



EUROPEAN
SPALLATION
SOURCE



SasView : A Small Angle Scattering Analysis Software Package

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



Science & Technology Facilities Council
ISIS

NIST

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



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

The screenshot shows the Trac web interface for SasView. The top navigation bar includes links for Wiki, Timeline, Roadmap, Browse Source, View Tickets (selected), New Ticket, Search, Admin, and Tags. Below the navigation bar, there's a section for "(3) Active Tickets by Milestone" with a search bar and a "Max items per page" dropdown set to 100. The main content area displays a table of tickets, categorized by milestone. The first table is for "Milestone Admin Tasks" and the second is for "Milestone SasView 4.1.0". Both tables have columns for Ticket, Summary, Component, Version, Type, Owner, Status, and Created.

Ticket	Summary	Component	Version	Type	Owner	Status	Created
#219	easy developer setup	SasView		task	Parker	new	2014-04-01
#299	write SasView Paper	SasView		task	new	2015-02-01	
#239	Need to verify UTK vs. Caltech license ownership	SasView		defect	butler	new	2014-04-05
#328	Create SasView organization and resolve ownership issues	SasView		defect	new	2015-02-15	
#699	Push new documentation to the website	SasView		defect	ajj	new	2016-10-05
#246	Fix problem with with dire install warnings from OS	SasView		task	new	2014-04-19	
#483	Create web page / section with list of publications using SasView.	SasView		task	new	2015-11-24	
#211	Reorganize users on daniel.chem.utk.edu	SasView		enhancement	butler	assigned	2014-03-30
#303	Integrate user and developer websites	SasView		enhancement	new	2015-02-12	
#304	Migrate mailing lists away from sourceforge	SasView		task	new	2015-02-12	
#362	Need to write trac wiki page of all services and locations etc	SasView		task	new	2015-02-22	
#494	Assure that the Qt licensing model is valid for SasView	SasView		task	new	2016-01-12	

Ticket	Summary	Component	Version	Type	Owner	Status	Created	
#426	Update scipy to 0.18.0	SasView		defect	wojciech	assigned	2016-08-23	
#585	Fix data upload to marketplace	SasView		defect	ajj	accepted	2016-10-04	
#583	Merge corfunc branch	SasView		task	ajj	accepted	2016-10-04	
#584	Merge file converter branch	SasView		task	ajj	accepted	2016-10-04	
#590	Update acknowledgement text in local_config.py when corfunc branch is merged	SasView		task	smk78	new	2016-10-04	
#591	Generate Zenodo DOI for 4.1 release when ready	SasView		task	ajj	accepted	2016-10-04	
#189	Save Project doesn't save state of simultaneous fit panel	SasView		defect	kryzys	accepted	2013-06-23	
#548	Remove MultiplicationModel.py once replacement from Sasmodels is available	SasView		defect	pkienle	assigned	2016-03-23	
#553	be_polyelectrolyte model docs	SasView		defect	richardh	new	2016-03-22	
#593	suspicious code in sasview 3.x rpa.cc	SasView		defect	butler	accepted	2016-07-18	
#524	custom models reloaded too often	SasView		defect	new	2016-08-19		
#639	Math not rendered without network connection (Windows)	SasView		defect	ajj	assigned	2016-08-30	
#653	SasView crashing when computer sleeps.	SasView		defect	new	2016-09-08		
#696	Investigate core shell bicelle model	SasView		defect	richardh	new	2016-10-05	
#422	Enhance help (non model) documentation	SasView		task	smk78	new	2015-06-05	
#240	Fix License.txt	SasView		defect	butler	assigned	2014-04-05	
#387	Need new tutorial documentation	SasView		defect	smk78	assigned	2015-03-22	
#415	Save Project and Save Analysis don't open on double clicking	SasView		defect	new	2015-05-12		
#535	Change category management to load from models rather than default json file	SasView		defect	new	2016-03-18		
#576	updated custom models not being recompiled	SasView		defect	wojciech	assigned	2016-05-20	
#589	Need to provide at least one custom model in plugins directory	SasView		defect	new	2016-07-04		
#597	Need to document Combine Batch Fit	SasView		defect	new	2016-07-24		
#638	Instrumental smearing not set automatically based on data	SasView		defect	new	2016-08-30		
#652	Logging is broken when "error while determining build number" is emitted	SasView		defect	wojciech	assigned	2016-09-08	
#663	errors in sasview.log from structure factor	SasView		defect	new	2016-09-21		
#665	opend wrong for long kernels	SasView		defect	new	2016-09-23		
#670	allow multiple array dispersity parameters	SasView		defect	new	2016-09-28		
#674	custom model name and id must be the same	SasView		defect	new	2016-09-29		
#680	Write/enhance model writing documentation	sasmodels		defect	new	2016-10-04		
#681	Package dependencies	SasView		defect	new	2016-10-04		
#700	Add ANSTO logo to website footer	SasView		defect	smk78	new	2016-10-05	

Hosted by UT

Automated Builds build.sasview.org

The screenshot shows the Jenkins web interface for SasView. The top navigation bar includes links for People, Build History, and a search bar. Below the navigation bar, there's a section for "Build Queue" and "Build Executor Status". The main content area displays a table of builds, categorized by build type. The table has columns for S, W, Name, Last Success, Last Failure, and Last Duration. The builds are listed in a table with alternating blue and white rows.

S	W	Name	Last Success	Last Failure	Last Duration
●	☀	bumps_Ubuntu14.04_test	2 mo 0 days - #185	N/A	37 sec
●	☀	Periodictable-Ubuntu14.04_test	6 mo 22 days - #9	N/A	3.7 sec
●	☀	RefId_Ubuntu14.04_test	1 mo 12 days - #141	N/A	1 min 19 sec
●	☀	sasmodels_Ubuntu14.04_test	1 day 2 hr - #548	4 days 9 hr - #538	19 sec
●	☀	SasView_OSX10.10	3 hr 37 min - #324	N/A	12 min
●	☀	SasView_OSX10.10_Release	3 days 14 hr - #14	6 mo 0 days - #4	12 min
●	☀	SasView_OSX10.9	4 mo 25 days - #192	N/A	22 min
●	☀	SasView_OSX10.9_Release	6 mo 20 days - #9	6 mo 20 days - #9	12 min
●	☀	SasView_Ubuntu14.10	3 hr 45 min - #448	N/A	2 min 4 sec
●	☀	SasView_Win7	3 hr 14 min - #502	4 days 2 hr - #508	15 min
●	☀	SasView_Win7_Release	3 days 14 hr - #19	6 mo 20 days - #2	13 min
●	☀	SasView_Win7_Test	9 days 13 hr - #56	1 mo 18 days - #41	22 min

Hosted by ESS

Current Development Team

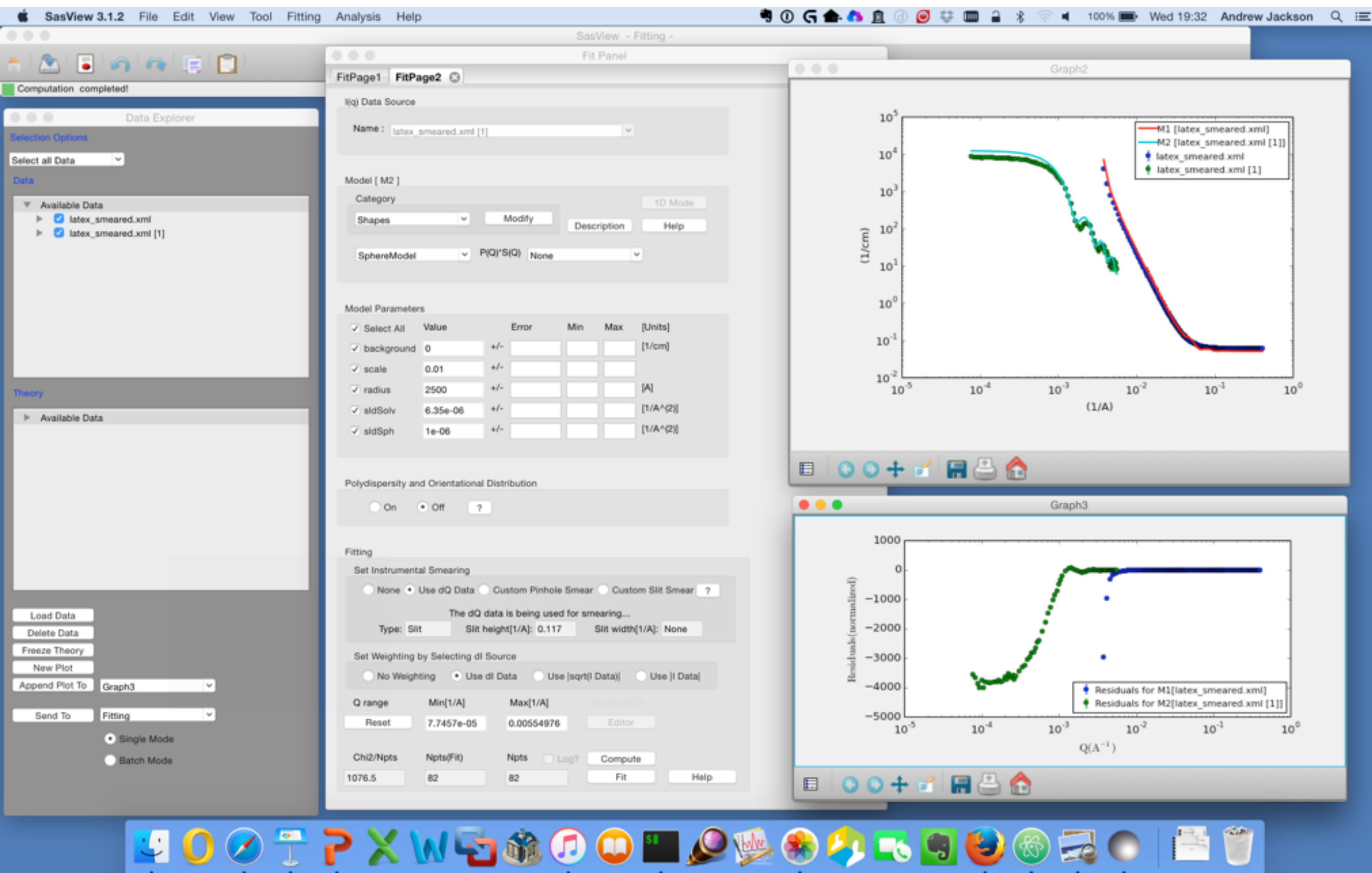
- Paul Butler (NIST)
- Mathieu Doucet (ORNL)
- Andrew Jackson (ESS)
- Steve King (ISIS)



- 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



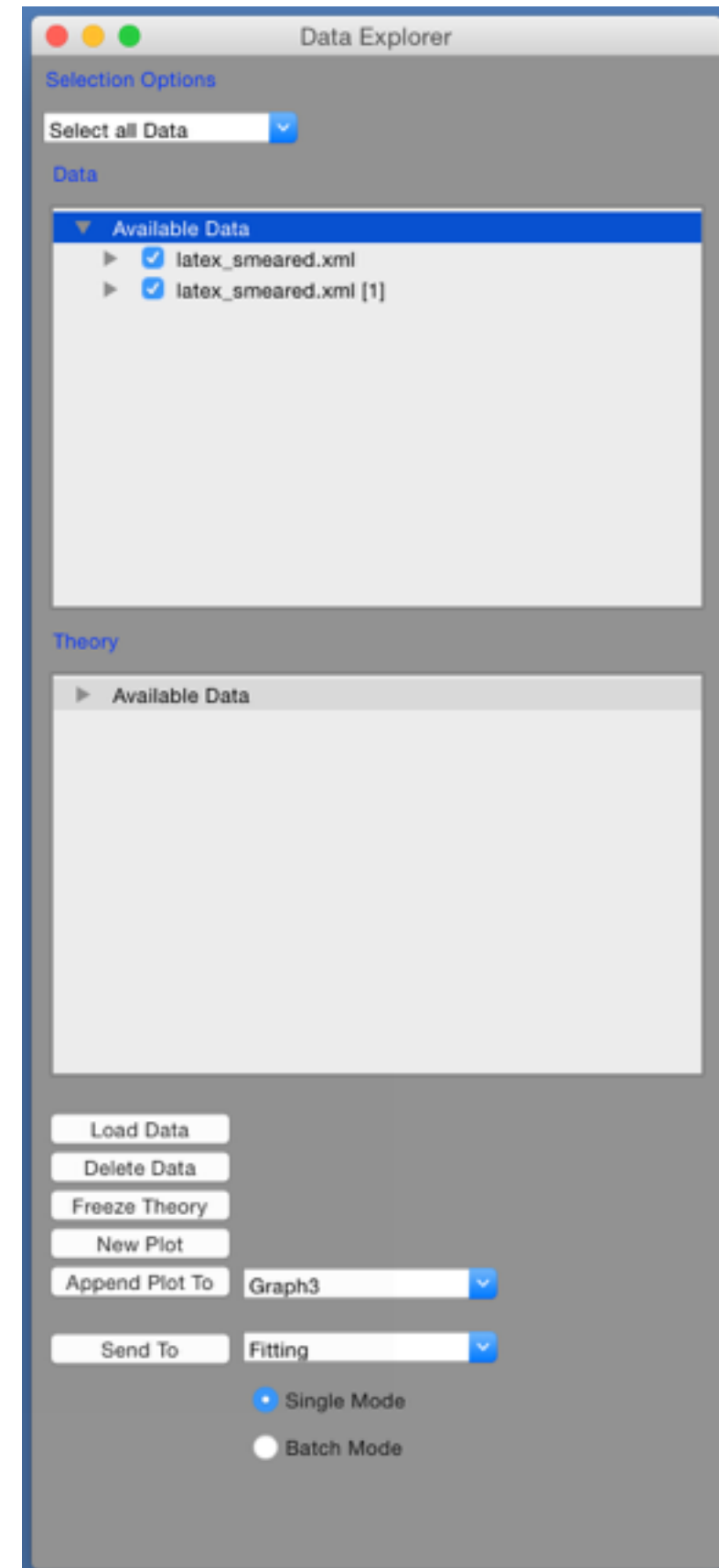
1D Analysis

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 Description Help

SphereModel

Model Parameters

<input checked="" type="checkbox"/> 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 dI Source

