EUROPEAN SPALLATION SOURCE

SasView

Data Analysis for Small Angle Scattering

Science & Technology Facilities Council
ISIS

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

Bundesanstalt für Materialforschung und -prüfung

A little history …

2006 2011 2012 2013 2014 2015 2016 2017 2018 2019

Heritage: NIST IGOR macros
SansView is DANSE project output
~ 8.5% of funds were for SANS

NIST Supported initial transition from NSF funding

Transition to Community project.

Move to GitHub
Rename to SasView

v3.0 released
v3.1 released

v4.0 released

v4.1 released

v4.2 released
v5.0b1 released
v4.2.1 released
v5.0b2 released

1st Code Camp at NIST April 2013

2nd Code Camp at ISIS April 2014

3rd Code Camp at ESS Feb 2015

4th Code Camp at TU Delft March 2016

5th Code Camp at ORNL Oct 2016

6th Code Camp at ILL/ESRF April 2017

7th Code Camp at DMSC October 2017

8th Code Camp at ESS Sept 2018

1st SasView User Meeting at SAS2018

9th Code Camp at ILL/ESRF March 2019

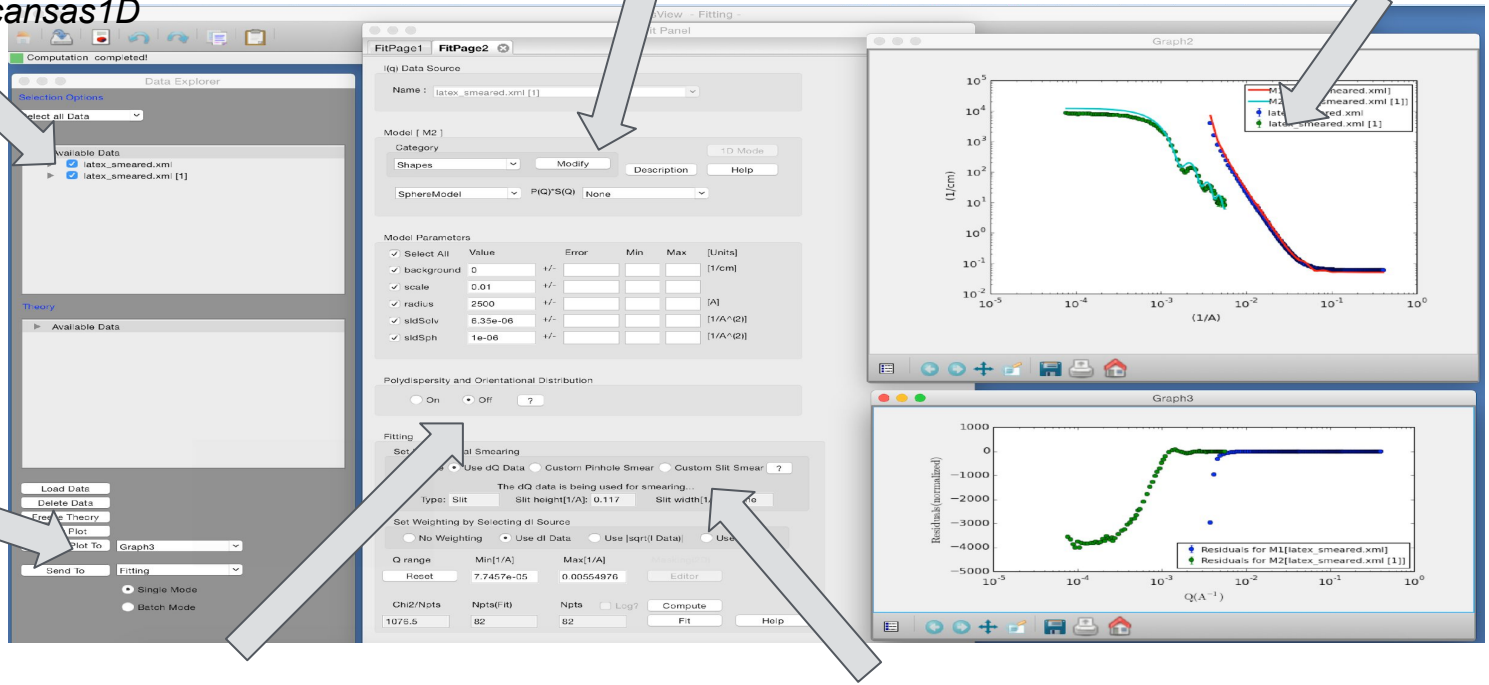
1D Analysis

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

2D Analysis

Fit panel - Active Fitting Optimizer: Levenberg-Marquardt

FitPage1

No data loaded

Model | Fit Options | Resolution | Polydispersity | Magnetism

Model

Category: Cylinder | Model name: cylinder | Structure factor: None

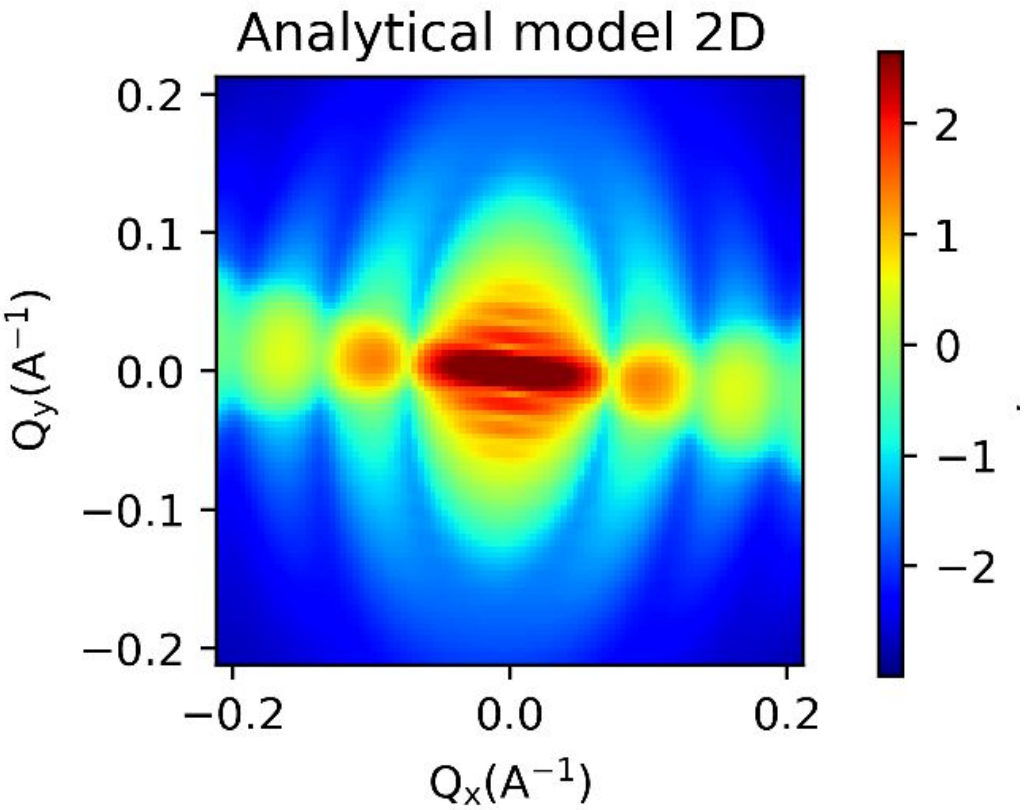
Parameter	Value	Min	Max	Units
scale	1.0	0.0	∞	
background	0.001	-∞	∞	cm^{-1}
cylinder				
sld	4	-∞	∞	$10^{-6}/Å^2$
sld_solvent	1	-∞	∞	$10^{-6}/Å^2$
radius	50	0.0	∞	Å
Polydispersity				
length	400	0.0	∞	Å
Polydispersity				
Distribution	0.1			gaussian
theta	60	-360.0	360.0	degrees
Polydispersity				
Distribution	10			gaussian
phi	85	-360.0	360.0	degrees
Polydispersity				
Distribution	10			gaussian

Options: Polydispersity, 2D view, Magnetism

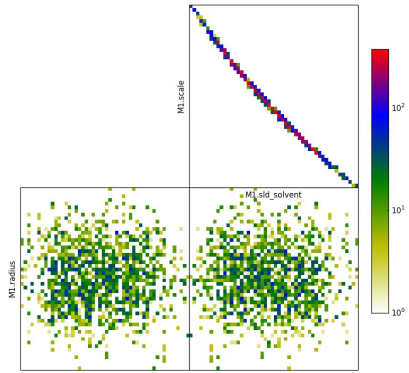
Fitting details: Min range 0.001 $Å^{-1}$; Max range 0.3 $Å^{-1}$; Smearing: None

