SASVIEW

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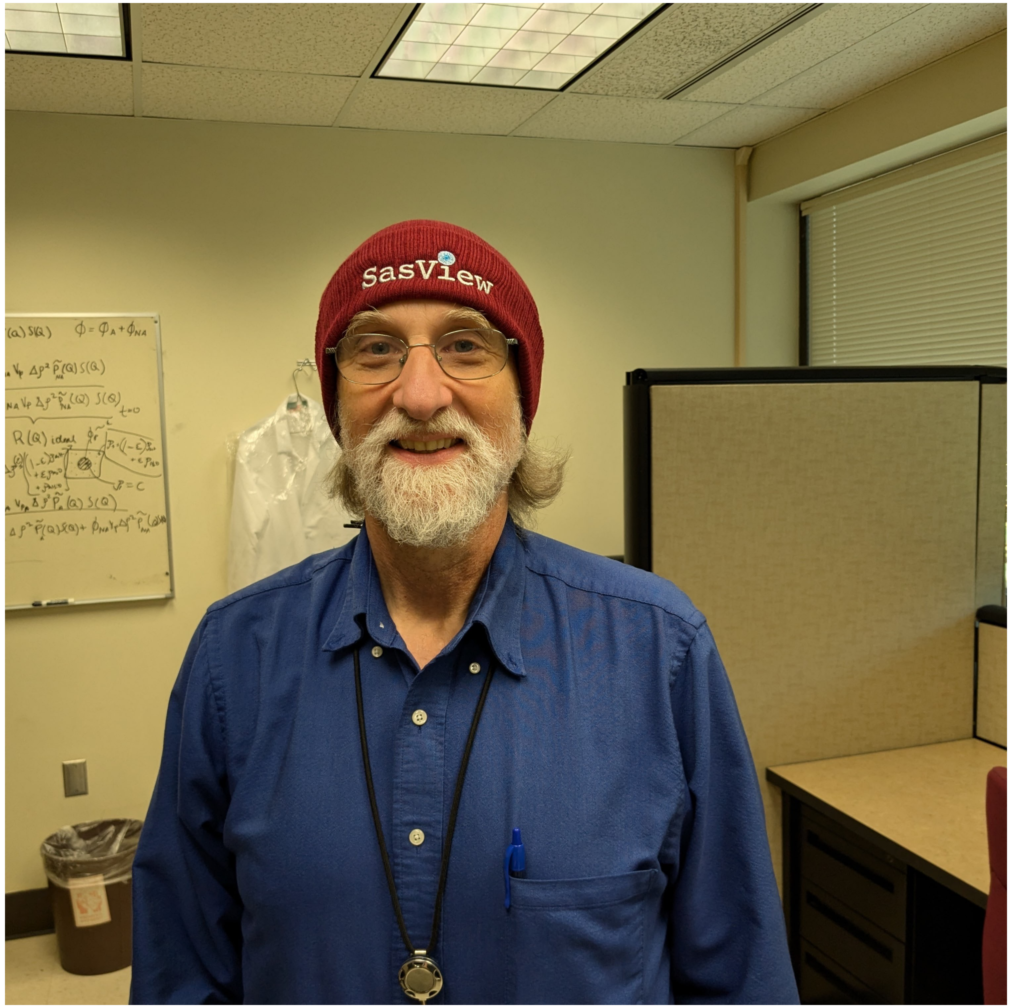
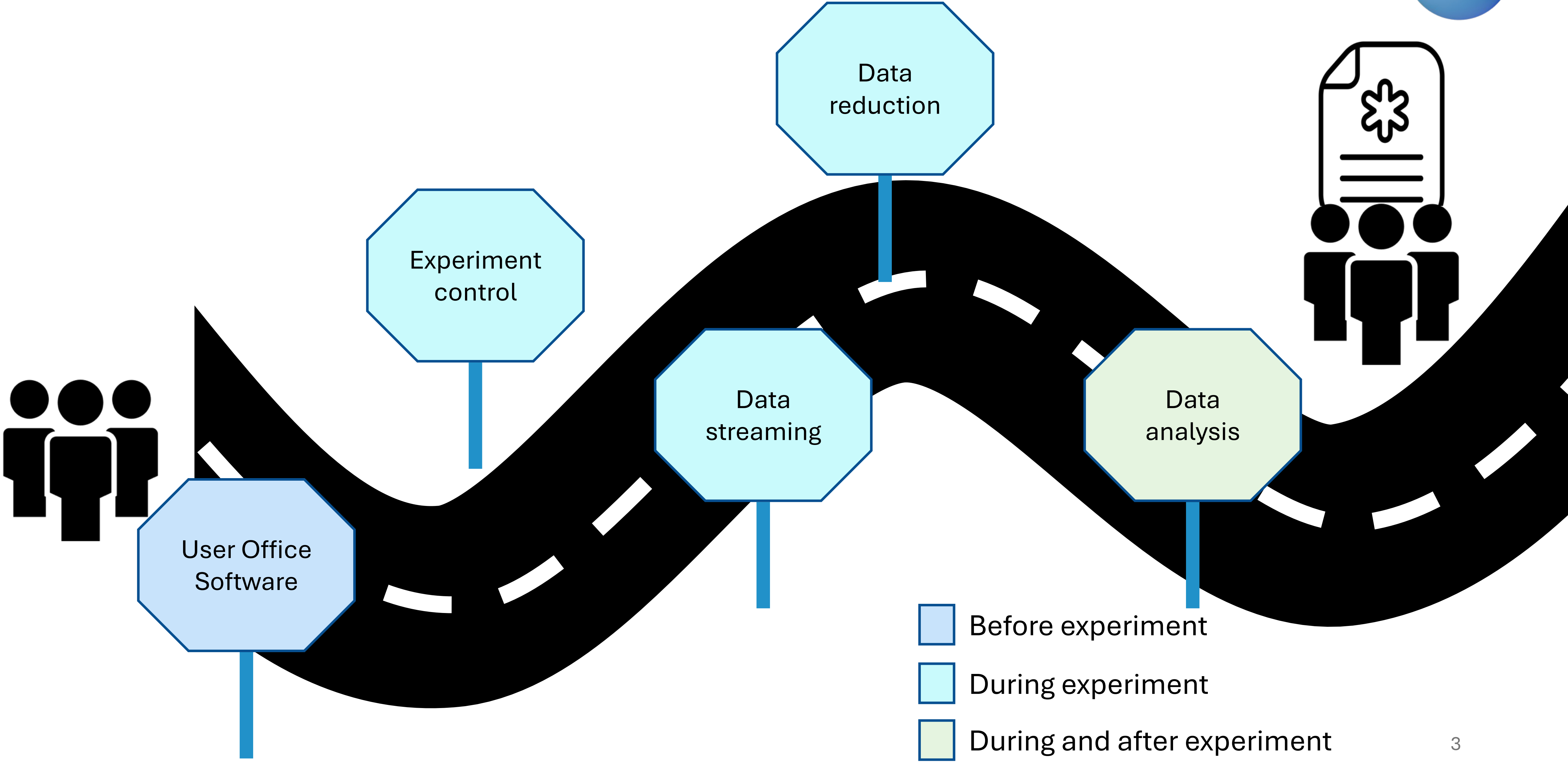
I will change the hat now…



Paul Butler, NIST

User Journey at Large-Scale Facility



User Office Software

Experiment control

Data streaming

Data reduction

Data analysis

Before experiment

During experiment

During and after experiment

Data analysis – facts of life

Data analysis is a part of the processing workflow

Reduced data on the disks is useless

User 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 to succeed!

