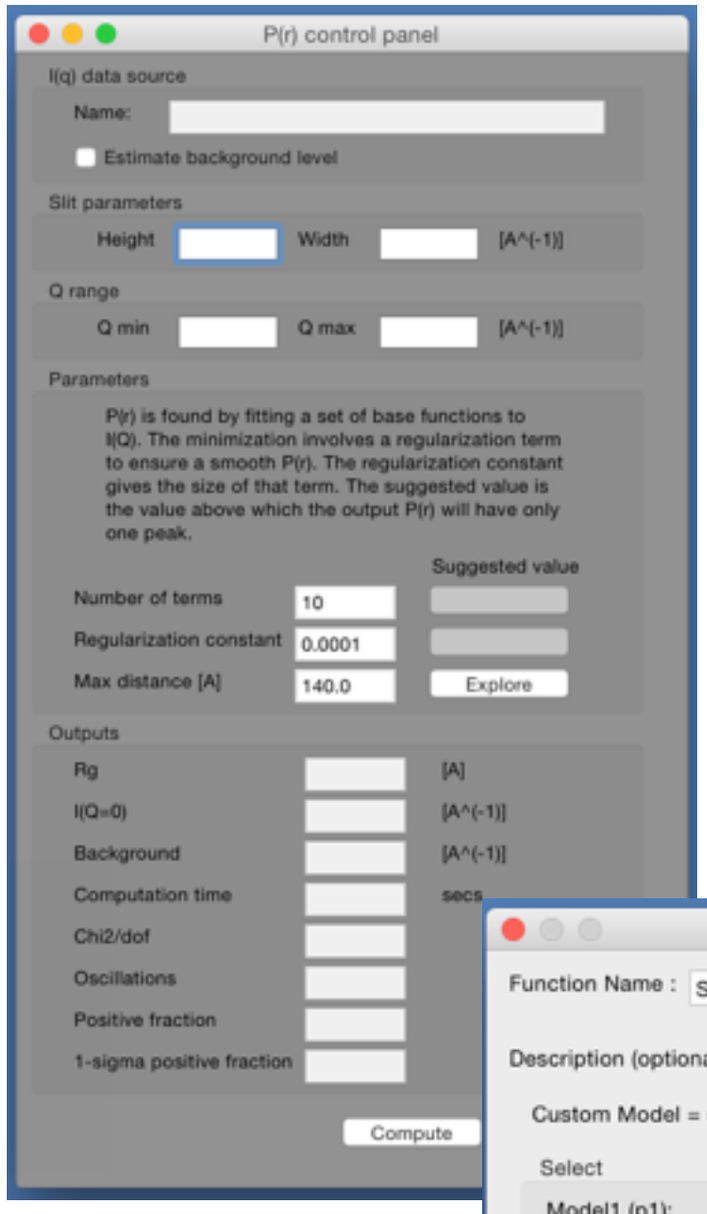
Other Features

Batch fitting …

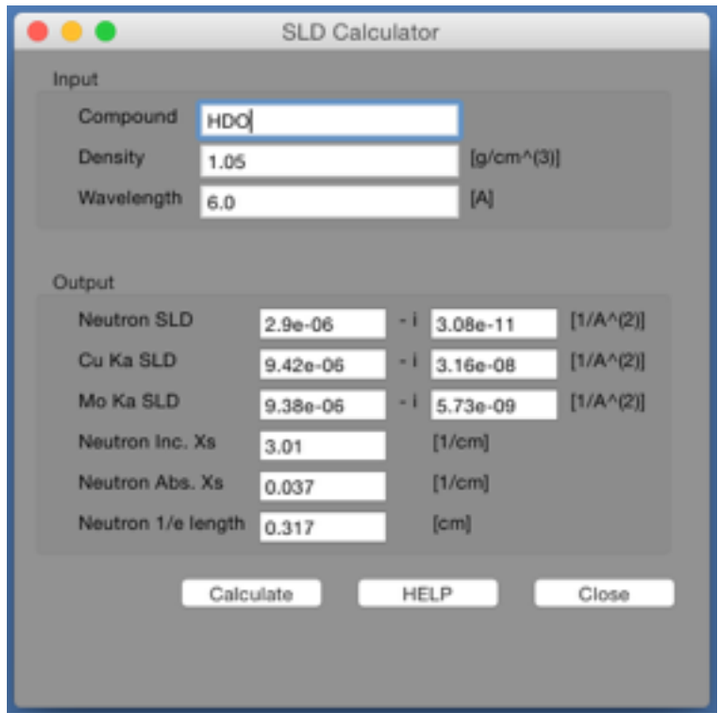


Other Features

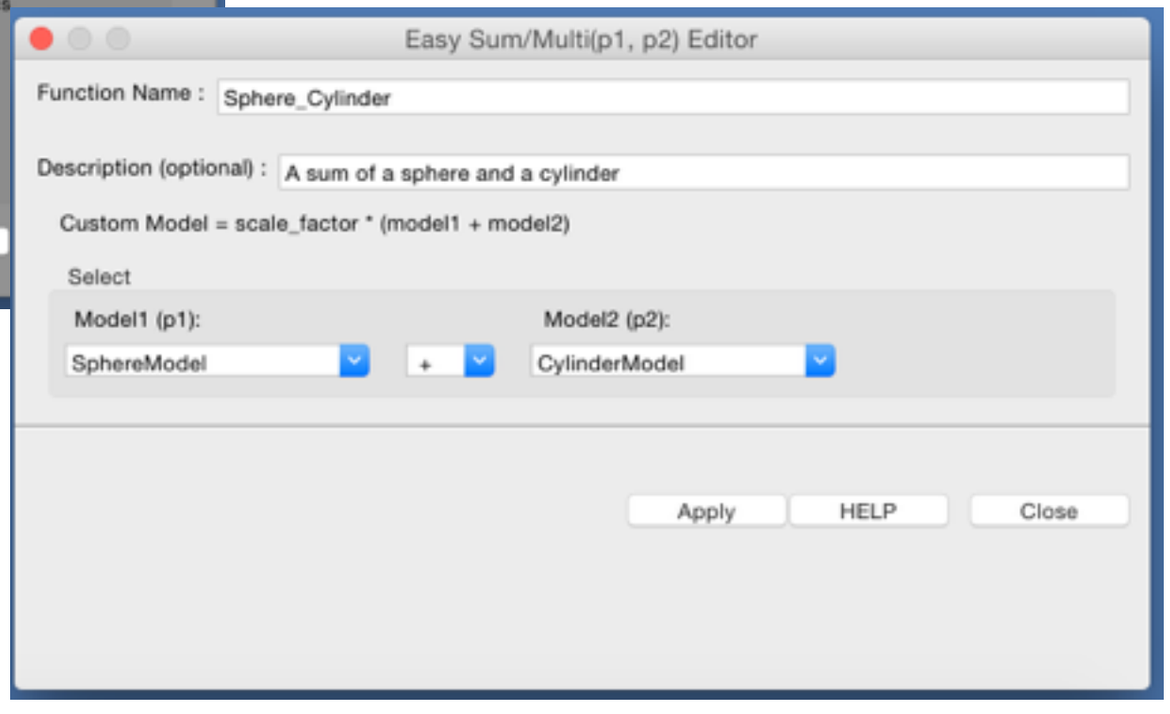
P(r) Inversion …



SLD Calculator …



Sum & Multiplication of Models …



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) = scale * q^(-power) + 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 4.0 is Out!

www.sasview.org

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

SESANS in sasmodels

Automatic transform of SANS model to P(z)

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

Return F(q) from models

Beta approximation

Coherent sums

Multi-GPU support

Documentation

Tutorials

Manual

Future ...

And much more!
See Roadmap and Tickets

Contributions Needed
All skill sets welcome
Models
Testing
Documentation
Admin and Infrastructure

Questions?