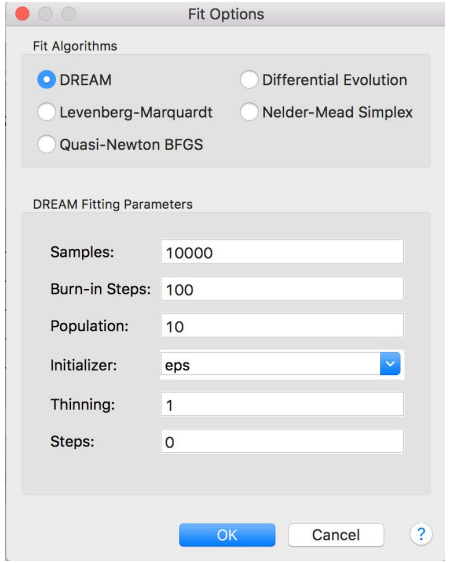
Fitting error: χ^2 24895

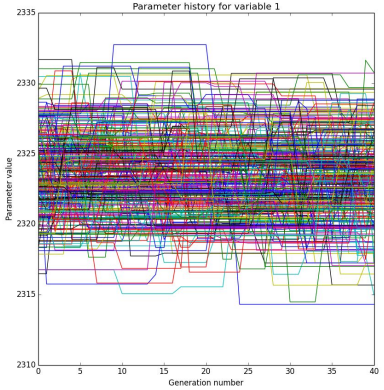
Show Plot | Fit | Help

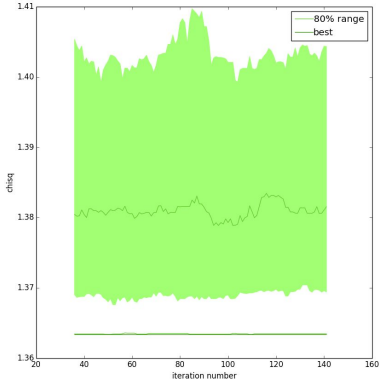


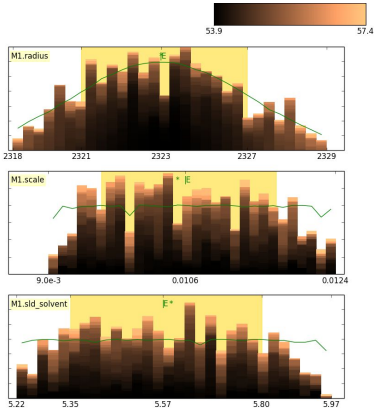
Fitting Algorithms





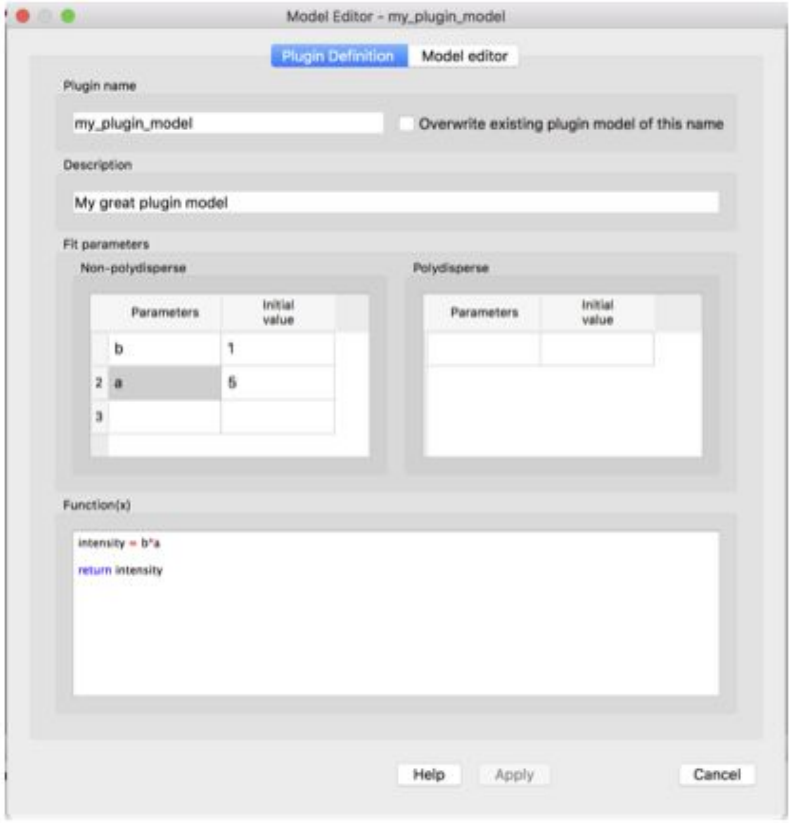






Uses bumps package from P. Kienzle

Plugin Model Editor



Python & C model files

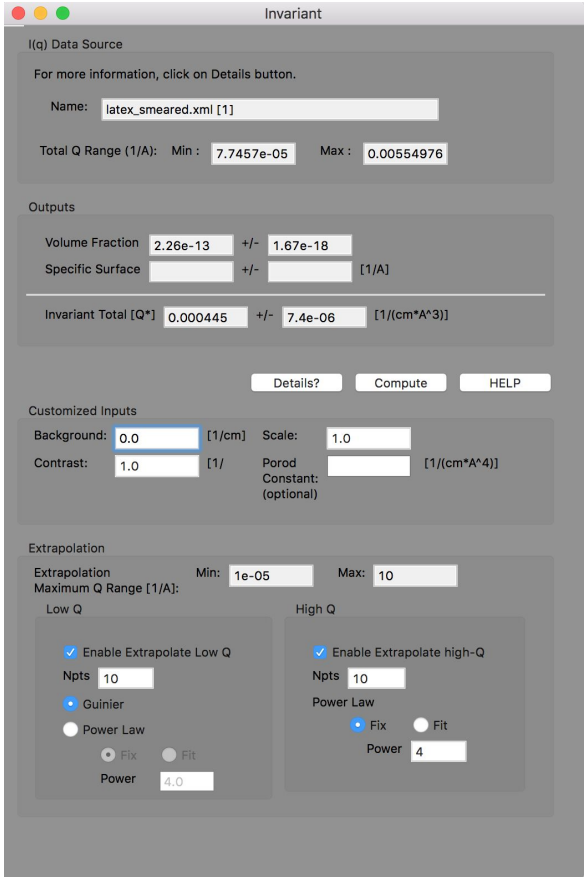
cylinder.py

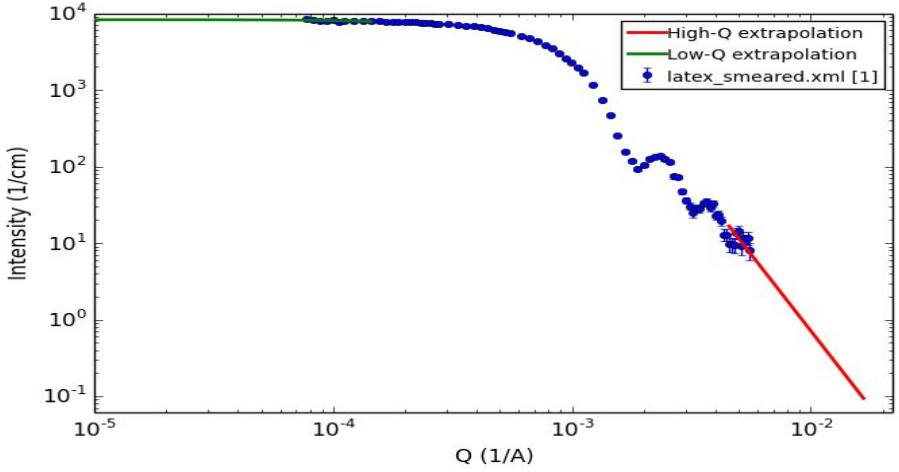
```
import ...

name = "cylinder"
title = "Right circular cylinder with uniform scattering length density."
description = """
     f(q,alpha) = 2*(sld - sld_solvent)*V*sin(qLcos(alpha)/2))
                  /[qLcos(alpha)/2]*J1(qRsin(alpha))/[qRsin(alpha)]

           P(q,alpha)= scale/V*f(q,alpha)^(2)+background
           V: Volume of the cylinder
           R: Radius of the cylinder
           L: Length of the cylinder
           J1: The bessel function
           alpha: angle between the axis of the
           cylinder and the q-vector for 1D
           :the ouput is P(q)=scale/V*integral
           from pi/2 to zero of...
           f(q,alpha)^(2)*sin(alpha)*dalpha + background
"""
category = "shape:cylinder"

#            [ "name", "units", default, [lower, upper], "type", "description"],
parameters = [["sld", "1e-6/Ang^2", 4, [-inf, inf], "sld",
               "Cylinder scattering length density"],
              ["sld_solvent", "1e-6/Ang^2", 1, [-inf, inf], "sld",
               "Solvent scattering length density"],
              ["radius", "Ang", 20, [0, inf], "volume",
               "Cylinder radius"],
              ["length", "Ang", 400, [0, inf], "volume",
               "Cylinder length"],
              ["theta", "degrees", 60, [-360, 360], "orientation",
               "cylinder axis to beam angle"],
              ["phi", "degrees", 60, [-360, 360], "orientation",
               "rotation about beam"],
             ]

source = ["lib/polevl.c", "lib/sas_J1.c", "lib/gauss76.c", "cylinder.c"]

def ER(radius, length):
    """
        Return equivalent radius (ER)
    """
    ddd = 0.75 * radius * (2 * radius * length + (length + radius) * (length + pi * radius))
```