The SasView approach

An open, collaborative, community development

- Community driven project
- Supported by 10 facilities, 40 contributors (~15 active at any one time)
- Small leadership team: Paul Butler (NIST), Steve King (ISIS), Wojciech Potrzebowski (SciLifeLab, formerly 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

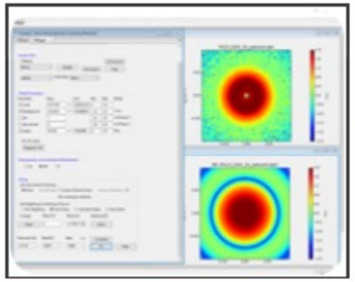
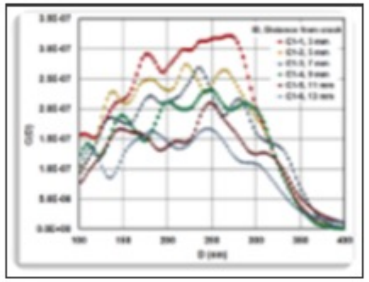
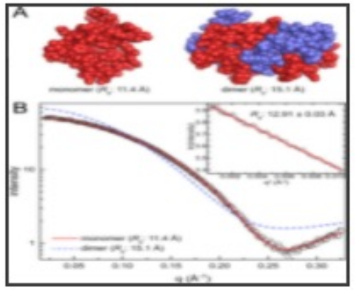
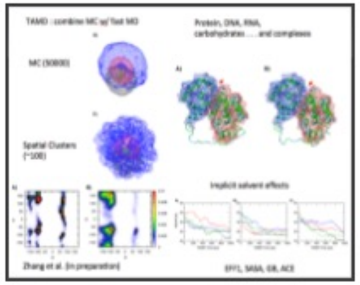
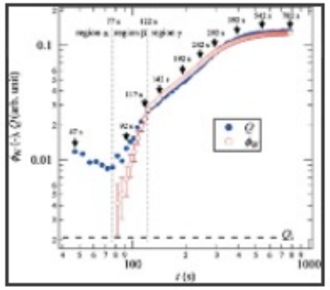
SasView collaboration

- Those who bring the resources (time, effort, funds) choose what to work on

- but cannot break existing experiences ...

Different approaches to SAS data analysis

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

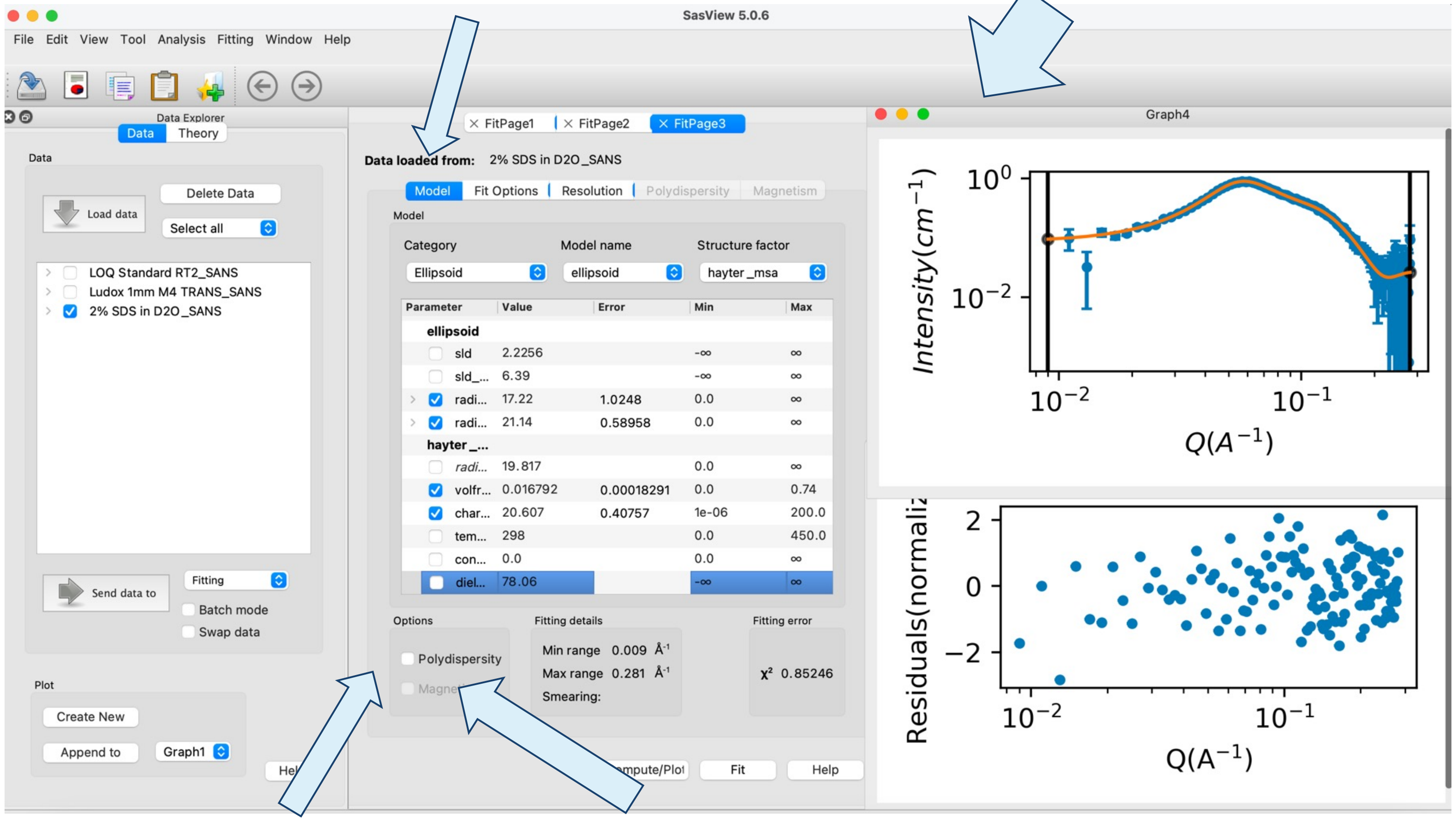
70+ models to explain data

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

Single, batch and simultaneous
1D and 2D fitting

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

Analysis Tool Choice
&
Plotting



□ 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:

