SasView

An
"open, collaborative, community development" platform for
Small Angle Scattering Data Analysis

SasView

Data Analysis eh?

…. So what exactly does that mean?

Only works on Reduced data

(All the instrumental artifacts are removed and only the science is left)
…. Sorta

Focus on analytical approaches for this package
…. Sorta

Whatever anybody puts into it
…. Sorta

A little history …

2006

Heritage: NIST IGOR macros
SansView is DANSE project output
~ 8.5% of funds were for SANS
+ BUMPS … see later

2011

2012 NIST Supported initial transition from NSF funding

2013 Transition to Community project.

1st Code Camp at NIST April 2013

2014

2nd Code Camp at ISIS April 2014

2015

Move to GitHub
Rename to SasView

v3.0 released
v3.1 released

3rd Code Camp at ESS Feb 2015

2016

4th Code Camp at TU Delft March 2016
5th Code Camp at ORNL Oct 2016

v4.0 released

v4.1 released

2017

6th Code Camp at ILL/ESRF April 2017

7th Code Camp at DMSC October 2017

8th Code Camp at ESS Sept 2018

2018

v5.0b1 released
v4.2 released

1st SasView User Meeting at SAS2018

v4.2.1 released
v5.0b2 released

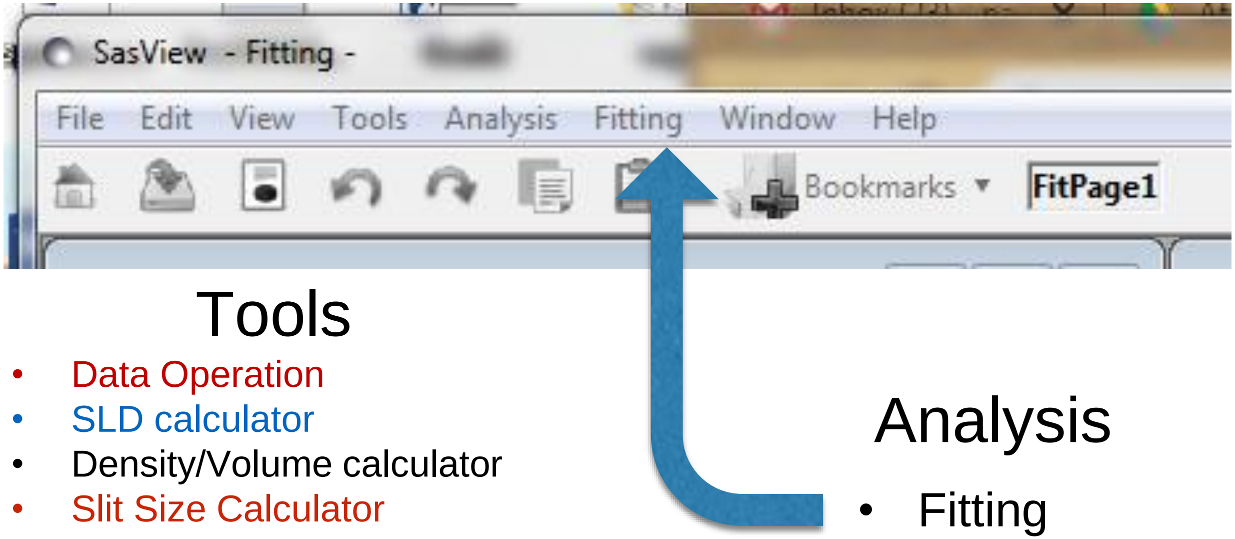
2019

9th Code Camp at ILL/ESRF March 2019

So …

What Can SasView Do Currently?

Perspectives on the data



Tools

- Data Operation
- SLD calculator
- Density/Volume calculator
- Slit Size Calculator
- Kiessig Thickness Calculator
- Q Resolution Estimator
- Generic Scattering calculator
- Orientation Viewer
- Python Shell/Editor
- Image Viewer
- File Converter

Analysis

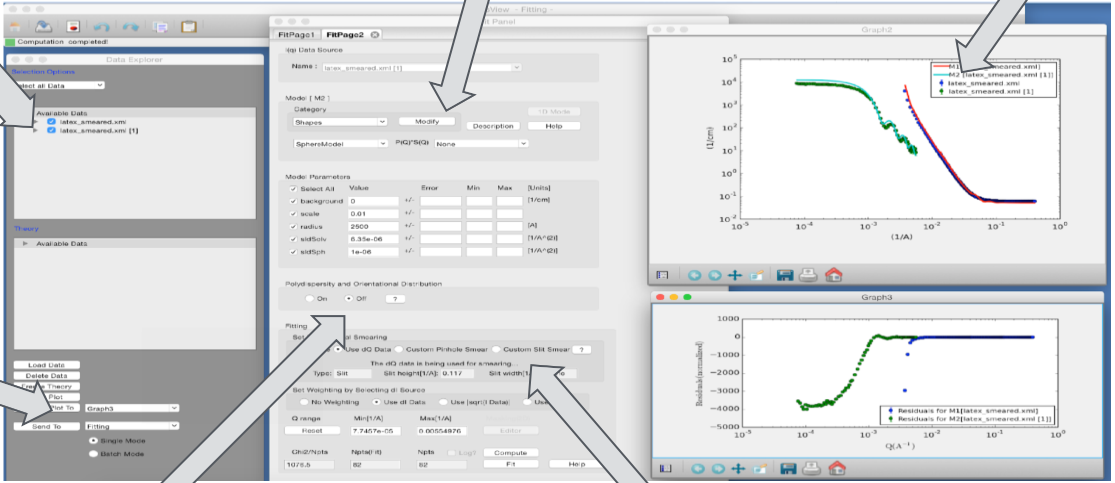
- Fitting
- Invariant
- Pr Inversion
- Correlation Function

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



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

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

Model Parameters

	Value		Error	Min	Max	[Units]
✓ Select All						
✓ 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
Instrumental Smearing: [✓ 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]:

Set Weighting by Selecting dI Source: No Weighting [✓ Use dI Data] Use |sqrt(I Data)|

Q range: Min[1/A] 7.7457e-05 Max[1/A] 0.00554976
Chi2/Npts: 1078.5 Npts(Fit): 82 Npts: 82
Compute Fit Help

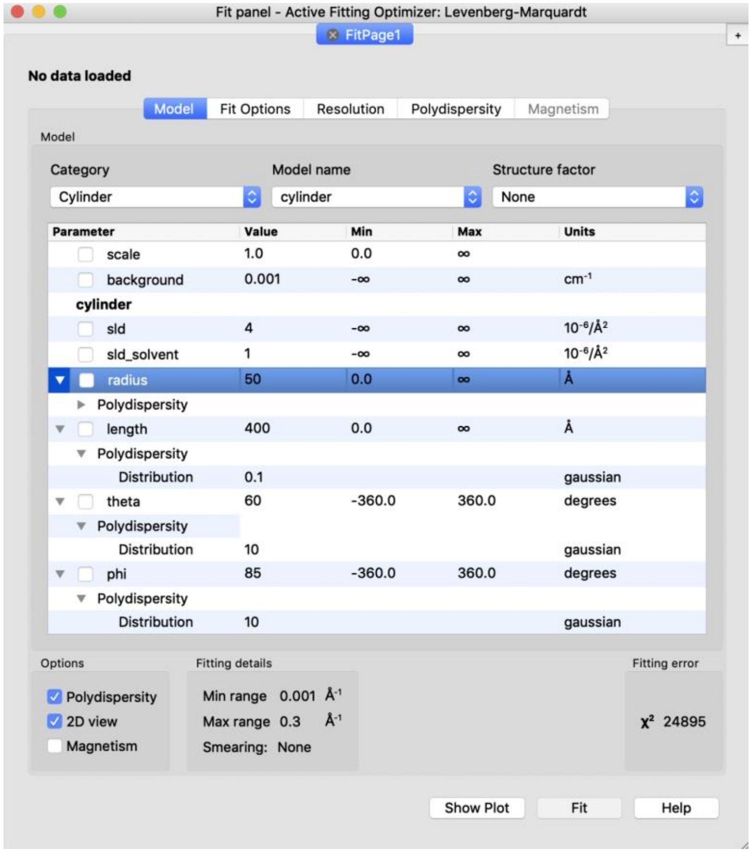
Legend (Graph2): M1 [latex_smeared.xml]; M2 [latex_smeared.xml [1]]; latex_smeared.xml; latex_smeared.xml [1]
Legend (Graph3): Residuals for M1[latex_smeared.xml]; Residuals for M2[latex_smeared.xml [1]]

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

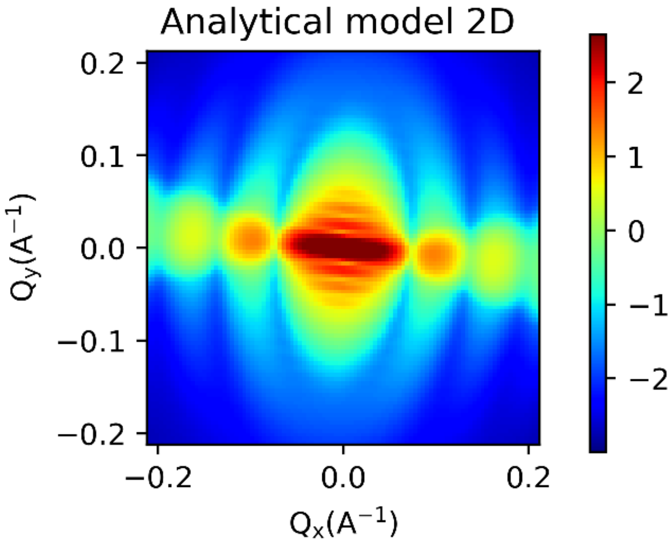
Min range 0.001 Å^{-1}

Max range 0.3 Å^{-1}

Smearing: None

Fitting error

χ^2 24895

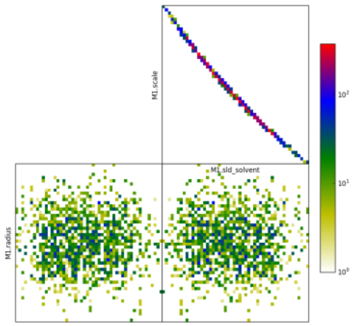


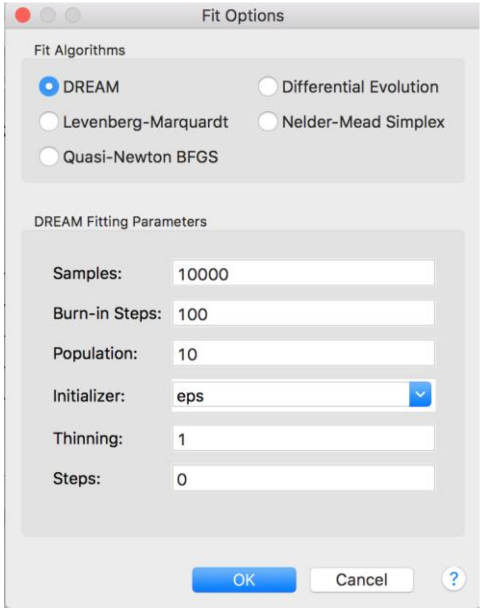
Orientational polydispersity = “jitter”

Decouples the frame for the object’s orientation with respect to the beam and the “jitter” around the axis of the object.