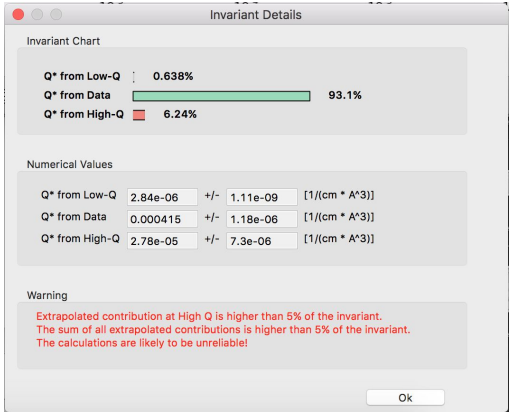
cylinder.c

```
#define INVALID(v) (v.radius<0 || v.length<0)

static double
form_volume(double radius, double length)
{
    return M_PI*radius*radius*length;
}

static double
fq(double qab, double qc, double radius, double length)
{
    return sas_2J1x_x(qab*radius) * sas_sinx_x(qc*0.5*length);
}

static double
orient_avg_1D(double q, double radius, double length)
{
    // translate a point in [-1,1] to a point in [0, pi/2]
    const double zm = M_PI_4;
    const double zb = M_PI_4;

    double total = 0.0;
    for (int i=0; i<GAUSS_N ;i++) {
        const double theta = GAUSS_Z[i]*zm + zb;
        double sin_theta, cos_theta; // slots to hold sincos function output
        // theta (theta,phi) the projection of the cylinder on the detector plane
        SINCOS(theta , sin_theta, cos_theta);
        const double form = fq(q*sin_theta, q*cos_theta, radius, length);
        total += GAUSS_W[i] * form * form * sin_theta;
    }
    // translate dx in [-1,1] to dx in [lower,upper]
    return total*zm;
}

static double
Iq(double q,
    double sld,
    double solvent_sld,
    double radius,
    double length)
{
    const double s = (sld - solvent_sld) * form_volume(radius, length);
    return 1.0e-4 * s * s * orient_avg_1D(q, radius, length);
}
```