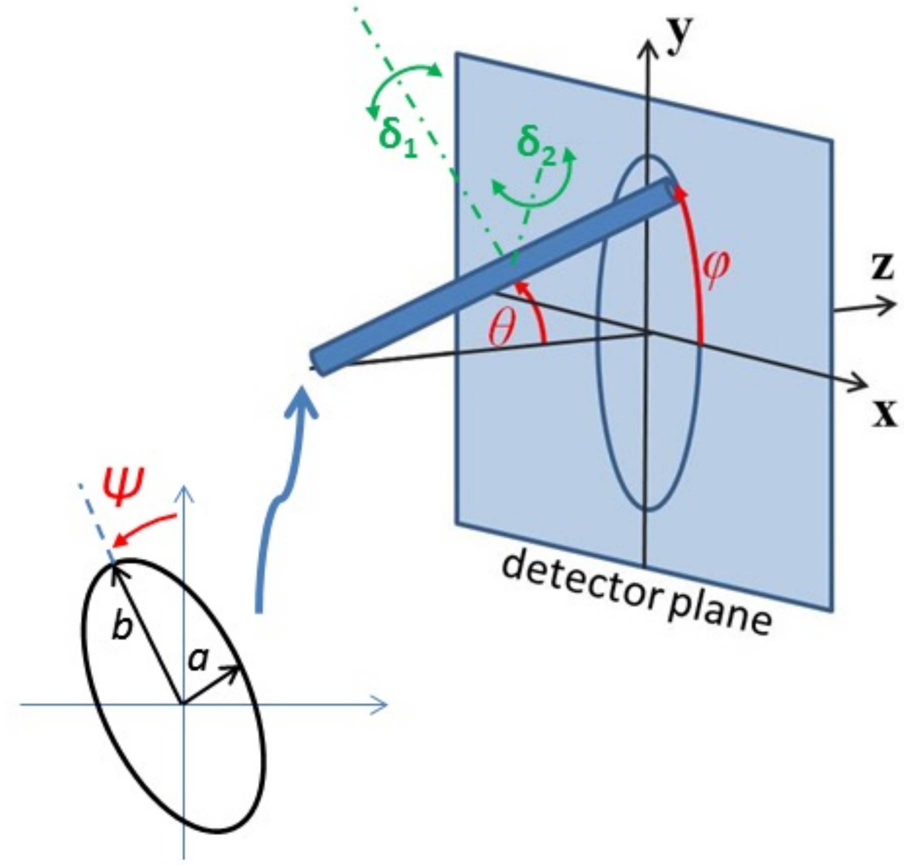
Fitting error

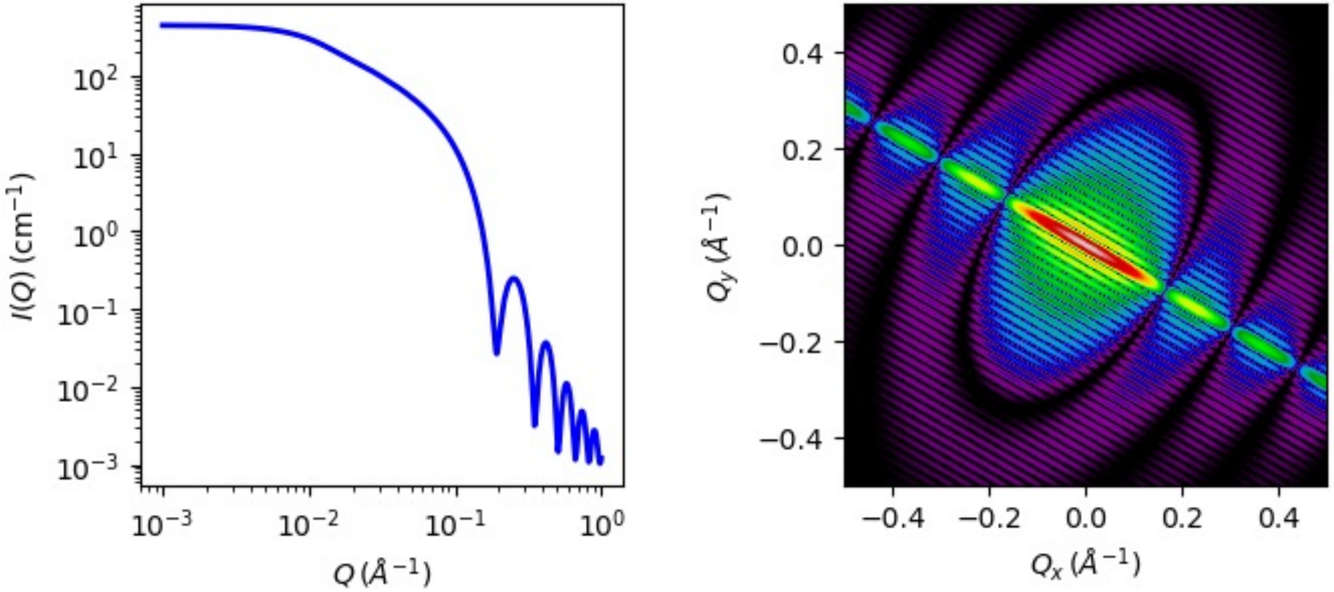
χ^2 0.85246

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

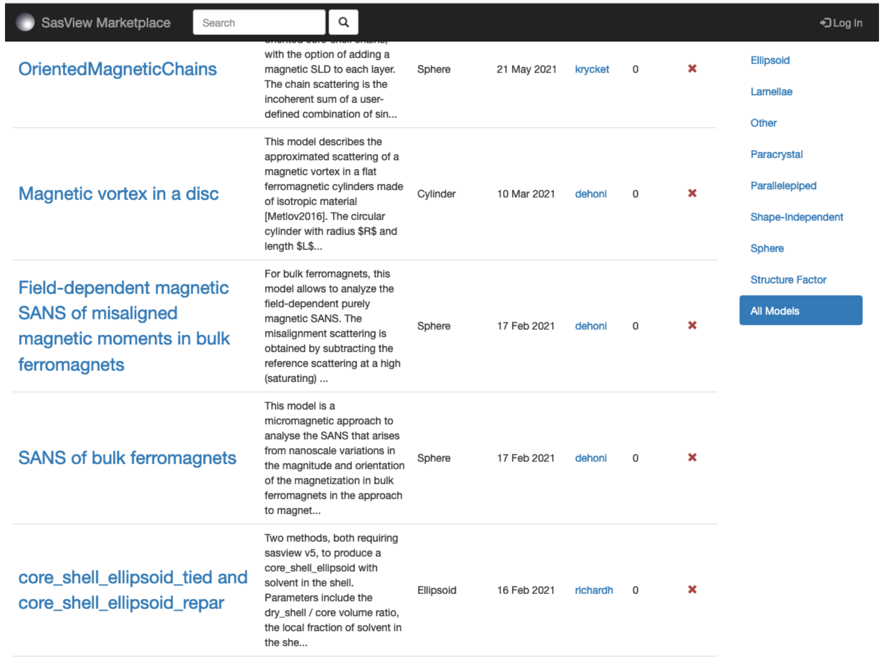




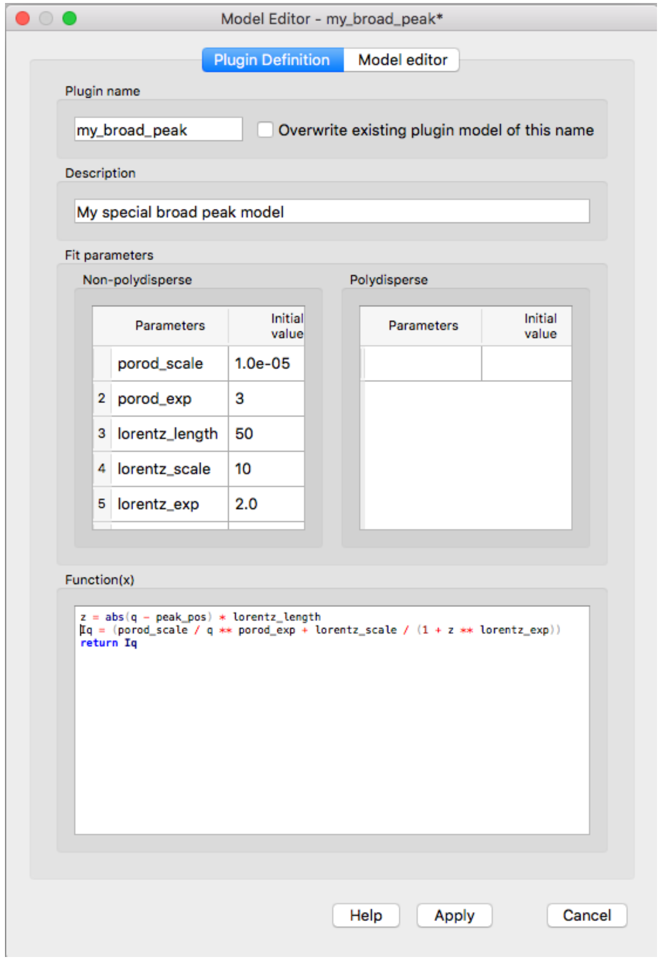