Turning on GPU Option highly recommended for fitting

Fitting Algorithms



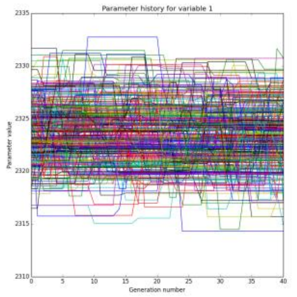

Fit Options

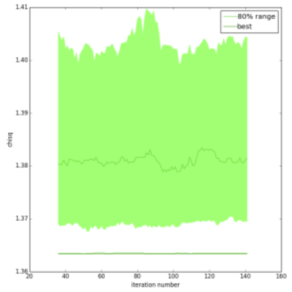
Fit Algorithms

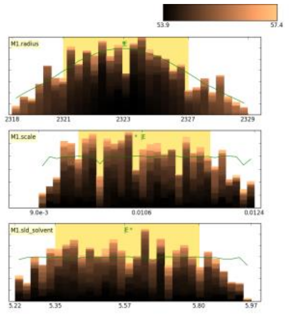
[✓ DREAM] Differential Evolution Levenberg-Marquardt Nelder-Mead Simplex Quasi-Newton BFGS

DREAM Fitting Parameters

Samples:	10000
Burn-in Steps:	100
Population:	10
Initializer:	eps
Thinning:	1
Steps:	0

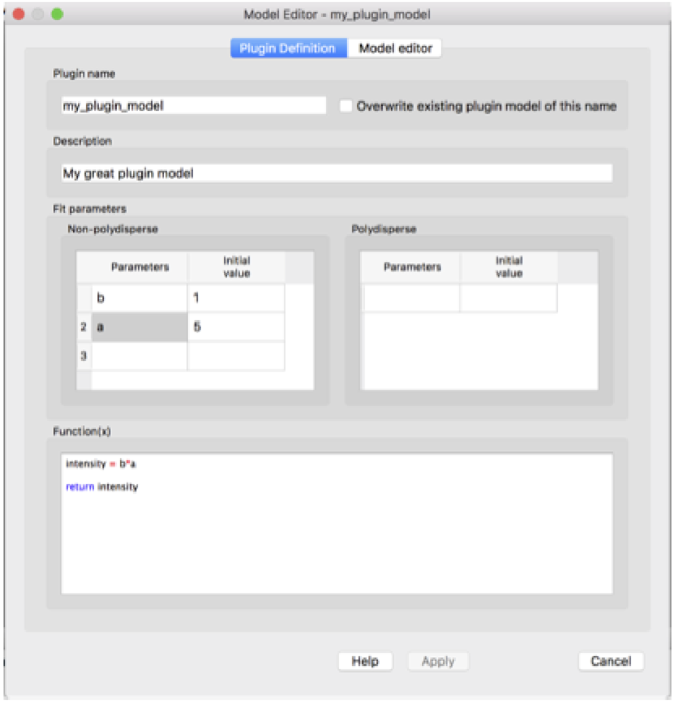






Uses bumps package from P. Kienzle
(also has DANSE origins)

Plugin Model Editor



Plugin name

my_plugin_model

Overwrite existing plugin model of this name

Description

My great plugin model

Fit parameters

Non-polydisperse

	Parameters	Initial value
	b	1
2	a	5
3		

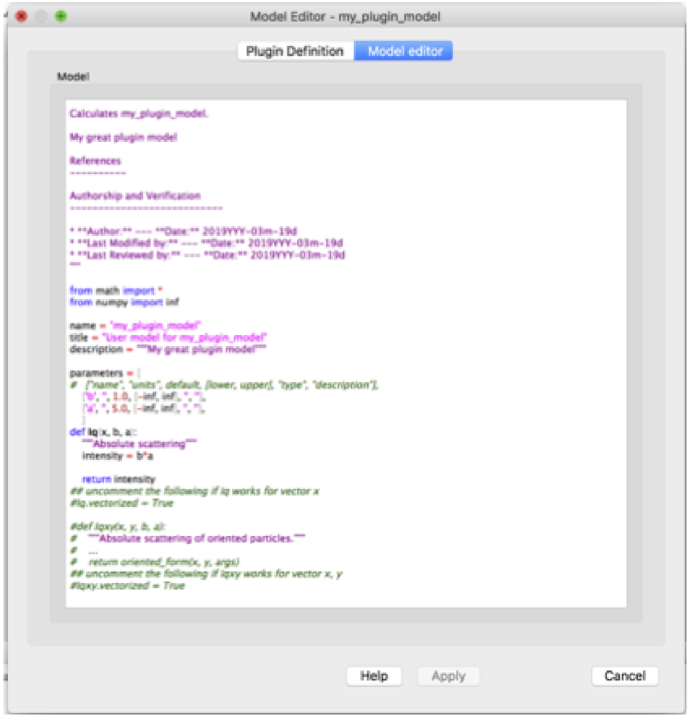
Polydisperse

Parameters	Initial value

Function(x)

```
intensity = b*a

return intensity
```



Model

```
Calculates my_plugin_model.

My great plugin model

References
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Authorship and Verification
----------------------------

* **Author:** --- **Date:** 2019YYY-03m-19d
* **Last Modified by:** --- **Date:** 2019YYY-03m-19d
* **Last Reviewed by:** --- **Date:** 2019YYY-03m-19d
"""


from math import *
from numpy import inf

name = "my_plugin_model"
title = "User model for my_plugin_model"
description = """My great plugin model"""

parameters = [
#   ["name", "units", default, [lower, upper], "type", "description"],
    ['b', '', 1.0, [-inf, inf], '', ''],
    ['a', '', 5.0, [-inf, inf], '', ''],
    ]
def Iq(x, b, a):
    """Absolute scattering"""
    intensity = b*a

    return intensity
## uncomment the following if Iq works for vector x
#Iq.vectorized = True

#def Iqxy(x, y, b, a):
#    """Absolute scattering of oriented particles."""
#    ...
#    return oriented_form(x, y, args)
## uncomment the following if Iqxy works for vector x, y
#Iqxy.vectorized = True
```
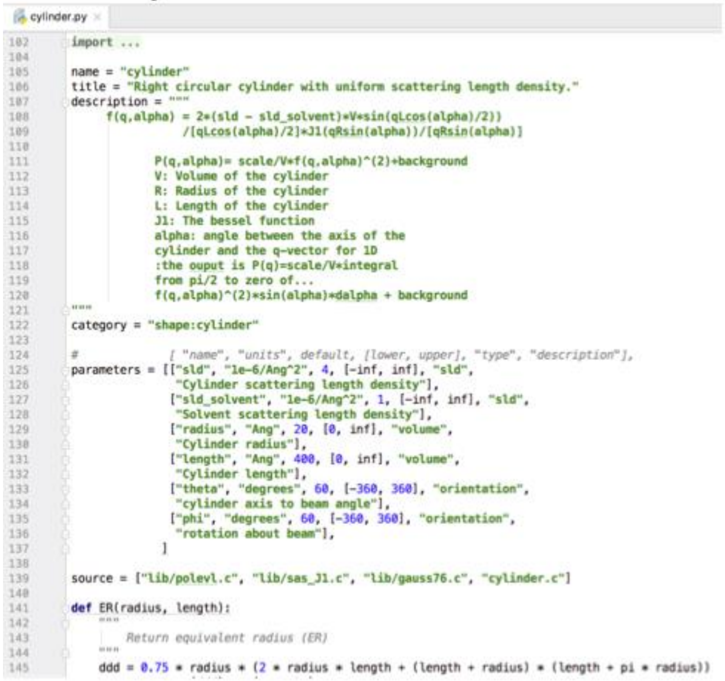
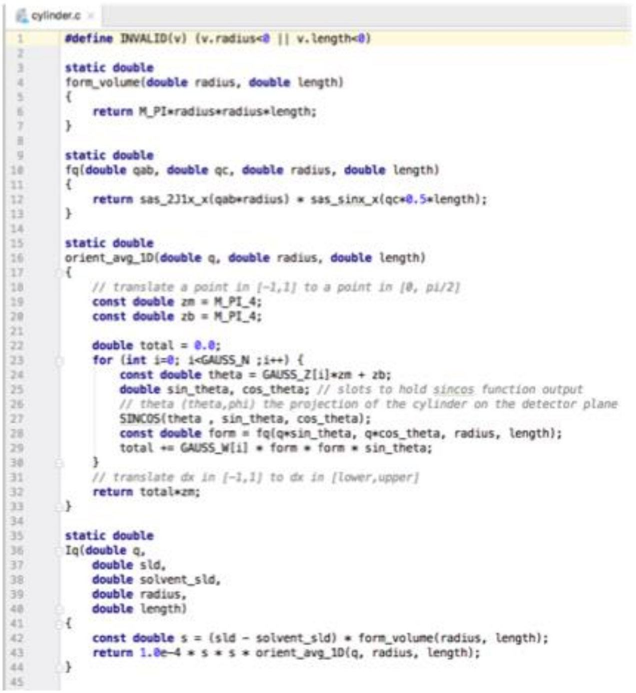

