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Facilities Council

ISIS Neutron and
Muon Source

Welcome





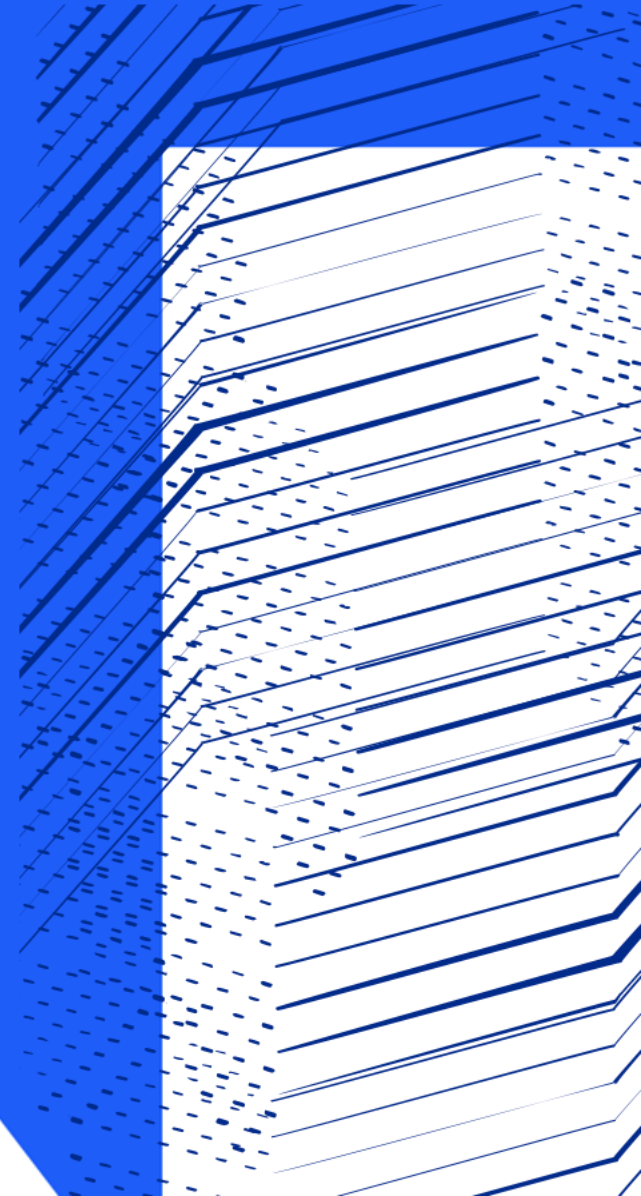
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SasView:

A 'Swiss Army Knife' for SAS Data Analysis

Dr Stephen King



Outline

1 What is Data Analysis?

And what it is not!

2 Data Formats

A possibly dull, but important, consideration!

3 Options for Data Analysis

Where to start!