☐ No Weighting ☒ Use dI Data ☐ Use |sqrt(I Data)| ☐ Use |I Data|

Q range Min[1/Å] Max[1/Å] Masking(Q)

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 ...



Fit Panel

FitPage1 FitPage2

I(q) Data Source

Name: latex_smeared.xml [1]

Model [M2]

Category: Shapes

SphereModel None

Model Parameters

<input checked="" type="checkbox"/> 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 dI Source

☐ No Weighting ☒ Use dI Data ☐ Use |sqrt(I Data)| ☐ Use |I Data|

Q range Min[1/Å] Max[1/Å]

7.7457e-05 0.00554976

Chi2/Npts Npts(Fit) Npts ☐ Log?

1076.5 82 82

1D Analysis

Send to fitting ...

Select a model ...

Set parameters ...

Use resolution ...

The screenshot shows the 'Fit Panel' window with the following sections:

- I(q) Data Source:** Name: latex_smeared.xml [1]
- Model [M2]:** Category: Shapes, Modify, Description, Help. Model: SphereModel, P(Q)*S(Q), None.
- Model Parameters:** A table with columns: Select All, Value, Error, Min, Max, [Units].

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 dI Source: No Weighting ☐ Use dI Data ☒ Use |sqrt(I Data)| ☐ Use |I Data| ☐. Q range: Min[1/Å]: 7.7457e-05, Max[1/Å]: 0.00554976, Masking(Q): Editor. Chi2/Npts: 1076.5, Npts(Fit): 82, Npts: 82, Log? ☐ Compute, Fit, Help.

1D Analysis

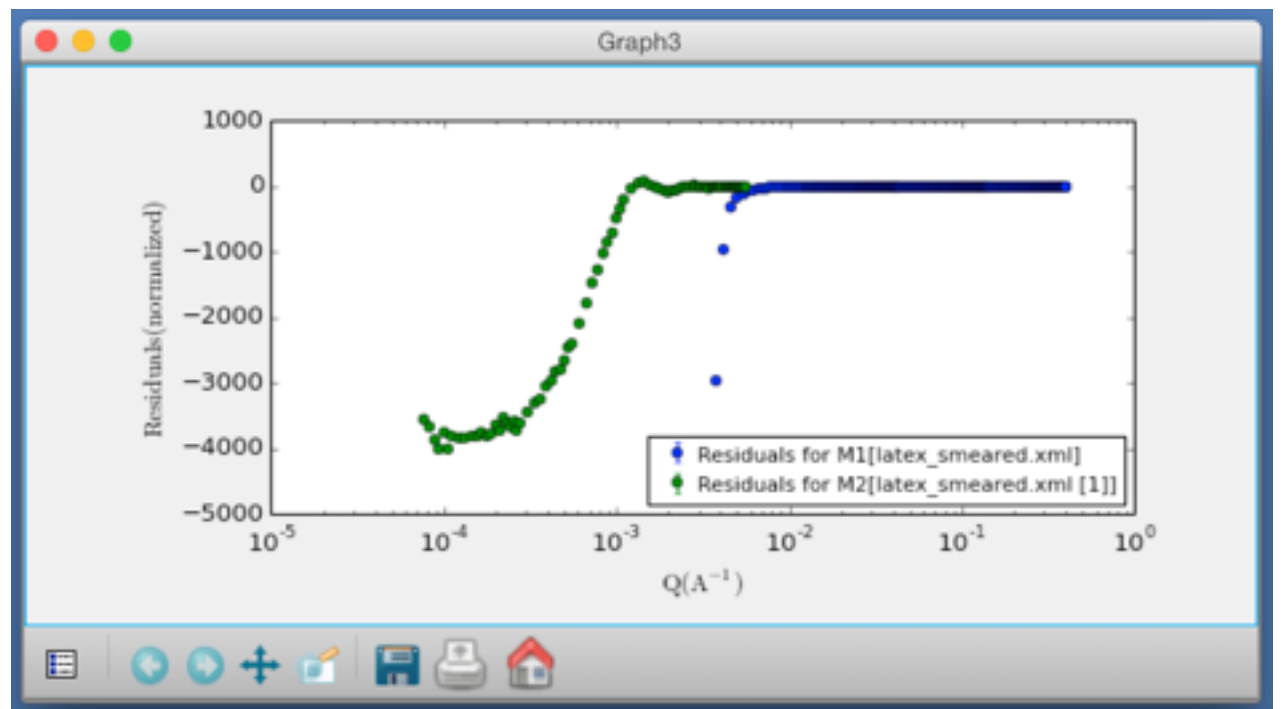
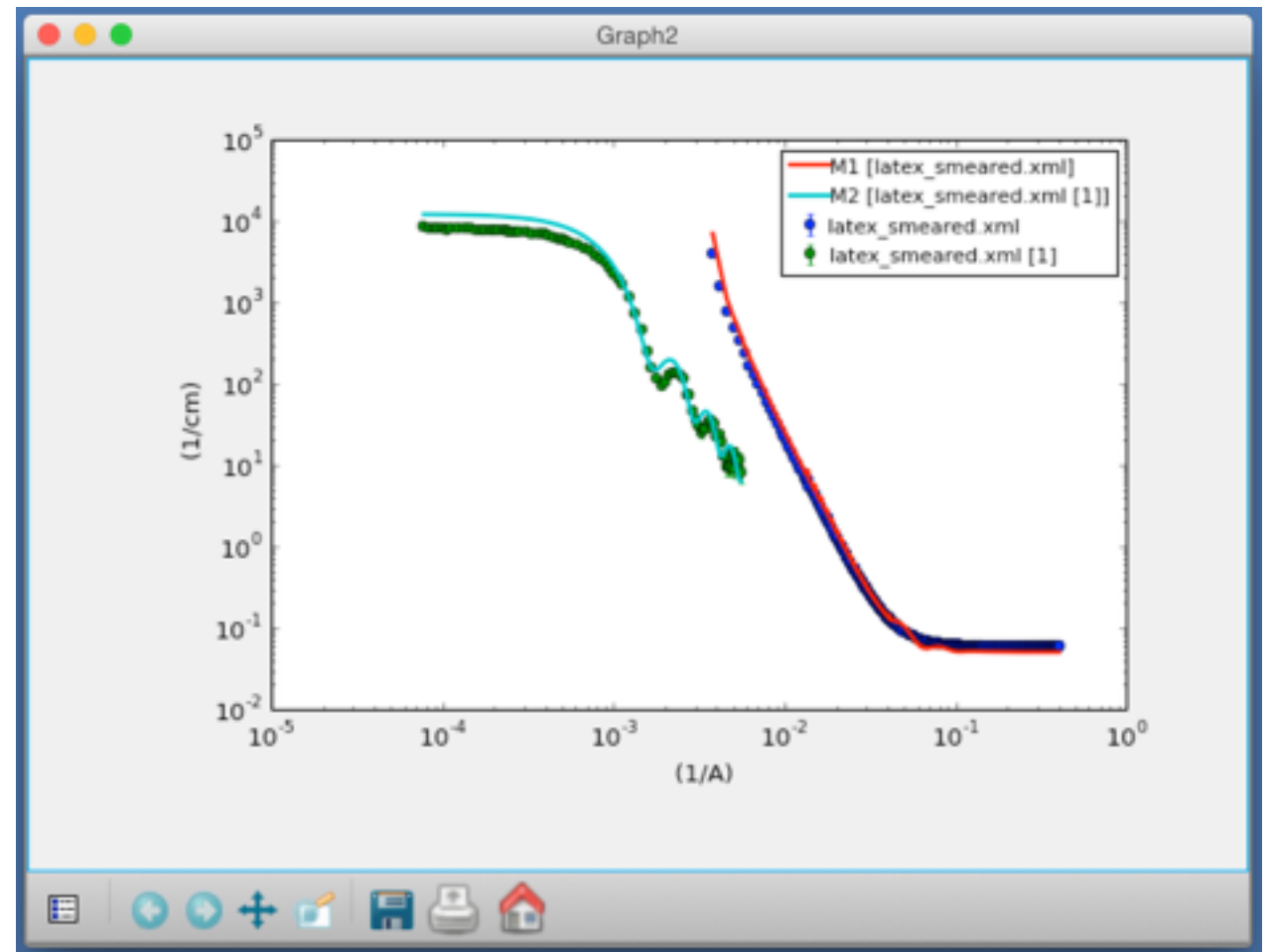
Send to fitting ...

Select a model ...

Set parameters ...

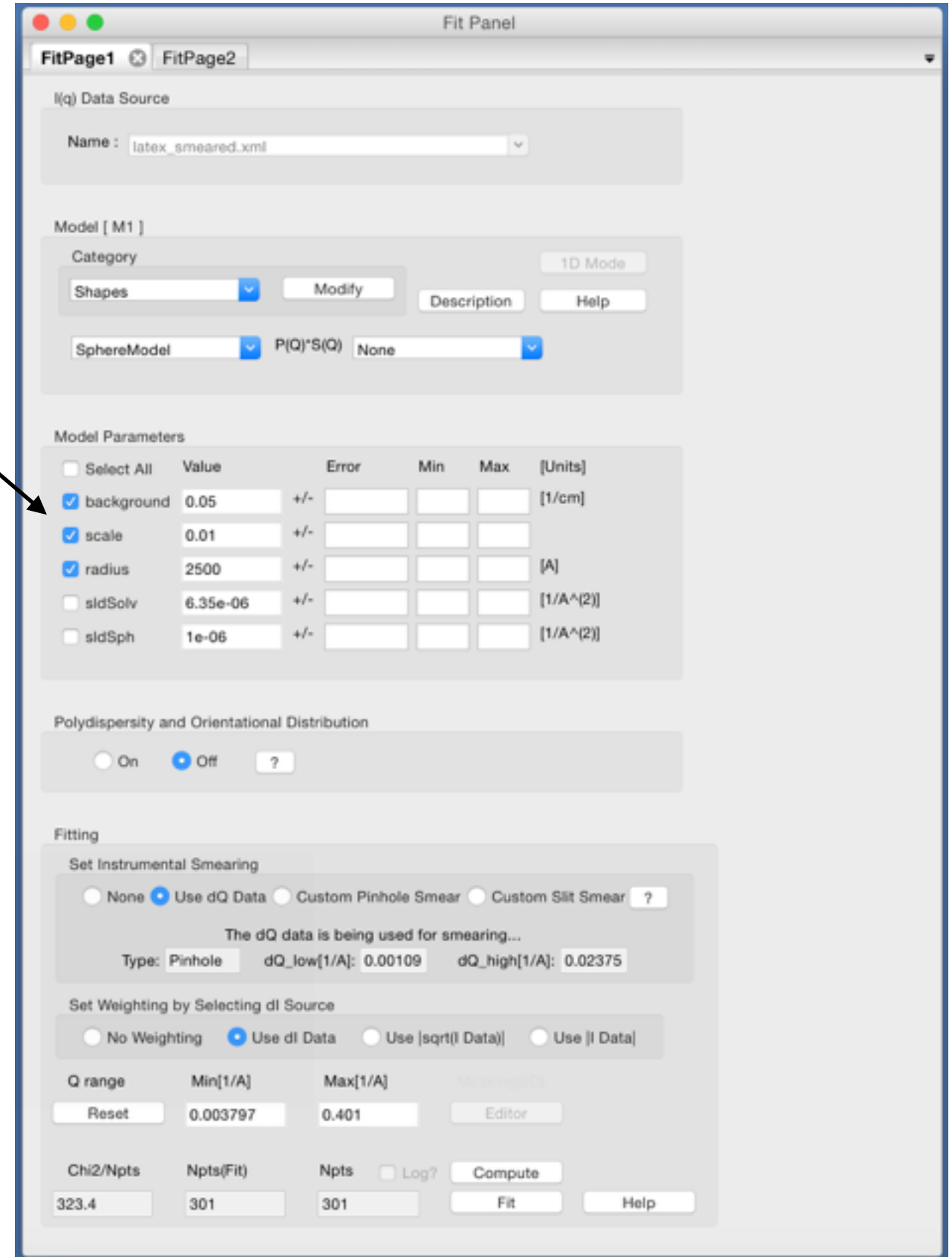
Use resolution ...