Python & C model files



cylinder.py

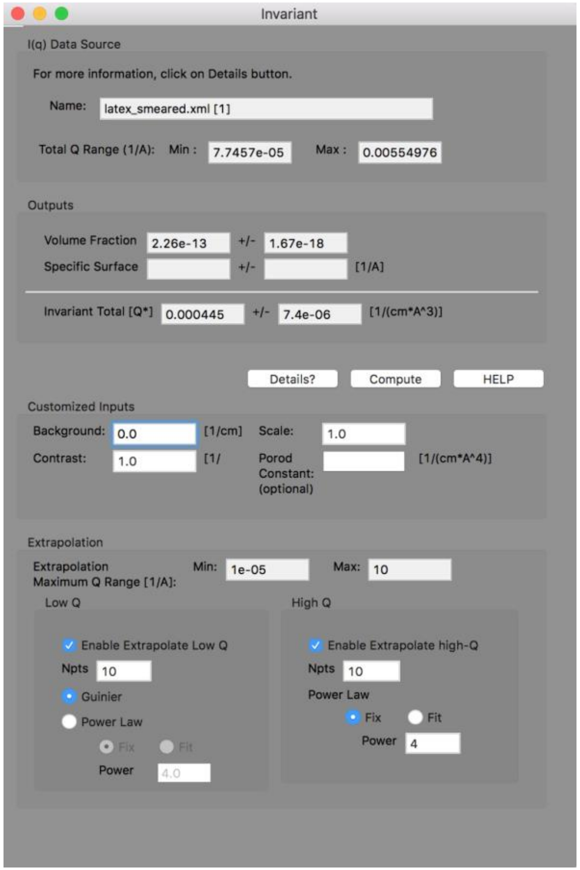
```python
import ...

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

```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



Invariant

I(q) Data Source

For more information, click on Details button.

Name: latex_smeared.xml [1]

Total Q Range (1/A): Min : 7.7457e-05 Max : 0.00554976

Outputs

Volume Fraction	2.26e-13	+/-	1.67e-18	
Specific Surface		+/-		[1/A]
Invariant Total [Q*]	0.000445	+/-	7.4e-06	[1/(cm*A^3)]

Customized Inputs

Background: 0.0 [1/cm] Scale: 1.0

Contrast: 1.0 [1/ Porod Constant: (optional) [1/(cm*A^4)]

Extrapolation

Extrapolation Maximum Q Range [1/A]: Min: 1e-05 Max: 10

Low Q

✓ Enable Extrapolate Low Q

Npts 10

● Guinier

○ Power Law

● Fix ○ Fit

Power 4.0

High Q

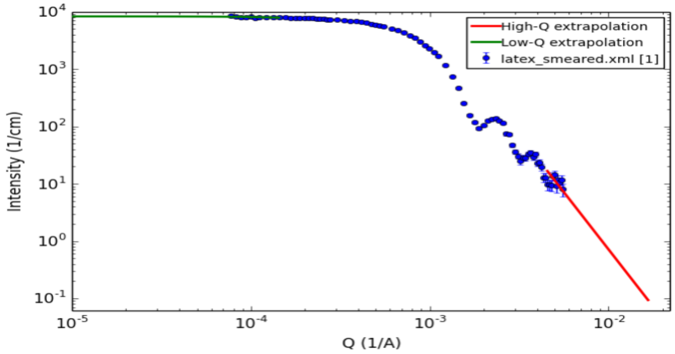
✓ Enable Extrapolate high-Q

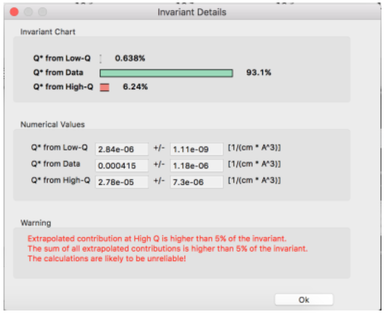
Npts 10

Power Law

● Fix ○ Fit

Power 4





Invariant Details

Invariant Chart

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

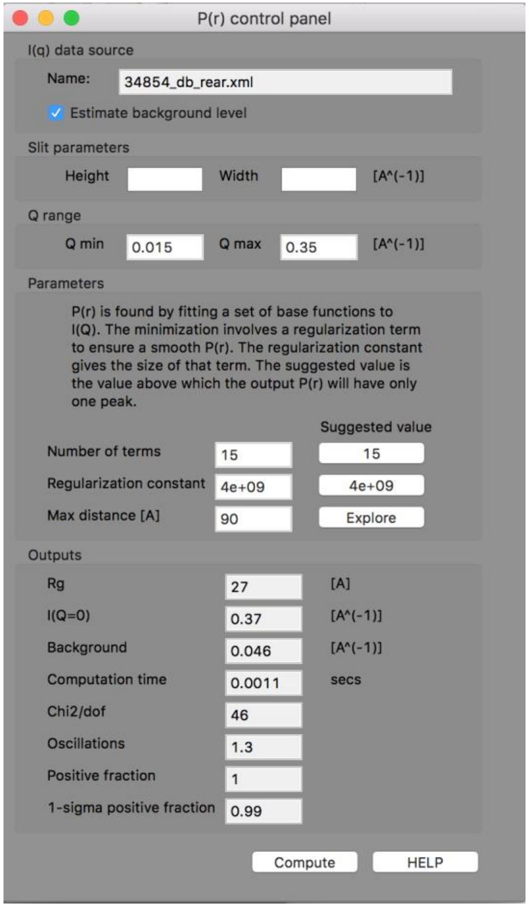
Numerical Values

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

P(r) Inversion



P(r) control panel

I(q) data source

Name:	34854_db_rear.xml

[✓] Estimate background level

Slit parameters

Height		Width		[A^(-1)]

Q range

Q min	0.015	Q max	0.35	[A^(-1)]

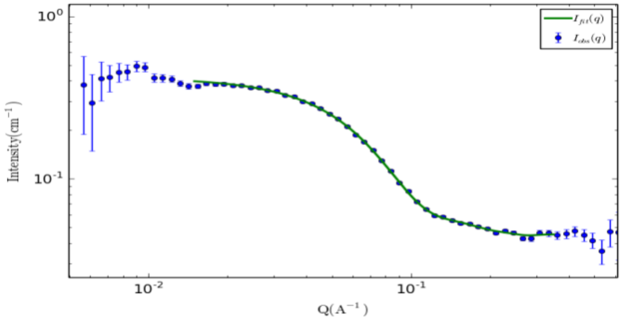
Parameters

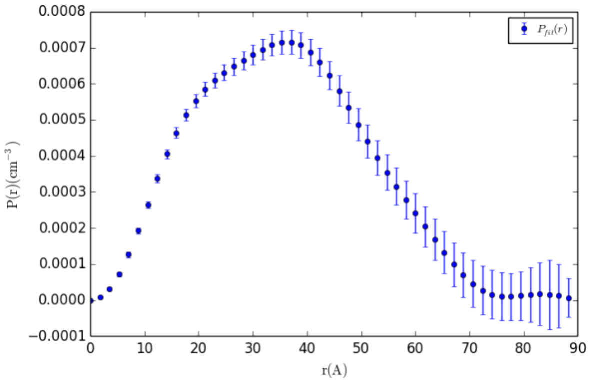
P(r) is found by fitting a set of base functions to I(Q). The minimization involves a regularization term to ensure a smooth P(r). The regularization constant gives the size of that term. The suggested value is the value above which the output P(r) will have only one peak.

		Suggested value
Number of terms	15	15
Regularization constant	4e+09	4e+09
Max distance [A]	90	Explore

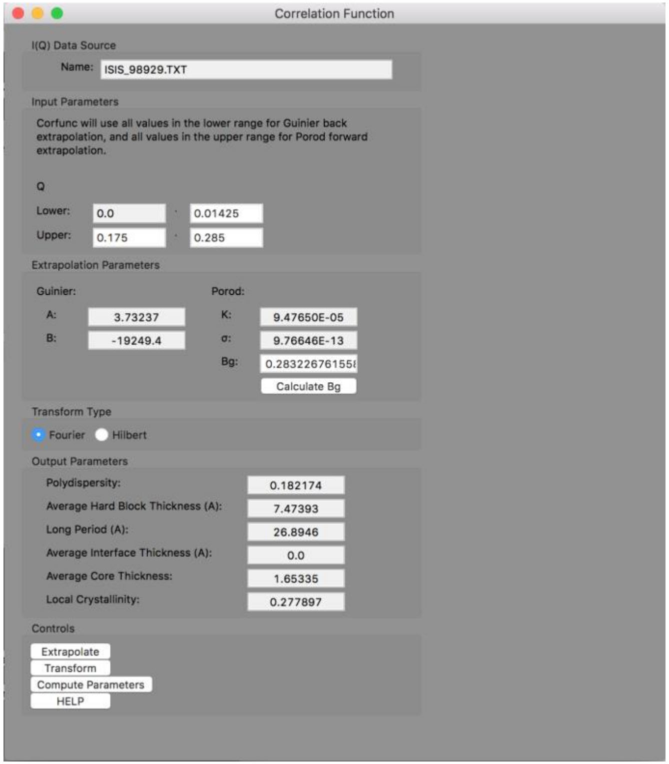
Outputs

Rg	27	[A]
I(Q=0)	0.37	[A^(-1)]
Background	0.046	[A^(-1)]
Computation time	0.0011	secs
Chi2/dof	46	
Oscillations	1.3	
Positive fraction	1	
1-sigma positive fraction	0.99	





Correlation Function Analysis (new!)



I(Q) Data Source

Name: ISIS_98929.TXT

Input Parameters

Corfunc will use all values in the lower range for Guinier back extrapolation, and all values in the upper range for Porod forward extrapolation.

