



Writing Models in SasView

A Contributing to SasView workshop Tutorial

Paul Butler
Virtually Dec 9, 2021



Program

- Just in case ... a bit about what SasView is today
 - What the program “is” and “is not”
 - What the program can do
 - SasView support resources available
- A bit of historical background and current status
- The SasView collaborative model
- Quizz: What is the shape of the future?
- Tutorial:
 - Very brief Introduction
 - a step by step walk through
 - from: general equation
 - To: reparameterization
 - ... and everything in between?

For complete

See YouTube channel video by Steve King!!:

https://www.youtube.com/watch?v=Sbzf_wdlPnQ

Scripting Tutorial next Thursday, Dec 16

Led by Wojciech Potrzebowski

A platform for Small Angle Scattering Data Analysis

SasView



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

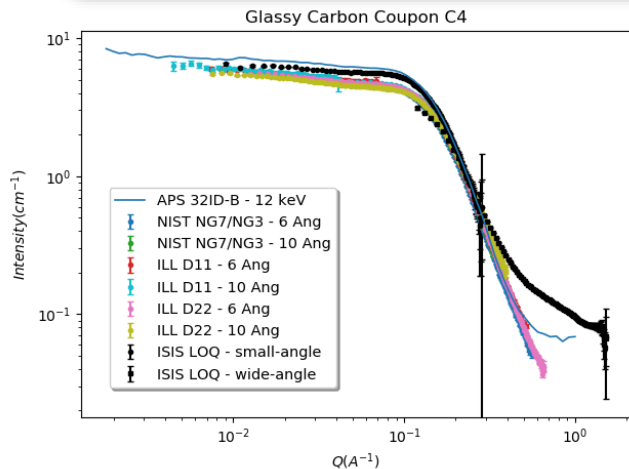
Whatever anybody puts into it

.... Sorta



Experimental Data Flow

Reduced data should be reproducible anywhere!

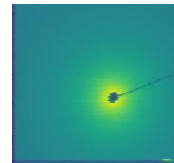


<http://www.cansas.org>

Instrument-
dependent
data



Instrument-
independent
data



Data Acquisition System



'raw' data file
(NXS)



Data Reduction Programs
(e.g. *Mantid*)



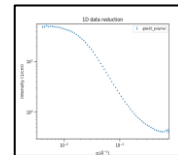
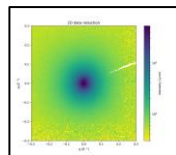
reduced data file
(1D: HDF / XML / TXT; 2D: HDF / TXT)