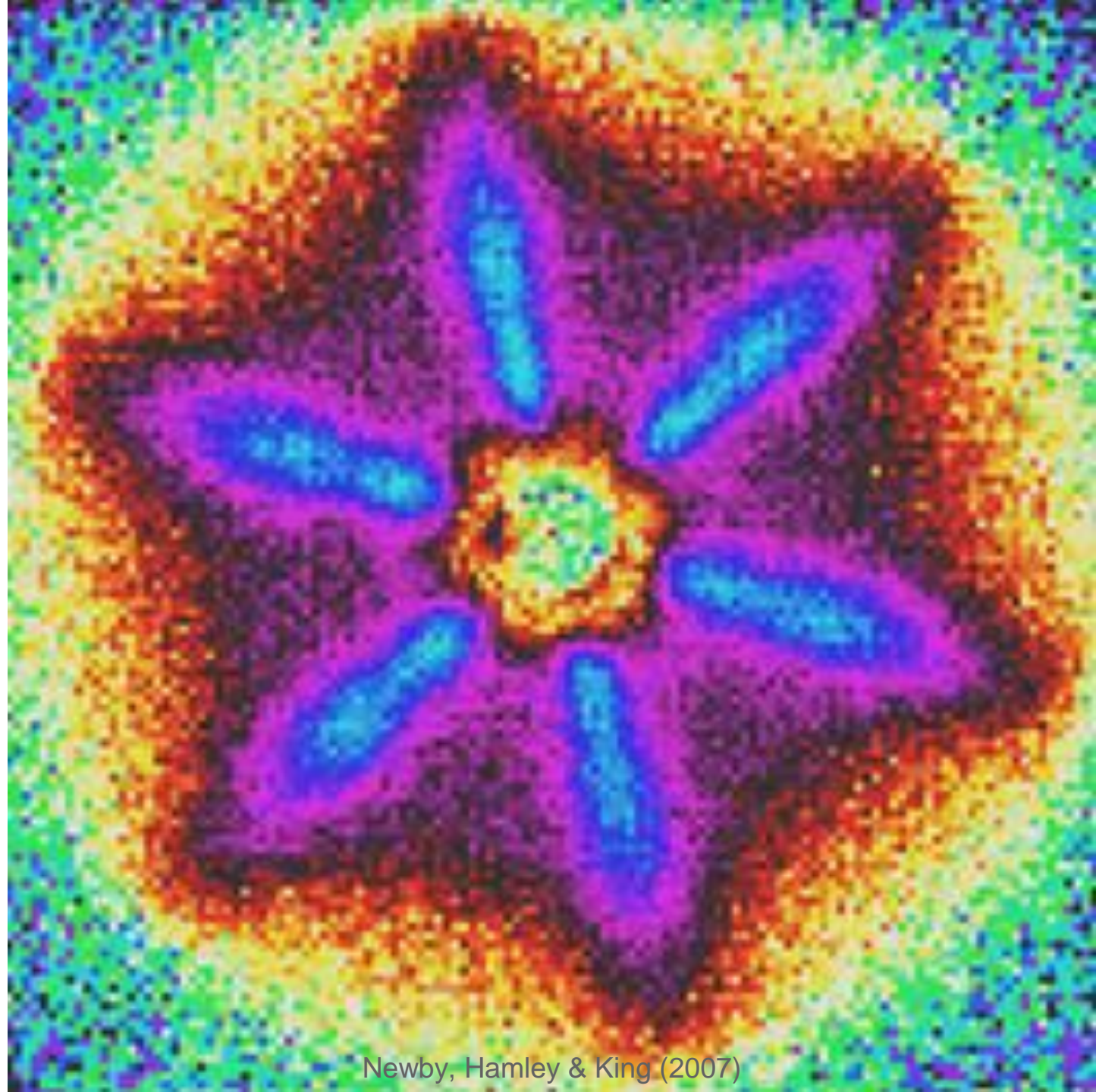
4 The SasView Collaboration

And how you can contribute!

5 Demonstrations of SasView

Including Model-Fitting 101

6 Questions?





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What is Data Analysis?

Two quotes...

“Data analysis is a process of inspecting, cleansing, transforming, and modeling data with the goal of discovering useful information, informing conclusions, and supporting decision-making.”

Wikipedia

“...a way of drawing inductive inferences from data and distinguishing the signal (the phenomenon of interest) from the noise (statistical fluctuations) present in the data...”

Shamoo & Resnik (OUP, 2003)

Key:

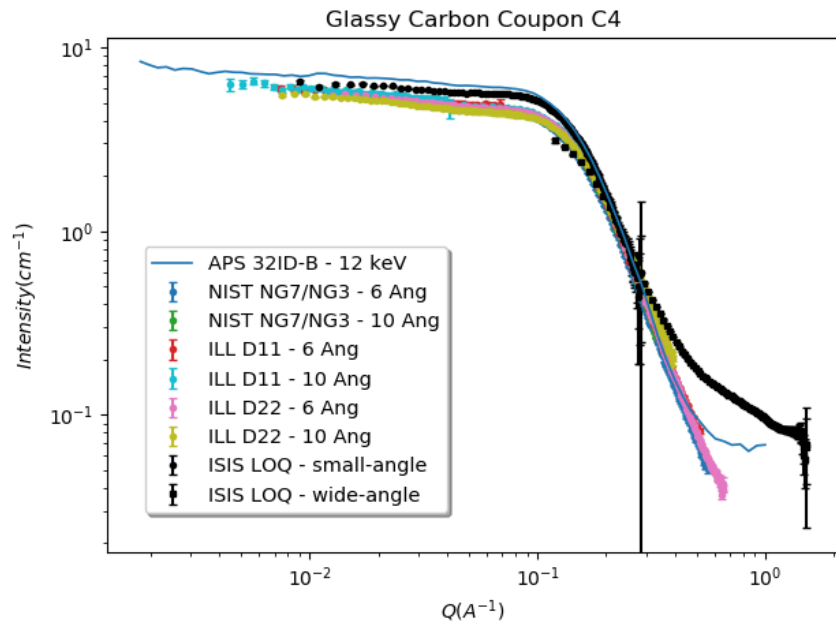
outcomes

methods

issues

Experimental Data Flow

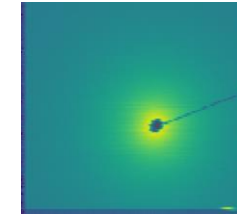
Reduced data should be reproducible anywhere!



<http://www.cansas.org>

Instrument-
dependent
data

Instrument-
independent
data



Data Acquisition System

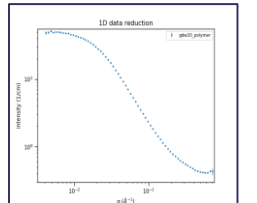
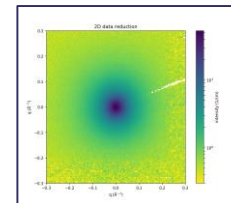
'raw' data file
(NXS)

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

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

Data Analysis Programs

Paper / Thesis





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Reduced Data Formats

Possible Types of Data

Real data:

- the scattering data; 1D (*intensity vs Q*) / 2D (*intensity vs $Q_{parallel,x}$ vs $Q_{perpendicular,y}$*)
- the associated uncertainties
- maybe *transmission vs λ* from TOF-SANS

Meta data:

- identifying date, time, user, instrument, sample, reduction software & version, ...

