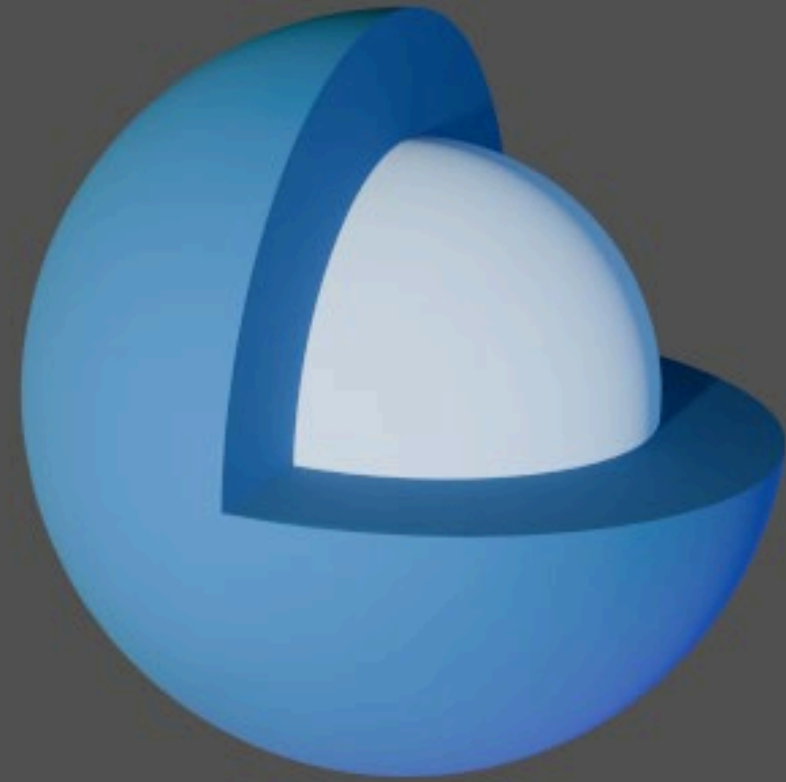




The SasView Organization

‘Disciplined and Professional’