1D and 2D cylinder model

Plugin models

- 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

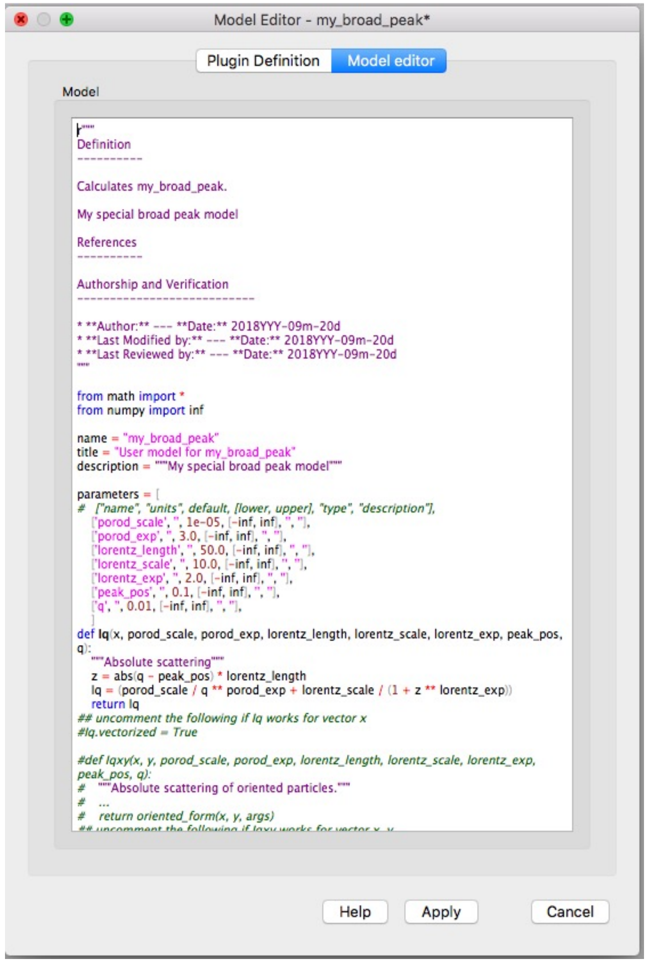
	Parameters	Initial value
	porod_scale	1.0e-05
2	porod_exp	3
3	lorentz_length	50
4	lorentz_scale	10
5	lorentz_exp	2.0