Non-neutron data:

- parameters 'scanned' during the course of a measurement (e.g. T , P , $\dot{\gamma}$, θ , etc)
- simultaneous ancillary measurements (e.g. DLS correlation functions)
- simulation data

Possible Types of Data Format

‘Minimalist’ (e.g. ‘plain text’, TXT, DAT, CSV*):

- typically just contains some numbers + a header if you are lucky!

Self-describing (e.g. XML, CanSAS1D):

- uses ‘tags’ to order and describe the data/metadata to an agreed structure

Hierarchical (e.g. HDF, NXcanSAS):

- also self-describing, but fully portable (no outside information needed)
- can contain a mix of data types (‘a file-system-in-a-file’)

SasView inputs many of these (and more)!

* Beware the semi-colon ; !

The CanSAS Standards

CanSAS1D

- v1.0 released May 2009
- v1.1 released Mar 2013
- for 1D reduced data only
- XML-based (.xml)
- still human-readable

<http://www.cansas.org/formats/canSAS1d/1.1/doc/>

NXcanSAS

- v1.0 released Jan 2017
- for nD reduced data
- HDF5-based (.h5)
- NeXus-structured
- not human-readable

<http://www.cansas.org/wgwiki/index.php/NXcanSAS>

<https://www.nexusformat.org/>

<https://www.hdfgroup.org/downloads/hdfview/> (free!)

HDF® VIEW





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Options for SAS Data Analysis

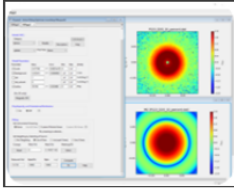
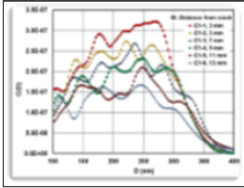
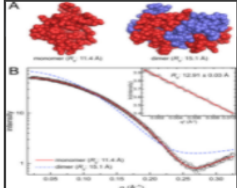
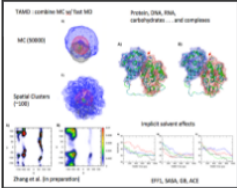
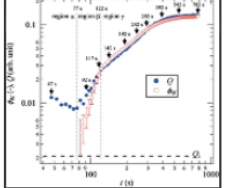
Many Options!

But:

- not every option is needed every time!
- often one option will suffice

Influences:

- what you want to know
- the data quality
- your field/speciality

Model-Fitting Methods	Real-Space Methods	Ab-initio Methods	MC/MD Methods	Other Methods
 <p>Example of 2D model-fitting using the SasView application</p>	 <p>Cavity size distributions in a steel weldment as derived from SANS 10.1179/1743284714Y.00000000577</p>	 <p>Ab-initio modelling of polcalcine constrained by SAXS 10.1002/pro.3376</p>	 <p>MC & TAMD modelling of proteins constrained by SANS 10.1016/j.jmngm.2017.02.010</p>	 <p>Time evolution of the invariant during crystallisation of P4MP1 10.1038/pj.2012.204</p>
<p>This approach uses iterative optimisation to match the calculated scattering from a model function describing the scattering objects to the measured scattering data. Each iteration one or more physical parameters describing the model (e.g. concentration, size, scattering length density) are adjusted.</p>	<p>This approach uses mathematical transformations (e.g. Fourier Transforms) to convert the measured scattering data in reciprocal-space (i.e. in Q-space) into a function in real-space. Typical outputs are density correlation functions, volume fraction distributions, and size distributions.</p>	<p>This approach uses iterative optimisation to match the calculated scattering from assemblies of spheres or from a 3D 'shape envelope function' to the measured scattering data. Each iteration the number and/or position of the spheres, or the curvature of the envelope function, is adjusted.</p>	<p>This approach uses iterative optimisation in combination with Monte Carlo (MC) and/or Molecular Dynamics (MD) techniques or RRT searches to match a calculated 'atomistic level' structure for the scattering objects to the measured scattering data.</p>	<p>Other approaches to data analysis may involve identifying, for example: any Q-dependencies in the measured data, particular patterns in the Q-values of any peaks present, asymptotic extrapolations, calculation of the integral under the measured data (the 'invariant'), or the intensity at Q=0.</p>

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



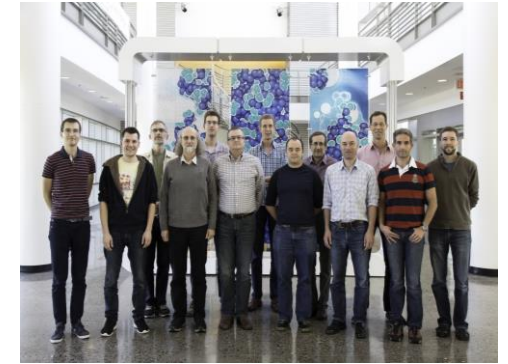
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The SasView Collaboration