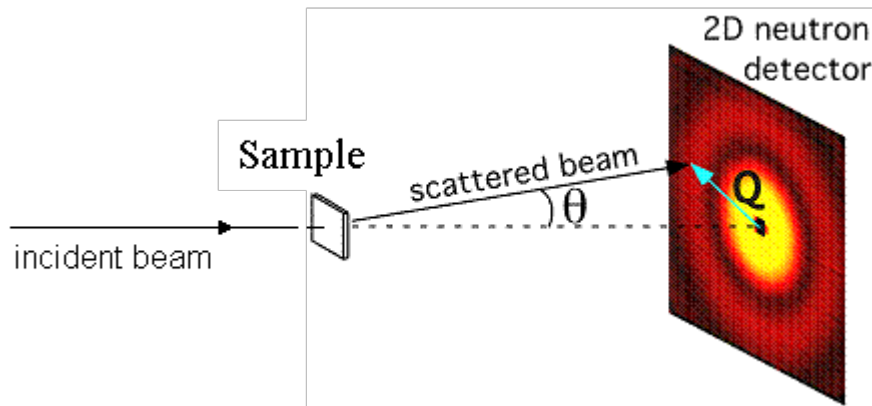
Jeff Krzywón



SASVIEW

ALL ANGLE SCATTERING ANALYSIS TOOLKIT

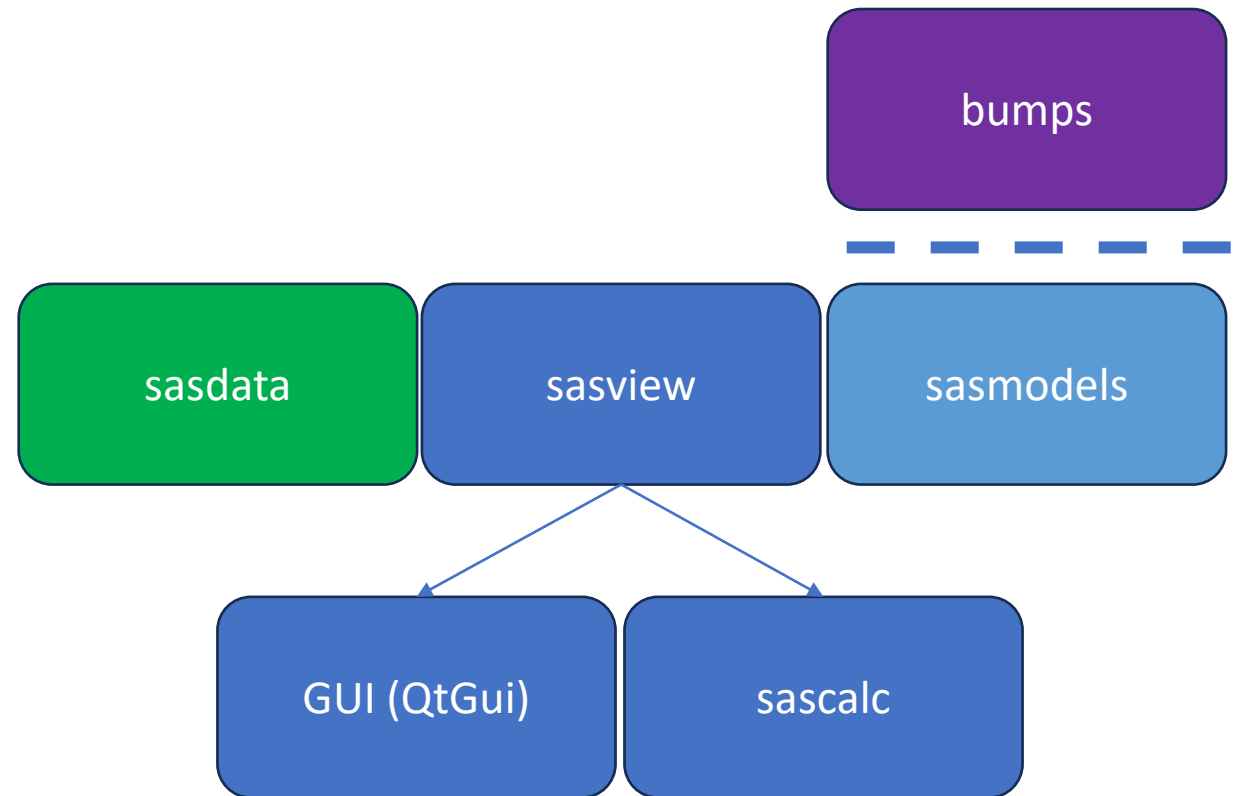
What is SasView



A Small Angle Scattering
Data Analysis tool for
SAS data in inverse
space and SESANS data
in correlation space

Code Structure

- sasmodels (on pypi)
 - Analytical models for various shapes and structures
 - Applies dispersity and resolution
 - Runs fits using bumps
- sasdata (on pypi)
 - Package to handle data import/export, data management, and data manipulations
- sasview (working release coming to pypi soon)
 - Overlap between GUI and sascalc



History



2006

2011

2012

NIST Supported initial transition from NSF funding

2013

Transition to Community project.

1st Code Camp at NIST April 2013

2014

v3.0 released (SansView)

2nd Code Camp at ISIS April 2014

2015

3rd Code Camp at ESS Feb 2015

2016

v4.0 released (SasView with sasmodels)

4th Code Camp at Delft March 2016



5th Code Camp at ORNL Oct 2016

2019

1st SasView User Meeting at SAS 2018

v5.0.0 released (Move from wx to Qt)

