SAXS and SANS data analysis with SasView

hands-on session at FASEM school

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It’s time to start downloading…

(If you haven’t done it yet)

Download The Latest Release Version of SasView

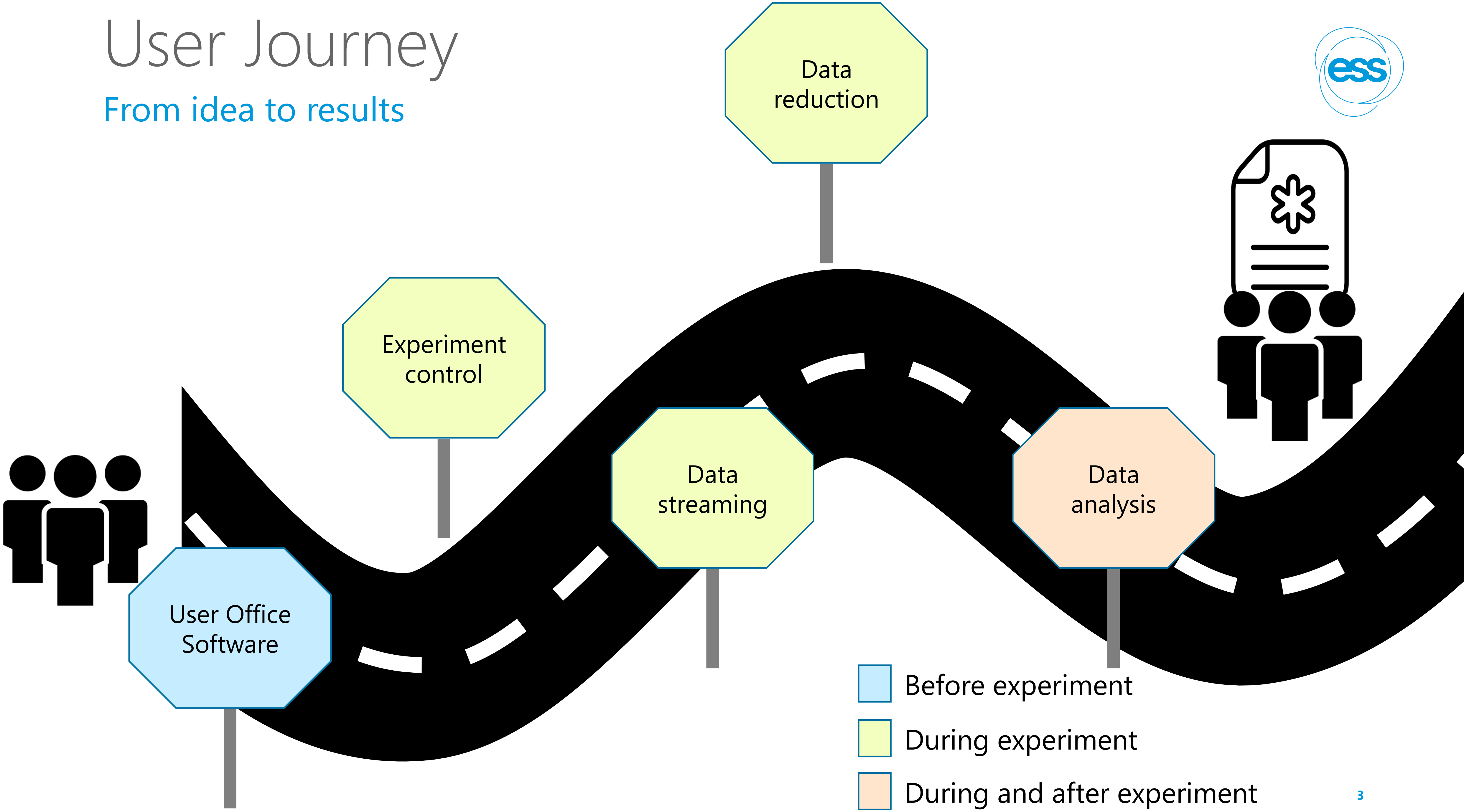
Version 5

Released June 6, 2023.
See what's new!

https://github.com/SasView/sasview/releases/tag/v5.0.6

User Journey

From idea to results



User Office Software

Experiment control

Data streaming

Data reduction

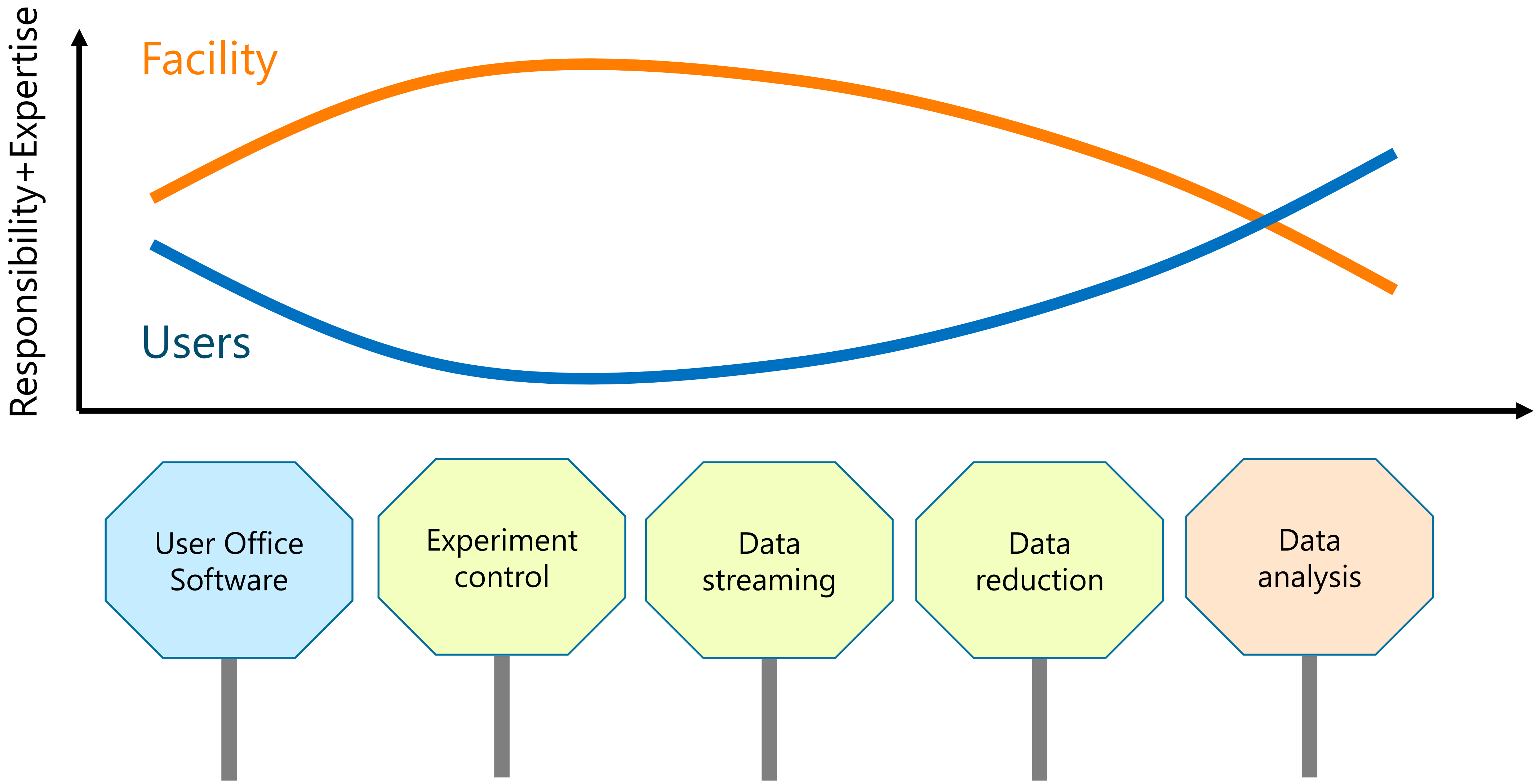
Data analysis

🟦 Before experiment

🟩 During experiment

🟧 During and after experiment

User Journey



Data analysis

Facts of life

Data analysis is part of the processing workflow

Reduced data on the disks is useless

Users expertise is critical for successful data analysis

Facilities should support data analysis software but shouldn’t fully drive the process

->We need open and collaborative software tools in order to succeed!

The SasView approach

An open, collaborative, community development

- Community driven project
- Supported by 9 facilities, 40 contributors (~15 active at any one time)
- Small leadership team: Paul Butler (NIST), Steve King (ISIS), Wojciech Potrzebowski (ESS)
- Biweekly calls
- Regular SasView camps and hackathons

- Hosted on github: https://github.com/SasView/sasview

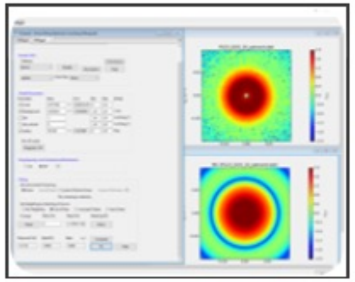
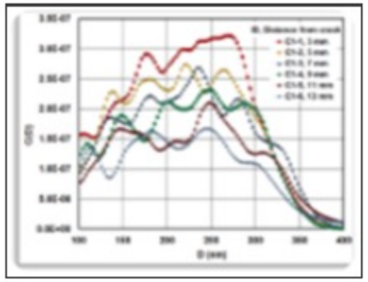
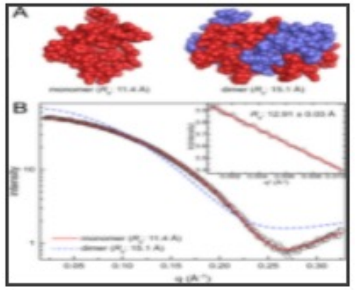
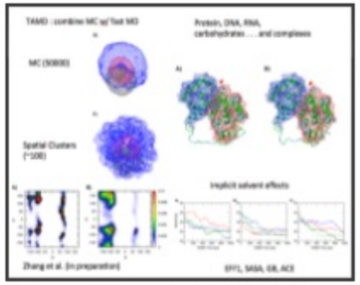
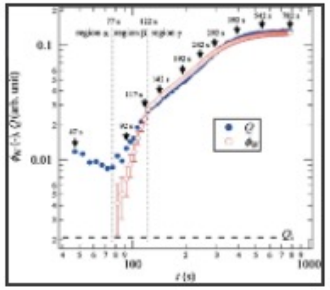
Pictures from Code Camps: V, VI, VIII, X

www.sasview.org

Data analysis

Few different options for SAS data

Not in SasView scope

Model-Fitting Methods	Real-Space Methods	~~Ab-Initio Methods~~	~~MC/MD Methods~~	Other Methods
 *Example of 2D model-fitting using the SasView application*	 *Cavity size distributions in a steel weldment as derived from SANS* *10.1179/1743284714Y.0000000577*	 *Ab-initio modelling of polcalcin constrained by SAXS* *10.1002/pro.3376*	 *MC & TAMD modelling of proteins constrained by SANS* *10.1016/j.jmgm.2017.02.010*	 *Time evolution of the invariant during crystallisation of P4MP1* *10.1038/pj.2012.204*

https://www.isis.stfc.ac.uk/Pages/SANSdataanalysisOverview.aspx

Typical SasView workflow

For reduced data:

Load and plot experimental data

Define a model (form and structure factor) with parameters

Fit the parameters so that model matches experimental data

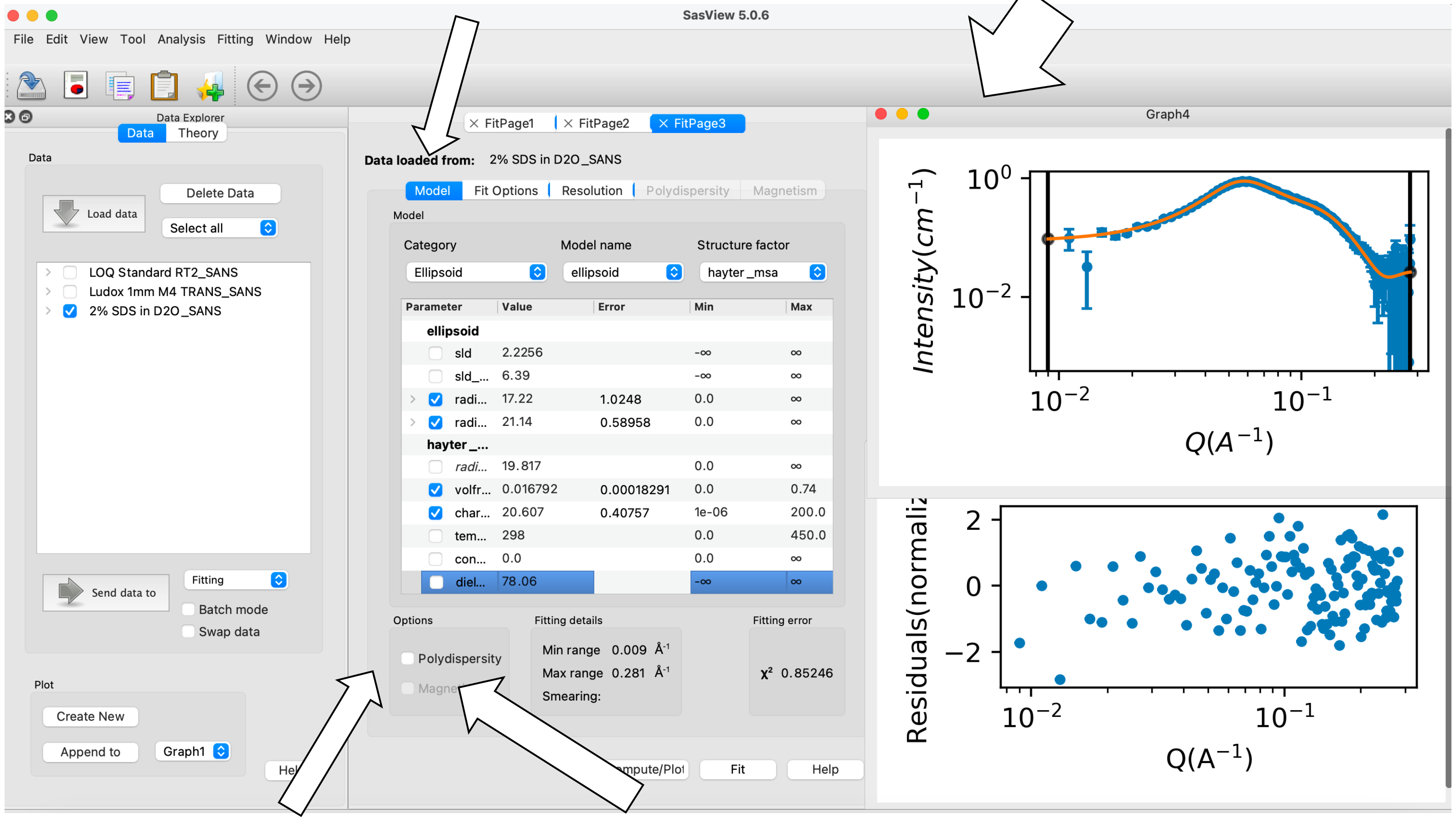
Draw scientific conclusions and publish results!

Fitting in SasView

70+ models to explain data

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

Single, batch and simultaneous
1D and 2D fitting



☐ LOQ Standard RT2_SANS
☐ Ludox 1mm M4 TRANS_SANS
☑ 2% SDS in D2O_SANS

Data loaded from: 2% SDS in D2O_SANS

Model

Category	Model name	Structure factor
Ellipsoid	ellipsoid	hayter _msa

Parameter	Value	Error	Min	Max
ellipsoid				
☐ sld	2.2256		-∞	∞
☐ sld_...	6.39		-∞	∞
☑ radi...	17.22	1.0248	0.0	∞
☑ radi...	21.14	0.58958	0.0	∞
hayter _...				
☐ *radi...*	19.817		0.0	∞
☑ volfr...	0.016792	0.00018291	0.0	0.74
☑ char...	20.607	0.40757	1e-06	200.0
☐ tem...	298		0.0	450.0
☐ con...	0.0		0.0	∞
☐ diel...	78.06		-∞	∞

Fitting details
Min range 0.009 $Å^{-1}$
Max range 0.281 $Å^{-1}$
Smearing:

Fitting error
χ^2 0.85246

Data management
Common data formats supported, including NXCansas & *cansas1D*

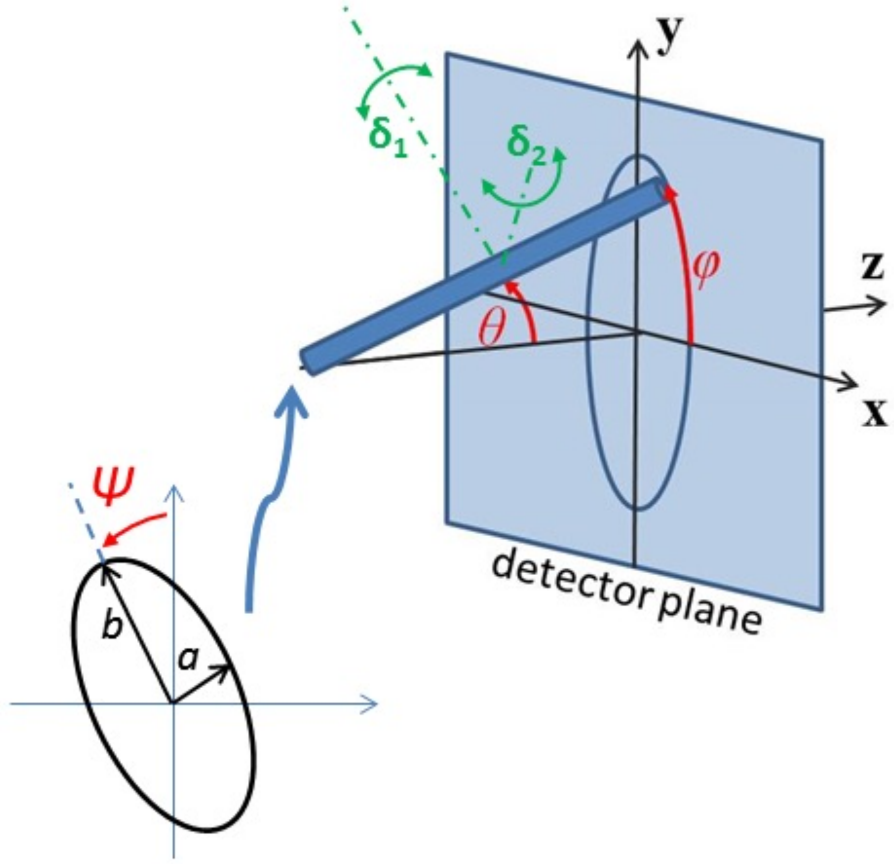
Analysis Tool Choice
&
Plotting

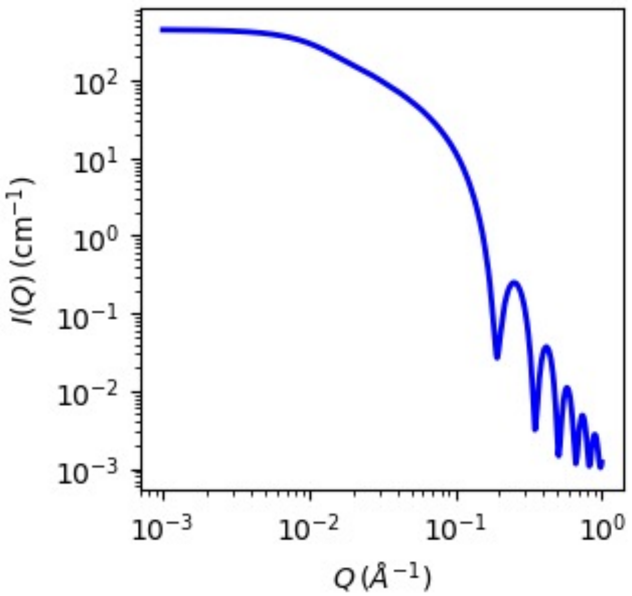
Polydispersity (choice of distribution and distribution parameters)