Status of SasView

- 2006; originates in NSF *DANSE* project
- 2013; transitions into a community project
- ~40 contributors from 9 organisations (~15 active at any one time)
- twice monthly zoom calls
- regular 'camps' & 'hackathons'
- small management team:
Paul Butler (NIST), Mathieu Doucet (ORNL),
Andrew Jackson/Wojciech Potrzebowski (ESS),
Steve King (ISIS)

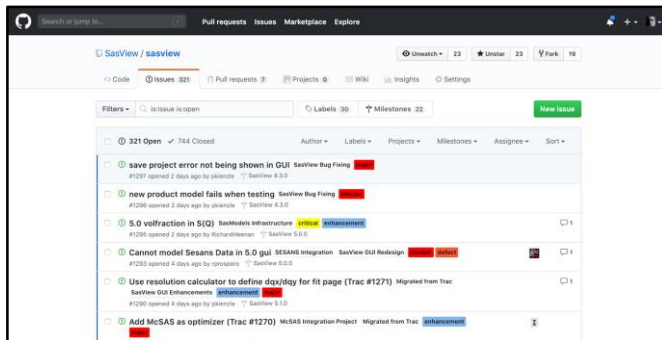


Open, Collaborative, Community Development

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

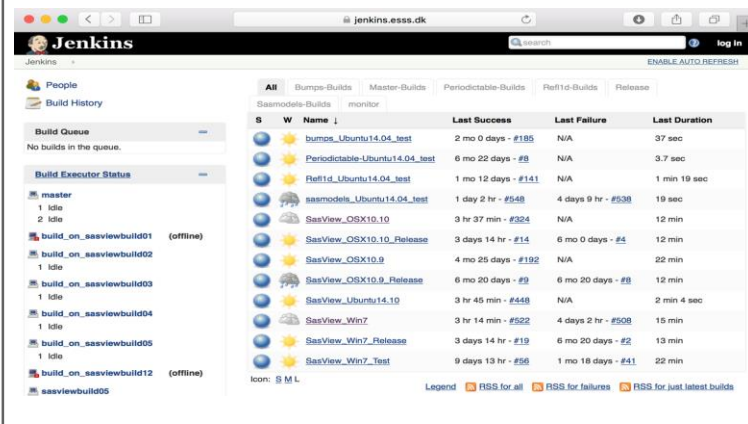
Rolling 5 Year Roadmap

Code Hosting, Issue Tracking & Developer Wiki on Github



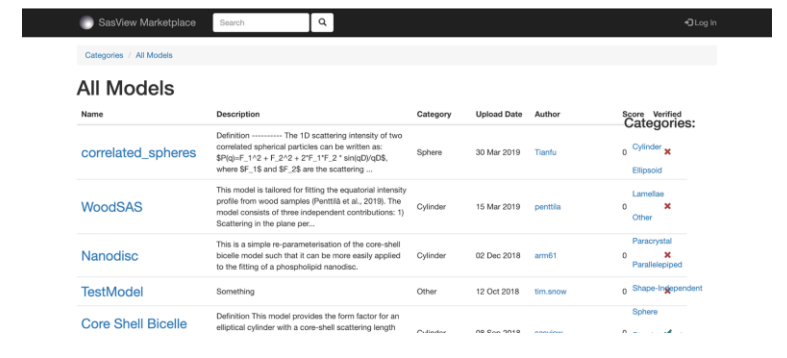
<https://github.com/SasView>

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

DOI for each release

The screenshot shows the Zenodo community page for 'SasView - Data Analysis for Small Angle Scattering'. The page features a search bar, 'Upload' and 'Communities' buttons, and 'Log in' and 'Sign up' links. Below the header, the title 'SasView - Data Analysis for Small Angle Scattering' is displayed. A 'Recent uploads' section includes a search bar and a list of uploads. The first upload is 'SasView version 5.0.1', dated February 7, 2020, with 'Software' and 'Open Access' tags. It lists numerous authors and a detailed description of the release. The second upload is 'SasView version 4.2', dated September 9, 2018, also with 'Software' and 'Open Access' tags. The third upload is 'SasView version 4.1.2', dated August 12, 2017, with 'Software' and 'Open Access' tags. A 'New upload' button is visible on the right side of the page.

zenodo Search Upload Communities Log in Sign up

SasView - Data Analysis for Small Angle Scattering

Recent uploads

Search SasView - Data Analysis for Small Angle Scattering

February 7, 2020 (v1) Software Open Access View

SasView version 5.0.1

Doucet, Mathieu; Cho, Jae Hie; Alina, Gervaise; Attala, Ziggy; Bakker, Jurrian; Bouwman, Wim; Butler, Paul; Campbell, Kieran; Cooper-Benun, Torin; Durniak, Celine; Forster, Laura; Gonzales, Miguel; Heenan, Richard; Jackson, Andrew; King, Stephen; Kienzie, Paul; Krzywion, Jeff; Nielsen, Torben; O'Driscoll, Lewis; Potrzebowski, Wojciech; Prescott, Stewart; Ferraz Leal, Ricardo; Rozycko, Piotr; Snow, Tim; Washington, Adam;

5.0.1 release

Uploaded on March 3, 2020

September 9, 2018 (4.2.0) Software Open Access View

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; Kienzie, Paul; Krzywion, 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 View

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; Kienzie, Paul; Krzywion, 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 #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

New upload

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

Want your upload to appear in this community?