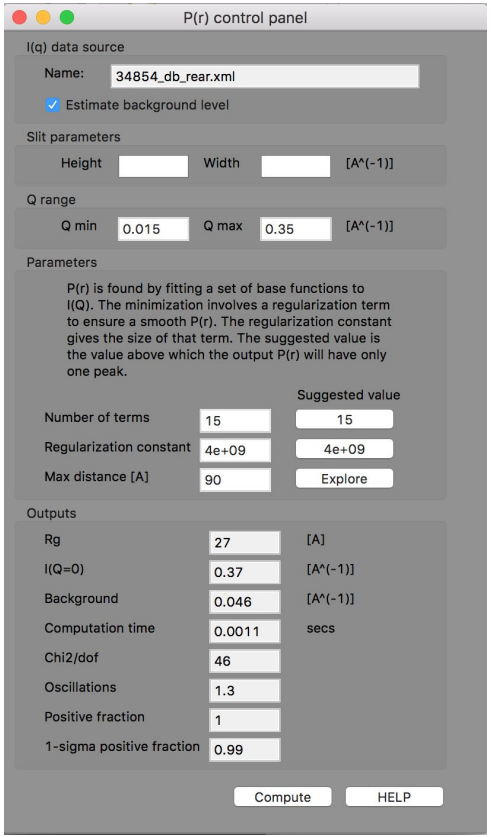
Invariant Calculation

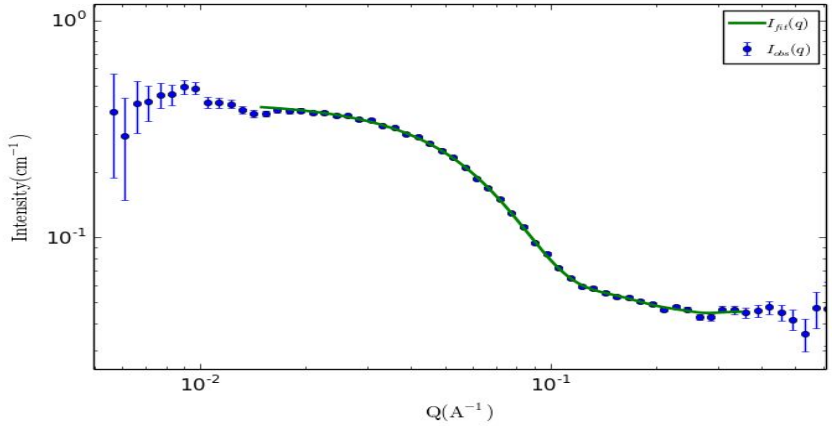


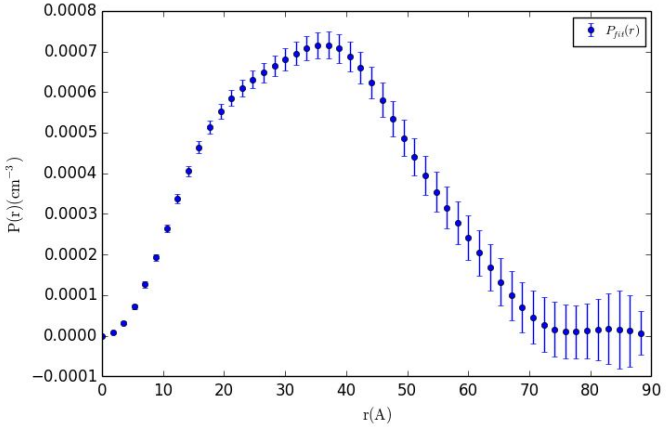




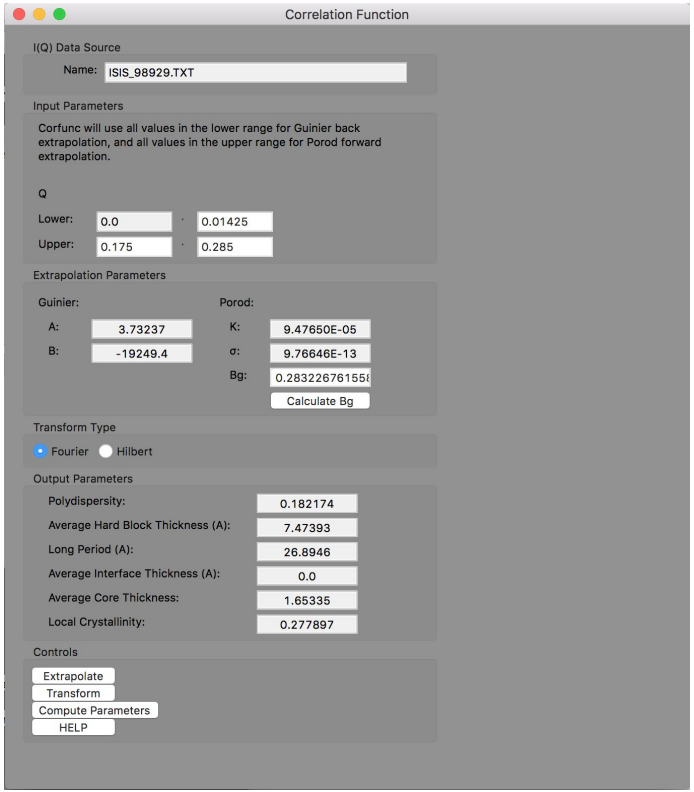
P(r) Inversion

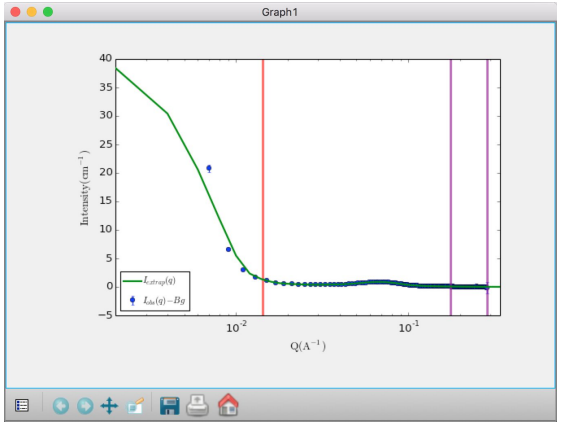


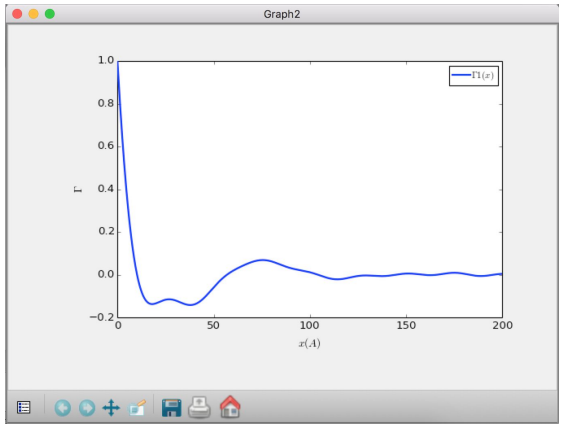




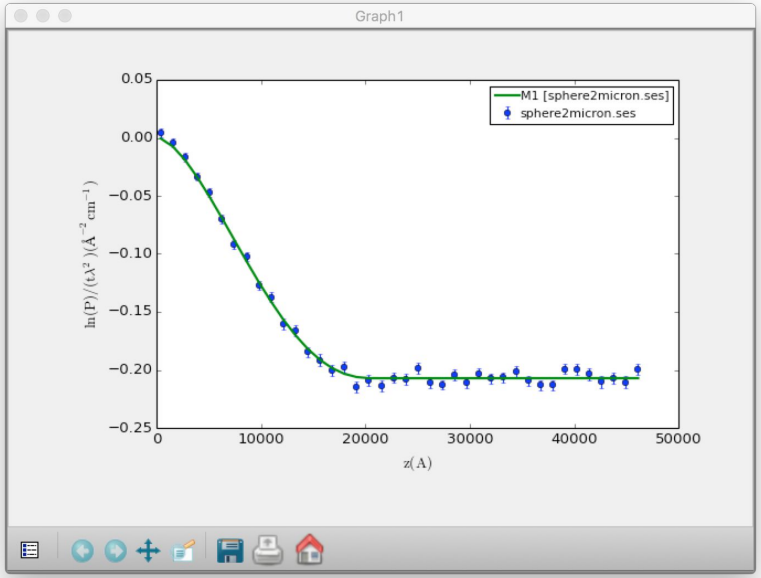
Correlation Function Analysis (new!)

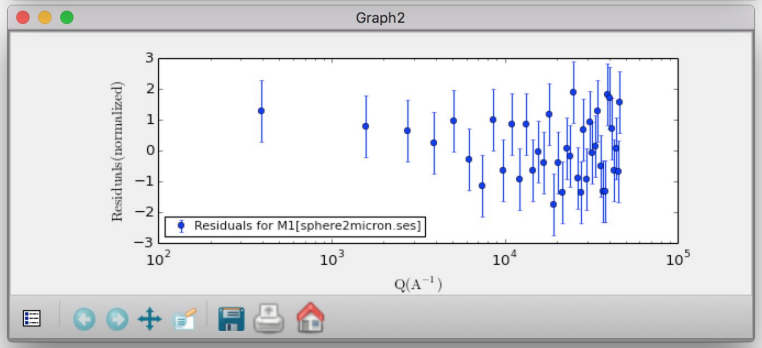






SESANS Analysis





Automatic Hankel Transform of SANS models

(TU Delft & ISIS)

How We Work

Open, Collaborative, Community Development

Code is open source and publicly hosted at Github

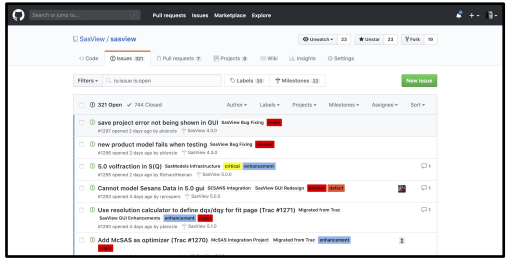
Released under BSD 3-clause license

Bug and Enhancement Ticket System

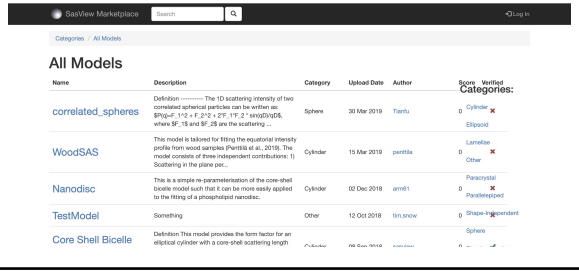
Bi-weekly developer calls **Code Camps** **5 Year Roadmap**

Model Marketplace DOI for each release

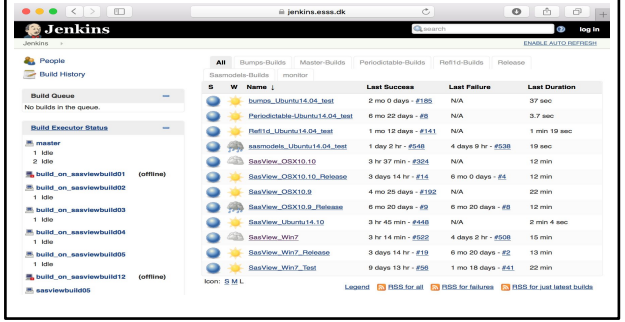
Code Hosting, Task and bug tracking, and developer/user wiki
Github



Model Marketplace for users to share their models
marketplace.sasview.org



Automated Builds
build.sasview.org



http://www.sasview.org

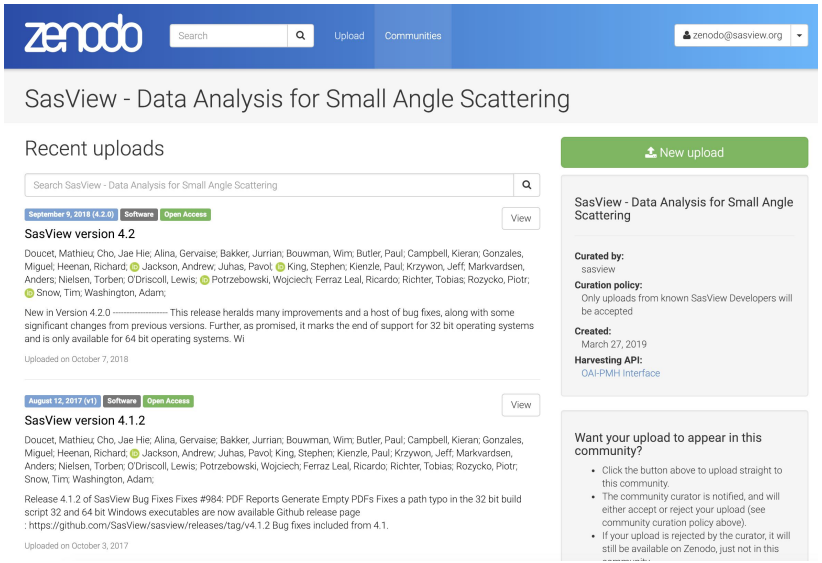
http://github.com/SasView

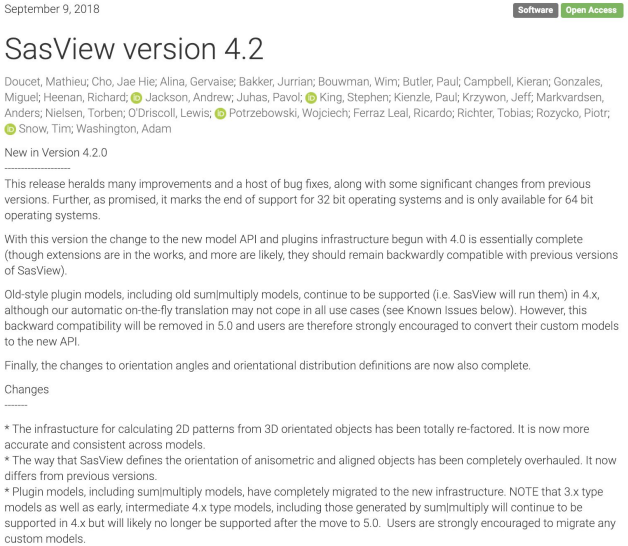
How We Work

Open, Collaborative, Community Development

DOI for each release

https://zenodo.org/communities/sasview-analysis





http://www.sasview.org

http://github.com/SasView

How We Work

Open, Collaborative, Community Development

DOI for each release

https://zenodo.org/communities/sasview-analysis

Publication date:
September 9, 2018

DOI:
DOI 10.5281/zenodo.1412041

Grants:
European Commission:
- SINE2020 - World class Science and Innovation with Neutrons in Europe 2020 – SINE2020 (654000)

Alternate identifiers:
https://github.com/SasView/sasview/releases/tag/v4.1.2

Communities:
SasView - Data Analysis for Small Angle Scattering

License (for files):
BSD 3-Clause "New" or "Revised" License

Files (405.4 MB)

Name	Size	
SasView-4.2.0-MacOSX.dmg md5:b0c68251297d8ae56c90354af5b206a9	196.9 MB	Download
sasview-4.2.0.tar md5:de9803768bf49f2f5d61e671ef33b1c6	66.0 MB	Download
sasview-4.2.0.zip md5:590672685fd4bb7840f0dfaad0b61d54	42.4 MB	Preview Download
setupSasView-4.2.0-x64.exe md5:3b10af1557127f6eb31f427b9549f6d1	100.0 MB	Download

http://www.sasview.org

http://github.com/SasView

How We Work

Open, Collaborative, Community Development

We work together towards common goals formulated through community input, with two guiding principles ...