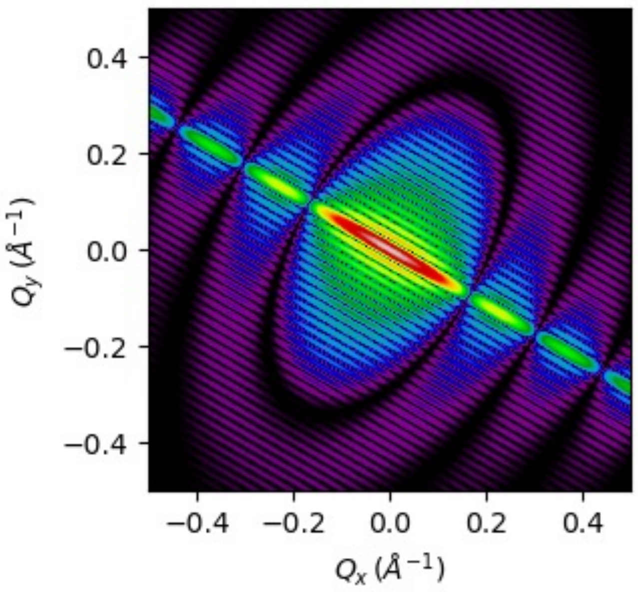
Resolution smearing (pinhole and slit)
Automatically from data or provide parameters

2D fitting

For oriented or magnetic particles





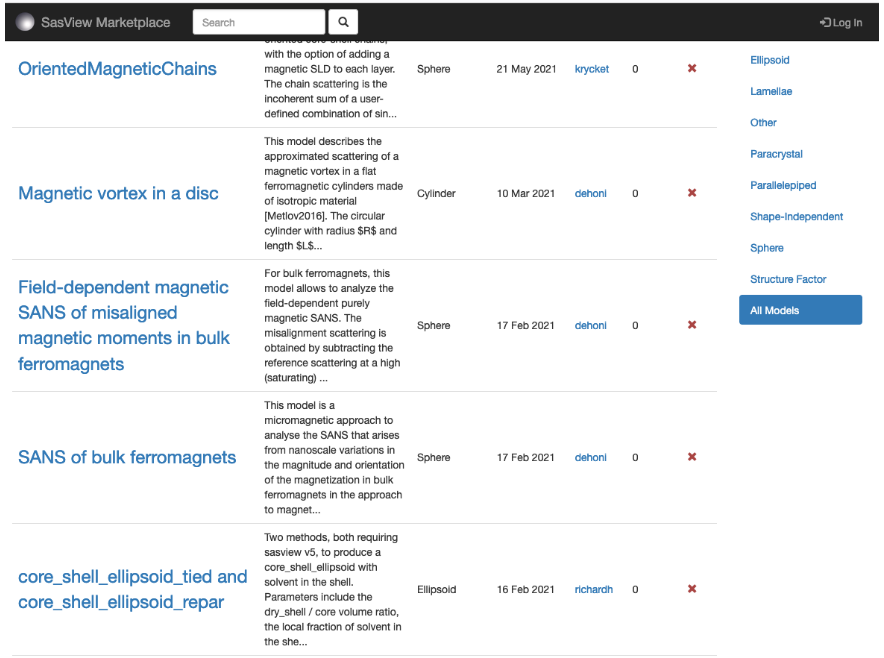


1D and 2D cylinder model

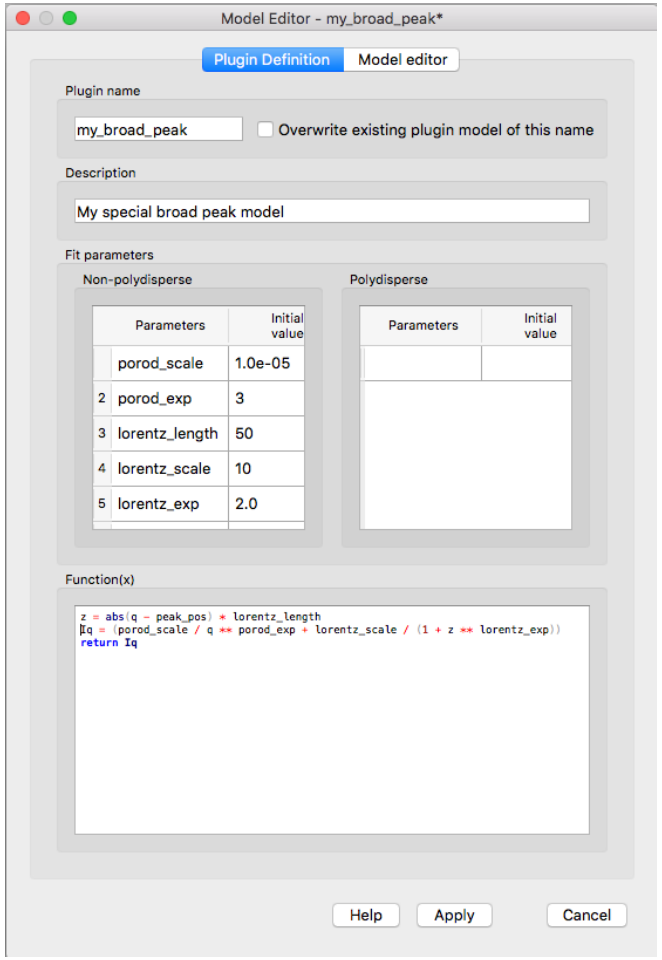
Plugin models

SasView provides tools and infrastructure for custom/plugin models

- Dedicated editor
- Syntax and performance testing
- Directly available in SasView ecosystem
- Community developed models can be deposited to marketplace: https://marketplace.sasview.org/



OrientedMagneticChains	with the option of adding a magnetic SLD to each layer. The chain scattering is the incoherent sum of a user-defined combination of sin...	Sphere	21 May 2021	krycket	0	✖
Magnetic vortex in a disc	This model describes the approximated scattering of a magnetic vortex in a flat ferromagnetic cylinders made of isotropic material [Metlov2016]. The circular cylinder with radius R and length L...	Cylinder	10 Mar 2021	dehoni	0	✖
Field-dependent magnetic SANS of misaligned magnetic moments in bulk ferromagnets	For bulk ferromagnets, this model allows to analyze the field-dependent purely magnetic SANS. The misalignment scattering is obtained by subtracting the reference scattering at a high (saturating) ...	Sphere	17 Feb 2021	dehoni	0	✖
SANS of bulk ferromagnets	This model is a micromagnetic approach to analyse the SANS that arises from nanoscale variations in the magnitude and orientation of the magnetization in bulk ferromagnets in the approach to magnet...	Sphere	17 Feb 2021	dehoni	0	✖
core_shell_ellipsoid_tied and core_shell_ellipsoid_repar	Two methods, both requiring sasview v5, to produce a core_shell_ellipsoid with solvent in the shell. Parameters include the dry_shell / core volume ratio, the local fraction of solvent in the she...	Ellipsoid	16 Feb 2021	richardh	0	✖



Plugin name: my_broad_peak

☐ Overwrite existing plugin model of this name

Description: My special broad peak model

Fit parameters

Non-polydisperse

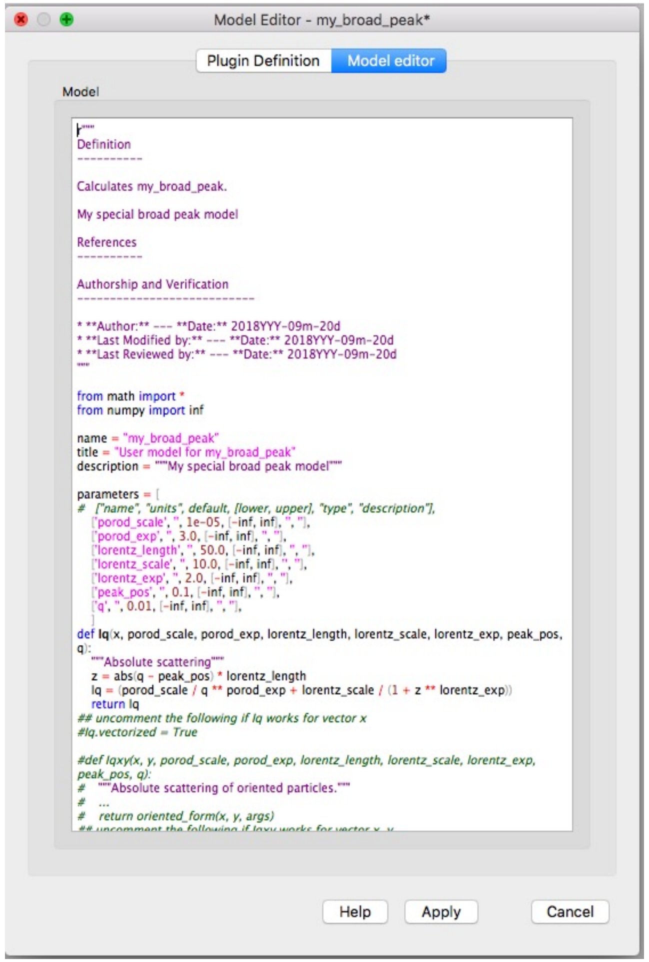
	Parameters	Initial value
1	porod_scale	1.0e-05
2	porod_exp	3
3	lorentz_length	50
4	lorentz_scale	10
5	lorentz_exp	2.0

Polydisperse

Parameters	Initial value

Function(x)

```
z = abs(q - peak_pos) * lorentz_length
Iq = (porod_scale / q ** porod_exp + lorentz_scale / (1 + z ** lorentz_exp))
return Iq
```



Model

```
r"""
Definition
----------

Calculates my_broad_peak.

My special broad peak model

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

* **Author:** --- **Date:** 2018YYY-09m-20d
* **Last Modified by:** --- **Date:** 2018YYY-09m-20d
* **Last Reviewed by:** --- **Date:** 2018YYY-09m-20d
"""

from math import *
from numpy import inf

name = "my_broad_peak"
title = "User model for my_broad_peak"
description = """My special broad peak model"""

parameters = [
#   ["name", "units", default, [lower, upper], "type", "description"],
    ['porod_scale', '', 1e-05, [-inf, inf], '', ''],
    ['porod_exp', '', 3.0, [-inf, inf], '', ''],
    ['lorentz_length', '', 50.0, [-inf, inf], '', ''],
    ['lorentz_scale', '', 10.0, [-inf, inf], '', ''],
    ['lorentz_exp', '', 2.0, [-inf, inf], '', ''],
    ['peak_pos', '', 0.1, [-inf, inf], '', ''],
    ['q', '', 0.01, [-inf, inf], '', ''],
    ]
def Iq(x, porod_scale, porod_exp, lorentz_length, lorentz_scale, lorentz_exp, peak_pos,
q):
    """Absolute scattering"""
    z = abs(q - peak_pos) * lorentz_length
    Iq = (porod_scale / q ** porod_exp + lorentz_scale / (1 + z ** lorentz_exp))
    return Iq
## uncomment the following if Iq works for vector x
#Iq.vectorized = True

#def Iqxy(x, y, porod_scale, porod_exp, lorentz_length, lorentz_scale, lorentz_exp,
peak_pos, q):
#    """Absolute scattering of oriented particles."""
#    ...
#    return oriented_form(x, y, args)
```

Which model should I use?