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
```



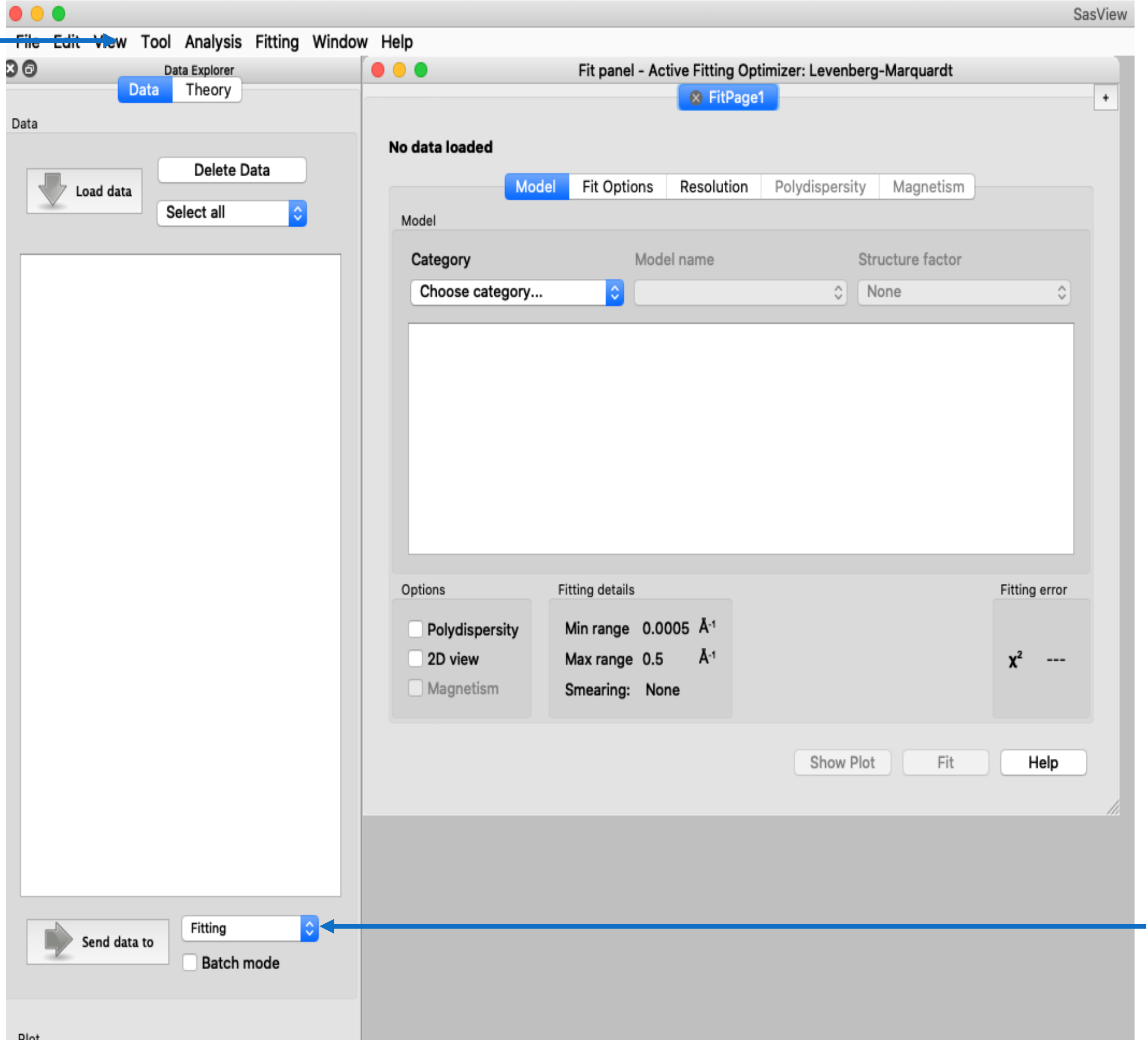
Model

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

Calculates my_broad_peak.

My special broad peak model

References
----------

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)
## uncomment the following if Iqxy works for vector x, y
```

Other SasView functionality

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

Category: Choose category...

Structure factor: None

□ Polydispersity

□ 2D view

□ Magnetism

Min range 0.0005 Å^{-1}

Max range 0.5 Å^{-1}

Smearing: None

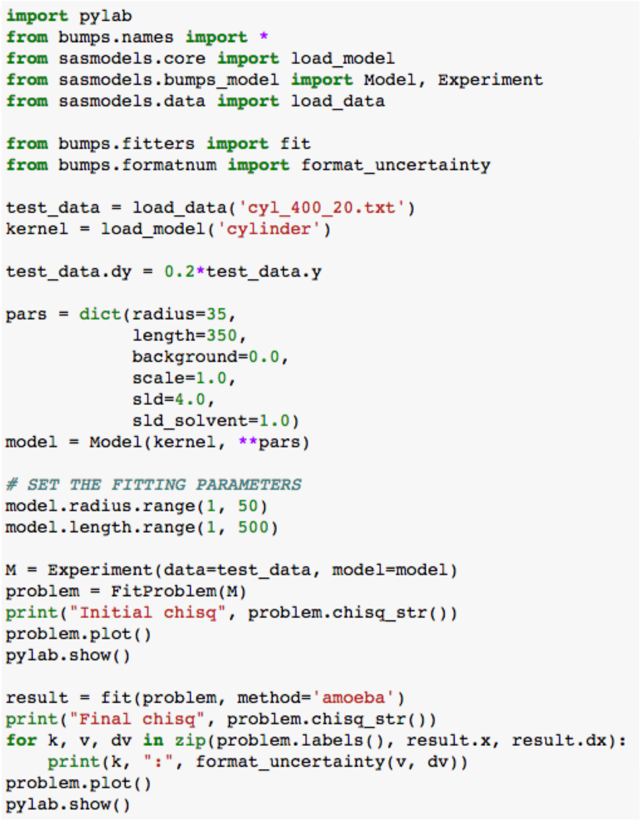
χ^2 ---

Analysis

- Fitting
- Invariant
- Pr Inversion
- Correlation Function

Beyond Graphical User Interface (GUI)

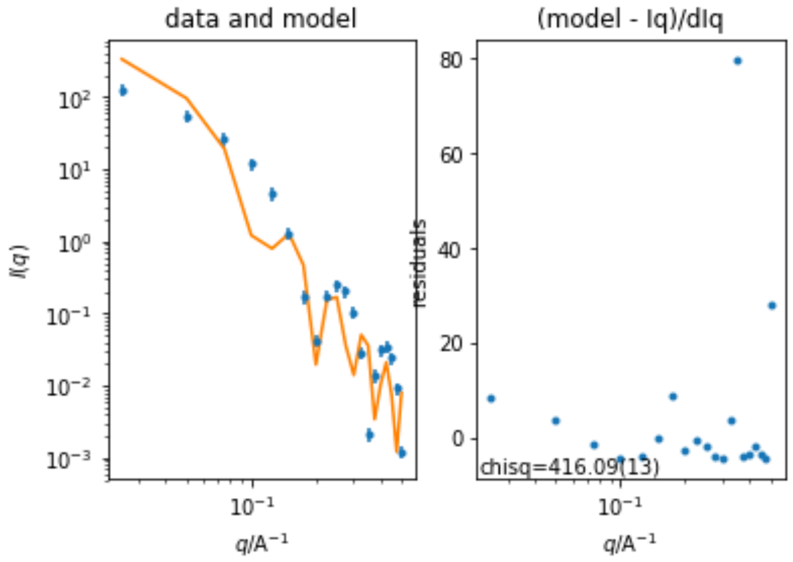
- Useful for batch jobs and reproducibility
- Scripts can be run on computer cluster



```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()
```