He who pays the piper …
Those who bring the resources (time and effort, or funds to buy time and effort) choose what to work on.

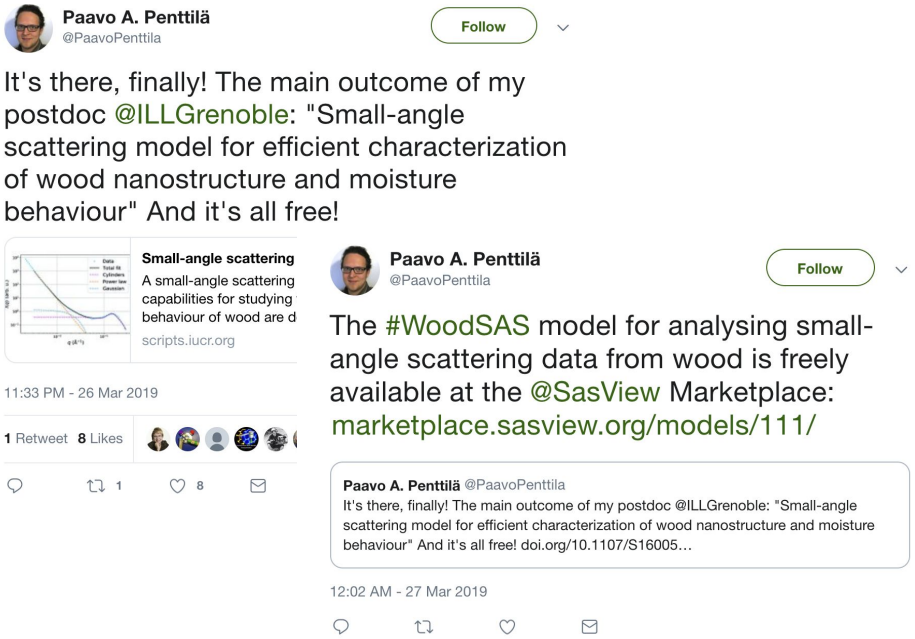
You break it, you bought it ...
You are not allowed to break what is already there for others. If you break it, you fix it.

http://www.sasview.org

http://github.com/SasView

How We Work

Open, Collaborative, Community Development



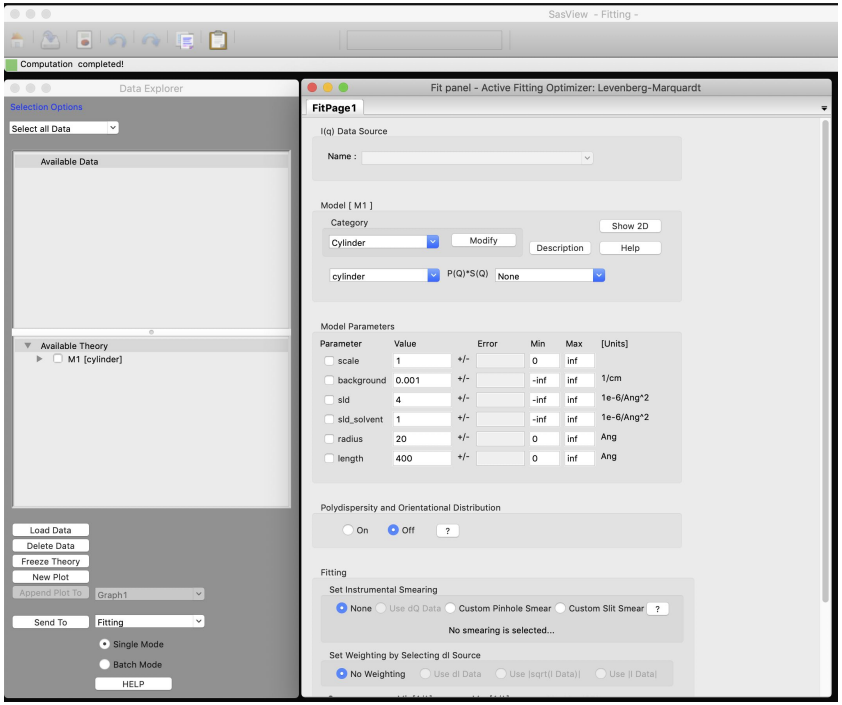
Ask not what the community is going to do for you,
ask what you can do for the community