How does it look?



1D Analysis

Choose which parameters to fit ...



The screenshot shows the 'Fit Panel' window with the following sections:

- l(q) Data Source:** Name: latex_smeared.xml
- Model [M1]:** Category: Shapes, 1D Mode button, Modify, Description, Help. SphereModel selected, P(Q)*S(Q) None.
- Model Parameters:** A table with checkboxes for selecting parameters to fit.
- Polydispersity and Orientational Distribution:** On (radio button), Off (radio button), ? (button).
- Fitting:** Set Instrumental Smearing: None (radio button), Use dQ Data (radio button), Custom Pinhole Smear (radio button), Custom Slit Smear (radio button), ? (button). The dQ data is being used for smearing... Type: Pinhole, dQ_low[1/A]: 0.00109, dQ_high[1/A]: 0.02375. Set Weighting by Selecting dI Source: No Weighting (radio button), Use dI Data (radio button), Use |sqrt(I) Data| (radio button), Use |I Data| (radio button). Q range: Reset, Min[1/A]: 0.003797, Max[1/A]: 0.401, Masking(Q): Editor. Chi2/Npts: 323.4, Npts(Fit): 301, Npts: 301, Log? (checkbox), Compute, Fit, Help.

<input type="checkbox"/> Select All	Value	Error	Min	Max	[Units]
<input checked="" type="checkbox"/> background	0.05	+/-			[1/cm]
<input checked="" type="checkbox"/> scale	0.01	+/-			
<input checked="" type="checkbox"/> radius	2500	+/-			[Å]
<input type="checkbox"/> sldSolv	6.35e-06	+/-			[1/Å ²]
<input type="checkbox"/> sldSph	1e-06	+/-			[1/Å ²]

1D Analysis

Choose which parameters to fit ...

... and press the Fit button!

The screenshot shows the 'Fit Panel' window with two tabs: 'FitPage1' and 'FitPage2'. The 'FitPage1' tab is active. The interface includes the following sections:

- I(q) Data Source:** A dropdown menu showing 'latex_smeared.xml'.
- Model [M1]:**
 - Category:** A dropdown menu showing 'Shapes'.
 - Modify:** A button.
 - Description:** A button.
 - Help:** A button.
 - SphereModel:** A dropdown menu.
 - P(Q)*S(Q):** A dropdown menu showing 'None'.
- Model Parameters:** A table with columns: Select All, Value, Error, Min, Max, [Units].

Select All	Value	Error	Min	Max	[Units]
<input checked="" type="checkbox"/>	background	0.05	+/-		[1/cm]
<input checked="" type="checkbox"/>	scale	0.01	+/-		
<input checked="" type="checkbox"/>	radius	2500	+/-		[Å]
<input type="checkbox"/>	sldSolv	6.35e-06	+/-		[1/Å ²]
<input type="checkbox"/>	sldSph	1e-06	+/-		[1/Å ²]
- Polydispersity and Orientational Distribution:** Radio buttons for 'On', 'Off' (selected), and '?'. A '?' button is also present.
- Fitting:**
 - Set Instrumental Smearing:** Radio buttons for 'None', 'Use dQ Data' (selected), 'Custom Pinhole Smear', and 'Custom Slit Smear'. A '?' button is also present.
 - The dQ data is being used for smearing...**
 - Type:** Pinhole
 - dQ_low[1/Å]:** 0.00109
 - dQ_high[1/Å]:** 0.02375
 - Set Weighting by Selecting dI Source:** Radio buttons for 'No Weighting', 'Use dI Data' (selected), 'Use [sqrt(I) Data]', and 'Use |I Data|'.
 - Q range:** Min[1/Å] (0.003797), Max[1/Å] (0.401), and a 'Reset' button.
 - Chi2/Npts:** 323.4
 - Npts(Fit):** 301
 - Npts:** 301
 - Compute:** A button highlighted with a red box.
 - Fit:** A button.
 - Help:** A button.

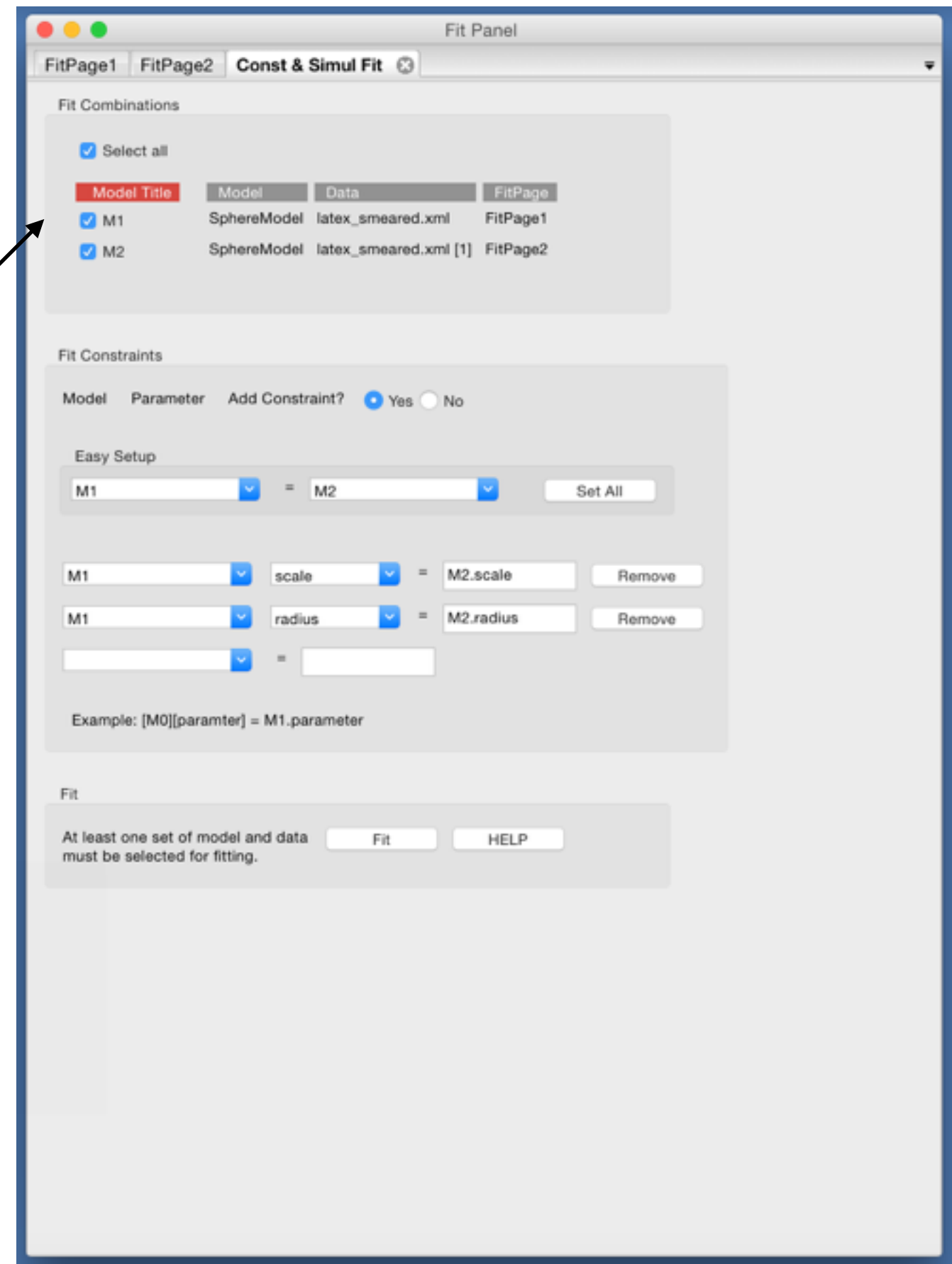
Constraints / Simultaneous Fit

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 ...

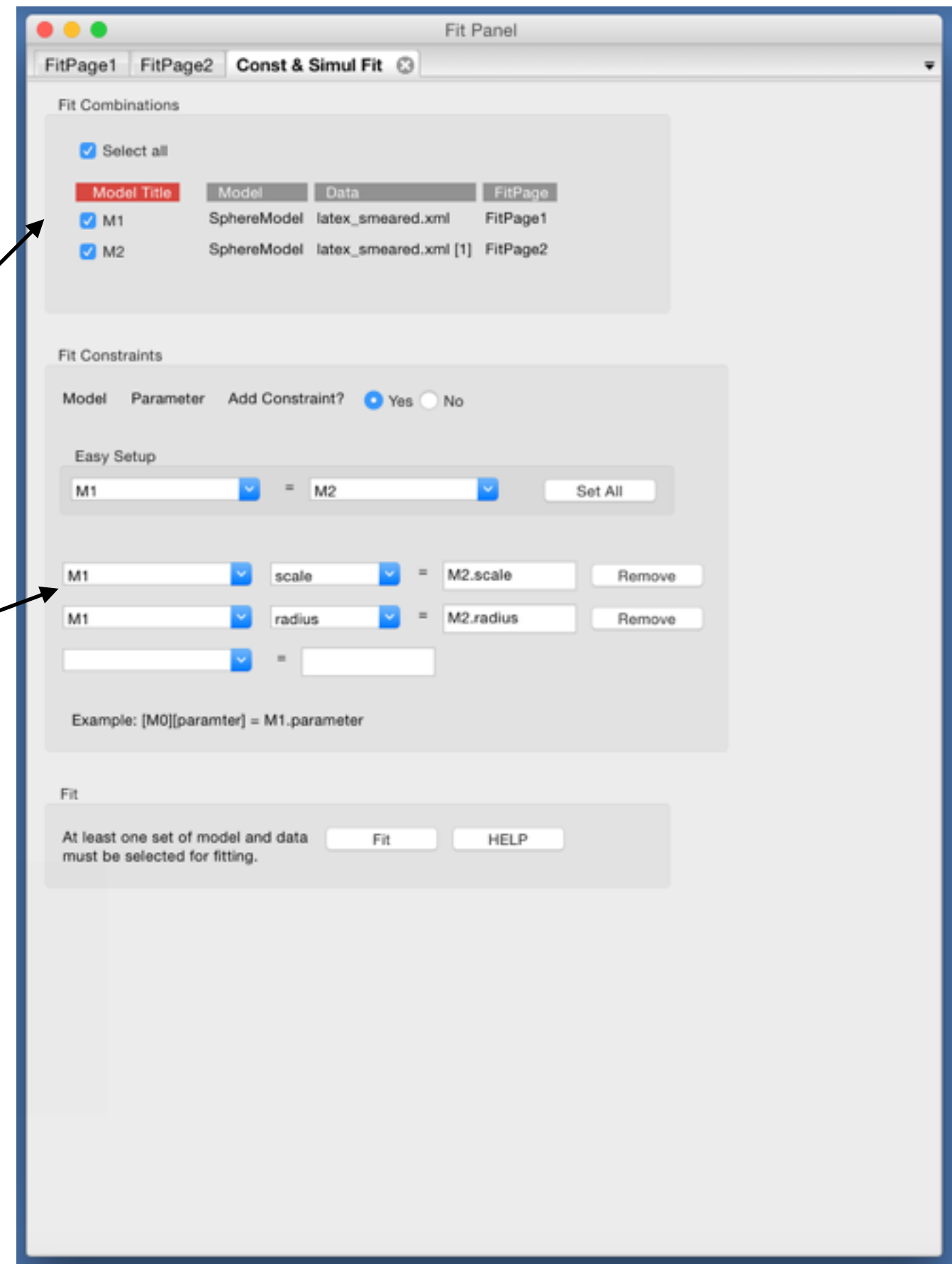


Constraints / Simultaneous Fit

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

Set up a simultaneous fit ...