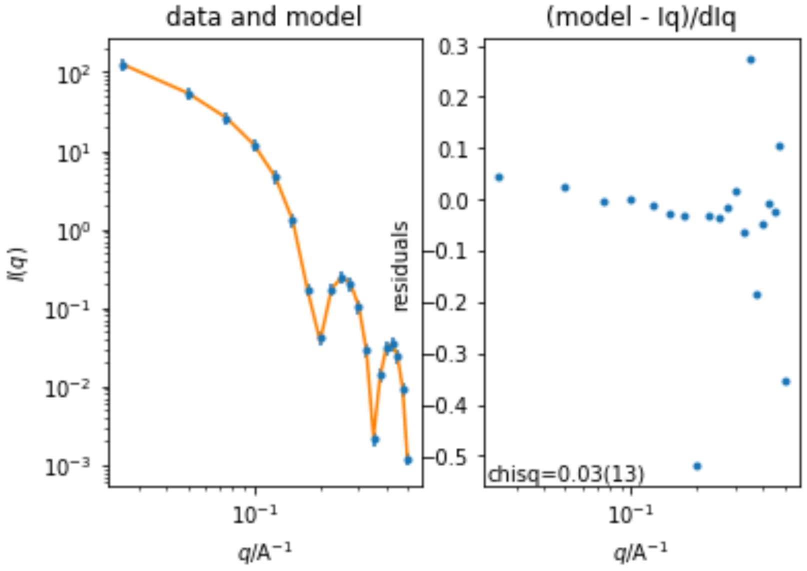
Before fit

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



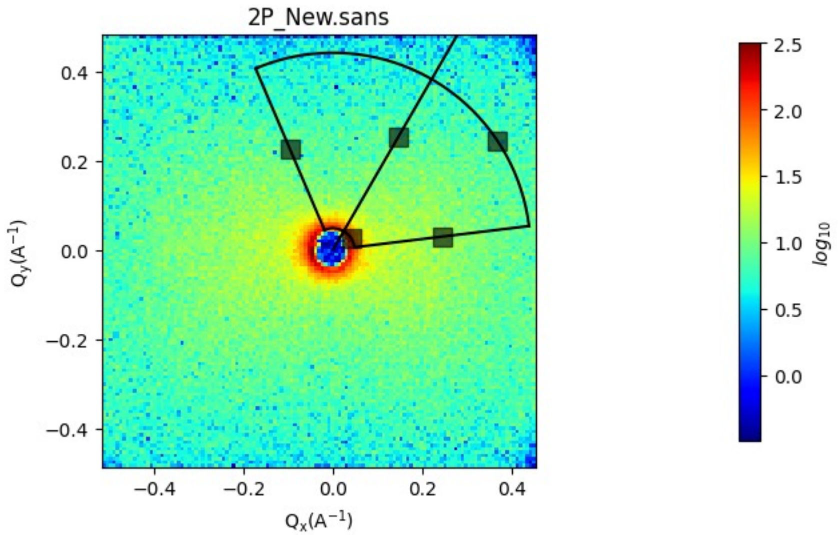
After fit

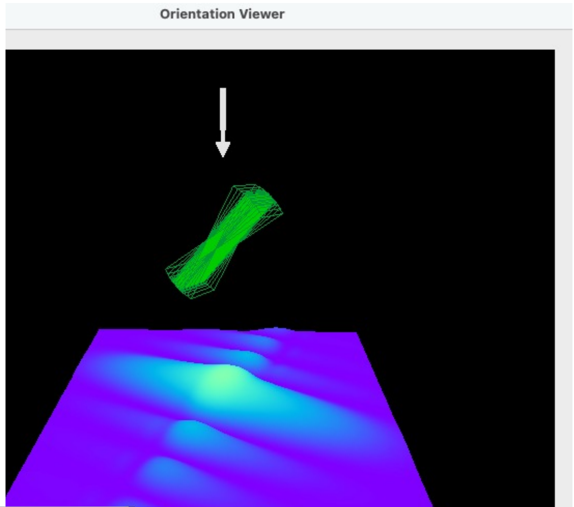
```
Final chisq 0.03(13)
length : 464.9(55)
radius : 19.977(64)
```