9th Code Camp at ILL/ESRF March 2019

2020

1st Virtual Code Camp March 2020*

1st Virtual Hackathon May 2020

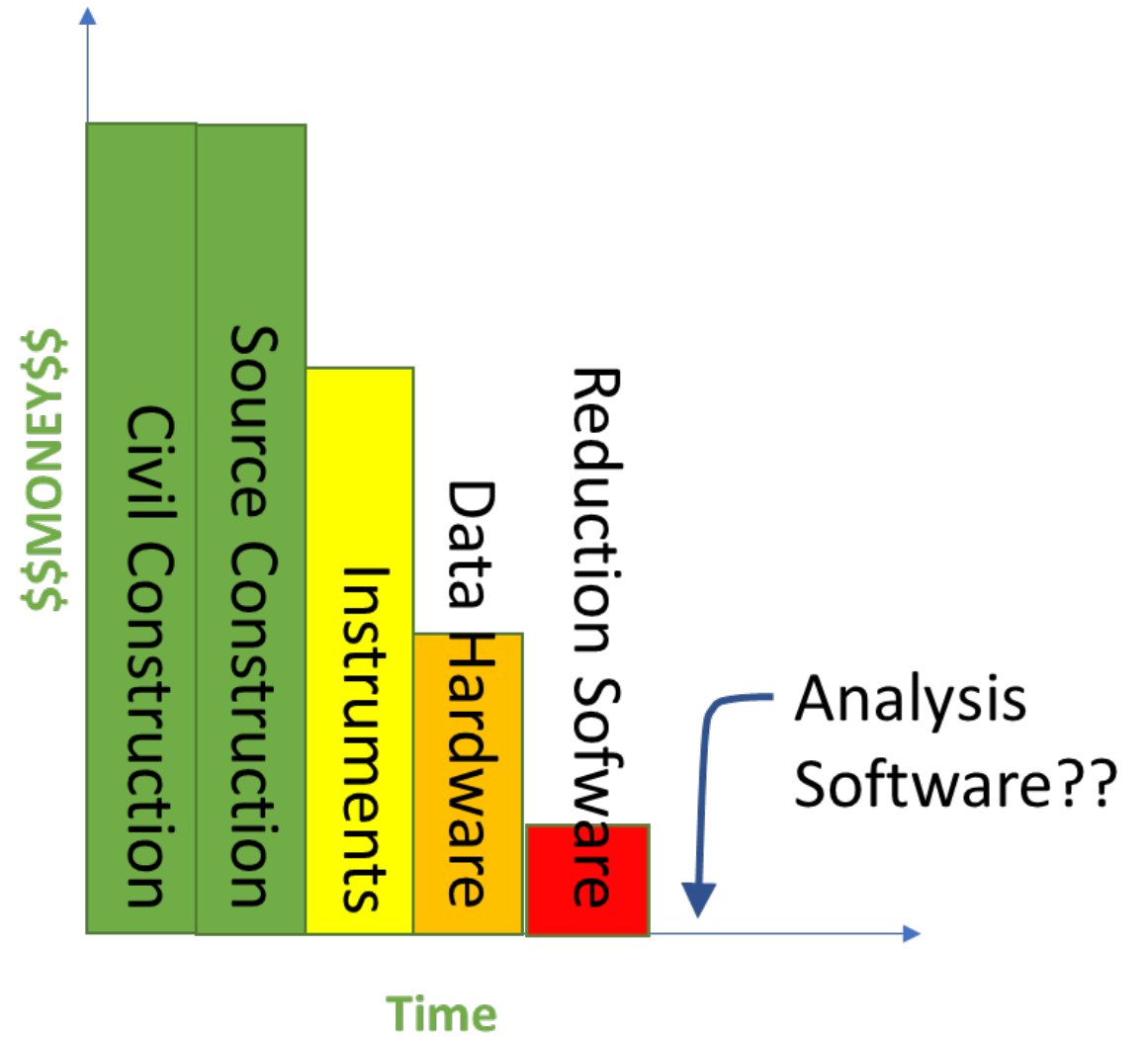
2024

v6.0.0 (sasdata separation)
(Sept/Oct 2024) (in Beta)

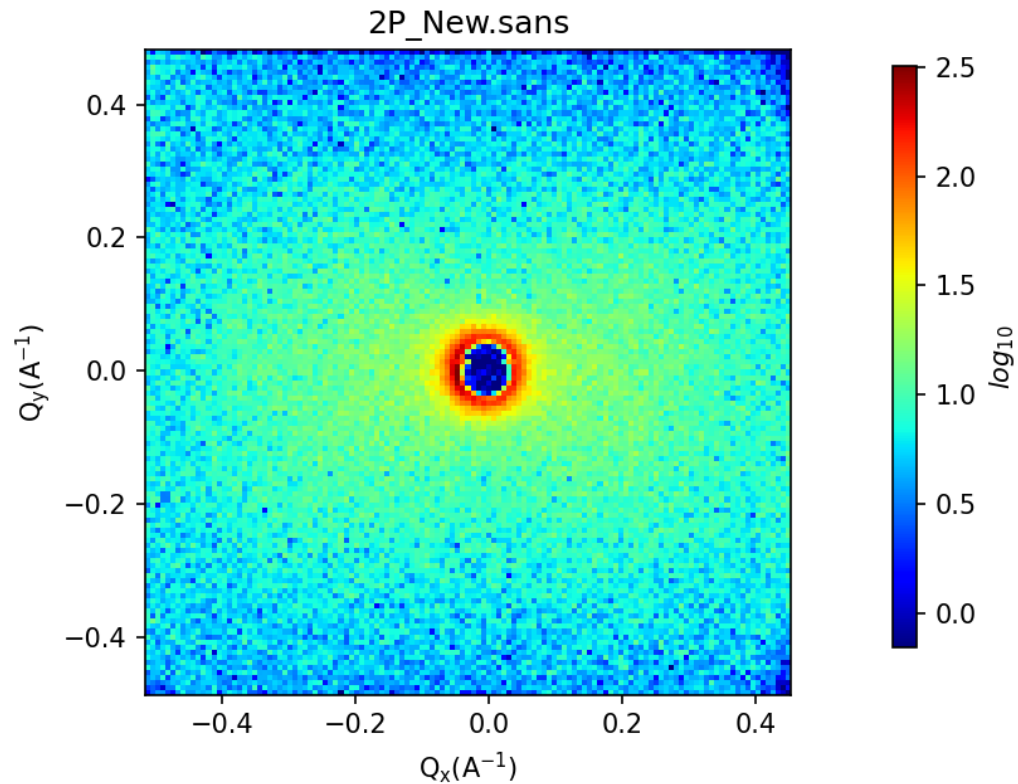
1st Contributor Camp January 2024

Addressing Resources Through Community

- Analysis
 - What is it?
 - Whose job is it?
 - What are the limits?