One needs to start somewhere…

Prior knowledge

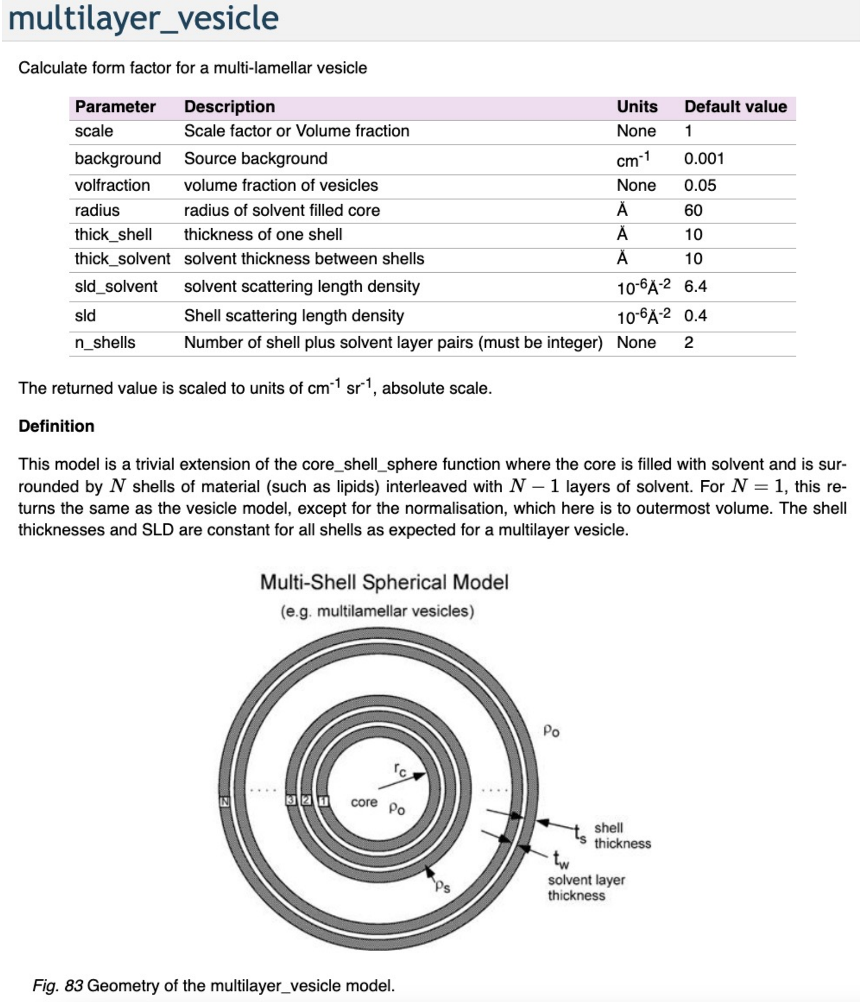
Literature search

SasView documentation

Usually, more than one model fits

Model-free analysis

Machine Learning



multilayer_vesicle

Calculate form factor for a multi-lamellar vesicle

Parameter	Description	Units	Default value
scale	Scale factor or Volume fraction	None	1
background	Source background	cm^{-1}	0.001
volfraction	volume fraction of vesicles	None	0.05
radius	radius of solvent filled core	Å	60
thick_shell	thickness of one shell	Å	10
thick_solvent	solvent thickness between shells	Å	10
sld_solvent	solvent scattering length density	$10^{-6}Å^{-2}$	6.4
sld	Shell scattering length density	$10^{-6}Å^{-2}$	0.4
n_shells	Number of shell plus solvent layer pairs (must be integer)	None	2

The returned value is scaled to units of cm^{-1} sr^{-1}, absolute scale.

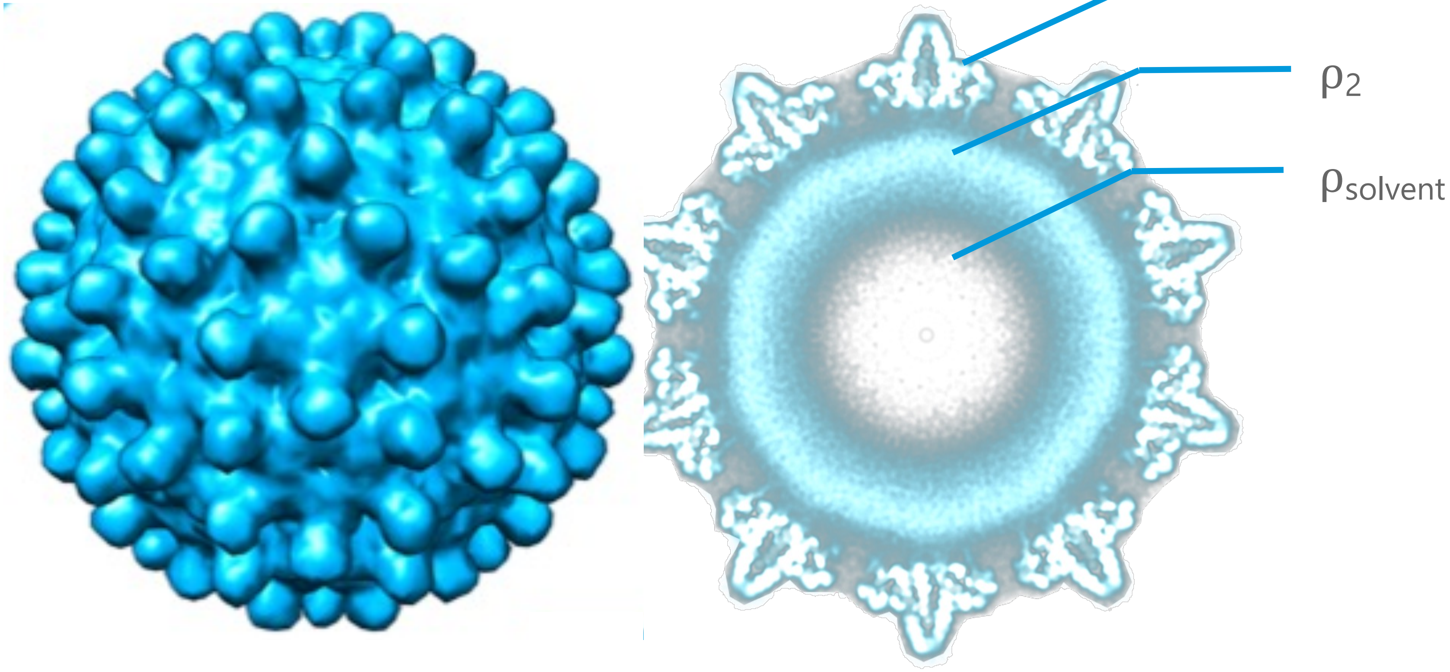
Definition

This model is a trivial extension of the core_shell_sphere function where the core is filled with solvent and is surrounded by N shells of material (such as lipids) interleaved with $N-1$ layers of solvent. For $N=1$, this returns the same as the vesicle model, except for the normalisation, which here is to outermost volume. The shell thicknesses and SLD are constant for all shells as expected for a multilayer vesicle.

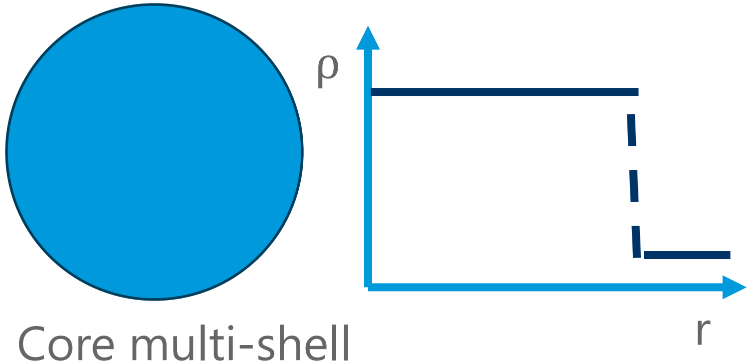
Fig. 83 Geometry of the multilayer_vesicle model.

Which model should I use?

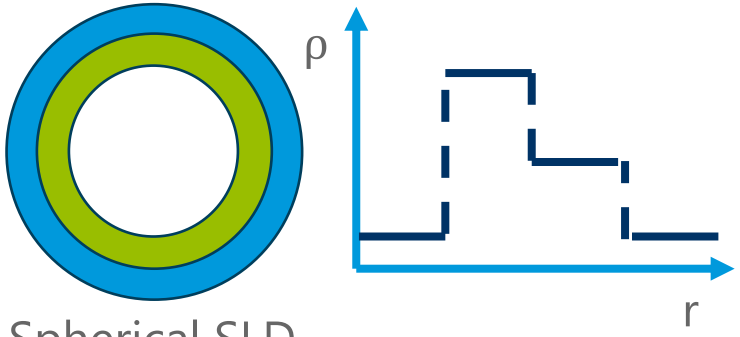
How to represent a virus capsid?