- Click the button above to upload a record directly to this community. To add one of your existing records to the community, edit the record, add this community under the 'Communities' section, save, and finally publish.
- The community curator will then be notified to either accept or reject your upload (see community curation policy below).
- If your upload is rejected by the curator, it will still be available on Zenodo, just not in this community.

The screenshot shows the Zenodo release page for 'SasView version 5.0.4'. The page features a search bar, 'Upload' and 'Communities' buttons, and 'Log in' and 'Sign up' links. Below the header, the title 'SasView version 5.0.4' is displayed. The page includes a list of authors, a 'Contact person(s)' section, a 'Data manager(s)' section, and a 'Researcher(s)' section. A 'Work package leader(s)' section is also present. The release is dated April 15, 2021, and is tagged as 'Software' and 'Open Access'. The page shows 24 views and 3 downloads. A table lists the files for download, including 'SasView-5.0.4-Linux.tar.gz', 'SasView-5.0.4-MacOSX.dmg', and 'setupSasView-5.0.4-Win64.exe'. The page also displays the DOI '10.5281/zenodo.4467703' and the license 'BSD 3-Clause "New" or "Revised" License'. A 'Versions' section shows the release history.

zenodo Search Upload Communities Log in Sign up

April 15, 2021 Software Open Access

SasView version 5.0.4

Doucet, Mathieu; Cho, Jae Hie; Alina, Gervaise; Attala, Ziggy; Bakker, Jurrian; Bouwman, Wim; Butler, Paul; Campbell, Kieran; Cooper-Benun, Torin; Durniak, Celine; Forster, Laura; Gonzalez, Miguel; Heenan, Richard; Jackson, Andrew; King, Stephen; Kienzie, Paul; Krzywion, Jeff; Murphy, Ryan; Nielsen, Torben; O'Driscoll, Lewis; Potrzebowski, Wojciech; Prescott, Stewart; Ferraz Leal, Ricardo; Rozycko, Piotr; Snow, Tim; Washington, Adam

Contact person(s)

Potrzebowski, Wojciech; Jackson, Andrew

Data manager(s)

Parsons, Drew; Rakitin, Maksim

Other(s)

Taylor, Jonathan; Udby, Linda

Researcher(s)

Anuchitanukul, Atjit; Corona, Patrick; Juhas, Pavol; Knudsen, Mikkel; Gilbert, Peter; Krueger, Susan; McKerns, Mike; Mothander, Karolina; Narayanan, Theyencheri; Porcar, Lionel; Pozzo, Lilo; Rennie, Adrian; Teixeira, Susana; Weigandt, Katie

Supervisor(s)

Fragneto, Giovanna; Markvardsen, Anders

Work package leader(s)

Fultz, Brent; Rod, Thomas Holm

5.0.4 release

Files (747.7 MB)

Name	Size	Download
SasView-5.0.4-Linux.tar.gz	239.9 MB	Download
md5fab6c0df8d3f6a997c04dae30ee5f68		
SasView-5.0.4-MacOSX.dmg	231.9 MB	Download
md5a8268fef50b0f94253c208e98b836f4		
setupSasView-5.0.4-Win64.exe	276.0 MB	Download
md57c0dd9981acc7eb2be81639771f08050		

Base Citations 0

24 views 3 downloads See more details...

Indexed in OpenAIRE

Publication date: April 15, 2021

DOI: 10.5281/zenodo.4467703

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/v5.0.4>

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

Versions

Version 1 10.5281/zenodo.4467703 Apr 15, 2021

Cite all versions? You can cite all versions by using the DOI 10.5281/zenodo.4467702. This DOI represents all versions, and will always resolve to the latest one. Read more.

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

Open, Collaborative, Community Learning

- 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 consists of four overlapping images:

- Slack Channel:** A screenshot of the #general channel in the SasView Slack workspace. It shows a list of channels on the left, a search bar at the top, and a message from Michael Zhang dated Thursday, April 15th.
- Twitter Profile:** A screenshot of the SasView (@SasView) Twitter profile. It includes the profile picture, name, handle, bio, website (sasview.org), and follower/following counts.
- Documentation Page:** A screenshot of the SasView 5.0.4 documentation page, specifically the 'Loading Data' section. It contains a table of contents, a list of topics, and detailed instructions on how to load data into the application.
- FAQ Page:** A screenshot of the SasView FAQ page, titled 'FAQ', which provides answers to common questions about the software.

Open, Collaborative, Community Learning

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- users@sasview.org

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



Go to each FitPage in turn and select the 'core' sphere model. The three theory curves will be added to the graph.

Parameter	Value
radius	0.000000
thickness	0.000000
volume fraction	0.000000
contrast	0.000000
background	0.000000



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 * [M] parameter_name`.

As we are assuming the volume fraction of droplets in each sample was different, remove the two scale constraints. And because the different datasets represent samples containing different amounts of H & D (and therefore have different incoherent scattering contributions), also remove the two background constraints.