... with constraints



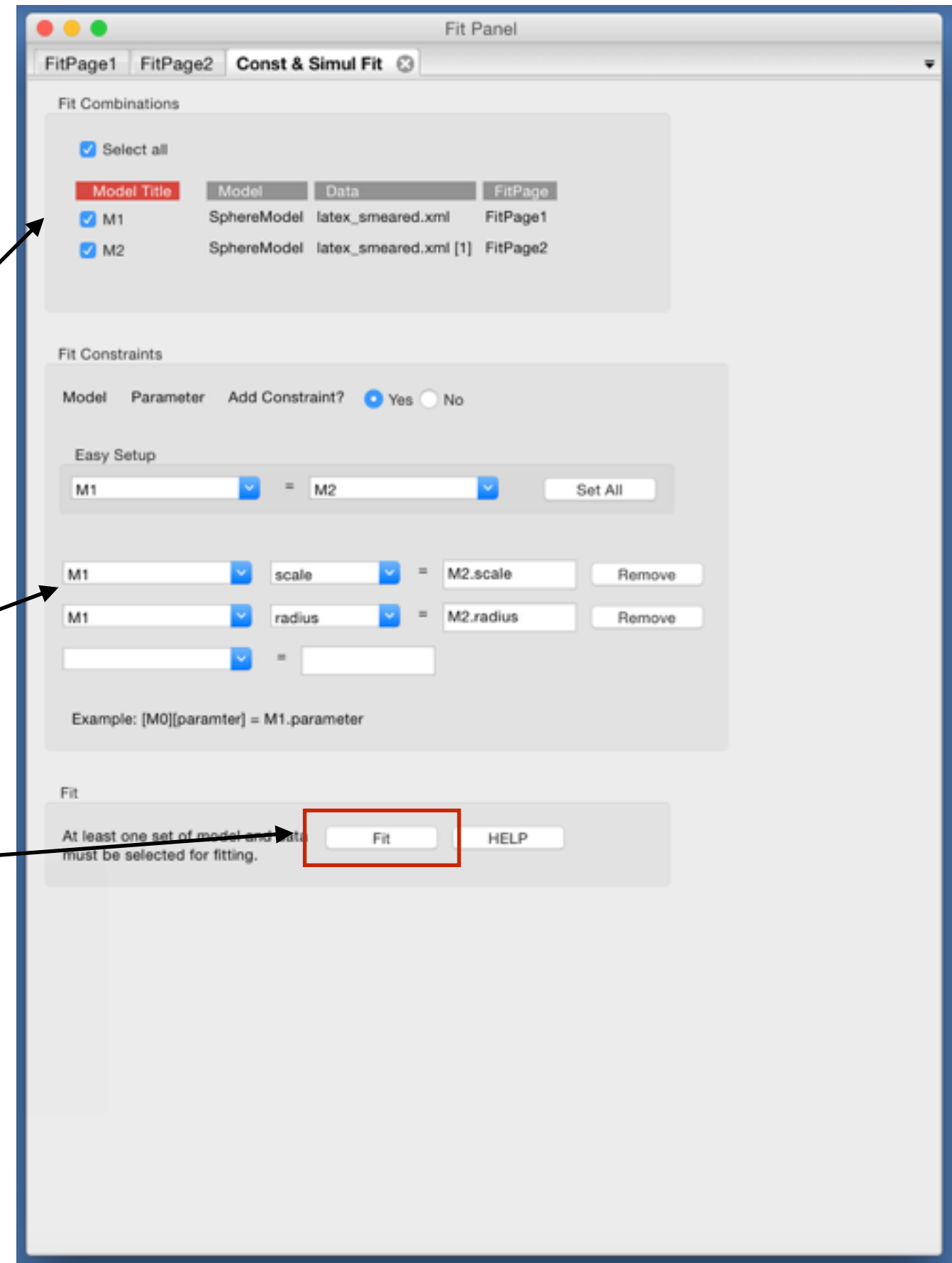
Constraints / Simultaneous Fit

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**

l(q) Data Source

Name: latex_smeared.xml [1]

Model [M2]

Category: Shapes 1D Mode

SphereModel None

Model Parameters

<input type="checkbox"/> Select All	Value	Error	Min	Max	[Units]
<input checked="" type="checkbox"/> background	2.6088	+/- 0.48857			[1/cm]
<input checked="" type="checkbox"/> scale	0.0075699	+/- 6.9289e-06			
<input checked="" type="checkbox"/> radius	2324	+/- 0.32602			[Å]
<input type="checkbox"/> sldSolv	6.35e-06	+/-			[1/Å ²]
<input 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 dI Source

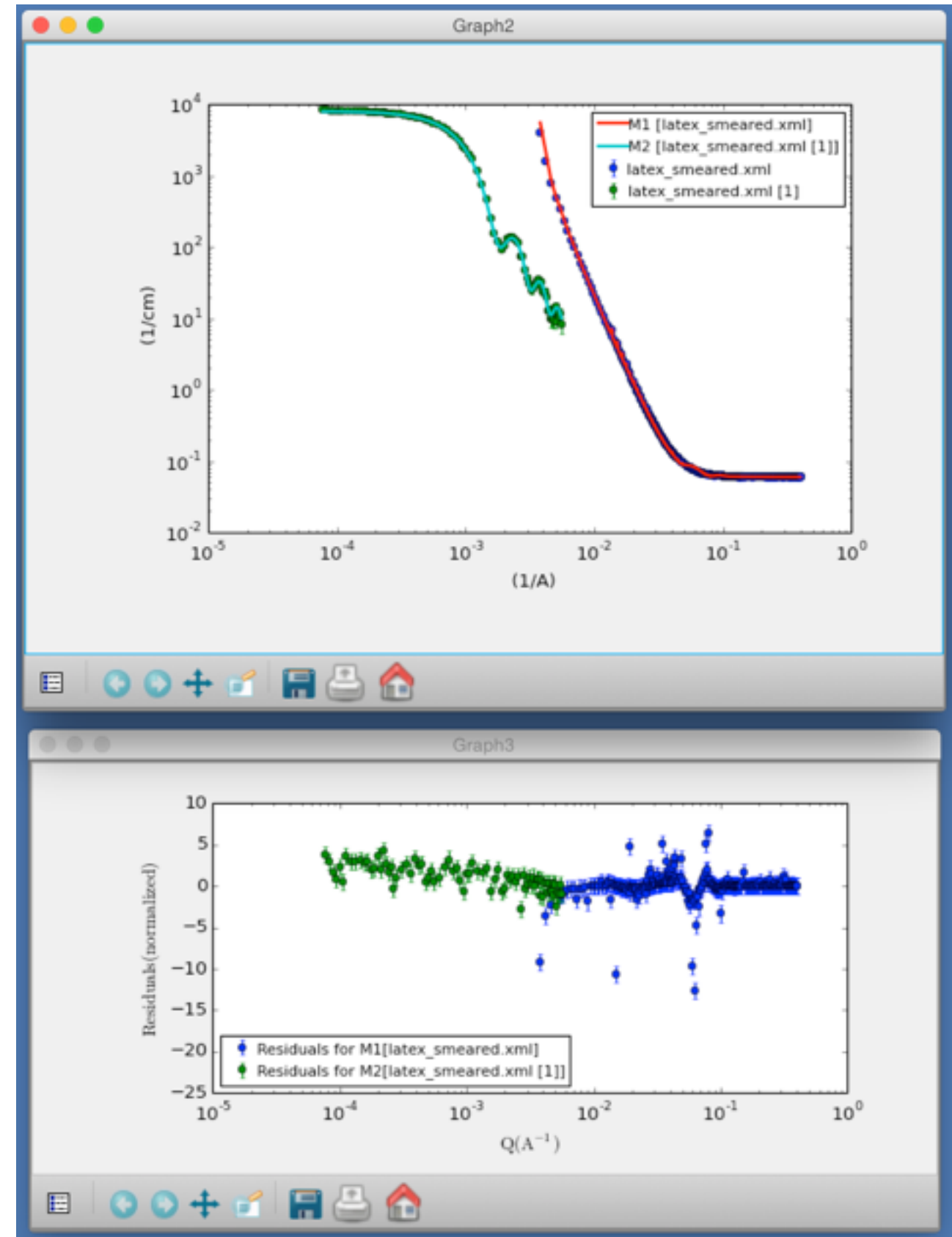
☐ No Weighting ☒ Use dI Data ☐ Use |sqrt(I Data)| ☐ Use |I Data|

Q range Min[1/Å] Max[1/Å]

7.7457e-05 0.00554976

Chi2/Npts Npts(Fit) Npts ☐ Log?

3.5962 82 82



2D Modelling

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

www.rsc.org/softmatter

PAPER

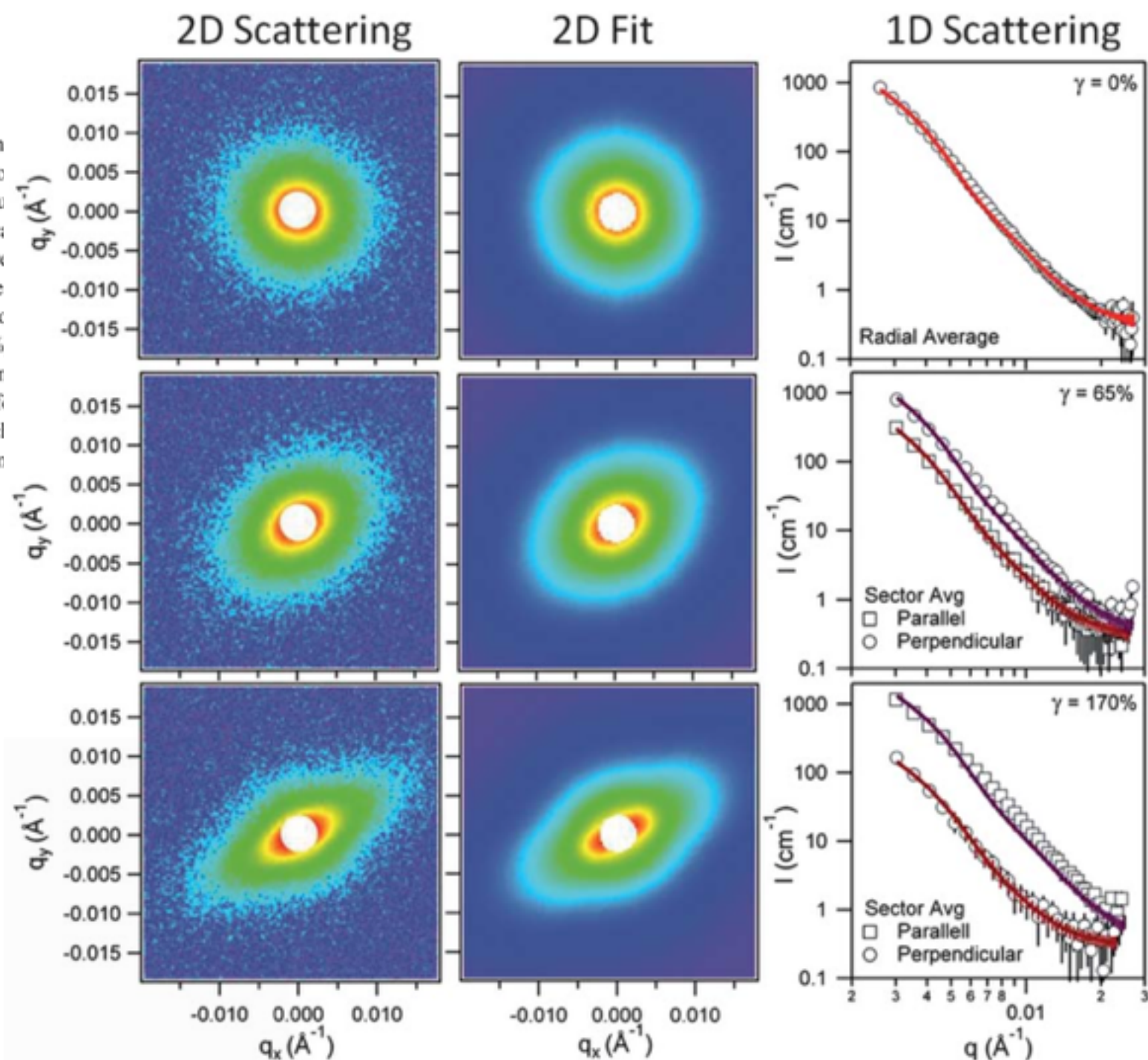
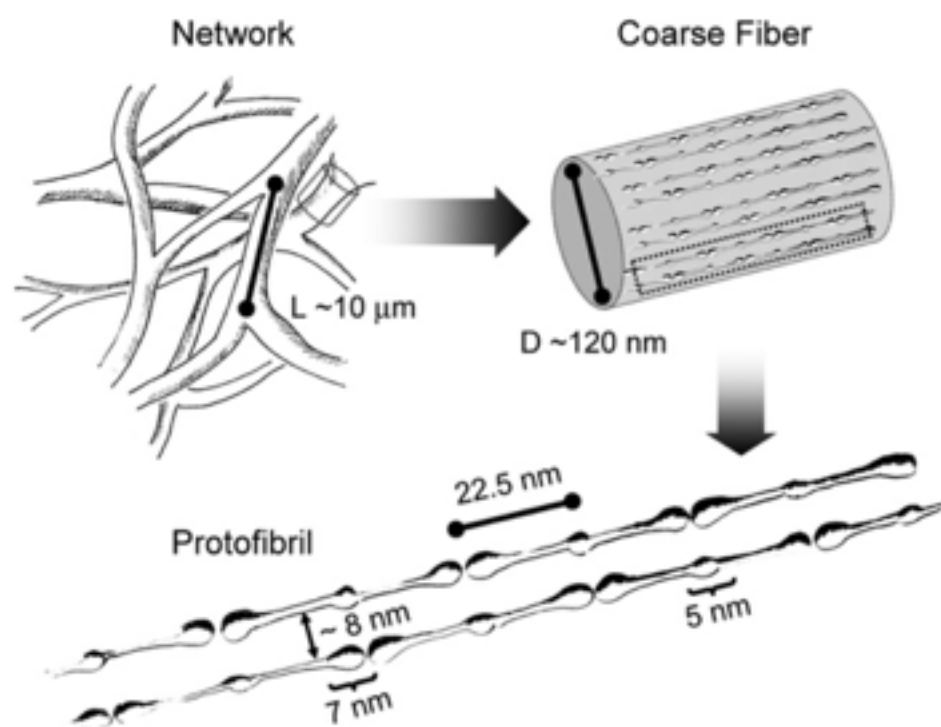
In situ neutron scattering study of structural transitions in fibrin networks under shear deformation