Q

Lower:	0.0	0.01425
Upper:	0.175	0.285

Extrapolation Parameters

Guinier:		Porod:	
A:	3.73237	K:	9.47650E-05
B:	-19249.4	σ:	9.76646E-13
		Bg:	0.28322676155

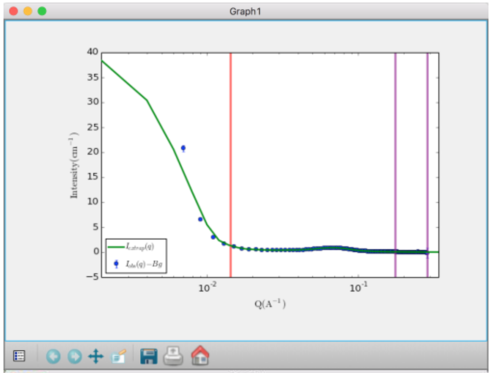
Transform Type

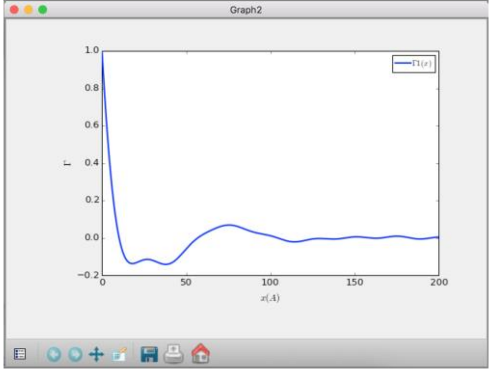
[✓ Fourier] Hilbert

Output Parameters

Polydispersity:	0.182174
Average Hard Block Thickness (A):	7.47393
Long Period (A):	26.8946
Average Interface Thickness (A):	0.0
Average Core Thickness:	1.65335
Local Crystallinity:	0.277897

Controls

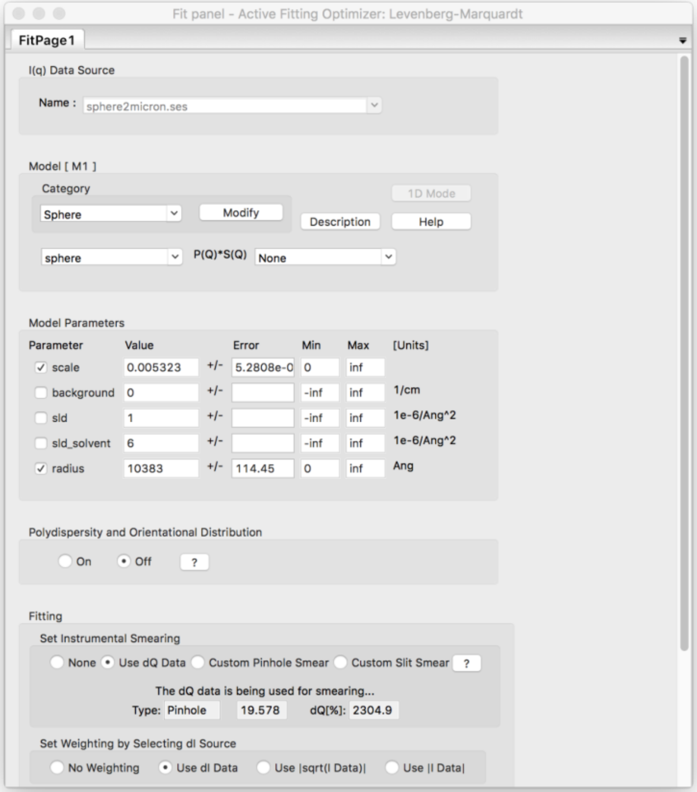




CCP13 (Fiber Diffraction) legacy code (Fortran)

(ISIS summer student)

SESANS Analysis



Fit panel - Active Fitting Optimizer: Levenberg-Marquardt

FitPage1

I(q) Data Source

Name : sphere2micron.ses

Model [M1]

Category: Sphere — Modify — 1D Mode — Description — Help

sphere — P(Q)*S(Q): None

Model Parameters

Parameter	Value		Error	Min	Max	[Units]
✓ scale	0.005323	+/-	5.2808e-0	0	inf	
background	0	+/-		-inf	inf	1/cm
sld	1	+/-		-inf	inf	1e-6/Ang^2
sld_solvent	6	+/-		-inf	inf	1e-6/Ang^2
✓ radius	10383	+/-	114.45	0	inf	Ang

Polydispersity and Orientational Distribution

On [✓ Off] ?

Fitting

Set Instrumental Smearing

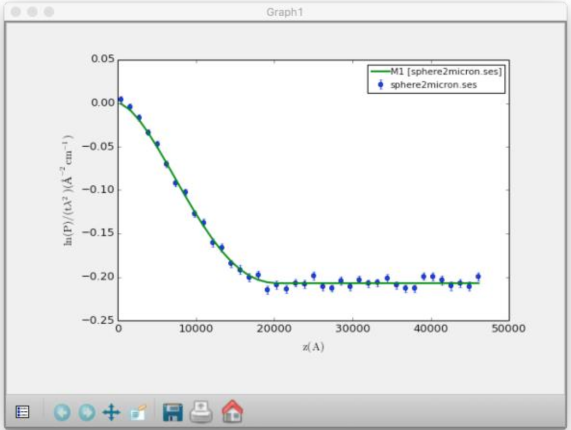
None [✓ Use dQ Data] Custom Pinhole Smear Custom Slit Smear ?

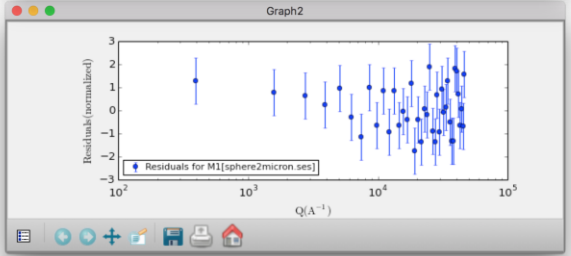
The dQ data is being used for smearing...

Type: Pinhole 19.578 dQ[%]: 2304.9

Set Weighting by Selecting dI Source

No Weighting [✓ Use dI Data] Use |sqrt(I Data)| Use |I Data|



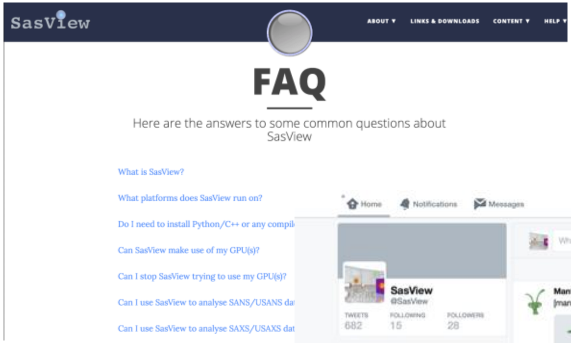


Automatic Hankel Transform of SANS models

(TU Delft & ISIS)

Resources, Education & Outreach

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



FAQ

Here are the answers to some common questions about SasView

What is SasView?

What platforms does SasView run on?

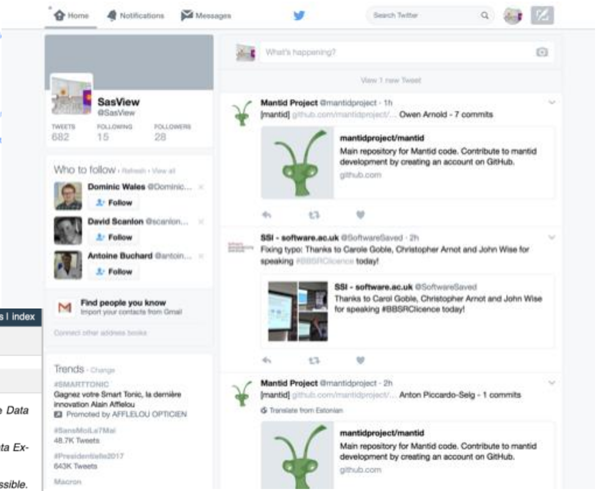
Do I need to install Python/C++ or any compil

Can SasView make use of my GPU(s)?

Can I stop SasView trying to use my GPU(s)?

Can I use SasView to analyse SANS/USANS da

Can I use SasView to analyse SAXS/USAXS dat



SasView @SasView

TWEETS 682 FOLLOWING 15 FOLLOWERS 28

Who to follow · Refresh · View all

Dominic Wales @Dominic... Follow

David Scanlon @scanlon... Follow

Antoine Buchard @antoin... Follow

Find people you know
Import your contacts from Gmail

Connect other address books

Trends · Change

#SMARTTONIC
Gagnez votre Smart Tonic, la dernière innovation Alain Afflelou
Promoted by AFFLELOU OPTICIEN

#SansMoiLe7Mai
48.7K Tweets

#Presidentielle2017
643K Tweets

Macron

Mantid Project @mantidproject · 1h
[mantid] github.com/mantidproject/... Owen Arnold - 7 commits

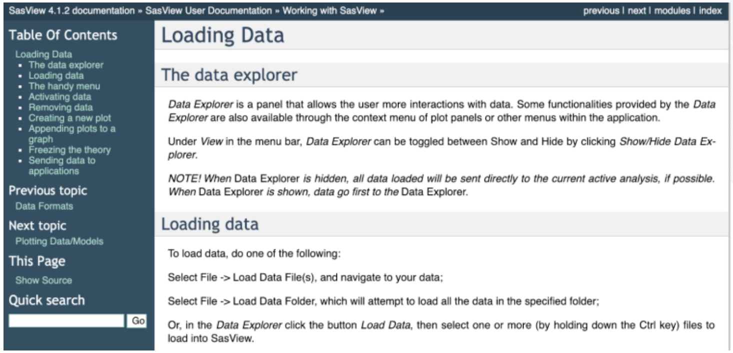
mantidproject/mantid
Main repository for Mantid code. Contribute to mantid development by creating an account on GitHub.
github.com

SSI - software.ac.uk @SoftwareSaved · 2h
Fixing typo: Thanks to Carole Goble, Christopher Arnot and John Wise for speaking #BBSRCIicence today!

SSI - software.ac.uk @SoftwareSaved
Thanks to Carol Goble, Christopher Arnot and John Wise for speaking #BBSRCIicence today!

Mantid Project @mantidproject · 2h
[mantid] github.com/mantidproject/... Anton Piccardo-Selg - 1 commits
Translate from Estonian

mantidproject/mantid
Main repository for Mantid code. Contribute to mantid development by creating an account on GitHub.
github.com


SasView 4.1.2 documentation » SasView User Documentation » Working with SasView » previous | next | modules | index

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- Appending plots to a graph
- Freezing the theory
- Sending data to applications

Previous topic
Data Formats

Next topic
Plotting Data/Models

This Page
Show Source

Quick search
Go

Loading Data

The data explorer

Data Explorer is a panel that allows the user more interactions with data. Some functionalities provided by the *Data Explorer* are also available through the context menu of plot panels or other menus within the application.