But as it is the 'shell' contrast (M1) which should provide the most sensitivity to the thickness parameter, we need to change the constraint equalities dealing with thickness to read:

M2 thickness = M1.thickness
M3 thickness = M1.thickness

So we now have constraints that look like this:



SasView
5 subscribers

SUBSCRIBE 5

HOME VIDEOS PLAYLISTS CHANNELS DISCUSSION ABOUT

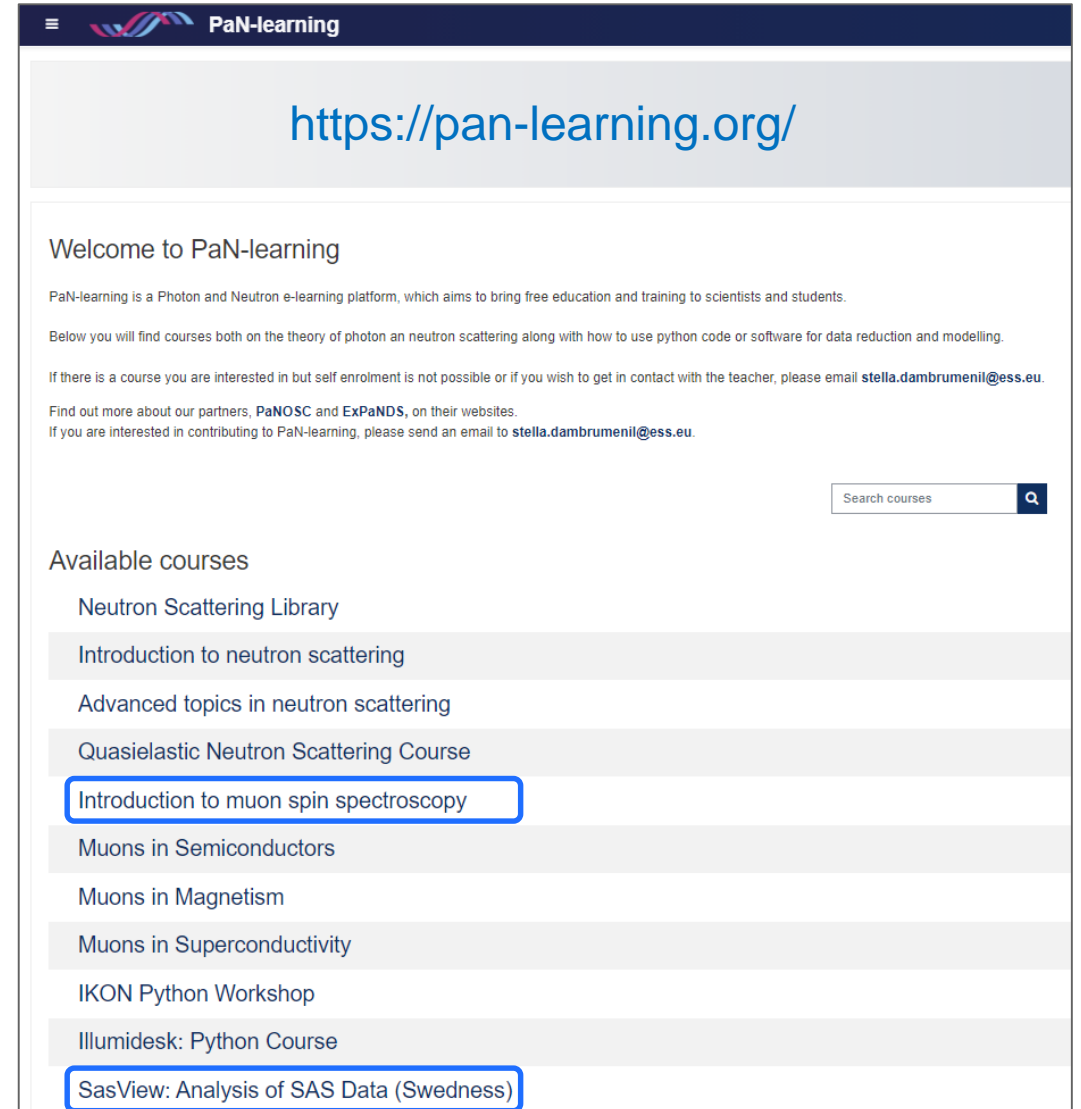
Uploads ▶ PLAY ALL

Video Title	Views	Time
Using the P(r) calculator in SasView	65 views	4:51
Scattering Length Density Calculator in SasView	43 views	1:28
Introduction to applying the beta approximation in...	23 views	7:27
Calculating the Scattering Invariant in SasView	29 views	4:01

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

*All the work of ISIS Sandwich
Student Michael Oakley*

A screenshot of the PaN-learning website. The header is dark blue with the PaN-learning logo and name. Below the header, the URL 'https://pan-learning.org/' is displayed in blue. The main content area is white and contains a welcome message, a description of the platform, and a list of available courses. The courses are listed in a table with alternating light and dark grey rows. The course 'Introduction to muon spin spectroscopy' is highlighted with a blue border. The course 'SasView: Analysis of SAS Data (Swedness)' is also highlighted with a blue border. A search bar is located on the right side of the page.