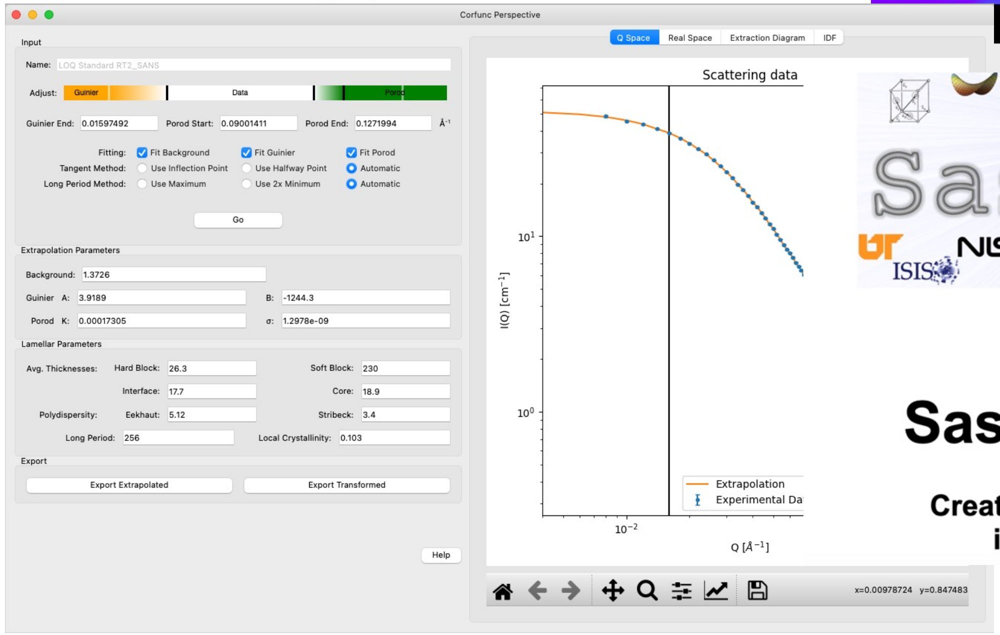


SasView 6.0.0-beta release

- 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

Adjust: Guinier | Data | Porod

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

Go

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

Export Extrapolated Export Transformed

Help

SasView Tutorials

Creating Custom Fitting Models in SasView Version 5.x

https://github.com/SasView/sasview/releases/tag/v6.0.0-beta-2

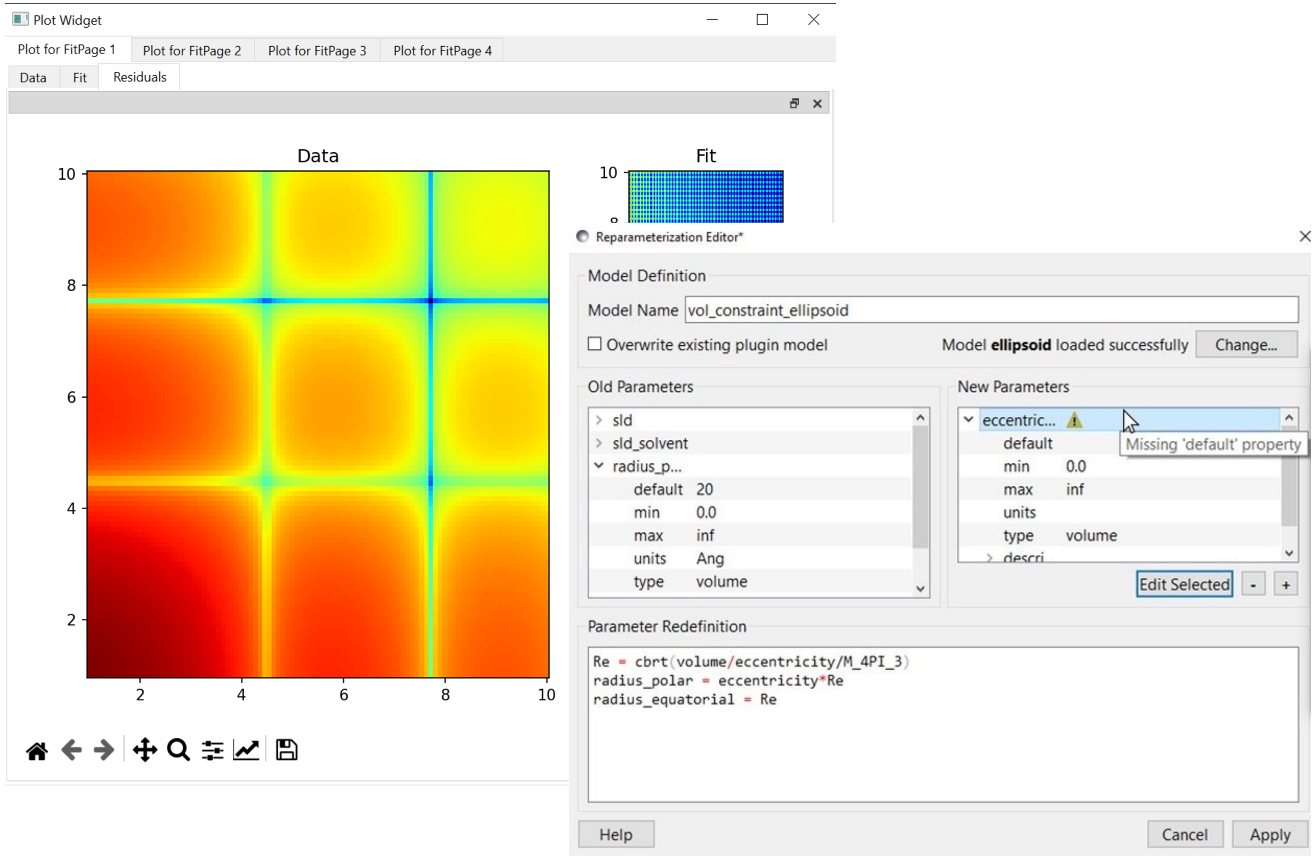
Examples of contributions

- Magnetic SANS community workshop
- Student projects
- Incorporating external software tools

Contributor camp, University of Delaware, January 2024

Student projects

- Improvements in:
  - Plotting
  - Data structure
  - Documentation
  - Plugin Editor
  - Slicers
  - Generic Scattering Calculator
- Web-based API
- Pore size distributions
- Simultaneous SAXS and SANS fitting



Model Name: vol_constraint_ellipsoid

☐ Overwrite existing plugin model

Model **ellipsoid** loaded successfully

Old Parameters:

sld	
sld_solvent	
radius_p...	
default	20
min	0.0
max	inf
units	Ang
type	volume

New Parameters:

eccentric...	
default	
min	0.0
max	inf
units	
type	volume
descri...	

Missing 'default' property

```
Re = cbrt(volume/eccentricity/M_4PI_3)
radius_polar = eccentricity*Re
radius_equatorial = Re
```

Iestyn Cadwallader-Jones, Nouhalia Agouzal, Dorian Lozano, Julius Karliczek (ILL), Ellis Hewis, James Crake-Merani, Ruben Lopes (ISIS), Alex Zheng (NIST), Brayden Miller (NIST), Xael Shan (NIST), Anita Zhang (Princeton), Kristian Lytje (Arhus University)

Magnetic SANS workshops

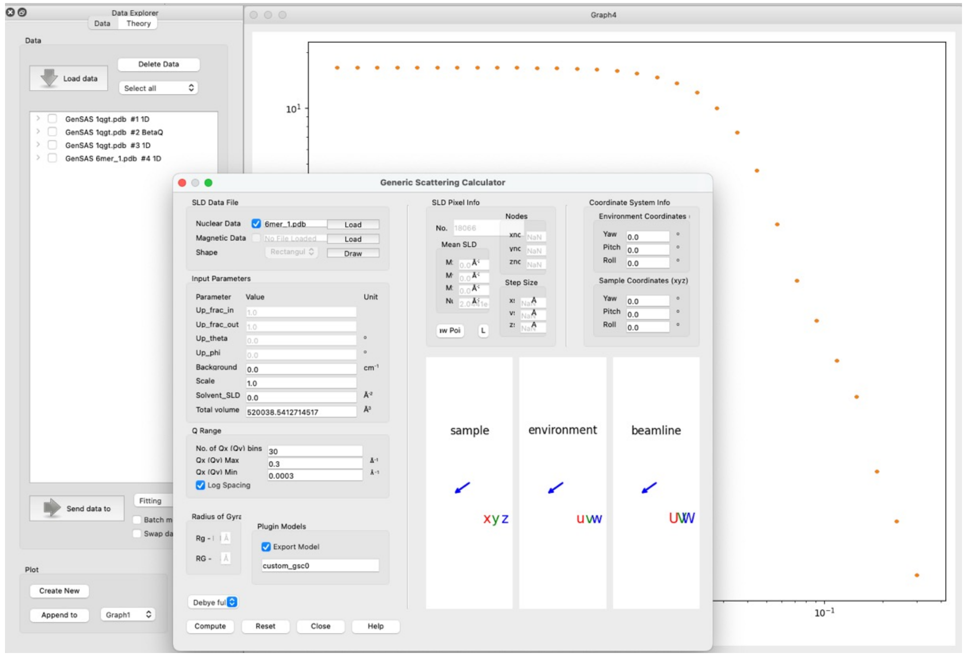
- 2-day in-person workshop in 2022
- 1-day follow-up hybrid workshop in 2023
- Participants from universities and facilities
- Gather requirements for Magnetic SANS data analysis
- A number of GitHub issues created
- Ongoing work on slicers and porting MuMag functionality (**Michael Adams**, Univ. of Luxembourg)