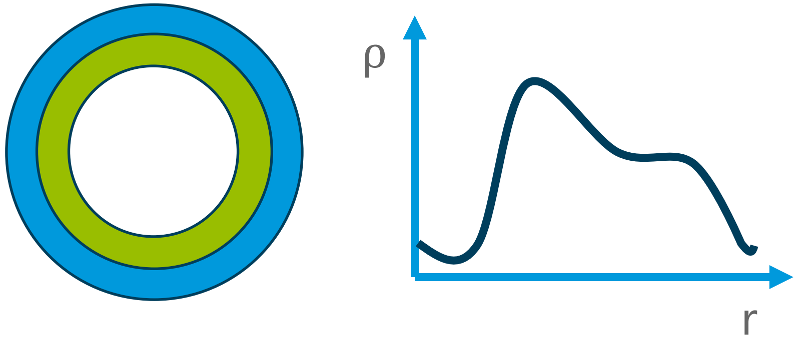
- Sphere



- Core multi-shell



- Spherical SLD

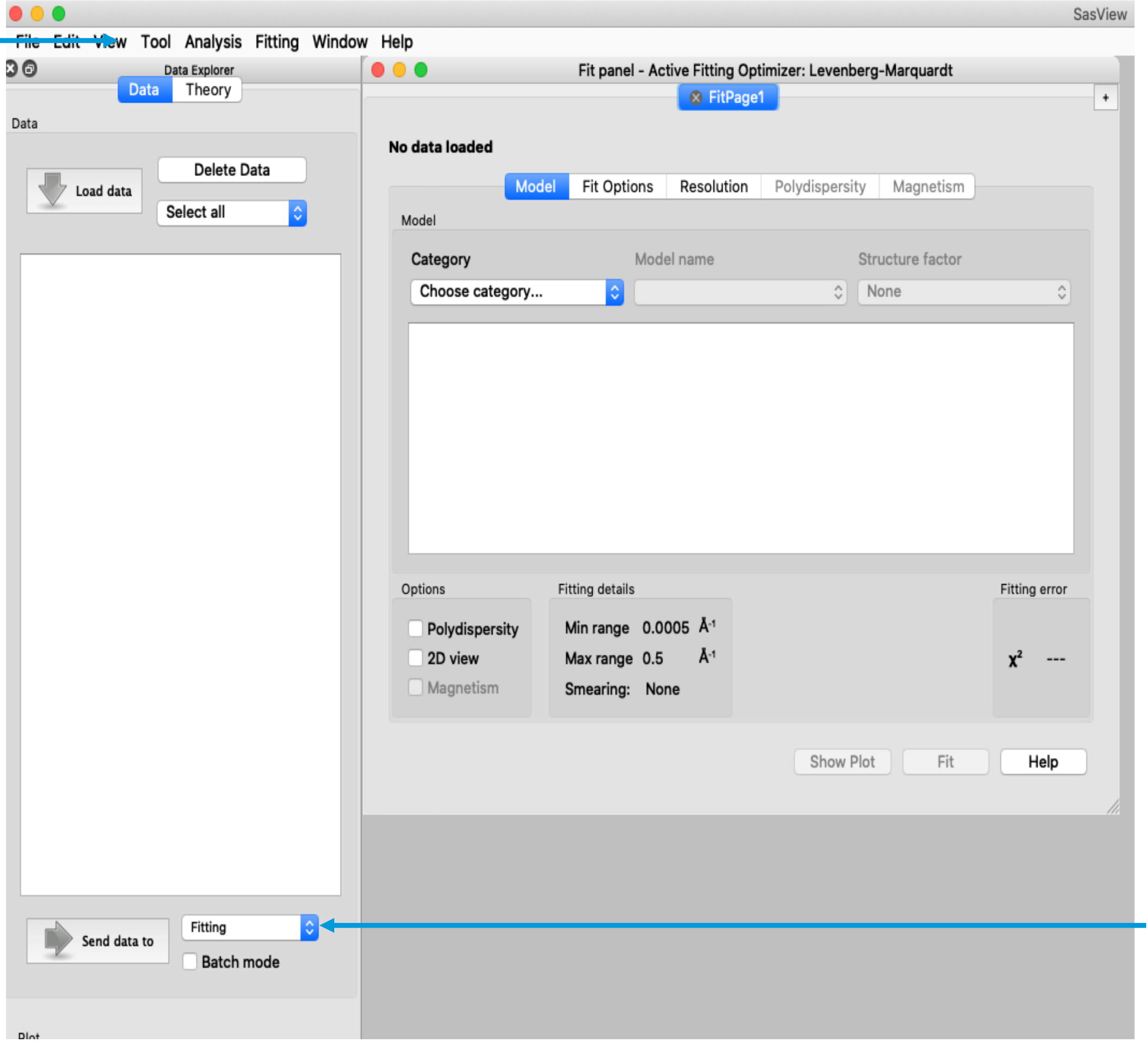


Other SasView functionality

Various utility tools and calculators

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



Fit panel - Active Fitting Optimizer: Levenberg-Marquardt

No data loaded

Min range 0.0005 $Å^{-1}$

Max range 0.5 $Å^{-1}$

Smearing: None

χ^2 ---

Analysis

- Fitting
- Invariant
- Pr Inversion
- Correlation Function

Beyond Graphical User Interface (GUI)

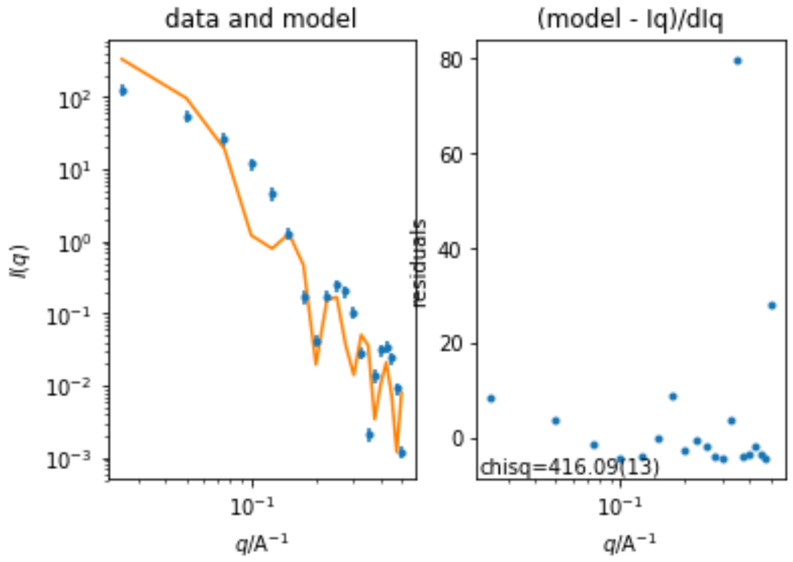
Running SasView from script

- Useful for batch jobs and reproducibility
- Scripts can be run on computer cluster

```python
import pylab
from bumps.names import *
from sasmodels.core import load_model
from sasmodels.bumps_model import Model, Experiment
from sasmodels.data import load_data

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

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

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()
```

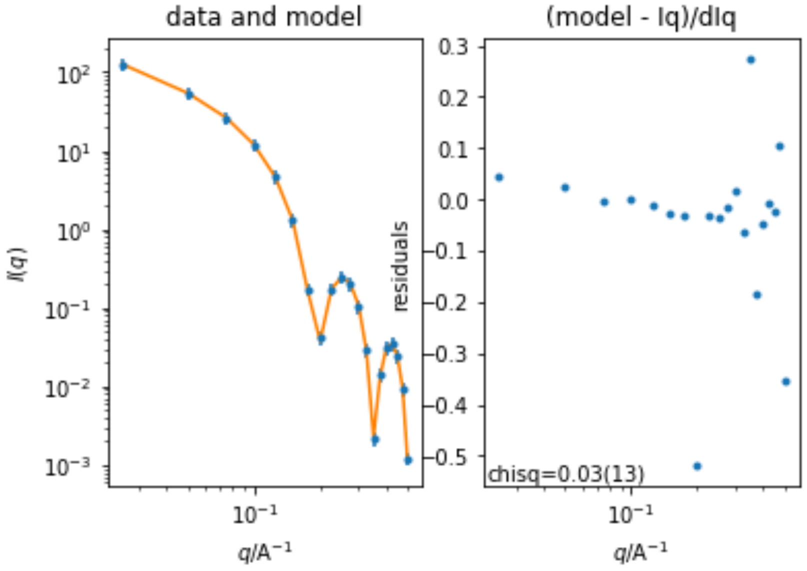
Before fit

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



After fit

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



Beyond Graphical User Interface (GUI)

How to start?

sasview

sasdata

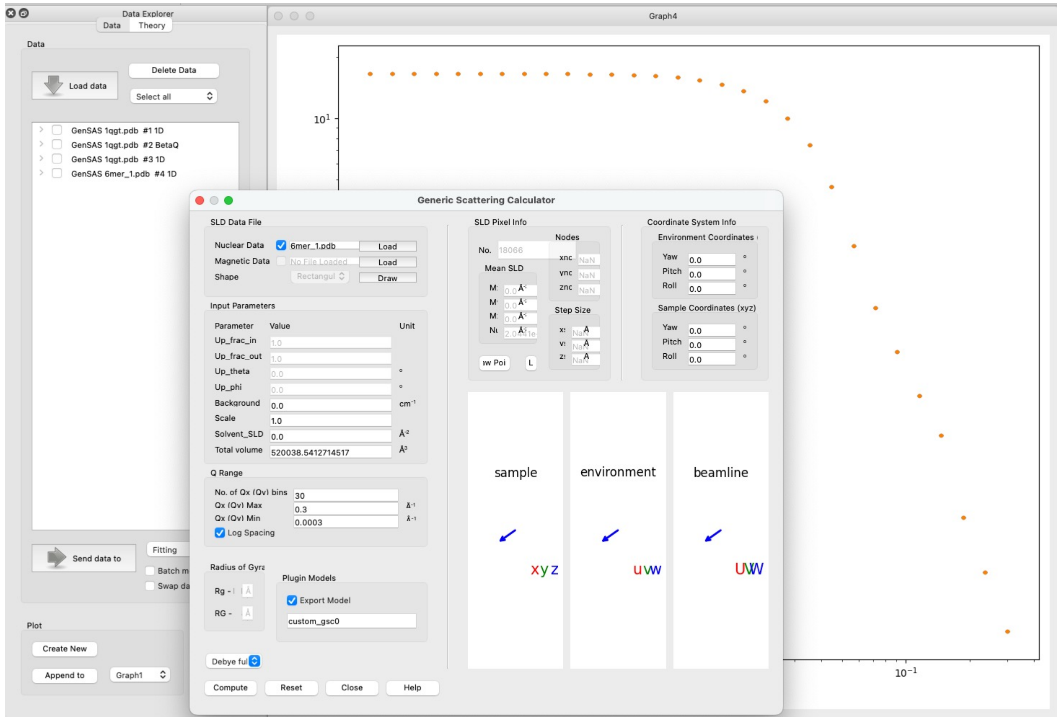
sasmodels

bumps

- Python installation
- For fitting, there is no need to install sasview
- *Pip install sasmodels sasdata*
- It can be run on computer clusters (also with GPU)