Data Analysis Programs

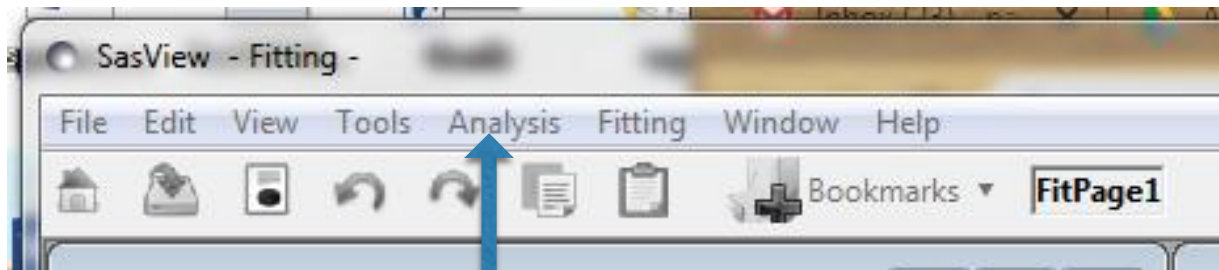


Paper / Thesis





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
NXCanvas & *cansas1D*

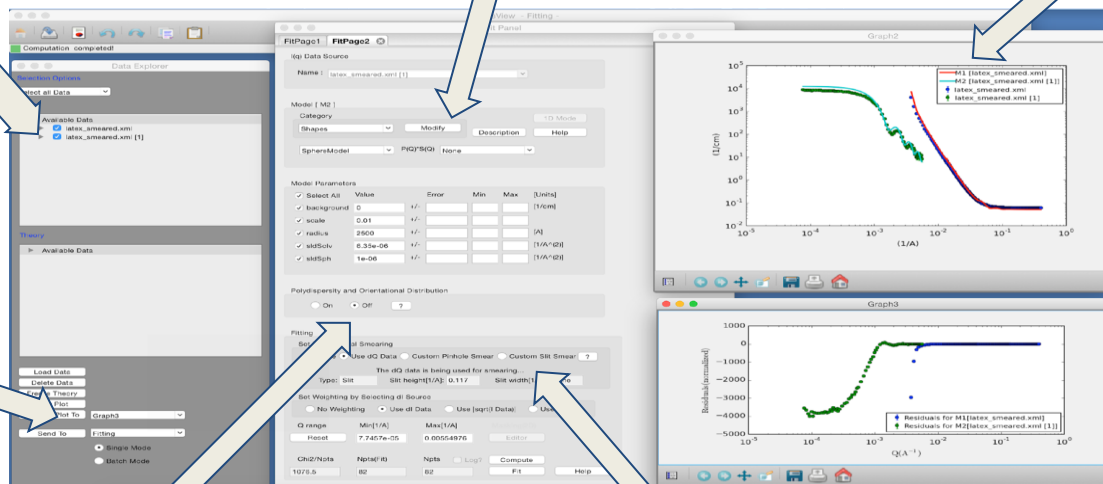
Wide choice of built-in models (> 70)
 $P(Q)$, $S(Q)$ & $P(Q)*S(Q)$

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

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

Parameter	Value	Min	Max	Units
<input type="checkbox"/> scale	1.0	0.0	∞	
<input type="checkbox"/> background	0.001	$-\infty$	∞	cm^{-1}
cylinder				
<input type="checkbox"/> sld	4	$-\infty$	∞	$10^{-6}/\text{\AA}^2$
<input type="checkbox"/> sld_solvent	1	$-\infty$	∞	$10^{-6}/\text{\AA}^2$
<input checked="" type="checkbox"/> radius	50	0.0	∞	\AA
Polydispersity				
<input type="checkbox"/> length	400	0.0	∞	\AA
Polydispersity				
Distribution	0.1			gaussian
<input type="checkbox"/> theta	60	-360.0	360.0	degrees
Polydispersity				
Distribution	10			gaussian
<input type="checkbox"/> phi	85	-360.0	360.0	degrees
Polydispersity				
Distribution	10			gaussian

Options

☒ Polydispersity
☒ 2D view
☐ Magnetism

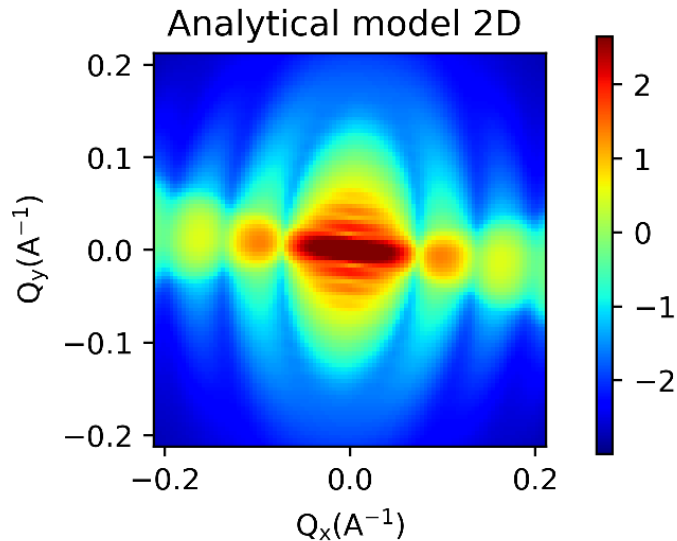
Fitting details

Min range: 0.001 \AA^{-1}
Max range: 0.3 \AA^{-1}
Smearing: None

Fitting error

χ^2 24895

Show Plot Fit Help



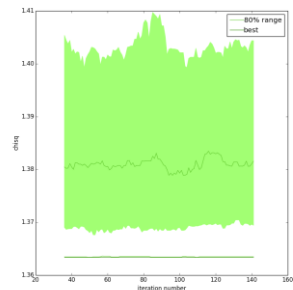
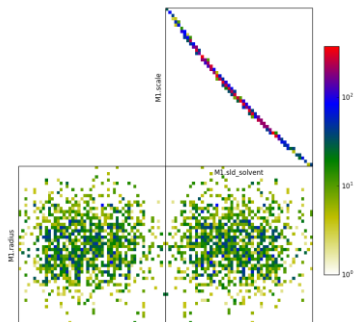
Orientational polydispersity = “jitter”