Under *View* in the menu bar, *Data Explorer* can be toggled between Show and Hide by clicking *Show/Hide Data Explorer.*

NOTE! When Data Explorer *is hidden, all data loaded will be sent directly to the current active analysis, if possible. When* Data Explorer *is shown, data go first to the* Data Explorer.

Loading data

To load data, do one of the following:

Select File -> Load Data File(s), and navigate to your data;

Select File -> Load Data Folder, which will attempt to load all the data in the specified folder;

Or, in the *Data Explorer* click the button *Load Data*, then select one or more (by holding down the Ctrl key) files to load into SasView.

Resources, Education & Outreach

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

Go to each FitPage in turn and select the **core_shell_sphere** model. The three theory curves will be added to the graph.

Enter the following SLD values in the appropriate FitPage's:

Contrast / SLD	*sld_core*	*sld_shell*	*sld_solvent*
'core'	+6.39×10^{-6} Å^{-2}	+0.62×10^{-6} Å^{-2}	-0.28×10^{-6} Å^{-2}
'shell'	+6.39×10^{-6} Å^{-2}	+0.62×10^{-6} Å^{-2}	+6.68×10^{-6} Å^{-2}
'drop'	-0.55×10^{-6} Å^{-2}	+0.62×10^{-6} Å^{-2}	+6.68×10^{-6} Å^{-2}

The objective of this simultaneous fit will be to find common values for the *radius* (of the droplet cores) and *thickness* (of the surfactant layer) parameters that provide a good solution to all three datasets.

(Depending on how meticulous the p
possible to find a common scale param
volume fraction of droplets in each sam

We now need to tell SasView that the
the *radius* for the 'shell' contrast data
contrast dataset, and so on. This is
constrain parameters that are free to c
thickness parameters. However, we
parameters so check those too.

Tip: Always check the parameters y
before opening the Constrained or Sim

Now go to the Menu Bar and click Fittin

In the Const & Simul Fit page, check the boxes under Model Title (or just Select all!) to select those theories that you want to construct constraints for. For this example, check all three theories. Then, in the section of the page called Fit Constraints, check the Yes radio button to Add Constraint.

To constrain all identically named parameters to fit simultaneously to the same value across all the selected theories we can use the Easy Setup drop-down buttons. There are, however, several ways that we can set up the constraint equalities. Here we shall use the 'core' contrast (M3) as the reference. So set M2 = M3 and click Set All. Then set M1 = M3 and click Set All.

Tip: If you need to scale parameter values between FitPage's then use the free-form constraint box below Easy Setup. The right-hand side of the equality can be of the form: scalar _ [Mi] parameter_name

, remove
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scattering

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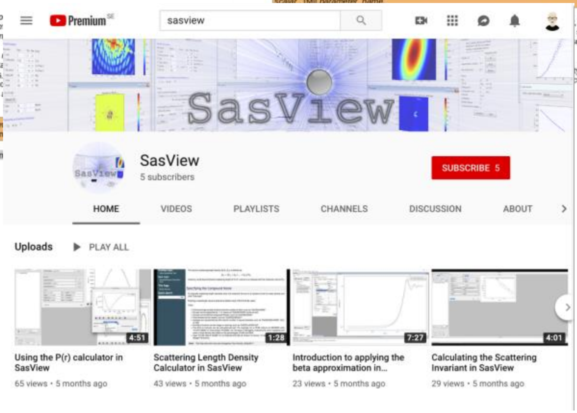

SasView
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Introduction to applying the beta approximation in... — 7:27 — 23 views • 5 months ago

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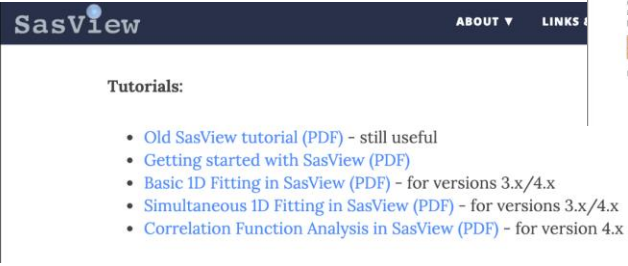

Tutorials:

- Old SasView tutorial (PDF) - still useful
- Getting started with SasView (PDF)
- Basic 1D Fitting in SasView (PDF) - for versions 3.x/4.x
- Simultaneous 1D Fitting in SasView (PDF) - for versions 3.x/4.x
- Correlation Function Analysis in SasView (PDF) - for version 4.x

Resources, Education & Outreach

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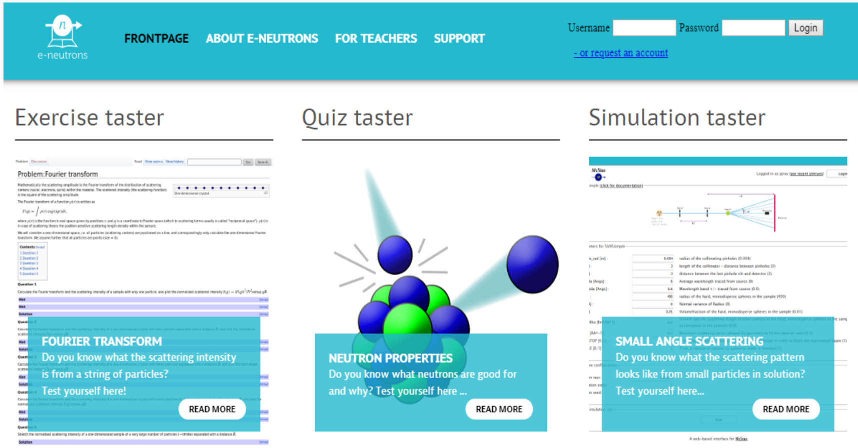
e-neutrons
FRONTPAGE
ABOUT E-NEUTRONS
FOR TEACHERS
SUPPORT
Username
Password
Login
- or request an account
Exercise taster
Quiz taster
Simulation taster
FOURIER TRANSFORM
Do you know what the scattering intensity is from a string of particles? Test yourself here!
READ MORE
NEUTRON PROPERTIES
Do you know what neutrons are good for and why? Test yourself here ...
READ MORE
SMALL ANGLE SCATTERING
Do you know what the scattering pattern looks like from small particles in solution? Test yourself here...
READ MORE

All the work of ISIS Sandwich Student Michael Oakley

Resources, Education & Outreach

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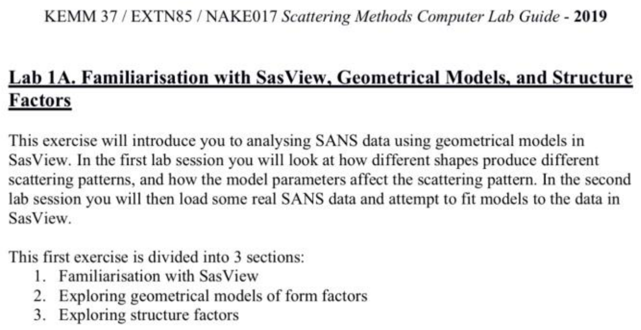


KEMM 37 / EXTN85 / NAKE017 *Scattering Methods Computer Lab Guide* - **2019**

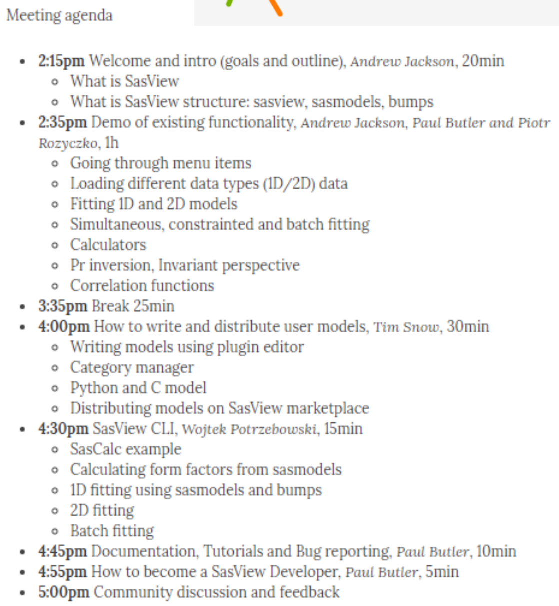
Lab 1A. Familiarisation with SasView, Geometrical Models, and Structure Factors

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

Resources, Education & Outreach

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- E-learning
- Twitter
- Slack
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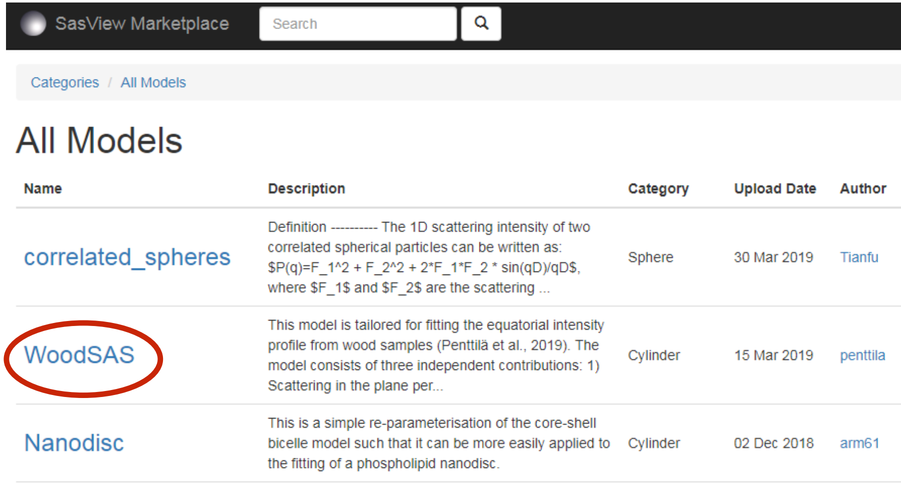
- (Marketplace)

All the work of ISIS Summer Student Lewis O'Driscoll

Uses mySQL & Postgress

8 models contributed by 7 authors in 2 years



All Models

Name	Description	Category	Upload Date	Author
correlated_spheres	Definition ---------- The 1D scattering intensity of two correlated spherical particles can be written as: $P(q)=F_1^2 + F_2^2 + 2*F_1*F_2 * sin(qD)/qD$, where F_1 and F_2 are the scattering ...	Sphere	30 Mar 2019	Tianfu
WoodSAS	This model is tailored for fitting the equatorial intensity profile from wood samples (Penttilä et al., 2019). The model consists of three independent contributions: 1) Scattering in the plane per...	Cylinder	15 Mar 2019	penttila
Nanodisc	This is a simple re-parameterisation of the core-shell bicelle model such that it can be more easily applied to the fitting of a phospholipid nanodisc.	Cylinder	02 Dec 2018	arm61

So …

Where is SasView Going?
What will it do for me?