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 hardening response of coarse fibrin networks by directly measuring the structural response of a fibrin gel to deformation. A special Couette shear cell is used to systematically probe the structure of a fibrin clot over strain values in the range of $\gamma = 1$ –170%. The SANS results indicate that the hardening response of coarse fibrin gels occurs in two distinct regions having different mechanical signatures that are separated by an intermediate strain softening regime ($\gamma < 10\%$) where there is a measurable increase in the shear modulus upon the application of strain. At higher strain values ($\gamma > 30\%$) the hardening regime is directly correlated to significant fiber alignment. The mean diameter determined directly from two-dimensional fits to the anisotropic scattering data is found to increase monotonically in the high-strain regime. The results suggest that the non-linear mechanical response of fibrin clots is the result of a reduction of lateral entropic fluctuations at low strain and of fiber alignment at higher strain values.



Fitting Algorithms

Fit Options

Fit Algorithms

☒ DREAM ☐ Differential Evolution

☐ Levenberg-Marquardt ☐ Nelder-Mead Simplex

☐ Quasi-Newton BFGS

DREAM Fitting Parameters

Samples: 10000

Burn-in Steps: 100

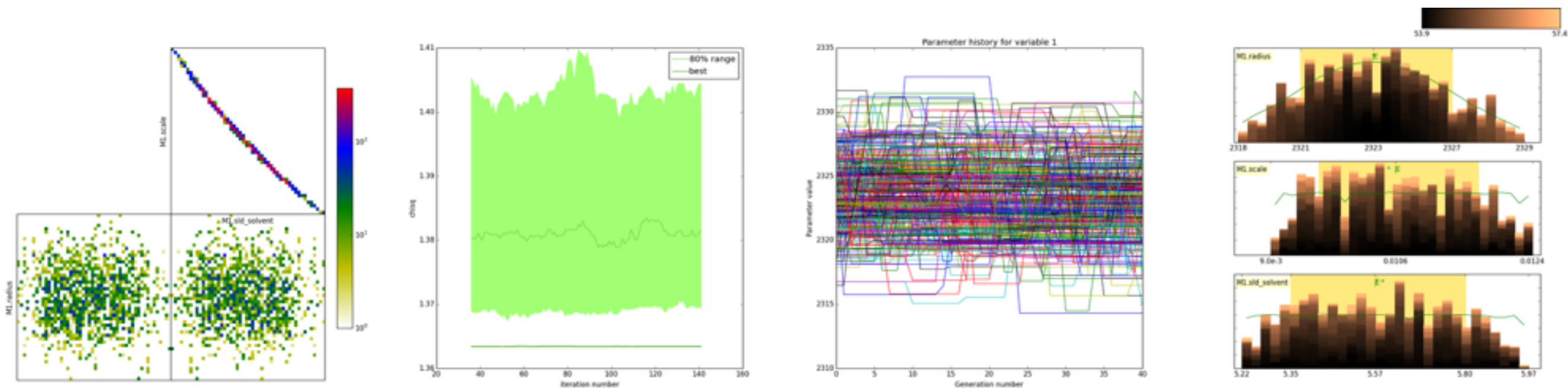
Population: 10

Initializer: eps

Thinning: 1

Steps: 0

OK Cancel ?



Fitting Algorithms

Fit Options

Fit Algorithms

☒ DREAM ☐ Differential Evolution

☐ Levenberg-Marquardt ☐ Nelder-Mead Simplex

☐ Quasi-Newton BFGS

DREAM Fitting Parameters

Samples: 10000

Burn-in Steps: 100

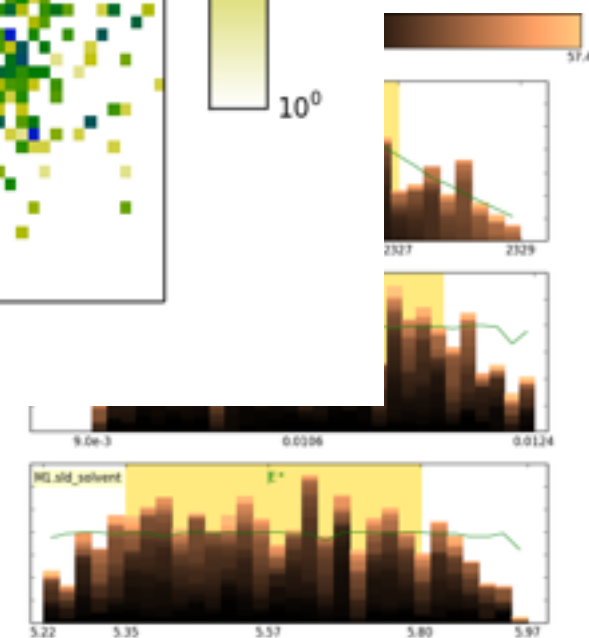
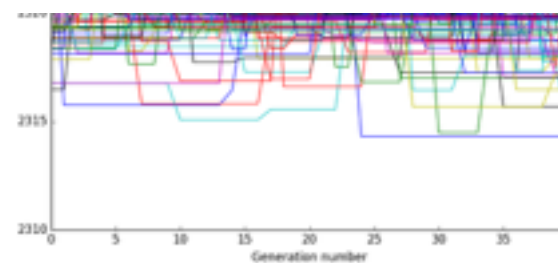
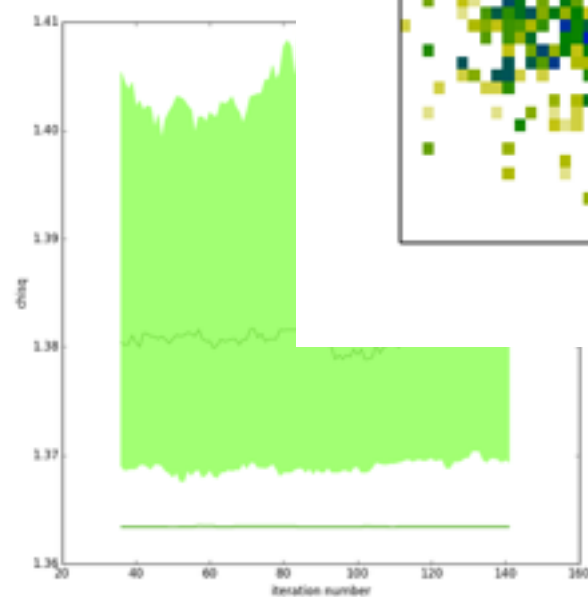
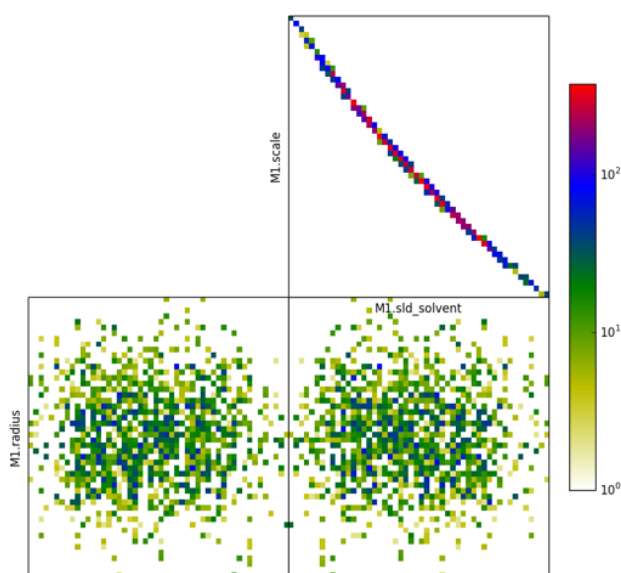
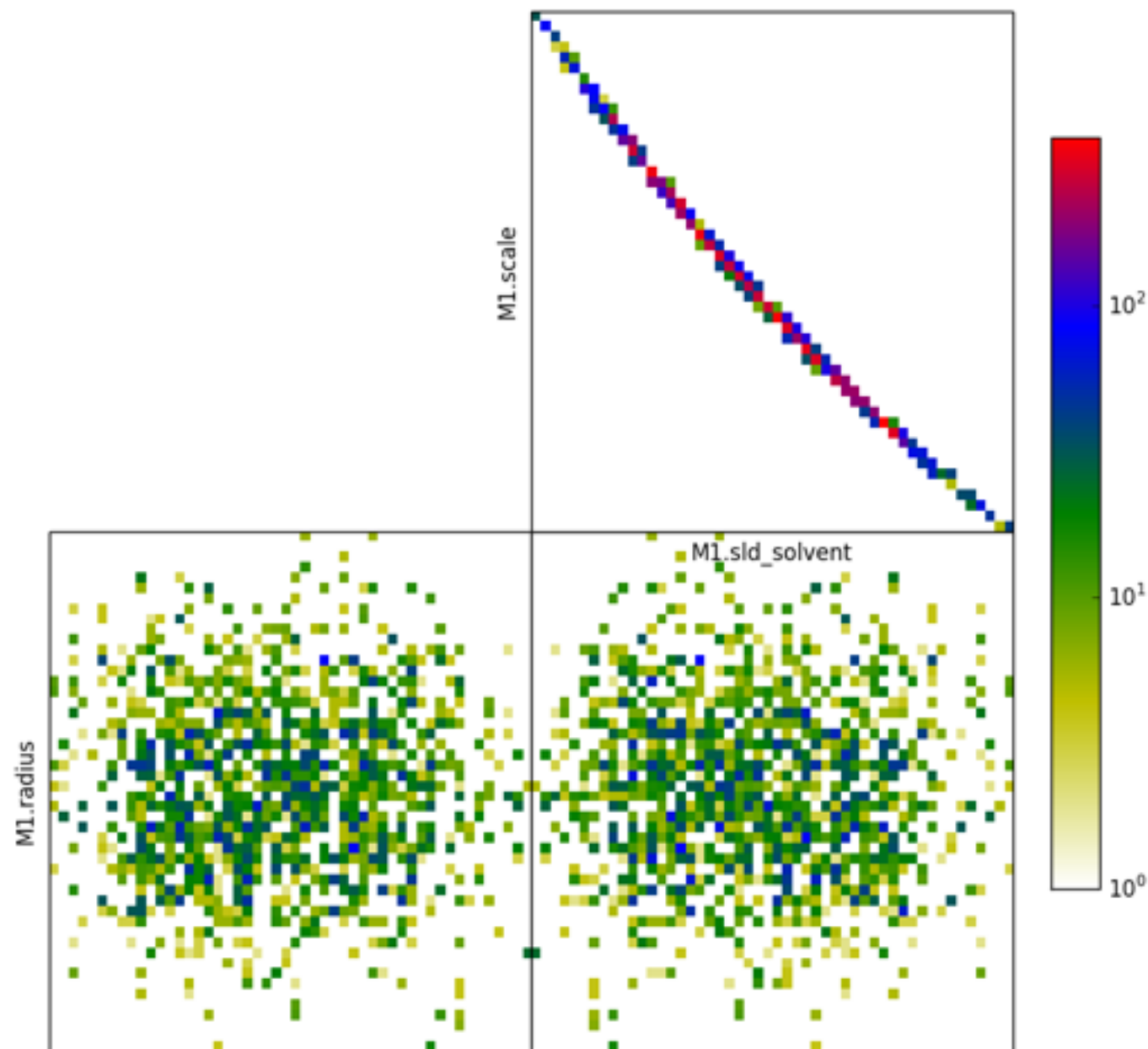
Population: 10

Initializer: eps

Thinning: 1

Steps: 0

OK Cancel ?