Generic Scattering calculator improvements

Available in SasView 6.0.0



Data Explorer

- GenSAS 1qgt.pdb #1 1D
- GenSAS 1qgt.pdb #2 BetaQ
- GenSAS 1qgt.pdb #3 1D
- GenSAS 6mer_1.pdb #4 1D

Generic Scattering Calculator

SLD Data File

Nuclear Data ☑ 6mer_1.pdb

Magnetic Data ☐ No File Loaded

Shape Rectangul

Input Parameters

Parameter	Value	Unit
Up_frac_in	1.0	
Up_frac_out	1.0	
Up_theta	0.0	°
Up_phi	0.0	°
Background	0.0	cm⁻¹
Scale	1.0	
Solvent_SLD	0.0	Å⁻²
Total volume	520038.5412714517	Å³

Q Range

No. of Qx (Qy) bins 30

Qx (Qy) Max 0.3 Å⁻¹

Qx (Qy) Min 0.0003 Å⁻¹

☑ Log Spacing

Plugin Models

☑ Export Model

custom_gsc0

Debye ful

SLD Pixel Info

No. 18066

Coordinate System Info

Environment Coordinates

Yaw 0.0 °

Pitch 0.0 °

Roll 0.0 °

Sample Coordinates (xyz)

Yaw 0.0 °

Pitch 0.0 °

Roll 0.0 °

Interacting bio-molecules

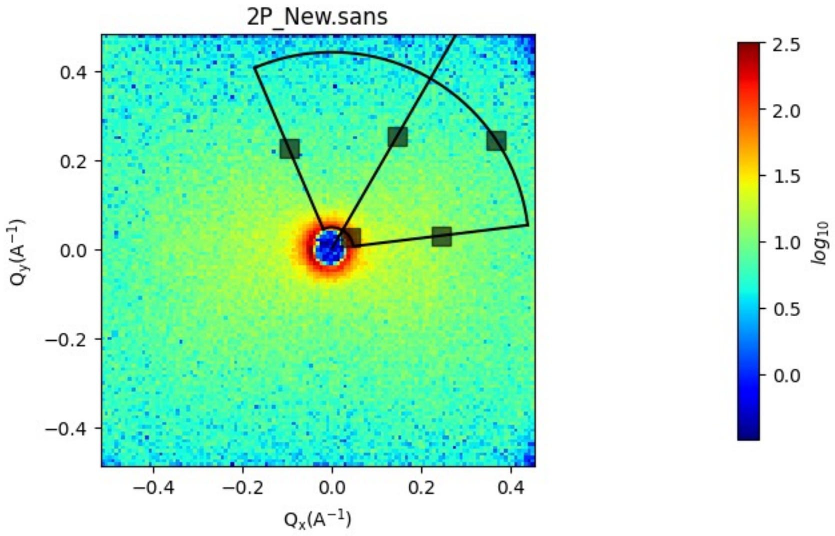
- Generate scattering profile from PDB file
- Save as a custom/plugin model
- Use for fitting with structure factors (including beta approximation)
- (PDB reader and engine refactored)
- (No hydration layer)

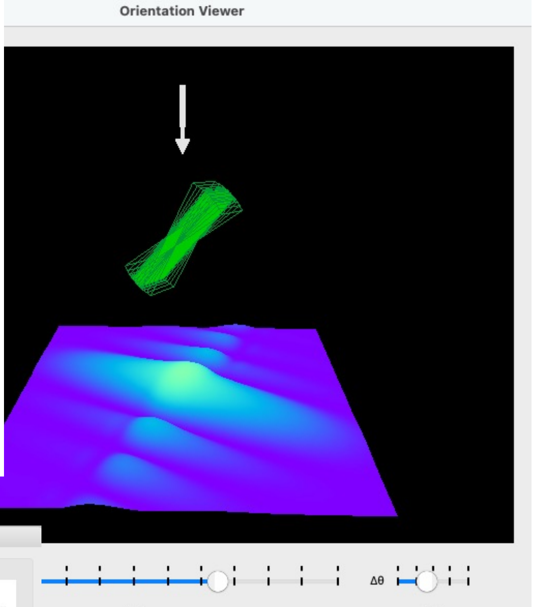
https://github.com/SasView/sasview/releases/tag/v6.0.0-alpha

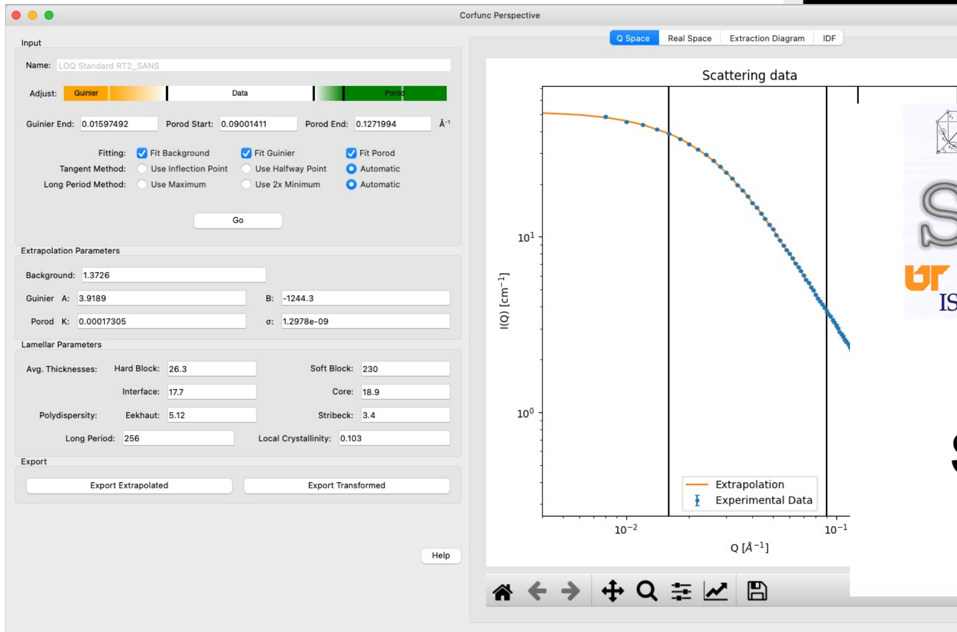
SasView 6.0.0-alpha release

Test at your own risk

- Orientation viewer available
- Corfunc perspective refactored
- Simultaneous fitting allows for a weighting scheme
- Preferences panel with display and plotting options
- Improved label handling on plots
- Residuals plots refactored
- PDB reader refactored
- Wedge slicer added
- Sasdata package separated
- Custom Model writing tutorial