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
- ☐ Levenberg-Marquardt
- ☐ Quasi-Newton BFGS
- ☐ Differential Evolution
- ☐ Nelder-Mead Simplex

DREAM Fitting Parameters

Samples: 10000

Burn-in Steps: 100

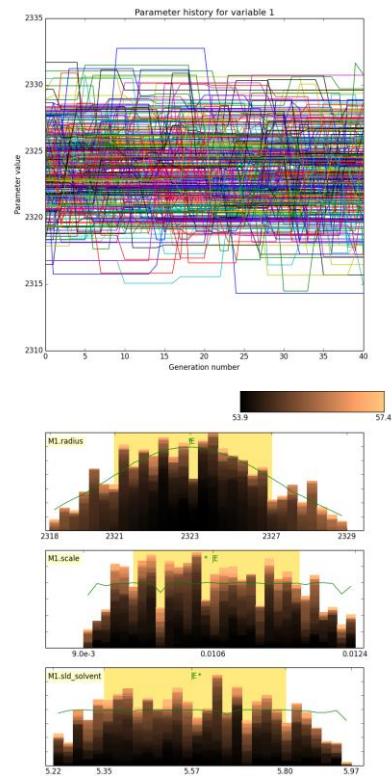
Population: 10

Initializer: eps

Thinning: 1

Steps: 0

OK Cancel ?



Uses bumps package from P. Kienzle
provides user choice of fitting engine
Conventional and Bayseian



Support Resources


- **Website**
- **Documentation**
 - in-program & online
- Written Tutorials
- Video Tutorials (YouTube)
- Taught Courses
 - scattering schools/workshops
 - university courses
- Bootcamps & regional workshops
- e-Learning
- **Slack**
- **Twitter**
- (Marketplace)
- **help@sasview.org**
- **users@sasview.org**

The collage displays four key support resources for SasView:

- Slack Channel:** A screenshot of the #general channel in the SasView Slack workspace. The sidebar shows options like Threads, All DMs, Mentions & reactions, Saved items, and a Slack Connect button. The main chat area shows a message from Michael Zhang dated Tuesday, May 18th, and a message from wpotrzebowski dated Wednesday, June 9th.
- Twitter Profile:** A screenshot of the SasView (@SasView) Twitter profile. It includes a bio stating "Software for analysis of small angle scattering modelling #SANS #SAXS", the website link sasview.org, and follower statistics (21 Following, 174 Followers).
- Documentation Page:** A screenshot of the SasView documentation website. It features a "Table of Contents" with sections like Loading Data, Data Formats, Previous topic, Next topic, This Page, and Quick search.
- FAQ Page:** A screenshot of the SasView FAQ page, titled "FAQ" and subtitled "Here are the answers to some common questions about SasView". It lists several common questions such as "What is SasView?", "What platforms does SasView run on?", and "Do I need to install Python/C++ or any compilers before I install SasView?".



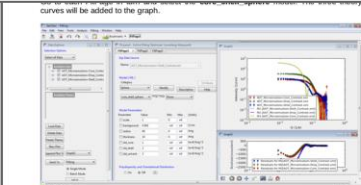
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- 
- A screenshot of a YouTube channel page for 'Princeton University'. The page shows a video titled 'SASVIEW: A Python-based software for analyzing small-angle scattering data'. The video player is visible, showing the video content. The channel name 'Princeton University' is at the top right. The video title is 'SASVIEW: A Python-based software for analyzing small-angle scattering data'. The video description is partially visible, mentioning 'SASVIEW is a Python-based software for analyzing small-angle scattering data'. The video player shows a thumbnail of the video content. The channel name 'Princeton University' is at the top right. The video title is 'SASVIEW: A Python-based software for analyzing small-angle scattering data'. The video description is partially visible, mentioning 'SASVIEW is a Python-based software for analyzing small-angle scattering data'. The video player shows a thumbnail of the video content.