PaN-learning

<https://pan-learning.org/>

Welcome to PaN-learning

PaN-learning is a Photon and Neutron e-learning platform, which aims to bring free education and training to scientists and students.

Below you will find courses both on the theory of photon and neutron scattering along with how to use python code or software for data reduction and modelling.

If there is a course you are interested in but self enrolment is not possible or if you wish to get in contact with the teacher, please email stella.dambrumenil@ess.eu.

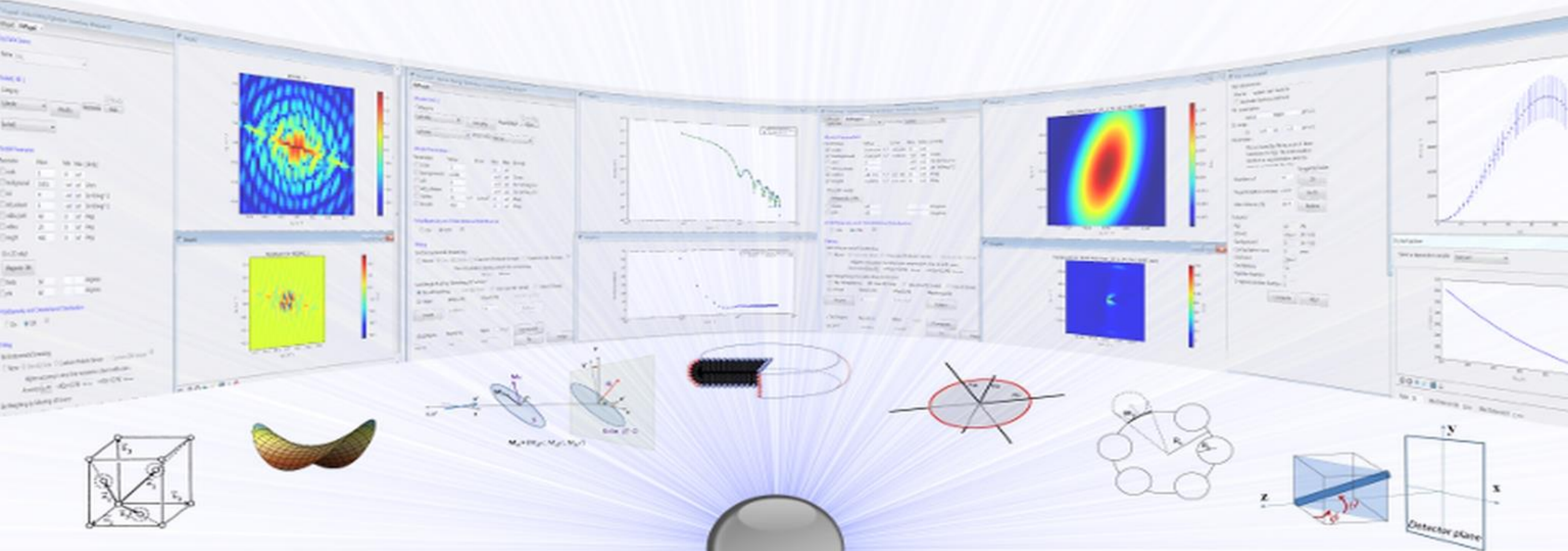
Find out more about our partners, **PaNOSC** and **ExPaNDS**, on their websites.

If you are interested in contributing to PaN-learning, please send an email to stella.dambrumenil@ess.eu.

Search courses

Available courses

Neutron Scattering Library
Introduction to neutron scattering
Advanced topics in neutron scattering
Quasielastic Neutron Scattering Course
Introduction to muon spin spectroscopy
Muons in Semiconductors
Muons in Magnetism
Muons in Superconductivity
IKON Python Workshop
Illumidesk: Python Course
SasView: Analysis of SAS Data (Swedness)



SasView

Model-Fitting 101

- The objective of model-fitting is to find a model solution (theory) that:
 - describes the **form** of the experimental data
 - offers minimal **uncertainty**
 - has **converged** nicely
- And above all is...

physically realistic !!!

“The fact, that A model fits your data, it is NOT proof that it is THE appropriate model.”