Scientific Software Development and The cyberinfrastructure revolution

- **Never enough resources to achieve the vision we have**
- **No resources for long term maintenance and support.**

Problem:

- To reap the benefit of investment in software developments requires foundational long term support.
- If entity that supports the development also must support the "maintenance" forever, the entity will soon cease to be able to fund new projects.

CONCLUSION: This paradigm is broken!!!

FACTS OF LIFE:

- **Resources are finite**
- **Needs are infinite**

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!

How We Work

Open, Collaborative, Community Development

Code is open source and publicly hosted at Github

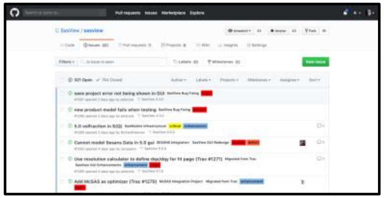
Released under BSD 3-clause license

Bug and Enhancement Ticket System

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

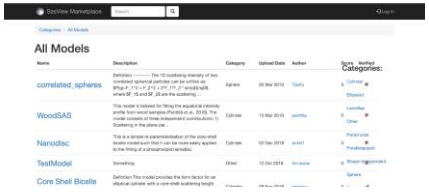
Model Marketplace DOI for each release

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



- save project error not being shown in GUI
- new product model fails when testing
- 5.0 volfraction in S(Q)
- Cannot model Sesans Data in 5.0 gui
- Use resolution calculator to define dqx/dqy for fit page (Trac #1271)
- Add McSAS as optimizer (Trac #1270)

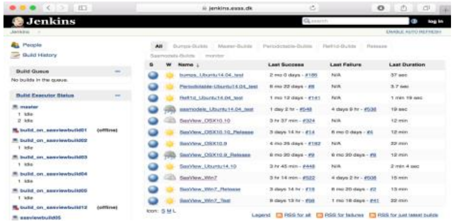
Model Marketplace for users to share their models
marketplace.sasview.org



All Models

Name	Description	Category	Upload Date	Author	Score	Verified
correlated_spheres	[illegible]	Sphere	[illegible] Mar 2019	[illegible]	[illegible]	✗
WoodSAS	This model is tailored for fitting the equatorial intensity profile from wood samples [illegible]	Cylinder	15 Mar 2019	[illegible]	[illegible]	✗
Nanodisc	This is a simple re-parameterisation of the core-shell bicelle model such that it can be more easily applied to the fitting of a phospholipid nanodisc.	Cylinder	02 Dec 2018	[illegible]	[illegible]	✗
TestModel	Something	Other	12 Oct 2018	[illegible]	[illegible]	✗
Core Shell Bicelle	Definition This model provides the form factor for an elliptical cylinder with a core-shell scattering length [illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Automated Builds
build.sasview.org



Name	Last Success	Last Failure	Last Duration
bumps_Ubuntu14.04_test	2 mo 0 days - #185	N/A	37 sec
Periodictable-Ubuntu14.04_test	8 mo 22 days - #8	N/A	3.7 sec
Refl1d_Ubuntu14.04_test	1 mo 12 days - #141	N/A	1 min 19 sec
sasmodels_Ubuntu14.04_test	1 day 2 hr - #540	4 days 9 hr - #536	19 sec
SasView_OSX10.10	3 hr 37 min - #324	N/A	12 min
SasView_OSX10.10_Release	3 days 14 hr - #14	8 mo 0 days - #4	12 min
SasView_OSX10.9	4 mo 26 days - #182	N/A	22 min
SasView_OSX10.9_Release	8 mo 20 days - #9	8 mo 20 days - #8	12 min
SasView_Ubuntu14.10	3 hr 45 min - #448	N/A	2 min 4 sec
SasView_Win7	3 hr 14 min - #522	4 days 2 hr - #508	15 min
SasView_Win7_Release	3 days 14 hr - #18	8 mo 20 days - #2	13 min
SasView_Win7_Test	8 days 13 hr - #98	1 mo 18 days - #41	22 min

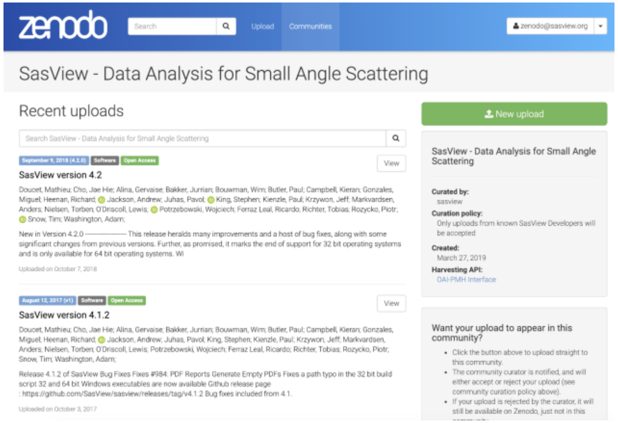
http://www.sasview.org http://github.com/SasView

How We Work

Open, Collaborative, Community Development

DOI for each release

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



SasView - Data Analysis for Small Angle Scattering

Recent uploads

September 9, 2018 (4.2.0) Software Open Access

SasView version 4.2

Doucet, Mathieu; Cho, Jae Hie; Alina, Gervaise; Bakker, Jurrian; Bouwman, Wim; Butler, Paul; Campbell, Kieran; Gonzales, Miguel; Heenan, Richard; Jackson, Andrew; Juhas, Pavol; King, Stephen; Kienzle, Paul; Krzywon, Jeff; Markvardsen, Anders; Nielsen, Torben; O'Driscoll, Lewis; Potrzebowski, Wojciech; Ferraz Leal, Ricardo; Richter, Tobias; Rozycko, Piotr; Snow, Tim; Washington, Adam;

New in Version 4.2.0 ------------------ This release heralds many improvements and a host of bug fixes, along with some significant changes from previous versions. Further, as promised, it marks the end of support for 32 bit operating systems and is only available for 64 bit operating systems. Wi

Uploaded on October 7, 2018

August 12, 2017 (v1) Software Open Access

SasView version 4.1.2

Doucet, Mathieu; Cho, Jae Hie; Alina, Gervaise; Bakker, Jurrian; Bouwman, Wim; Butler, Paul; Campbell, Kieran; Gonzales, Miguel; Heenan, Richard; Jackson, Andrew; Juhas, Pavol; King, Stephen; Kienzle, Paul; Krzywon, Jeff; Markvardsen, Anders; Nielsen, Torben; O'Driscoll, Lewis; Potrzebowski, Wojciech; Ferraz Leal, Ricardo; Richter, Tobias; Rozycko, Piotr; Snow, Tim; Washington, Adam;

Release 4.1.2 of SasView Bug Fixes Fixes #984: PDF Reports Generate Empty PDFs Fixes a path typo in the 32 bit build script 32 and 64 bit Windows executables are now available Github release page : https://github.com/SasView/sasview/releases/tag/v4.1.2 Bug fixes included from 4.1.

Uploaded on October 3, 2017

SasView - Data Analysis for Small Angle Scattering

Curated by: sasview

Curation policy: Only uploads from known SasView Developers will be accepted

Created: March 27, 2019

Harvesting API: OAI-PMH Interface

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- The community curator is notified, and will either accept or reject your upload (see community curation policy above).
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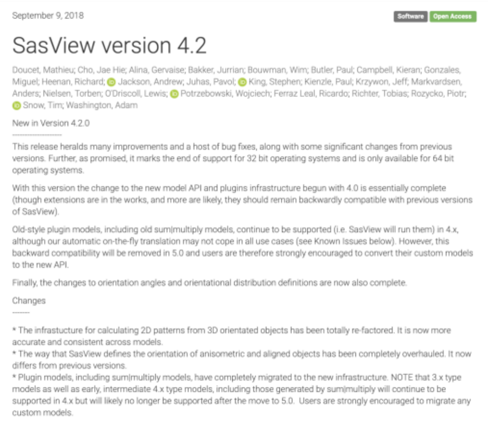


September 9, 2018 Software Open Access

SasView version 4.2

Doucet, Mathieu; Cho, Jae Hie; Alina, Gervaise; Bakker, Jurrian; Bouwman, Wim; Butler, Paul; Campbell, Kieran; Gonzales, Miguel; Heenan, Richard; Jackson, Andrew; Juhas, Pavol; King, Stephen; Kienzle, Paul; Krzywon, Jeff; Markvardsen, Anders; Nielsen, Torben; O'Driscoll, Lewis; Potrzebowski, Wojciech; Ferraz Leal, Ricardo; Richter, Tobias; Rozycko, Piotr; Snow, Tim; Washington, Adam

New in Version 4.2.0

This release heralds many improvements and a host of bug fixes, along with some significant changes from previous versions. Further, as promised, it marks the end of support for 32 bit operating systems and is only available for 64 bit operating systems.

With this version the change to the new model API and plugins infrastructure begun with 4.0 is essentially complete (though extensions are in the works, and more are likely, they should remain backwardly compatible with previous versions of SasView).

Old-style plugin models, including old sum|multiply models, continue to be supported (i.e. SasView will run them) in 4.x, although our automatic on-the-fly translation may not cope in all use cases (see Known Issues below). However, this backward compatibility will be removed in 5.0 and users are therefore strongly encouraged to convert their custom models to the new API.

Finally, the changes to orientation angles and orientational distribution definitions are now also complete.