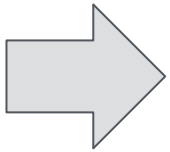
\- P. Butler, March 2019

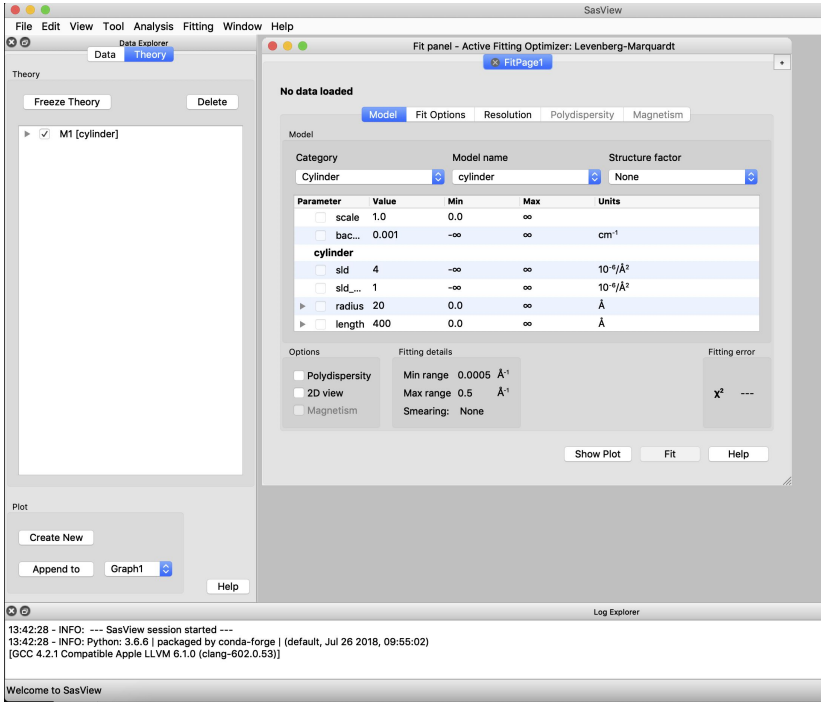
http://www.sasview.org

http://github.com/SasView

SINE 2020 Work - GUI



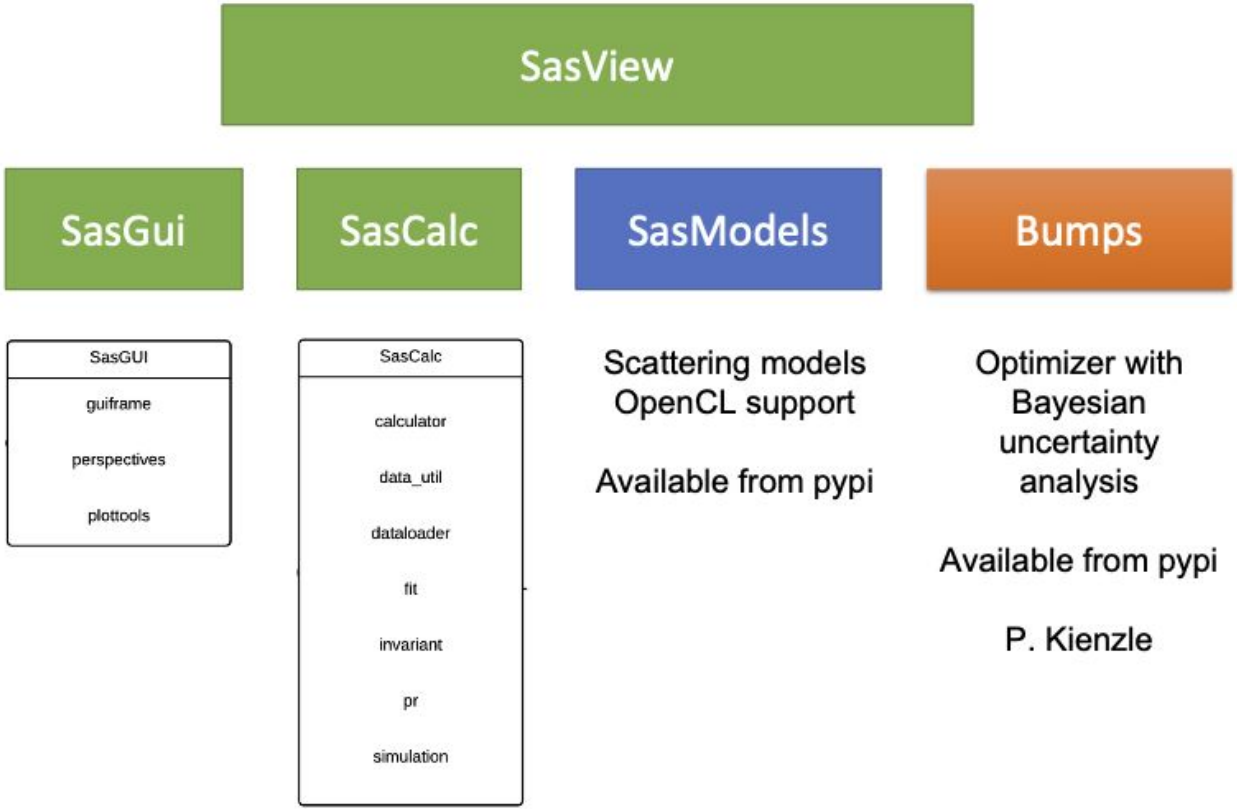




wxPython
Computation and GUI code mixed
"Organically developed" - hard for new developers

PyQT
Computation, GUI code, and models separated
Structured and documented - easier for new developers

SINE 2020 Work - Code Separation

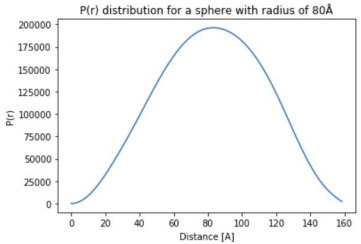


Jupyter Notebooks

SasCalc example

A simple example demonstarting pair distance distribution function P(r) inversion. In SasView it is calculated using Moore formula (1980)

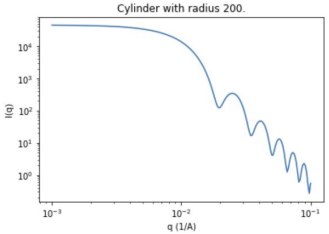
In [2]:
```
from sas.sascalc.dataloader.loader import Loader
from sas.sascalc.pr.invertor import Invertor
import matplotlib.pyplot as plt
import numpy as np

loader = Loader()
test_data = loader.load("sphere_80_err.txt")
x_data = test_data[0].x
y_data = test_data[0].y
z_data = test_data[0].dy

pr = Invertor()
pr.x = x_data
pr.y = y_data
pr.err = z_data

pr.alpha = 2.6e-5
pr.d_max = 160

#nfunc - number of base functions to use.
out, cov = pr.invert(nfunc=13)
pr_value = []
err_value = []
r = np.arange(0.0, pr.d_max, pr.d_max / pr.x.size)
for r_i in r:
    (value, err) = pr.pr_err(out, cov, r_i)
    pr_value.append(value)
    err_value.append(err)

plt.plot(r,pr_value)
plt.xlabel("Distance [A]")
plt.ylabel("P(r)")
plt.title('P(r) distribution for a sphere with radius of 80Å')
plt.show()
```



SasModels example

SasModels is a library of form and strcuture factor functions. The following example demonstrates how to generate a scattering pattern of a form factor of the cylinder model using sasmodels library. It requires sasmodels to be installed in the path.

In [35]:
```
from numpy import logspace
from matplotlib import pyplot as plt
from sasmodels.core import load_model
from sasmodels.direct_model import call_kernel

model = load_model('cylinder')
q = logspace(-3, -1, 200)
kernel = model.make_kernel([q])
Iq = call_kernel(kernel, dict(radius=200))
plt.loglog(q, Iq)
plt.xlabel('q (1/A)')
plt.ylabel('I(q)')
plt.title('Cylinder with radius 200.')
plt.show()
```

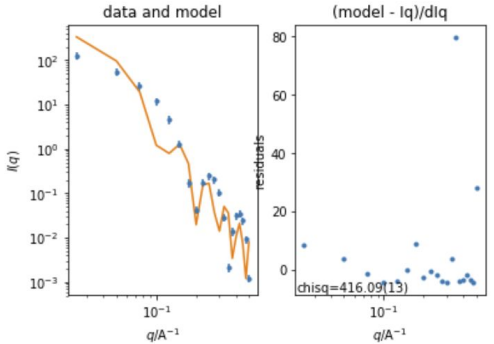


Jupyter Notebooks

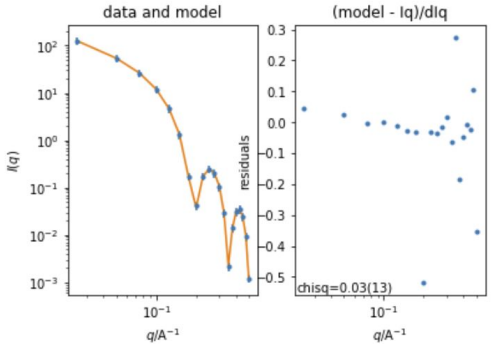
Fitting model function to data using bumps

The model functions from sasmodels can be used to fit experimental data. This can be done using bumps, which simillar to sasmodels is a separate package and needs to be installed in your path.

In [36]:
```
from sasmodels.core import load_model
from sasmodels.bumps_model import Model, Experiment
from sasmodels.data import load_data

from bumps.names import *
from bumps.fitters import fit
from bumps.formatnum import format_uncertainty

import pylab

test_data = load_data('cyl_400_20.txt')
kernel = load_model('cylinder')

#We set some errors for demonstration
test_data.dy = 0.2*test_data.y

pars = dict(radius=35,
            length=350,
            background=0.0,
            scale=1.0,
            sld=4.0,
            sld_solvent=1.0)
model = Model(kernel, **pars)

# SET THE FITTING PARAMETERS
model.radius.range(1, 50)
model.length.range(1, 500)

M = Experiment(data=test_data, model=model)
problem = FitProblem(M)
print("Initial chisq", problem.chisq_str())
problem.plot()
pylab.show()

result = fit(problem, method='amoeba')
print("Final chisq", problem.chisq_str())
for k, v, dv in zip(problem.labels(), result.x, result.dx):
    print(k, ":", format_uncertainty(v, dv))
problem.plot()
pylab.show()
```




```
Final chisq 0.03(13)
length : 464.9(55)
radius : 19.977(64)
```



The RoadMap

SasView 5 Year Roadmap

The purpose of building and operating large scattering facilities is to provide unique tools to answer new scientific questions with the final presentation of results (usually in the form of a paper) as the output. The biggest obstacle to that output is often the analysis of the acquired data. Data analysis software has been variously viewed as being in the domain of the scientist using the facility, a service to be provided by scattering facilities, or as the individual responsibility of the scientists running the facility beamlines. The result has been a proliferation of packages and libraries, many written and supported by one key person, often not as their primary responsibility [1].

Over the past decade several trends have contributed to exacerbate the analysis bottleneck: 1) As the techniques have matured the user pool has broadened. This combined with an apparent decrease in the overall level of programming taught to scientists, means that fewer users are capable of building their own analysis tools. 2) With the increasing maturity of the field, a large amount of basic modeling is well understood and developed. Even those capable of coding their own should not be wasting their time re-inventing the wheel but focus on new science and perhaps new analysis developments to enable that new science. 3) The quantity of data being produced by instruments and the complexity of the experiments being performed have increased. 4) Finally, as the general software landscape has moved towards increased quality of usability a
expectatio
data.

Late 2018 to mid 2019 (from code camp VIII - ESS) - Release 4.2, Release 5.0

The focus in this period will be on development and release of version 5.0 of SasView. In parallel version 4.2 and possibly 4.3 will be released providing a maintained, stable, release for current users of SasView. This managed transition from the 4.x series to the 5.x series will allow for extensive user testing of the 5.0 version prior to release. We expect to continue maintenance of the final 4.x release beyond the release of 5.0, with an eventual end-of-life for 4.x occurring with the 5.2 release.