Fitting Algorithms

Fit Options

Fit Algorithms

☒ DREAM ☐ Differential Evolution

☐ Levenberg-Marquardt ☐ Nelder-Mead Simplex

☐ Quasi-Newton BFGS

DREAM Fitting Parameters

Samples: 10000

Burn-in Steps: 100

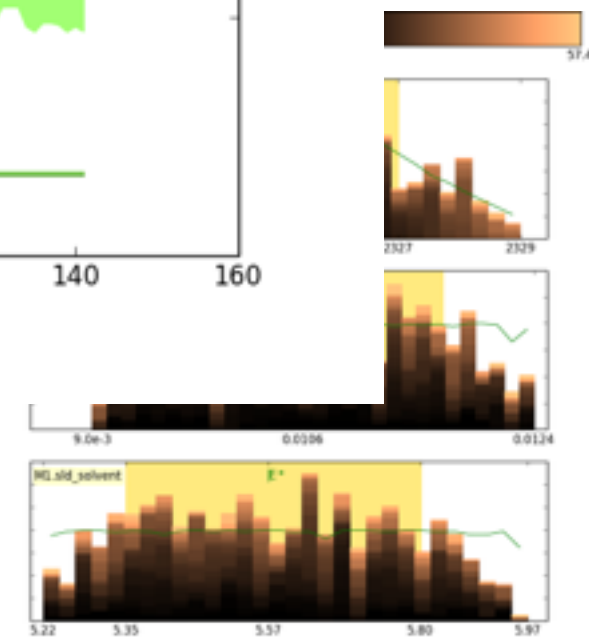
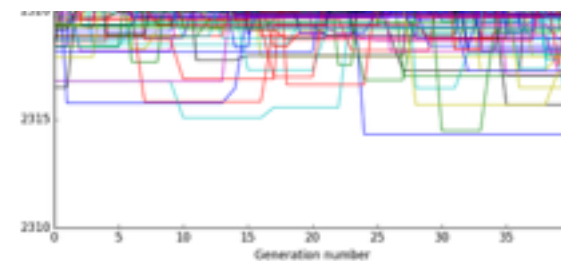
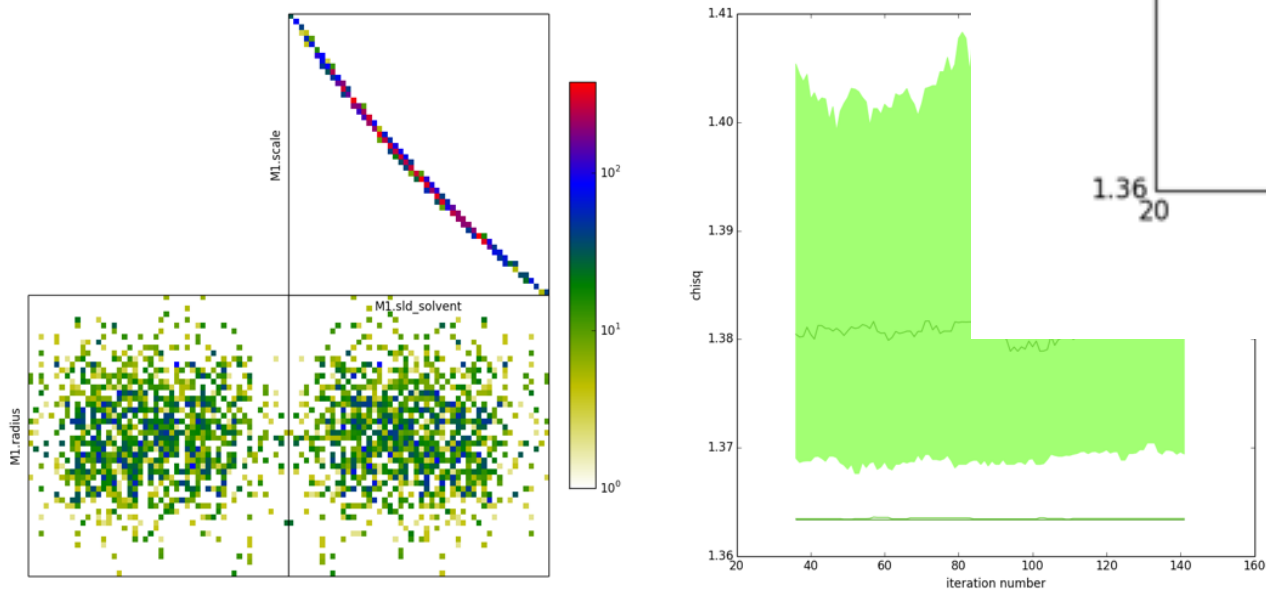
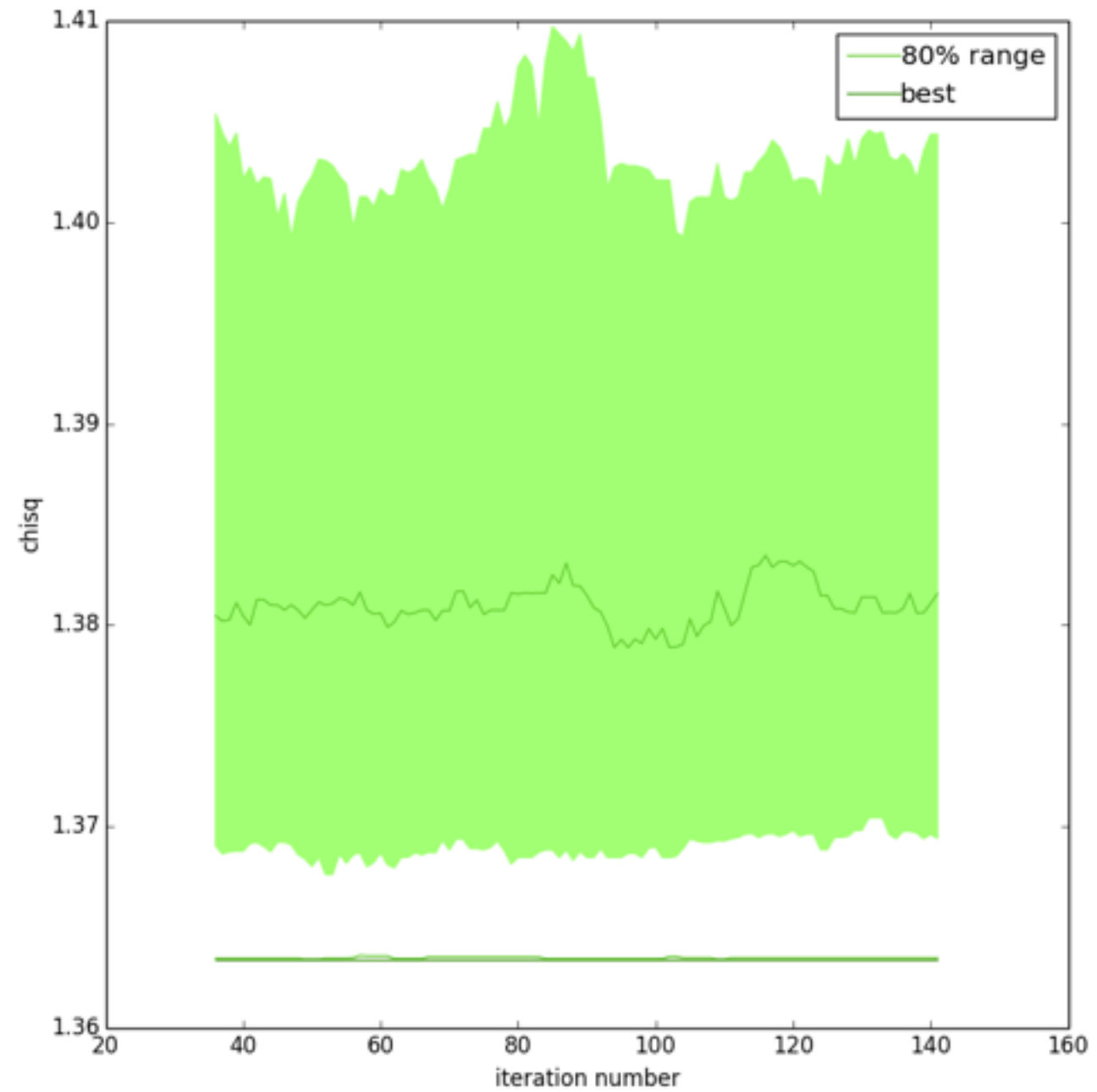
Population: 10

Initializer: eps

Thinning: 1

Steps: 0

OK Cancel ?