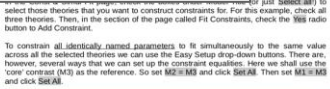
SasView
ABOUT ▼
LINKS & DOWNLOADS ▼
CONTENT ▼
HELP ▼

Tutorials:

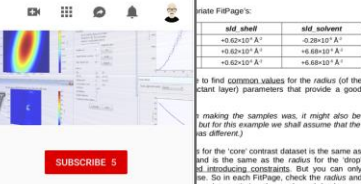
- [Old SasView tutorial \(PDF\)](#) - still useful
- [Getting started with SasView \(PDF\)](#)
- [Basic 1D Fitting in SasView \(PDF\)](#) - for versions 3.x/4.x
- [Simultaneous 1D Fitting in SasView \(PDF\)](#) - for versions 3.x/4.x
- [Correlation Function Analysis in SasView \(PDF\)](#) - for version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



This screenshot shows the 'Fit' tab in SasView. It displays a list of fit pages on the left, a central plot area with multiple data series and fit curves, and a right-hand panel with various fit parameters and statistics. The 'Fit' button is visible at the bottom.



This screenshot shows the 'Easy Setup' dialog box in SasView. It allows users to select theories (e.g., 'M2', 'M3') and constraints (e.g., 'M2=M3') for fitting. The 'Add Constraint' button is highlighted.



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SasView

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Scattering Length Density Calculator in SasView

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Calculating the Scattering Invariant in SasView

29 views • 5 months ago



Support Resources

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 - **e-Learning**
 - Slack
 - Twitter
 - (Marketplace)
-
- help@sasview.org
 - users@sasview.org

*All the work of ISIS Sandwich
Student Michael Oakley*

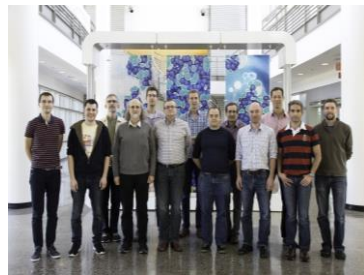


The screenshot shows the PaN-learning website. At the top, there is a dark blue header with the PaN-learning logo and name. Below the header, a light blue banner displays the URL <https://pan-learning.org/>. The main content area has a white background. It starts with a 'Welcome to PaN-learning' section, followed by a paragraph about the platform's mission. Below this is a search bar with the placeholder text 'Search courses'. The 'Available courses' section lists several courses: 'Neutron Scattering Library', 'Introduction to neutron scattering', 'Advanced topics in neutron scattering', 'Quasielastic Neutron Scattering Course', 'Introduction to muon spin spectroscopy' (highlighted with a red box), 'Muons in Semiconductors', 'Muons in Magnetism', 'Muons in Superconductivity', 'IKON Python Workshop', 'Illumidesk: Python Course', and 'SasView: Analysis of SAS Data (Swedness)' (highlighted with a red box).



History and Status of SasView

- 2006; originates in NSF *DANSE* project
- 2013; transitions into a community project
- 2016; Sine2020 project funded
- 2021; Essentially a “volunteer army”
- ~40 contributors from 9 organisations (~15 active at any one time)
- small management team:
Paul Butler (NIST), Wojciech Potrzebowski (ESS),
Steve King (ISIS), [Mathieu Doucet (ORNL), Andrew
Jackson (ESS)]





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



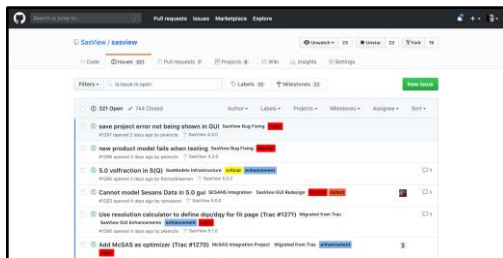
Open, Collaborative, Community Development