Full integration of the beta approximation work into 5.0 will be completed, with some limited beta approximation functionality being made available in 4.x.

The first SasView community meeting will be held at the SAS 2018 meeting in October 2018 providing SasView users and contributors with an introduction to the new functionality being made available in 5.0 and training on how to get involved in contributing to the SasView project. Building on this meeting a plan for expanding community interactions will be developed.

Release 4.2 and 5.0 will support separate plotting of the P(Q) and S(Q) components in a P*S

esign

the

Living document

Directs work for developers and helps find candidate projects for funding.

Discussed and updated at each Code Camp.

https://github.com/SasView/documents

Roadmap Late 2018 to mid 2019

- Move focus of all GUI efforts to the new Qt GUI Done. Major bug fixes only to 4.x GUI
- Parallel development and release tracks (5.x + 4.x) Working, but needs streamlining from 5.0 release
- Complete beta approximation work In testing
- New, more flexible interaction volumes/radii Underway?
- Community meeting at SAS 2018 Done
- Complete SasView paper Started
- Consolidate and extend training material - both written tutorials and hands-on training material. Ongoing
- Update model marketplace Needs developer
- Create plan for developing community interactions. Started
- Fixes to custom model editor to support polydispersity Done
- Incorporation of models from:
  a. SASFit[^7] Work done, but not shipping by default. https://github.com/SasView/sasfit-models
  b. Scatter[^8] (Förster - crystalline materials models primarily) In discussions with BornAgain team
- Project infrastructure cleanup:
  a. ticket review/cull given 5.0 release Ongoing
  b. possible move to GitHub issues. Underway
- Release
  a. 5.0 alpha (late 2018) Done
  b. 5.0 beta (early 2019) Done
  c. 5.0 (mid 2019) On track
  d. 4.2 Done

Not in roadmap for this period …

- Complete separation of sascalc package / headless usage

https://github.com/SasView/documents

SasView 4.x series - 4.2.1 current

www.sasview.org

Official Releases available for Windows, Mac, and Debian Linux

Models

New models

New model package (sasmodels)

Separation of models from GUI

Simpler addition of models by users

Speed! GPU and parallel processing

New, consistent approach to orientation distributions for 2D

Correlation Function Analysis

CCP13 corfunc algorithm

Documentation

Enhanced, updated documentation for models.

New Tutorials.

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

SasView – the Next Generation – 5.x

Parallel release of 4.x and 5.x until 5 series is stable.
5.0 beta2 release out now for testing!

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 → Release 5.0

Sasmodels Enhancements
Return F(q) from models → Target release - 5.0
Beta approximation
Coherent sums

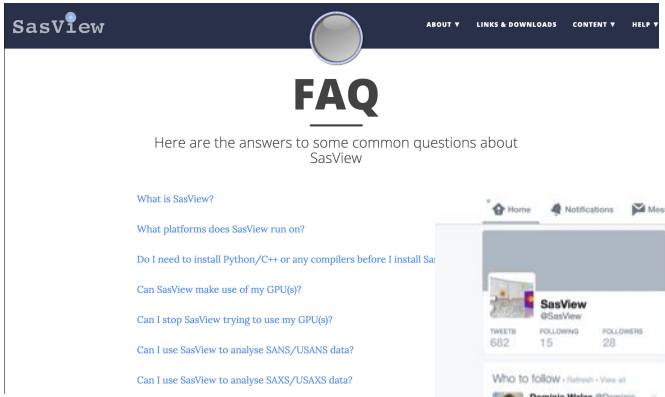
Constraints refactor → Target release - 5.1
Multi-GPU support
Inclusion of SasFit models → Target release - 5.0

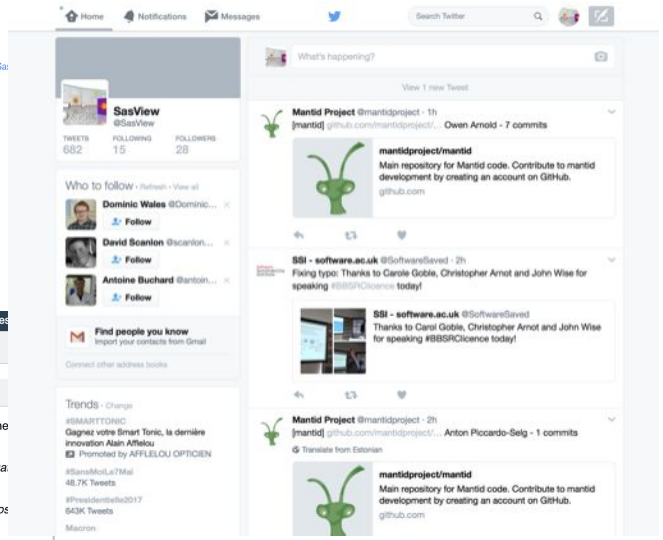
Integration of McSAS
Implementation of key models from Scatter → Target release - 5.1

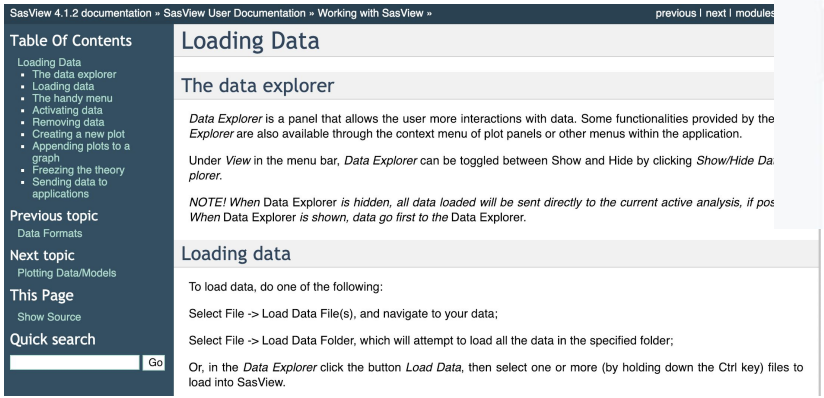
Documentation
Tutorials – written, interactive & video
Manual

Education & Outreach

- Website
- Documentation
- Written Tutorials
- Video Tutorials (YouTube)
- Taught courses
  - Scattering schools
  - University courses
- E-learning
- Bootcamps & Regional Workshops
- Twitter
- Slack
- (Marketplace)







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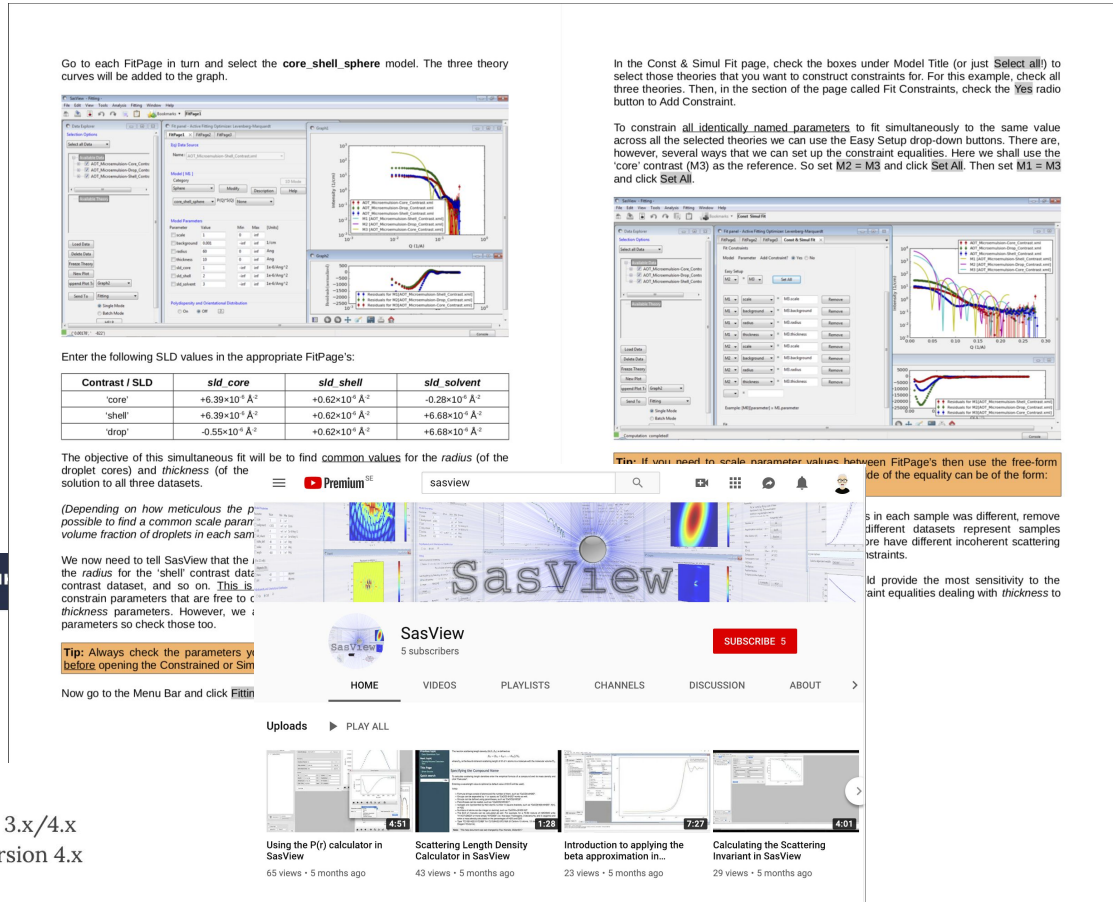