Input

Name: LOQ Standard RT2_SANS

Guinier End: 0.01597492 Porod Start: 0.09001411 Porod End: 0.1271994 Å^{-1}

Fitting: ☑ Fit Background ☑ Fit Guinier ☑ Fit Porod

Tangent Method: ○ Use Inflection Point ○ Use Halfway Point ● Automatic

Long Period Method: ○ Use Maximum ○ Use 2x Minimum ● Automatic

Extrapolation Parameters

Background: 1.3726

Guinier A: 3.9189 B: -1244.3

Porod K: 0.00017305 σ: 1.2978e-09

Lamellar Parameters

Avg. Thicknesses: Hard Block: 26.3 Soft Block: 230

Interface: 17.7 Core: 18.9

Polydispersity: Eekhaut: 5.12 Stribeck: 3.4

Long Period: 256 Local Crystallinity: 0.103

Export

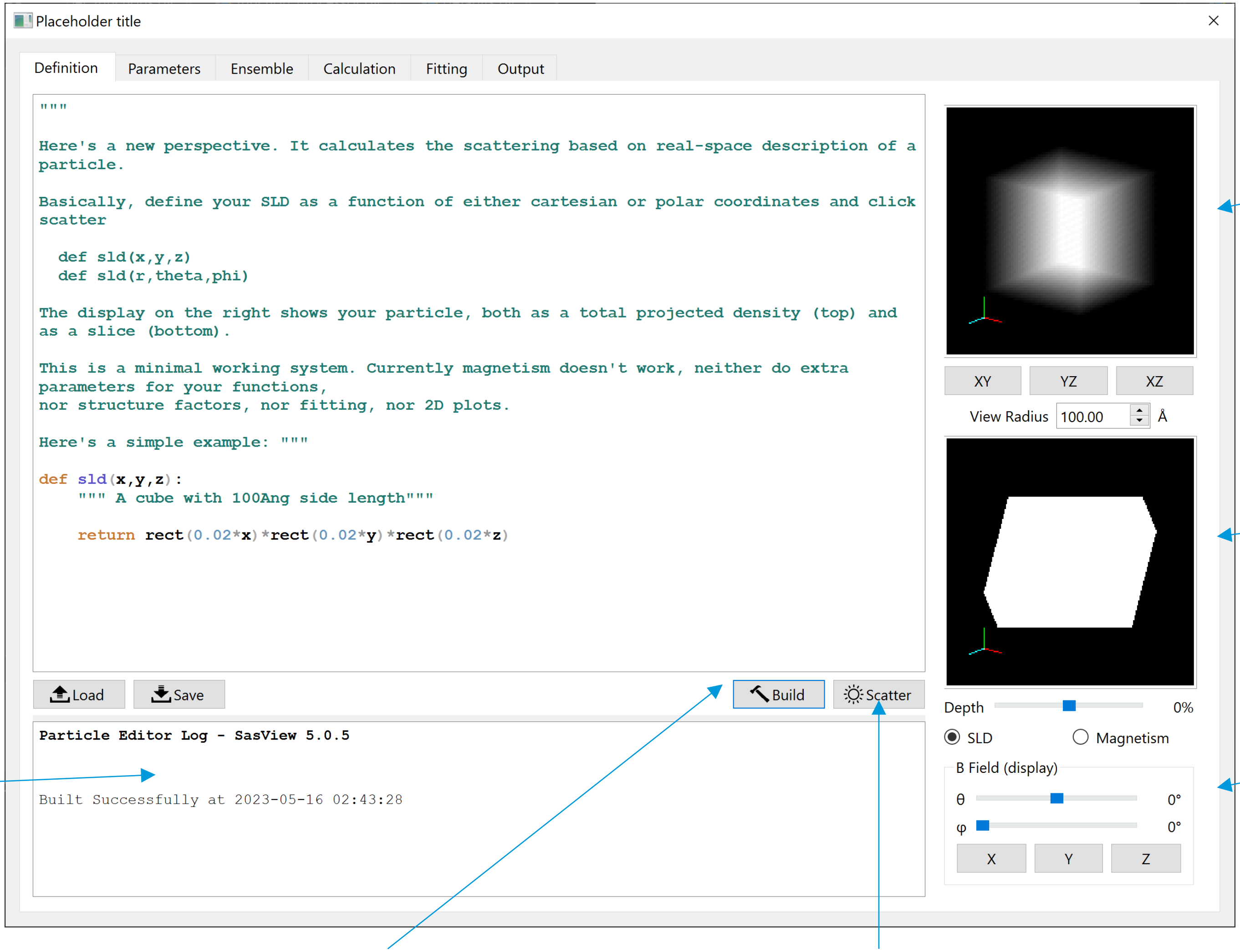
SasView Tutorials

Creating Custom Fitting Models in SasView Version 5.x

Particle Editor

Features beyond SasView-6.0.0

Define functions sld and (optionally) magnetism



```
"""

Here's a new perspective. It calculates the scattering based on real-space description of a
particle.

Basically, define your SLD as a function of either cartesian or polar coordinates and click
scatter

  def sld(x,y,z)
  def sld(r,theta,phi)

The display on the right shows your particle, both as a total projected density (top) and
as a slice (bottom).

This is a minimal working system. Currently magnetism doesn't work, neither do extra
parameters for your functions,
nor structure factors, nor fitting, nor 2D plots.

Here's a simple example: """

def sld(x,y,z):
    """ A cube with 100Ang side length"""

    return rect(0.02*x)*rect(0.02*y)*rect(0.02*z)
```

```
Particle Editor Log - SasView 5.0.5


Built Successfully at 2023-05-16 02:43:28
```

sld / magnetism "x-ray" projection

sld / magnetism cross section

Magnetic field controls for display

Feedback on code and calculations

"Recompile" and update display

Compute scattering

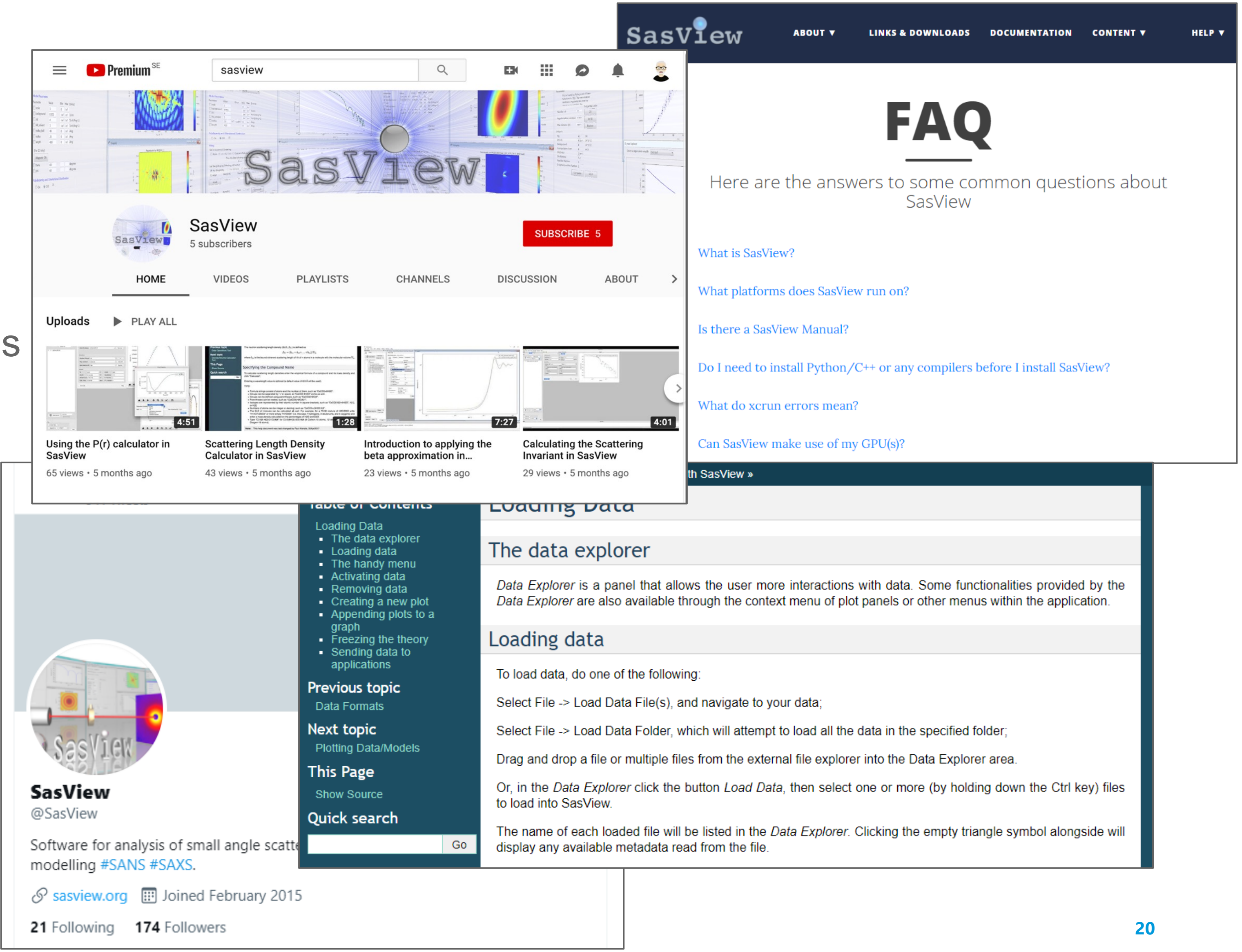
Lucas Willkins (ISIS)

SasView resources

Documentation and communication channels

- 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



Using the P(r) calculator in SasView
65 views • 5 months ago

Scattering Length Density Calculator in SasView
43 views • 5 months ago

Introduction to applying the beta approximation in...
23 views • 5 months ago

Calculating the Scattering Invariant in SasView
29 views • 5 months ago

FAQ

Here are the answers to some common questions about SasView

What is SasView?

What platforms does SasView run on?

Is there a SasView Manual?

Do I need to install Python/C++ or any compilers before I install SasView?

What do xcrun errors mean?

Can SasView make use of my GPU(s)?

Loading Data
- The data explorer
- Loading data
- The handy menu
- Activating data
- Removing data
- Creating a new plot
- 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

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.

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;

Drag and drop a file or multiple files from the external file explorer into the Data Explorer area.

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.

The name of each loaded file will be listed in the *Data Explorer*. Clicking the empty triangle symbol alongside will display any available metadata read from the file.

SasView
@SasView

Software for analysis of small angle scatte
modelling #SANS #SAXS.

sasview.org Joined February 2015

21 Following **174** Followers

How to contribute

You don’t have to be coding ninja to help out!

Respond to queries posted to help@sasview.org or github

Teach others how to get the best from SasView

Write and improve documentation

Write and record tutorials

Test SasView (over and over!) and write bug reports

Provide new plugin models

Deploy and improve automated testing

Review the code contributions of others

Develop code in Python3/C and PyQt/Matplotlib

www.sasview.org/contribute

Thank you!

On behalf of SasView community

SasView version 5.0.6

Doucet, Mathieu[1]; Cho, Jae Hie[2]; Alina, Gervaise[2]; Attala, Ziggy[3]; Bakker, Jurrian[4]; Beaucage, Peter[5]; Bouwman, Wim[6]; Bourne, Robert[3]; Butler, Paul[5]; Cadwallader-Jones, Iestyn[7]; Campbell, Kieran[8]; Cooper-Benun, Torin[3]; Durniak, Celine[9]; Forster, Laura[10]; Gilbert, Peter[5]; Gonzalez, Miguel[7]; Heenan, Richard[3]; Jackson, Andrew[9]; King, Stephen[3]; Kienzle, Paul[5]; Krzywon, Jeff[5]; Maranville, Brian[5]; Martinez, Nicolas[7]; Murphy, Ryan[5]; Nielsen, Torben[9]; O'Driscoll, Lewis[3]; Potrzebowski, Wojciech[9]; Prescott, Stuart[11]; Ferraz Leal, Ricardo[1]; Rozyczko, Piotr[9]; Snow, Tim[10]; Washington, Adam[3]; Wilkins, Lucas[3]; Wolf, Caitlyn[5]