Code is **open source** and **publicly hosted** at Github
Released under **BSD 3-clause license**

DOI for each release

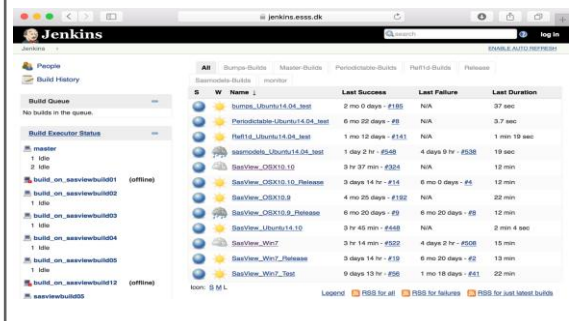
Rolling 5 Year Roadmap

Code Hosting, Issue Tracking & Developer Wiki on Github



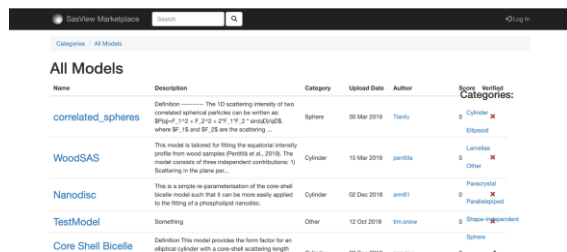
<https://github.com/SasView>

Automated Builds



<http://build.sasview.org/>

Model Marketplace for Users to share their models



<http://marketplace.sasview.org>



<https://www.sasview.org>





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.

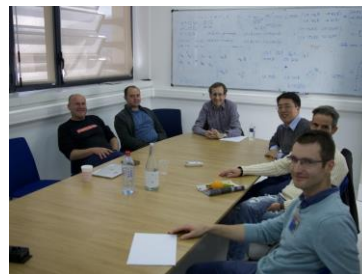
You break it, you bought it ...

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

Open, Collaborative, Community Development



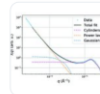
**Twice monthly zoom calls
Regular 'camps' & 'hackathons'**



Paavo A. Penttilä
@PaavoPenttila

Follow

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



Paavo A. Penttilä
@PaavoPenttila

Follow

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>



Quiz time

What will the Future SasView be able to do?



What to expect

We will be bold (or foolish)
and use SasView 5.0.5 beta.

No prior experience is required. However, a knowledge of SAS would be helpful along with a knowledge of enough maths to write the necessary functions

These few slides are intended to provide a quick orientation on a couple of fundamental aspects and on the outline of the demo tutorial. They are intended to be followed immediately by a live, hands-on, demo/tour using SasView to write models.



SOME FUNDAMENTALS

POSTULATE: creating a new model in SasView is EASY

- There is ZERO difference between built in model files and custom/plugin model files.
 - But there are some differences in how the GUI handles them...
- You do NOT need anything but SasView to create a model
 - Though it may help for complicated things
- You must know:
 - The equation you want to use ($I(Q) = \dots$ what?)
 - What are the adjustable parameters in that model
 - And then the complexities of polydispersity, orientation, integer parameters, “multiplicity” etc.



MORE FUNDAMENTALS

POSTULATE: creating a new model in SasView is EASY



There are three types of model files that can be used (ALL include *mymodel.py*). We will only cover two of them.

NOTE: SasView provides “magic” and tools specific to SAS data, and the models and GUI make assumptions about the data being SAS data. *HOWEVER*, fundamentally, SasView can fit/model any data with any equation that can be given analytically (DLS? Reflectivity?)

NOTE3: SasView 4.2 is no longer being worked on and will soon be obsolete.



THE PLAN

POSTULATE: creating a new model in SasView is EASY

- Write a simple python model (MODEL TYPE I) with no polydispersity
- Rewrite using special functions (and even other packages, e.g.scipy)
- Add polydispersity and the form_volume function
- Enable use with structure factor (effective radius)
- Rewrite in C (MODEL TYPE II and III)
- Using (and creating) C library functions
- Using cylinder model to look at orientation.
- Use of various other flags
- MAYBE .. multiplicity and Reparameterization.... A powerful new tool
- How to make the model available immediately to the community