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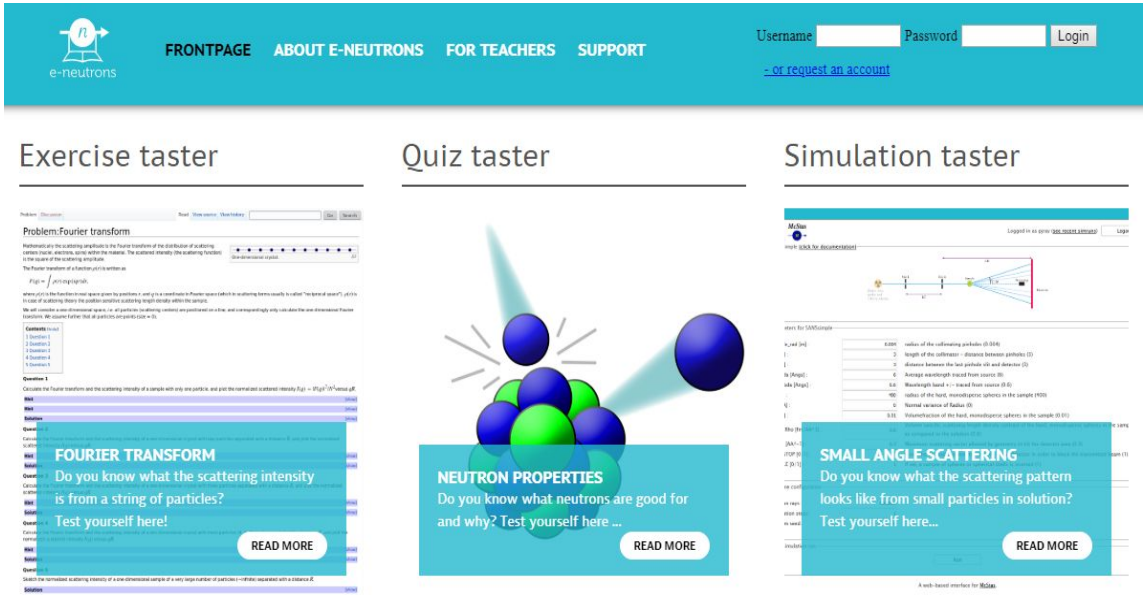

moodle AU

All the work of ISIS Sandwich Student Michael Oakley

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KEMM 37 / EXTN85 / NAKE017 *Scattering Methods Computer Lab Guide* - **2019**

Lab 1A. Familiarisation with SasView, Geometrical Models, and Structure Factors

This exercise will introduce you to analysing SANS data using geometrical models in SasView. In the first lab session you will look at how different shapes produce different scattering patterns, and how the model parameters affect the scattering pattern. In the second lab session you will then load some real SANS data and attempt to fit models to the data in SasView.

This first exercise is divided into 3 sections:

1. Familiarisation with SasView
2. Exploring geometrical models of form factors
3. Exploring structure factors

SAS2018
XVII International Small Angle Scattering Conference

Meeting agenda

- **2:15pm** Welcome and intro (goals and outline), *Andrew Jackson*, 20min
  - What is SasView
  - What is SasView structure: sasview, sasmodels, bumps
- **2:35pm** Demo of existing functionality, *Andrew Jackson, Paul Butler and Piotr Rozyczko*, 1h
  - Going through menu items
  - Loading different data types (1D/2D) data
  - Fitting 1D and 2D models
  - Simultaneous, constrainted and batch fitting
  - Calculators
  - Pr inversion, Invariant perspective
  - Correlation functions
- **3:35pm** Break 25min
- **4:00pm** How to write and distribute user models, *Tim Snow*, 30min
  - Writing models using plugin editor
  - Category manager
  - Python and C model
  - Distributing models on SasView marketplace
- **4:30pm** SasView CLI, *Wojtek Potrzebowski*, 15min
  - SasCalc example
  - Calculating form factors from sasmodels
  - 1D fitting using sasmodels and bumps
  - 2D fitting
  - Batch fitting
- **4:45pm** Documentation, Tutorials and Bug reporting, *Paul Butler*, 10min
- **4:55pm** How to become a SasView Developer, *Paul Butler*, 5min
- **5:00pm** Community discussion and feedback

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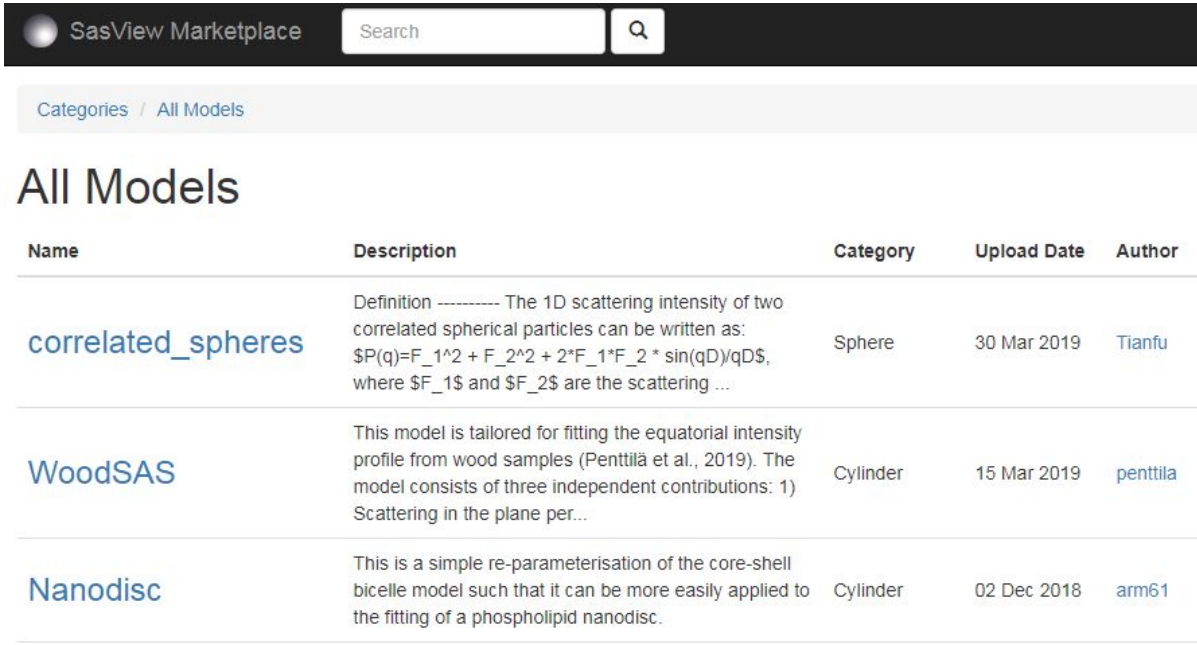
All the work of ISIS Summer Student Lewis O'Driscoll

Uses mySQL & Postgress

8 models contributed by
7 authors in 2 years



Come and Join the Fun!

Things people are saying about SansView/SasView

- *'SansView is a very helpful tool, very complete and easy to use'* - Niki
- *'I want to thank you for this amazing software. It's UI and options make the interpretation of spectra easier and faster'* - Philippe
- *'I really like the SasView software'* - Martin
- *'I have been using SasView as my software of choice for fitting SANS data, and I have been very happy with the software'* - Greg
- *'I have found SasView very easy to use and the batch fit function is a wonderful time saving tool. I can finally stop making painful excel macros!'* - Andrew
- *'I am a new user of SasView and I think it is a very useful and practical tool'* - Arnaud
- *'Within 30 seconds...I am completely converted to SasView!'* - Mike
- *'Thank you for creating and maintaining SasView. It is an incredibly helpful tool, and I use it regularly'* - Pasha
- *'All the best and thank you again to carry on such a good job on SasView'* - Niki
- *'Ooooh NICE PROGRAMME!! Hours of fun!'* - Stuart
- *'I love such amazing software so much. It help our researches a lot.'* - Po-Wei