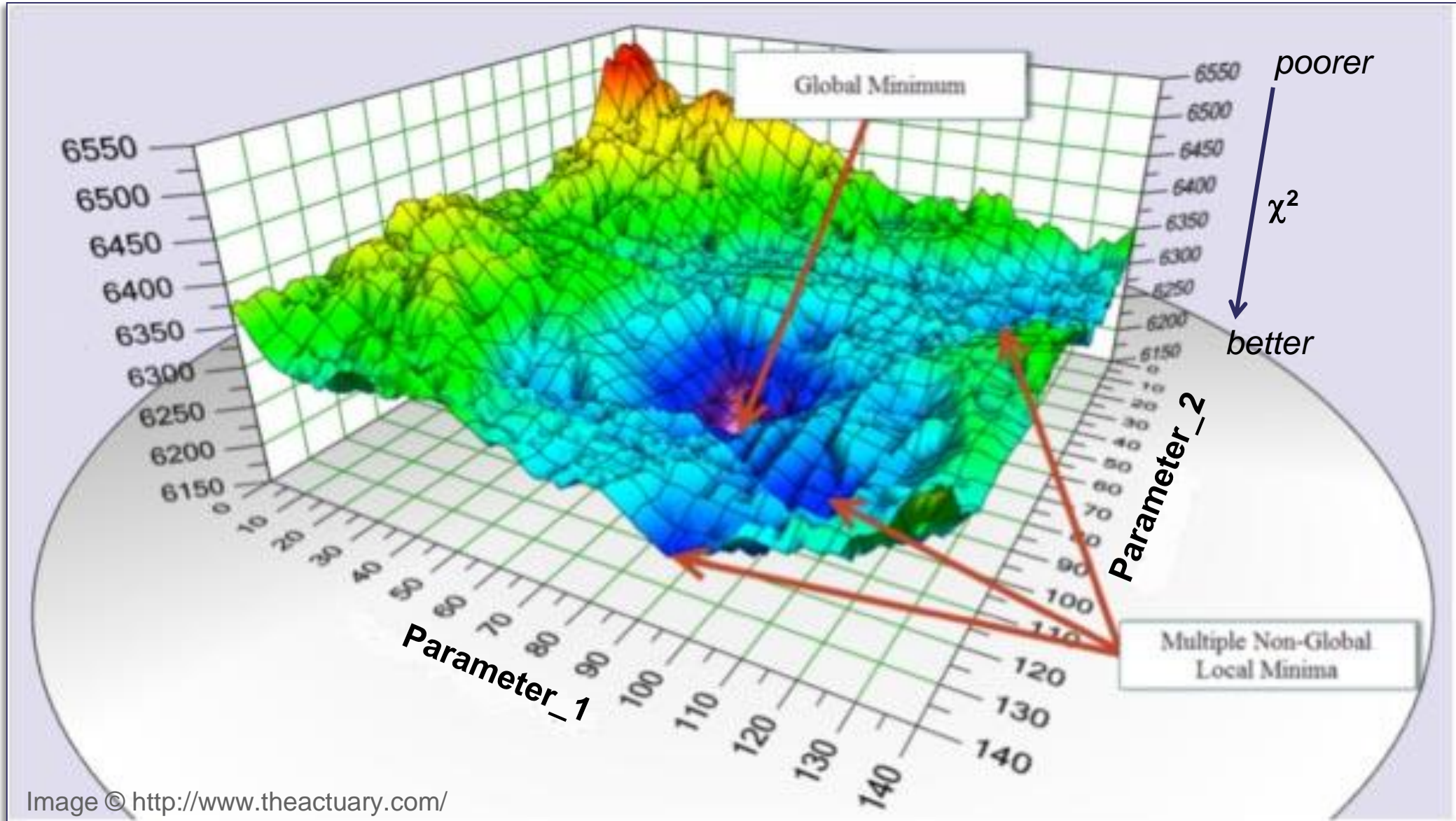
Jan Ilavsky, APS

Model-Fitting 101

- Wherever possible, select a model/parameters using *a priori* knowledge:
 - ancillary data (EM, DLS, *etc*)
 - published literature
- A model with **more parameters is not always better** than a model with fewer parameters!
- **Simultaneously fitting too many parameters** is generally **a bad idea!**
 - at least, until the program is homing in on a solution

Here's why...

Model-Fitting 101



Model-Fitting 101

- Finding the global minimum → **optimisation**
 - you can have **speed or robustness**, but not (generally-speaking) both!
- For speed: → **gradient-descent algorithms**
- For robustness: → **population algorithms**
 - also called 'evolutionary' or 'genetic' algorithms
 - **Bayesian (probability) algorithms**
- AI methods...

SasView features 5 optimisers...

SasView Optimisers

- **For speed: → gradient-descent algorithms**
 - *Levenberg-Marquardt*
 - the tried-and-trusted workhorse found in every model-fitting package
 - use when you have a reasonable fit in a minimum & want the best values
 - but beware it finding local minima
 - *Quasi-Newton BFGS*
- **In-between:**
 - *Nelder-Mead Simplex*
 - a good first choice (especially if your function is well-behaved)
- **For robustness: → population & Bayesian algorithms**
 - *Differential Evolution*
 - *DREAM*
 - use when you need a really robust fit &/or want to explore correlations

} ‘bumps’

<https://pypi.org/project/bumps/>
Paul Kienzle, NIST

<https://www.sasview.org/docs/user/qtgui/Perspectives/Fitting/optimizer.html>



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Time for a Demonstration!



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Thanks to:

The members of the
SasView Development Team



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Questions?

www.sasview.org

 [@SasView](https://twitter.com/SasView)

 sasview.slack.com

 help@sasview.org



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Thank you

www.sasview.org

 @SasView

 sasview.slack.com

 help@sasview.org