Changes

----

* The infrastucture for calculating 2D patterns from 3D orientated objects has been totally re-factored. It is now more accurate and consistent across models.
* The way that SasView defines the orientation of anisometric and aligned objects has been completely overhauled. It now differs from previous versions.
* Plugin models, including sum|multiply models, have completely migrated to the new infrastructure. NOTE that 3.x type models as well as early, intermediate 4.x type models, including those generated by sum|multiply will continue to be supported in 4.x but will likely no longer be supported after the move to 5.0. Users are strongly encouraged to migrate any custom models.

http://www.sasview.org

http://github.com/SasView

How We Work

Open, Collaborative, Community Development

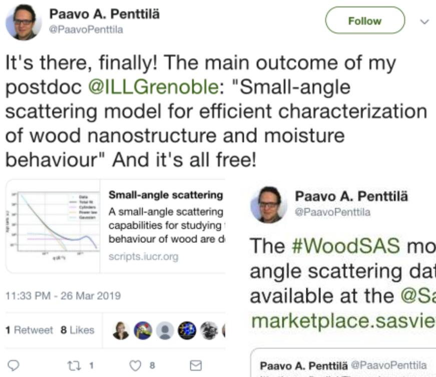
We work together towards common goals formulated through community input, with two guiding principles ...

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.

How We Work

Open, Collaborative, Community Development



Paavo A. Penttilä
@PaavoPenttila
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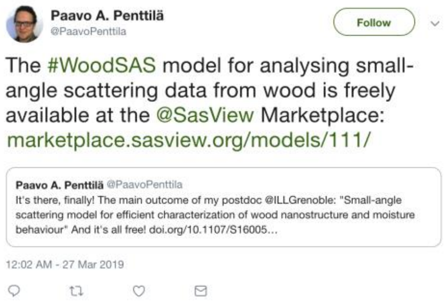
It's there, finally! The main outcome of my postdoc @ILLGrenoble: "Small-angle scattering model for efficient characterization of wood nanostructure and moisture behaviour" And it's all free!

Small-angle scattering
A small-angle scattering
capabilities for studying
behaviour of wood are d
scripts.iucr.org

11:33 PM - 26 Mar 2019

1 Retweet 8 Likes



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@PaavoPenttila
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The #WoodSAS model for analysing small-angle scattering data from wood is freely available at the @SasView Marketplace: marketplace.sasview.org/models/111/

Paavo A. Penttilä @PaavoPenttila
It's there, finally! The main outcome of my postdoc @ILLGrenoble: "Small-angle scattering model for efficient characterization of wood nanostructure and moisture behaviour" And it's all free! doi.org/10.1107/S16005…

12:02 AM - 27 Mar 2019

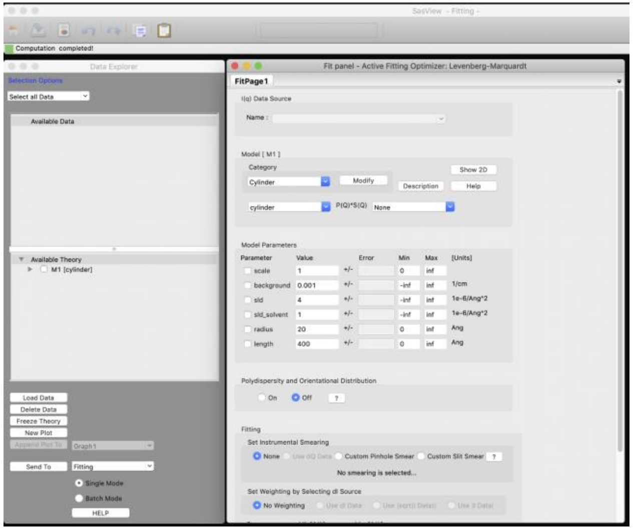
Ask not what the community is going to do for you,
ask what you can do for the community

- P. Butler, March 2019

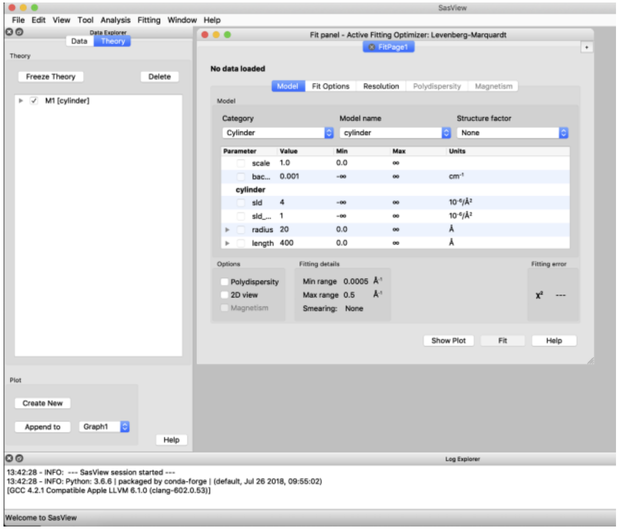
http://www.sasview.org

http://github.com/SasView

SINE 2020 Work - GUI



Parameter	Value		Error	Min	Max	[Units]
scale	1	+/-		0	inf	
background	0.001	+/-		-inf	inf	1/cm
sld	4	+/-		-inf	inf	1e-6/Ang*2
sld_solvent	1	+/-		-inf	inf	1e-6/Ang*2
radius	20	+/-		0	inf	Ang
length	400	+/-		0	inf	Ang



Parameter	Value	Min	Max	Units
scale	1.0	0.0	∞	
bac...	0.001	-∞	∞	cm^{-1}
cylinder				
sld	4	-∞	∞	$10^{-6}/Å^2$
sld_...	1	-∞	∞	$10^{-6}/Å^2$
radius	20	0.0	∞	Å
length	400	0.0	∞	Å

Min range 0.0005 $Å^{-1}$
Max range 0.5 $Å^{-1}$
Smearing: None

χ^2 ---

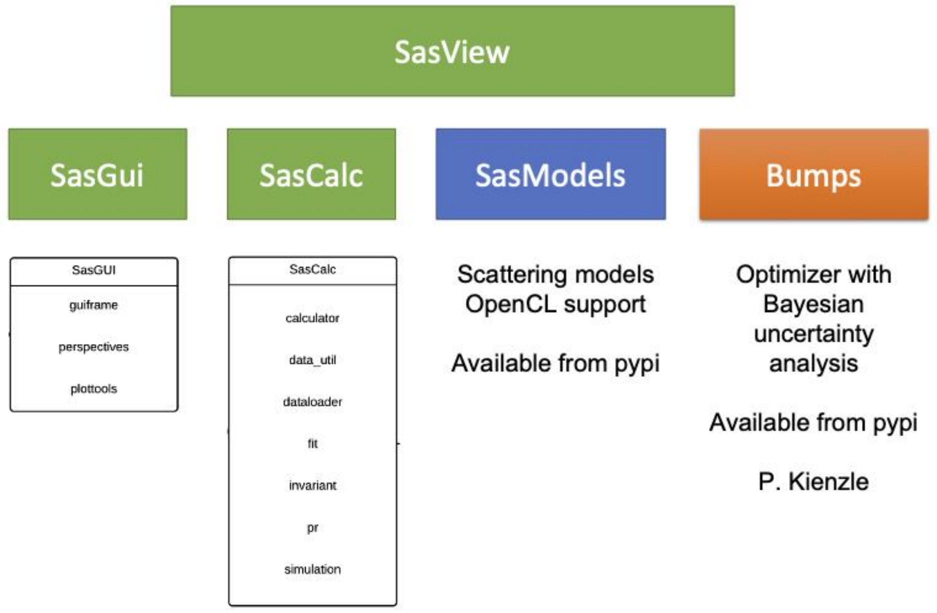
```
13:42:28 - INFO:  --- SasView session started ---
13:42:28 - INFO: Python: 3.6.6 | packaged by conda-forge | (default, Jul 26 2018, 09:55:02)
[GCC 4.2.1 Compatible Apple LLVM 6.1.0 (clang-602.0.53)]
```

Welcome to SasView

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



Scattering models
OpenCL support

Available from pypi

Optimizer with Bayesian uncertainty analysis

Available from pypi

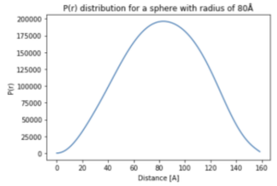
P. Kienzle

Jupyter Notebooks

SasCalc example

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

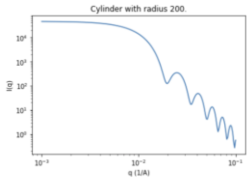
```
In [2]:  from sas.sascalc.dataloader.loader import Loader
         from sas.sascalc.pr.invertor import Invertor
         import matplotlib.pyplot as plt
         import numpy as np

         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()
```



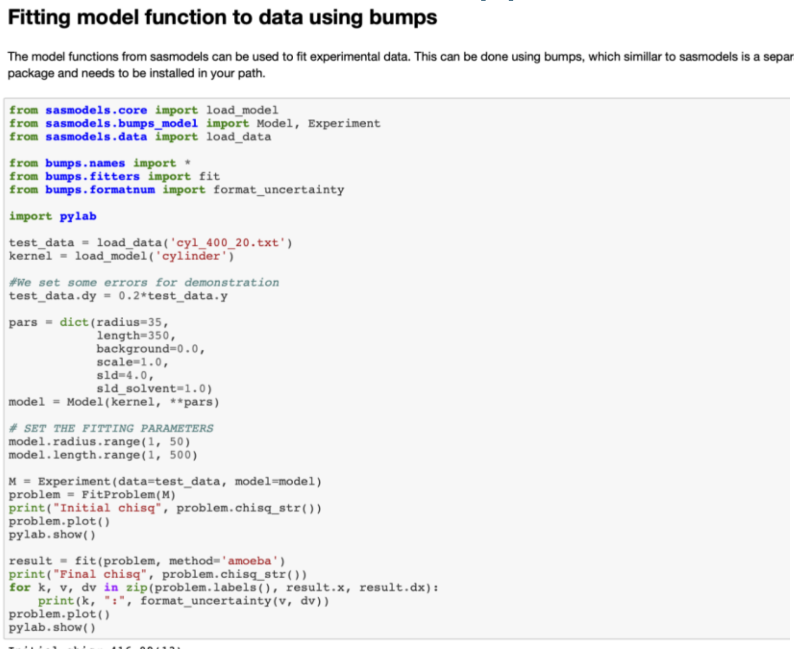
SasModels example

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

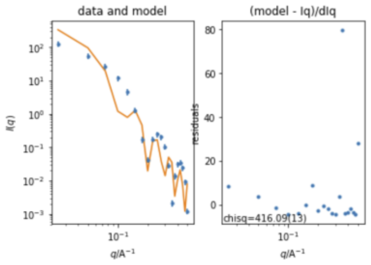


Fitting model function to data using bumps

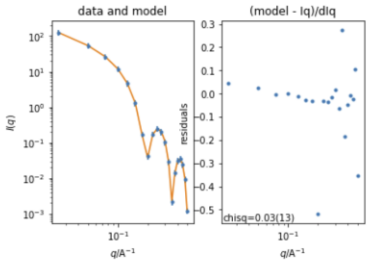
The model functions from sasmodels can be used to fit experimental data. This can be done using bumps, which simillar to sasmodels is a separate package and needs to be installed in your path.

```
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()
```