Fitting Algorithms

Fit Options

Fit Algorithms

☒ DREAM ☐ Differential Evolution

☐ Levenberg-Marquardt ☐ Nelder-Mead Simplex

☐ Quasi-Newton BFGS

DREAM Fitting Parameters

Samples: 10000

Burn-in Steps: 100

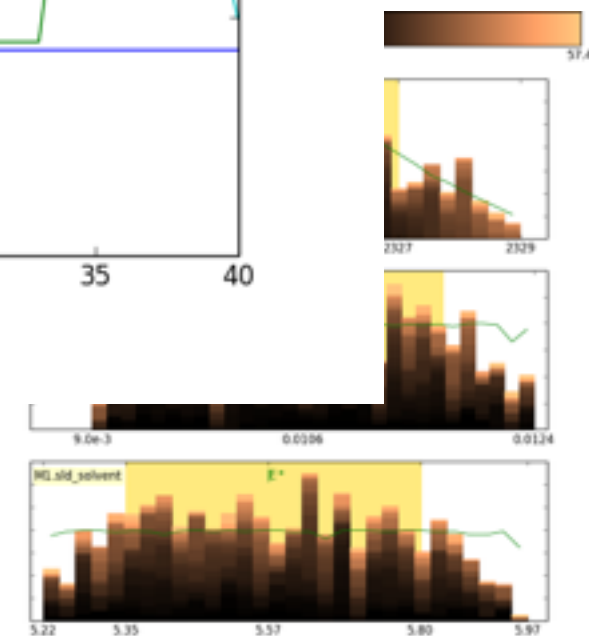
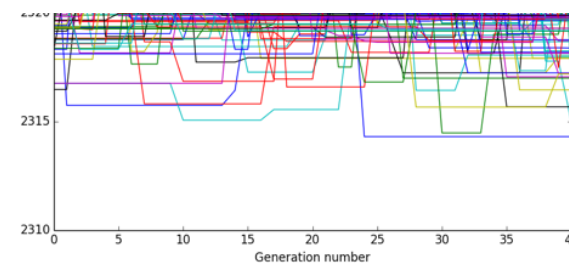
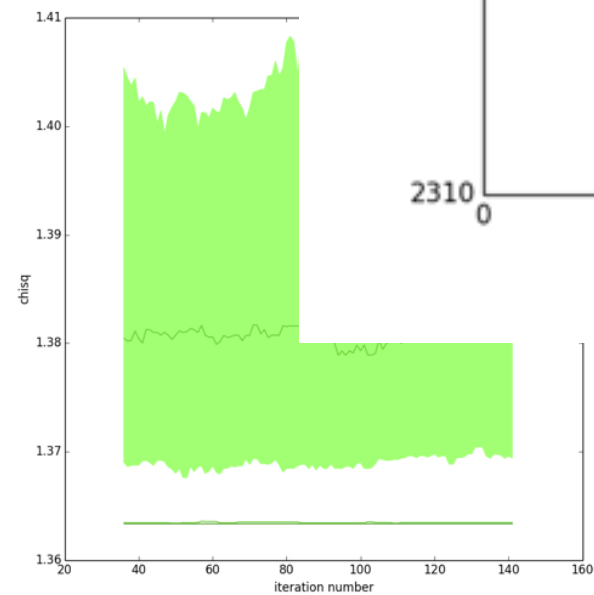
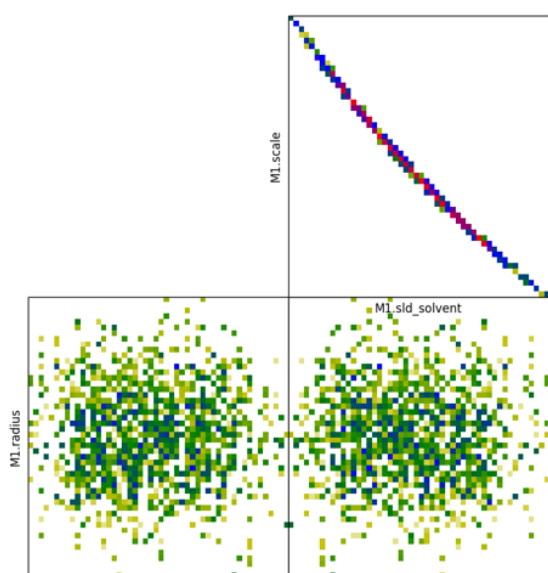
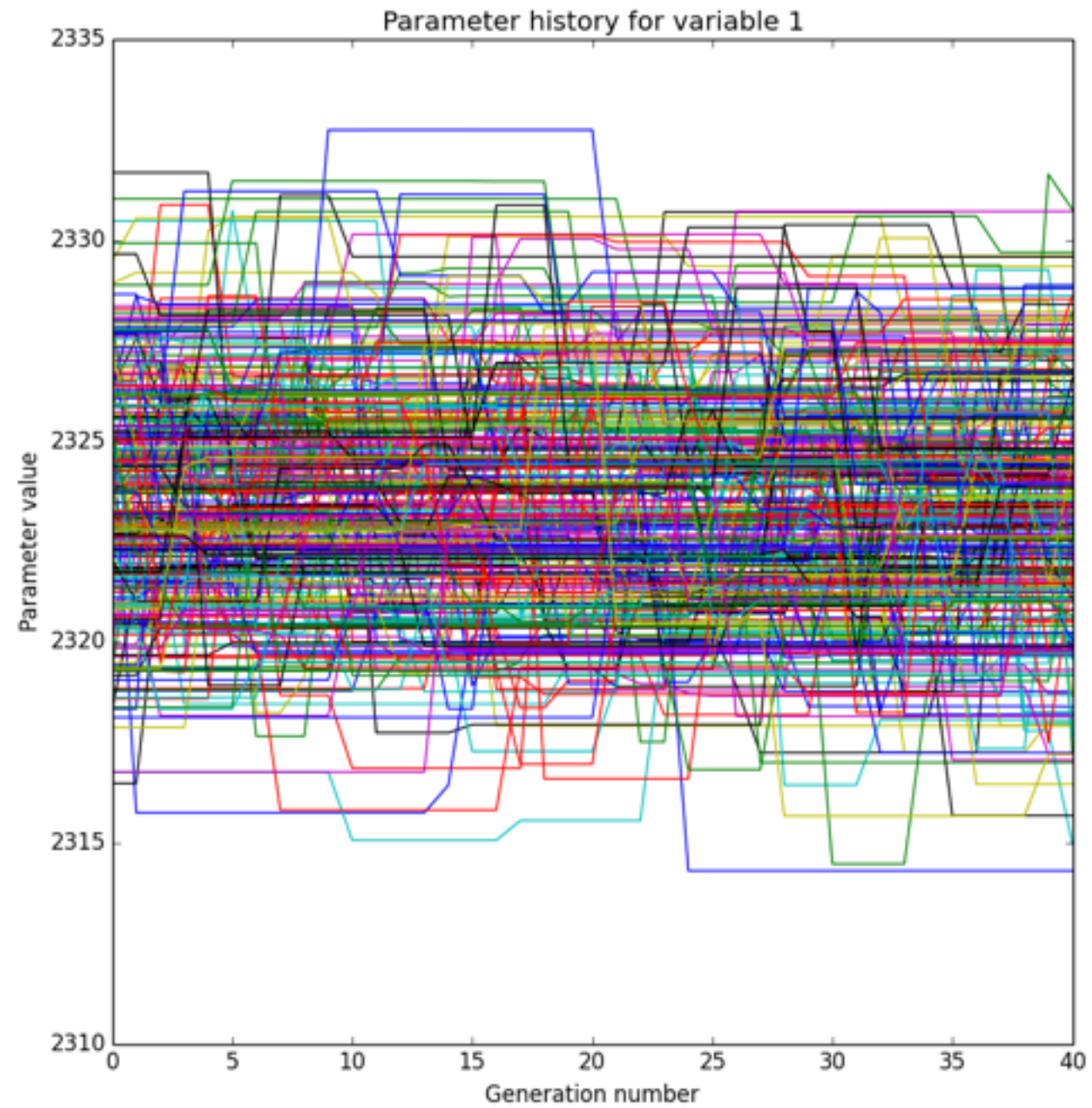
Population: 10

Initializer: eps

Thinning: 1

Steps: 0

OK Cancel ?



Fitting Algorithms

Fit Options

Fit Algorithms

☒ DREAM ☐ Differential Evolution

☐ Levenberg-Marquardt ☐ Nelder-Mead Simplex

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DREAM Fitting Parameters

Samples: 10000

Burn-in Steps: 100

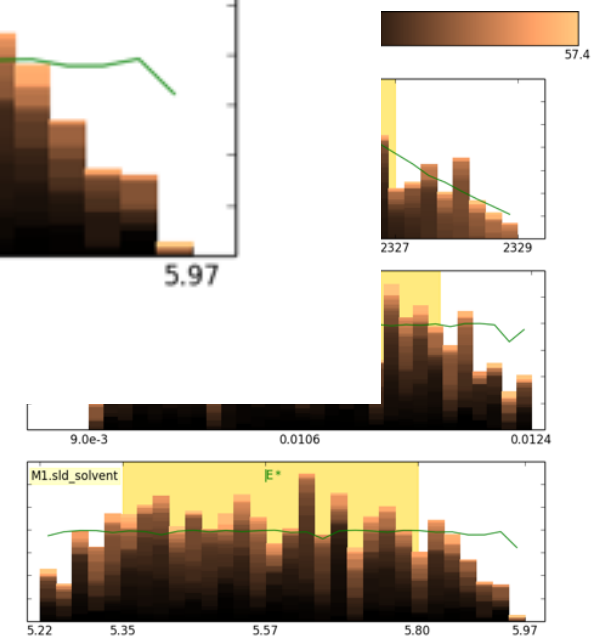
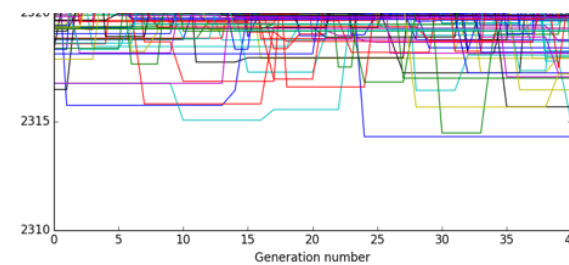
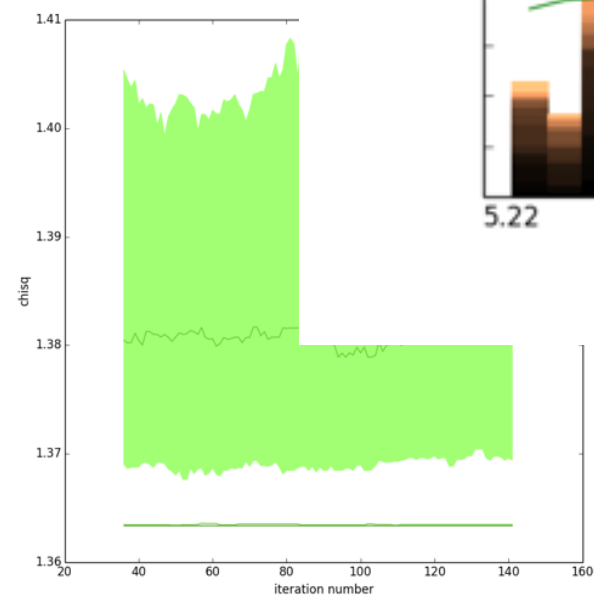
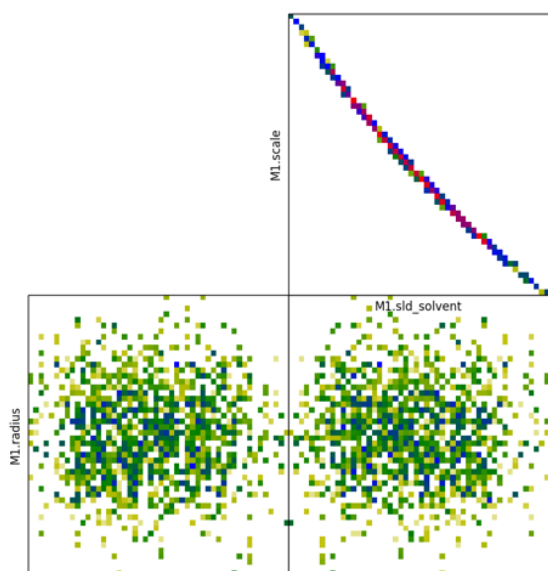
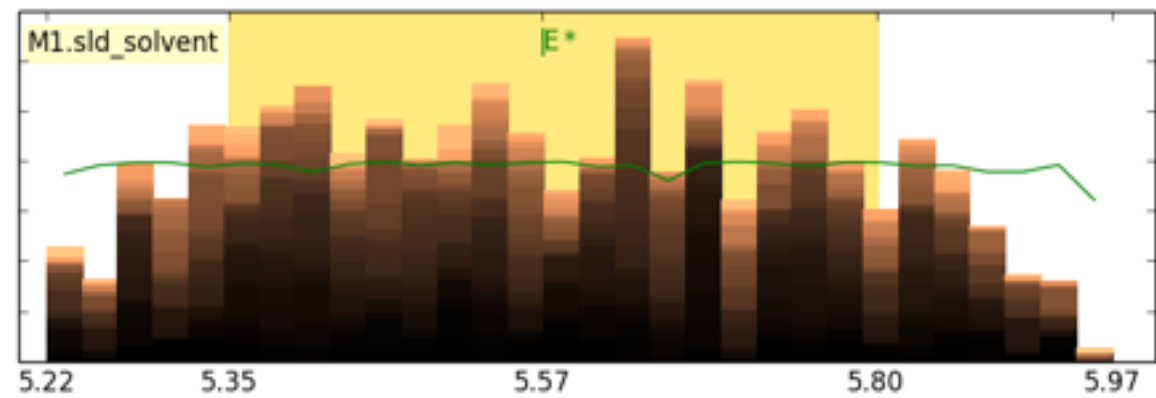
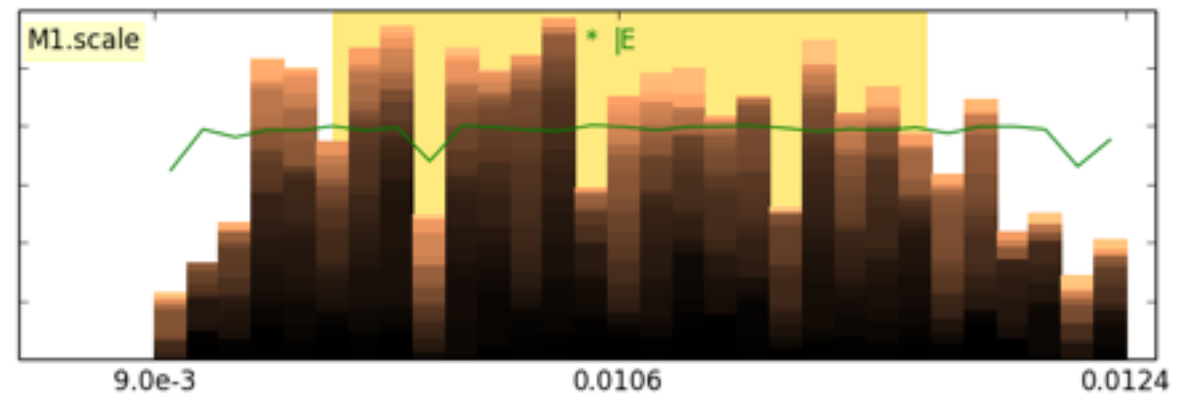
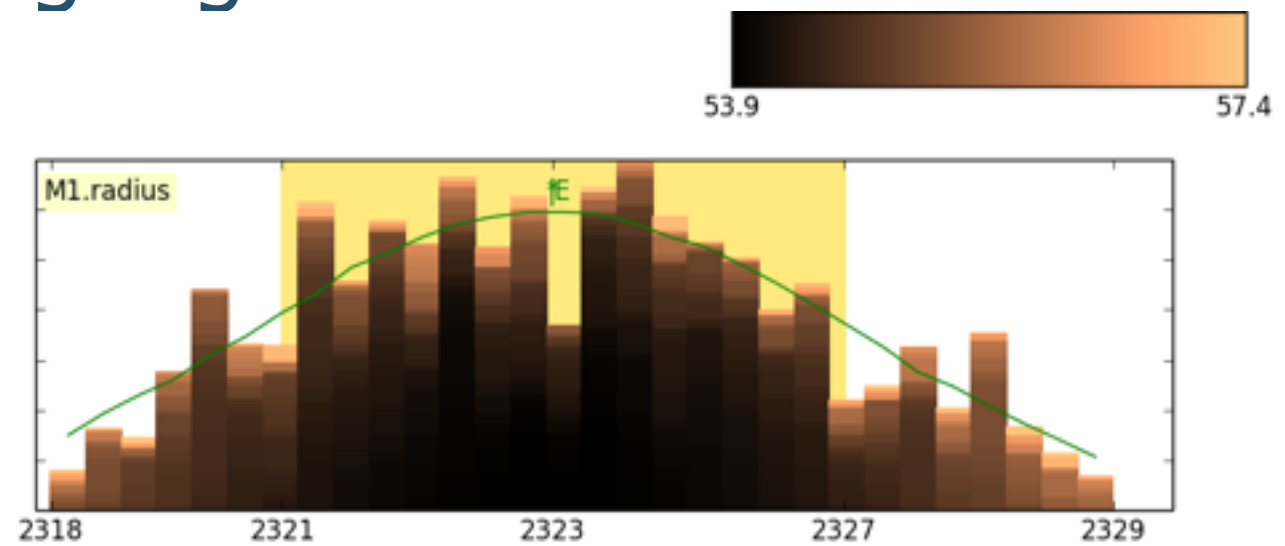
Population: 10