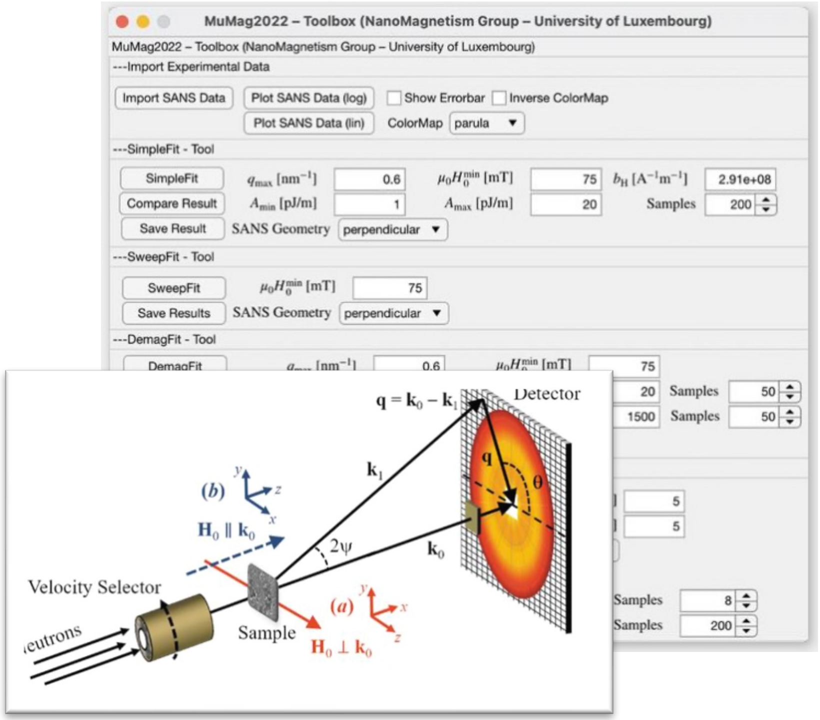
https://www.tandfonline.com/doi/full/10.1080/10448632.2022.2126691

Credit: Annika Stellhorn (ESS)

https://www.linxs.se/events/2023/1follow-up-magnetic-sans-data-and-software-h4crj

Incorporating external tools





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

K. Lytje and J. S. Pedersen Acta Cryst. (2024). D80, 493-505

Analyzing ferromagnets

- MuMag analyzes unpolarized total SANS data within the approach-to-saturation regime
- Matlab based GUI converted to SasView GUI

M. P. Adams, M. Bersweiler, E. M. Jefremovas and A. Michels J. Appl. Cryst. (2022). 55, 1055-1062,

How to get involved?

- Build up community/working group (like Magnetic SANS)
- Student projects
- Integrate own software libraries
- 5yr road map
- Project ideas (related to LOKI):
  - Rheo-SANS
  - SEC-SANS data treatment (ATSAS equivalent)
  - Improvements in scattering calculator for biomolecules
  - TOF resolution function (together with CanSAS)

www.sasview.org/contribute

Questions?

Thank you!

Features beyond 6.0.0 - particle editor

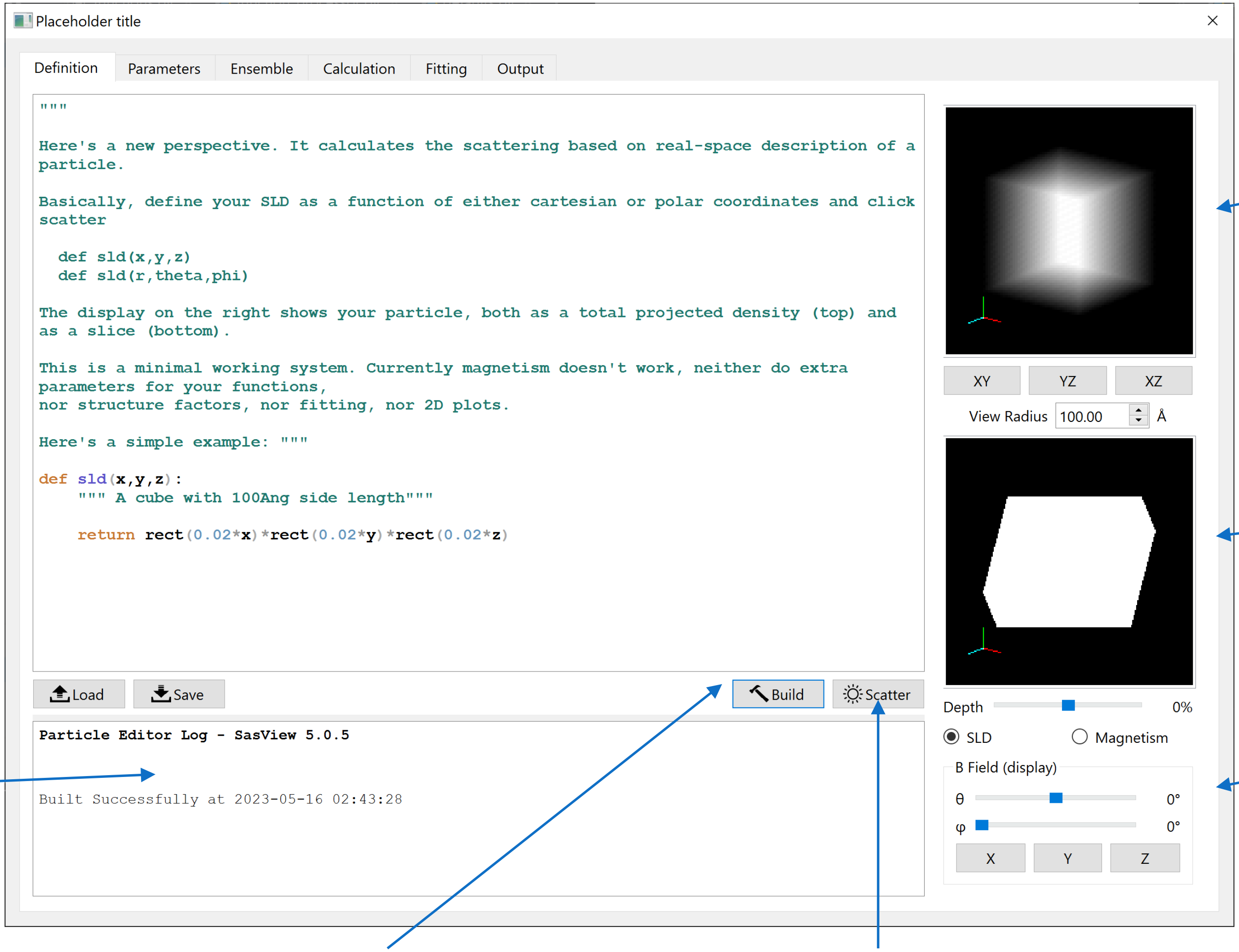
Define functions sld and (optionally) magnetism

sld / magnetism “x-ray” projection

sld / magnetism cross section

Feedback on code and calculations

Magnetic field controls for display



```
"""

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
```

“Recompile” and update display

Compute scattering