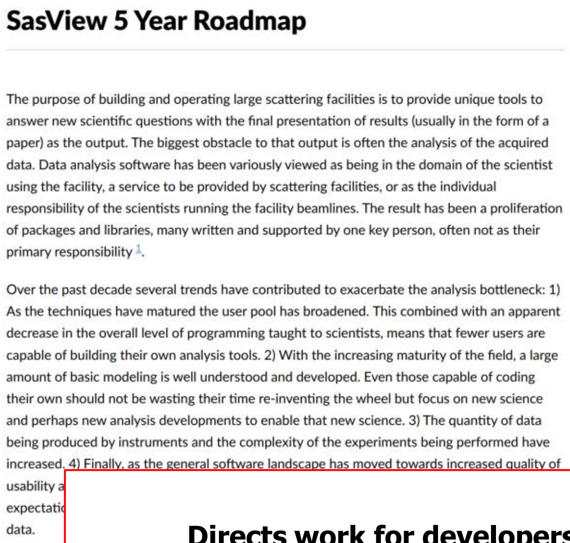
```
Initial chisq 416.09(13)
```



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



The RoadMap



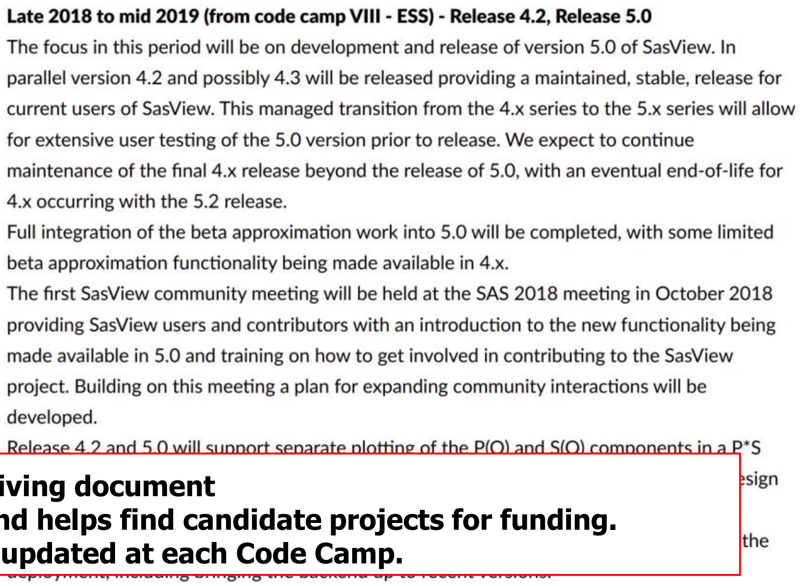
SasView 5 Year Roadmap

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

expectati

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

deployment, including bringing the backend up to recent versions.

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 beta-2 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 → Release 5.0
Provision of CLI & updated Python API

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

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

Integration of McSAS → Target release - 5.1
Integration of PyPrism?
Implementation of key models from Scatter
Documentation
Tutorials – written, interactive & video
Manual

And much more!
See Roadmap and Tickets

Status of contributor community

"Management" Team

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

- 9 facilities
- 40 contributors on github (does not count original team)
- about 15 "active" at any one time

New people … now getting student interest

- Dominique Dressen (Sabrina Dish student Colone Uni)
- Rachel Ford (Julia Kornfield student Caltech)
- CARR (Tianfu and Dongfeng)
- CSNS (could not come due to visa)
- NSLSII → conda forge and deploy on their instruments
- ALS using sasmodels
- Users submitting models to marketplace

So …

Where is SasView Going?
What will it do for me?

Saview Bootcamp? Training courses?

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

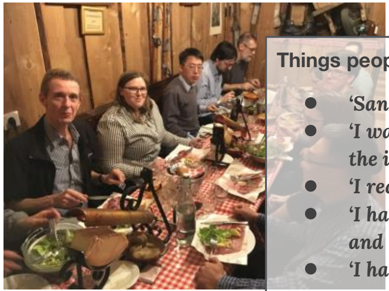
- Day One = Using SasView
  - morning = overview lectures
  - Afternoon = hands-on/tutorial
- Day Two = Write your own model - hands-on
- Day Three = using sasview via scripting
  - Morning = Python tutorial
  - Afternoon = Intro to scripting with Jupyter Notebook and using to script sasview
- Day Four = Contribute - preparation for code camp
  - includes contributing to tutorials, documentation, checking and fixing math, adding tests, reporting using issues, GUI framework code, marketplace database, etc.

https://github.com/SasView/documents/blob/master/Training/SasView_Boot_Camp/syllabus.md

http://www.sasview.org

http://github.com/SasView

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

Questions?

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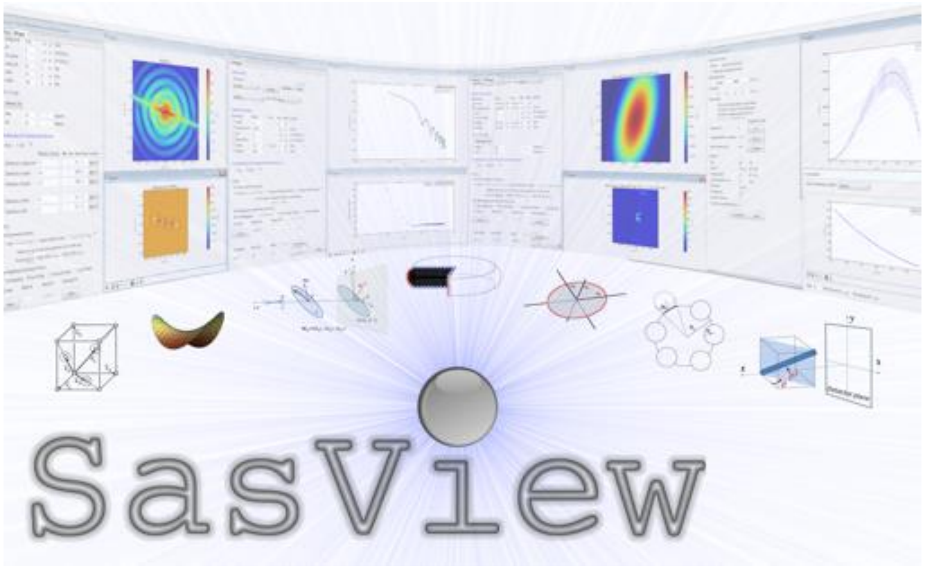


diamond

OAK RIDGE National Laboratory

ansto

EUROPEAN SPALLATION SOURCE

Science & Technology Facilities Council ISIS

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

BAM Bundesanstalt für Materialforschung und -prüfung

Roadmap Late 2019 to mid 2020

- Begin model fitting refactoring work to allow custom re-parameterization of models, allow reading in an array representing either PQ or SQ for P*S fits, fitting oriented model to 1D cuts including revisiting orientation definitions etc. Discussed at this code camp
- Complete architecture manual
- Begin work on refactoring constrained/simultaneous fits.
- Begin work on adding custom workflows identified as highest priority
- Work to update tutorials to support 5.x
- Begin work on advanced model fitting tutorial
- Usual bug fixes and other minor improvements as time and interest permit
- Integration of McSAS
- Begin work on generic O-Z solver
- Inclusion of PRISM^9 functionality
- Begin work to refactor/improve generic scattering calculator
- Improvements to custom model editors including features from compare.py
- Support for multi-GPU, multi-CPU and CPU/GPU computation

https://github.com/SasView/documents

Roadmap mid 2020 to mid 2024

- Refactor Simultaneous/Constrained fitting - significant changes in 5.0
- New Workflows
- Web UI (and Phone App)
- Headless - essentially done in 5.1?
- Intelligent limits/help ⇒ "AI" ?
- Add support for ASAXS
- Enable transparently running computational code remotely from within local GUI - dependent on headless

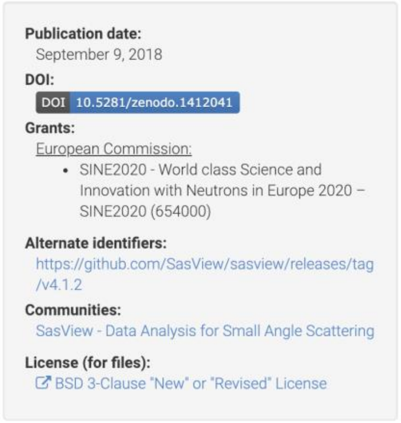
https://github.com/SasView/documents

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

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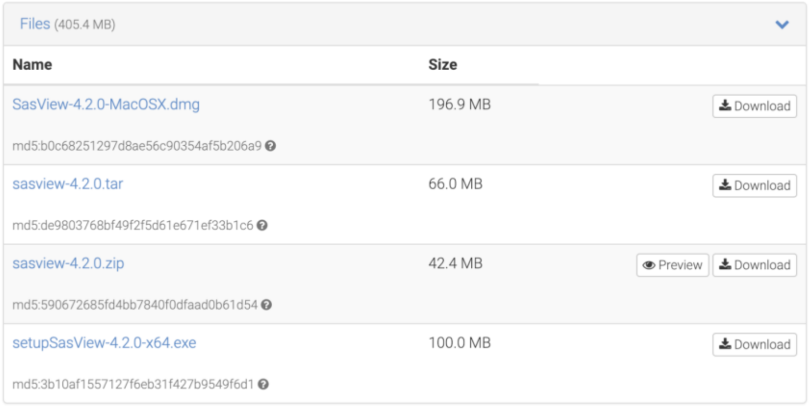

Files (405.4 MB)

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sasview-4.2.0.tar md5:de9803768bf49f2f5d61e671ef33b1c6	66.0 MB	Download
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setupSasView-4.2.0-x64.exe md5:3b10af1557127f6eb31f427b9549f6d1	100.0 MB	Download

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