https://zenodo.org/records/7581379

Hands-on session

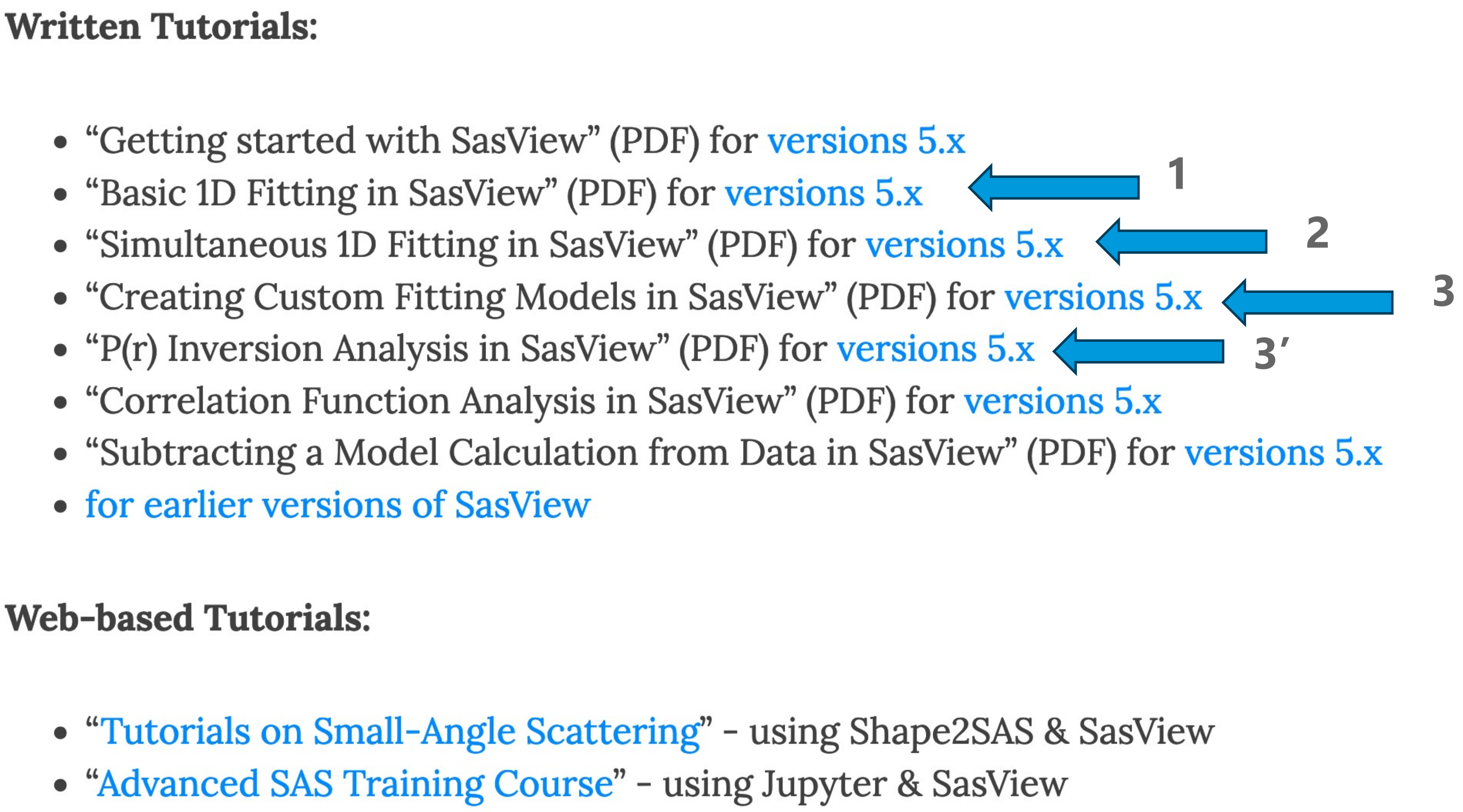
SasView Tutorials

Creating Custom Fitting Models in SasView Version 5.x

www.sasview.org

SasView Tutorials

https://www.sasview.org/documentation/



Written Tutorials:

- “Getting started with SasView” (PDF) for versions 5.x
- “Basic 1D Fitting in SasView” (PDF) for versions 5.x
- “Simultaneous 1D Fitting in SasView” (PDF) for versions 5.x
- “Creating Custom Fitting Models in SasView” (PDF) for versions 5.x
- “P(r) Inversion Analysis in SasView” (PDF) for versions 5.x
- “Correlation Function Analysis in SasView” (PDF) for versions 5.x
- “Subtracting a Model Calculation from Data in SasView” (PDF) for versions 5.x
- for earlier versions of SasView

Web-based Tutorials:

- “Tutorials on Small-Angle Scattering” - using Shape2SAS & SasView
- “Advanced SAS Training Course” - using Jupyter & SasView

Experimenting with SasView

Download SasView 6.0.0 and try out new features

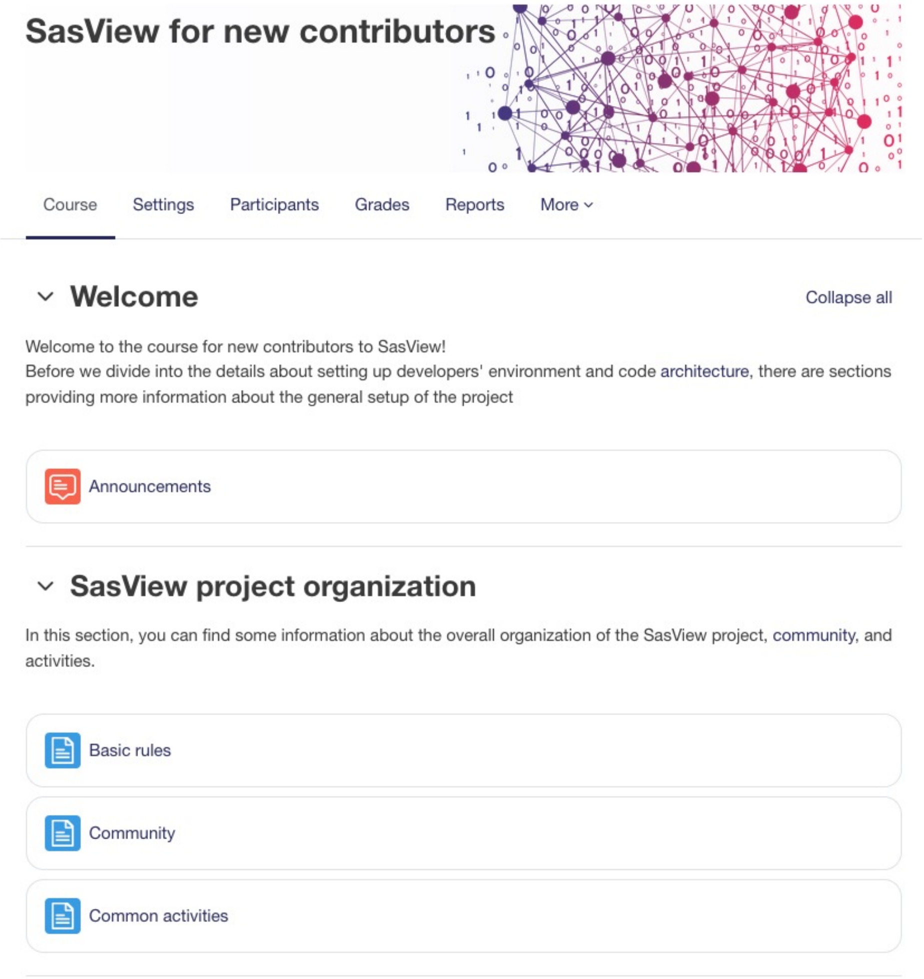
- https://github.com/SasView/sasview/releases/tag/v6.0.0-alpha

Run sasview from the script:

- Setup python environment
- Install required packages
- Play with some of the notebooks:
  - https://github.com/SasView/documents/tree/master/Notebooks

E-learning courses

https://e-learning.pan-training.eu/login/signup.php



SasView for new contributors

Welcome

Welcome to the course for new contributors to SasView!
Before we divide into the details about setting up developers' environment and code architecture, there are sections providing more information about the general setup of the project

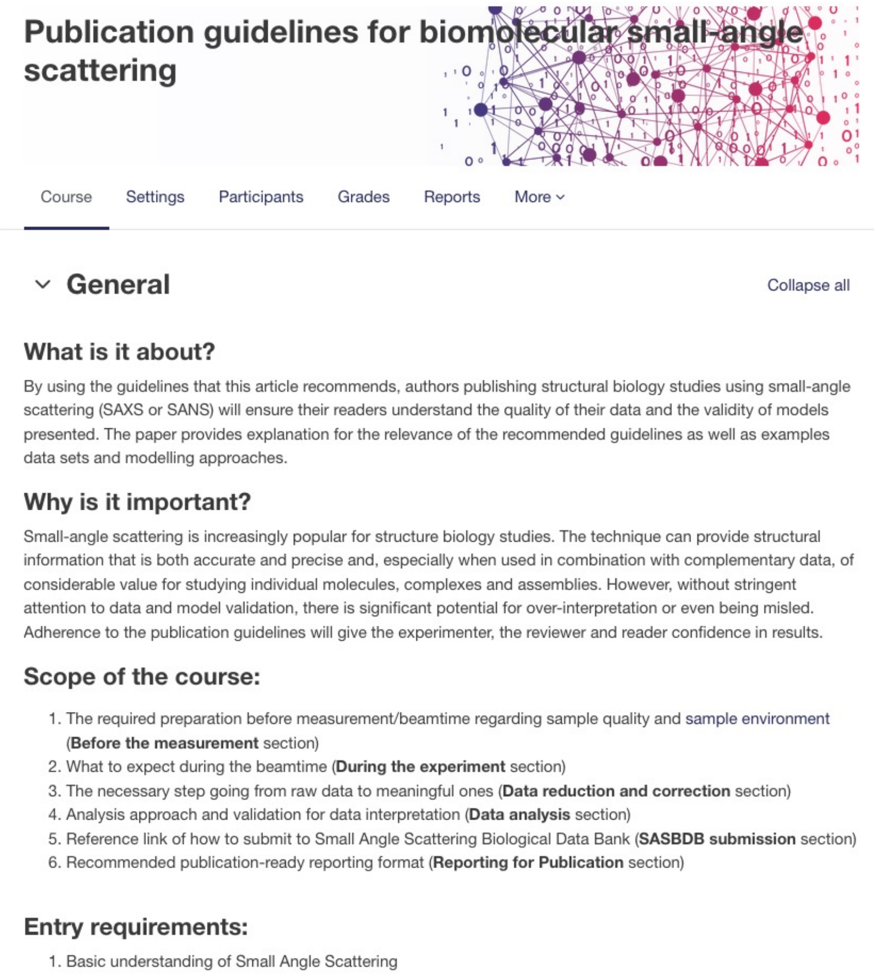
- Announcements

SasView project organization

In this section, you can find some information about the overall organization of the SasView project, community, and activities.

- Basic rules
- Community
- Common activities

https://e-learning.pan-training.eu/course/view.php?id=52



Publication guidelines for biomolecular small-angle scattering

General

What is it about?

By using the guidelines that this article recommends, authors publishing structural biology studies using small-angle scattering (SAXS or SANS) will ensure their readers understand the quality of their data and the validity of models presented. The paper provides explanation for the relevance of the recommended guidelines as well as examples data sets and modelling approaches.

Why is it important?

Small-angle scattering is increasingly popular for structure biology studies. The technique can provide structural information that is both accurate and precise and, especially when used in combination with complementary data, of considerable value for studying individual molecules, complexes and assemblies. However, without stringent attention to data and model validation, there is significant potential for over-interpretation or even being misled. Adherence to the publication guidelines will give the experimenter, the reviewer and reader confidence in results.

Scope of the course:

1. The required preparation before measurement/beamtime regarding sample quality and sample environment (**Before the measurement** section)
2. What to expect during the beamtime (**During the experiment** section)
3. The necessary step going from raw data to meaningful ones (**Data reduction and correction** section)
4. Analysis approach and validation for data interpretation (**Data analysis** section)
5. Reference link of how to submit to Small Angle Scattering Biological Data Bank (**SASBDB submission** section)
6. Recommended publication-ready reporting format (**Reporting for Publication** section)

Entry requirements:

1. Basic understanding of Small Angle Scattering

https://e-learning.pan-training.eu/course/view.php?id=120