Initializer: eps

Thinning: 1

Steps: 0

OK Cancel ?



Other Features

Batch fitting ...

Fit Panel

FitPage1 BatchPage1

I(q) Data Source

- Choose a file to set initial fit parameters -
- This panel is not designed to view individual fits. -

Name : P123_D2O_30_percent.xml

P123_D2O_30_percent.xml
P123_D2O_10_percent.xml
P123_D2O_40_percent.xml

Model

Category

Shape-Independent

Modify

Description

Help

1D Mode

Polydispersity and Orientational Distribution

On Off ?

Fitting

Set Instrumental Smearing

None Use dQ Data Custom Pinhole Smear Custom Slit Smear ?

No smearing is selected...

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] Masking(2D)

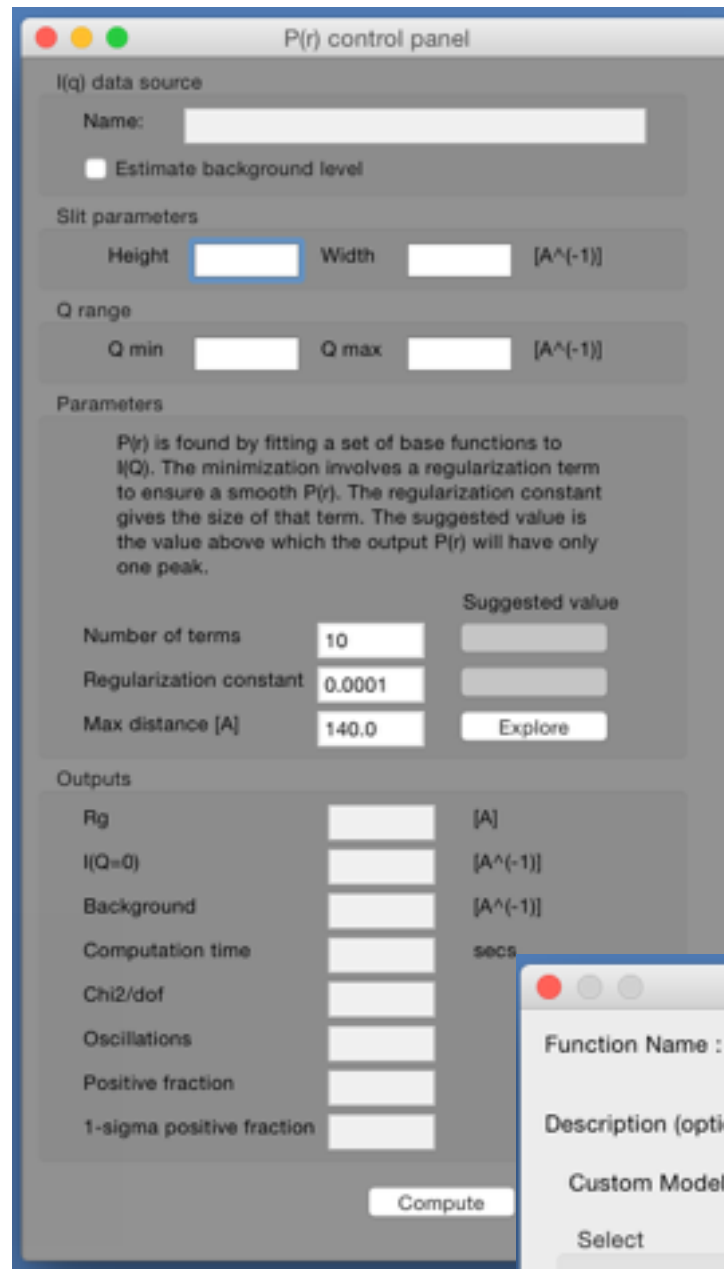
Reset 0.009 0.2545 Editor

Chi2/Npts Npts(Fit) Npts Log? Compute

- 124 124 Fit Help

Other Features

P(r) Inversion ...



P(r) control panel

I(q) data source
Name:
☐ Estimate background level

Slit parameters
Height Width [\AA^{-1}]

Q range
Q min Q max [\AA^{-1}]

Parameters
P(r) is found by fitting a set of base functions to I(Q). The minimization involves a regularization term to ensure a smooth P(r). The regularization constant gives the size of that term. The suggested value is the value above which the output P(r) will have only one peak.

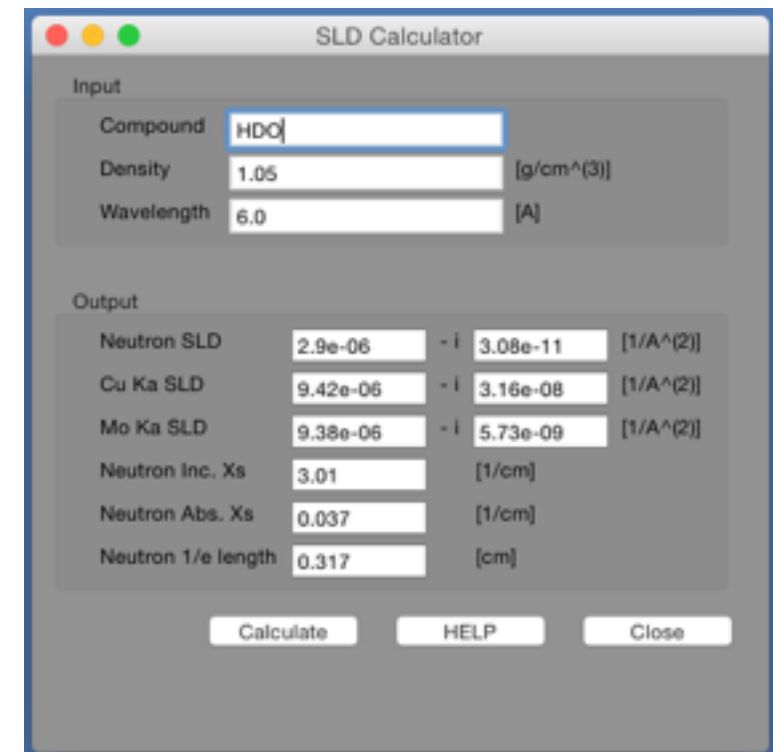
Number of terms Suggested value

Regularization constant

Max distance [\AA]

Outputs
Rg [\AA]
I(Q=0) [\AA^{-1}]
Background [\AA^{-1}]
Computation time secs
Chi2/dof
Oscillations
Positive fraction
1-sigma positive fraction

SLD Calculator ...

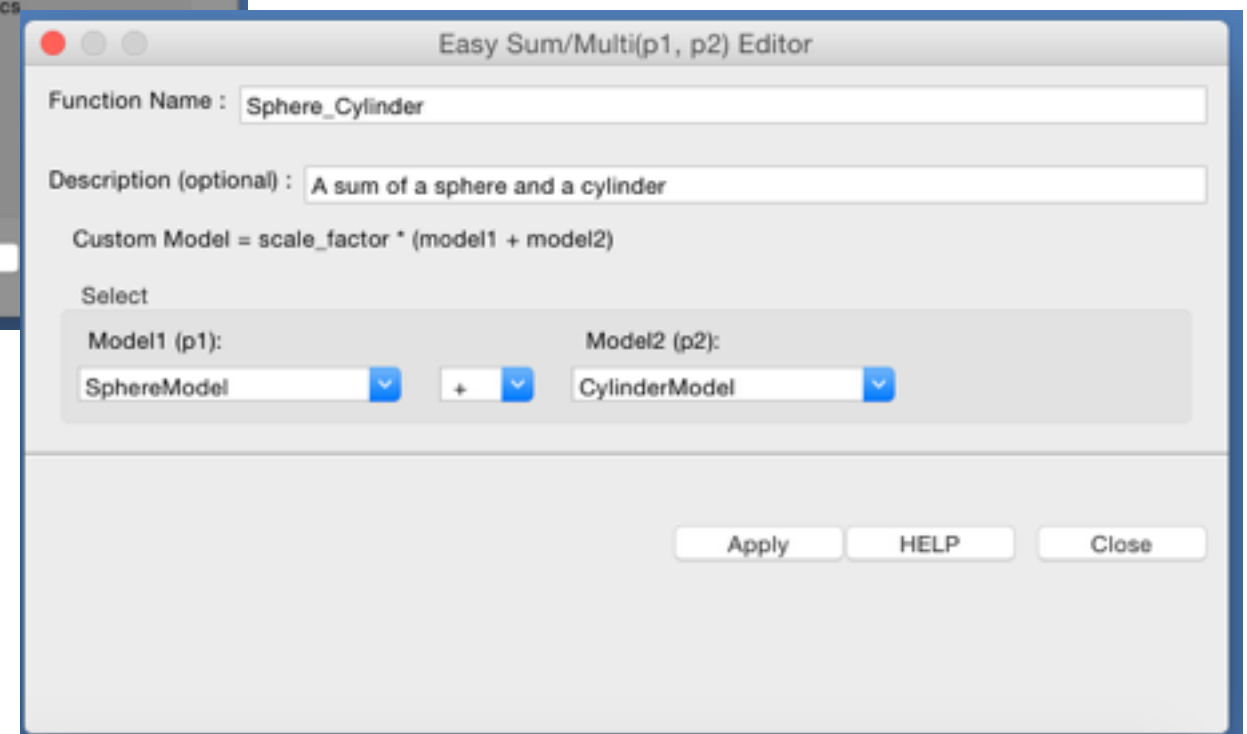


SLD Calculator

Input
Compound
Density [g/cm^3]
Wavelength [\AA]

Output
Neutron SLD - i [$1/\text{\AA}^2$]
Cu Ka SLD - i [$1/\text{\AA}^2$]
Mo Ka SLD - i [$1/\text{\AA}^2$]
Neutron Inc. Xs [$1/\text{cm}$]
Neutron Abs. Xs [$1/\text{cm}$]
Neutron 1/e length [cm]

Sum & Multiplication of Models ...



Easy Sum/Multi(p1, p2) Editor

Function Name :

Description (optional) :

Custom Model = scale_factor * (model1 + model2)

Select
Model1 (p1): + Model2 (p2):

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

- Documentation
- Description
- Parameters
- Calculation
- Tests

```
"""
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"
```

```
# ["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?