What is Analysis?



- Tools

- Generic Scattering Calculator to generate empirical models using PDB files (v6.0.0)
- SLD Calculator
- Q Resolution Estimator
- Various import/export methods
- Post-reduction averaging

- Analysis methods (perspectives)

- Fitting – Basic Model Fitting
- Invariant – Multi Phase Analysis
- $P(r)$ – Real Space Distributions
- Correlation Function – Real space

The SasView Approach

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

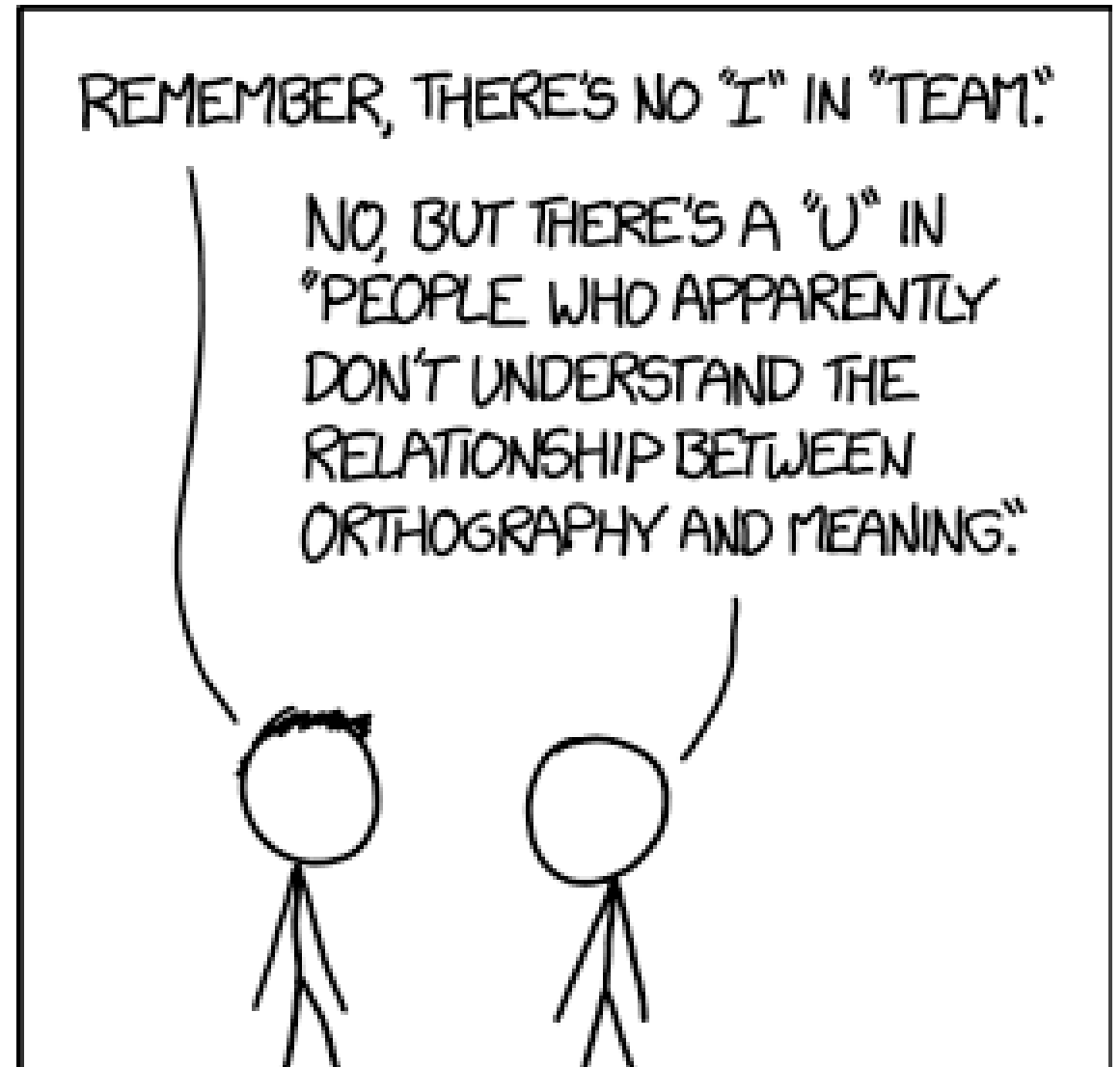
Work With Me, Not For Me

(and not dictate to me...)

- Nobody Owns SasView*
- Open Source
- Free to develop
 - Python and C

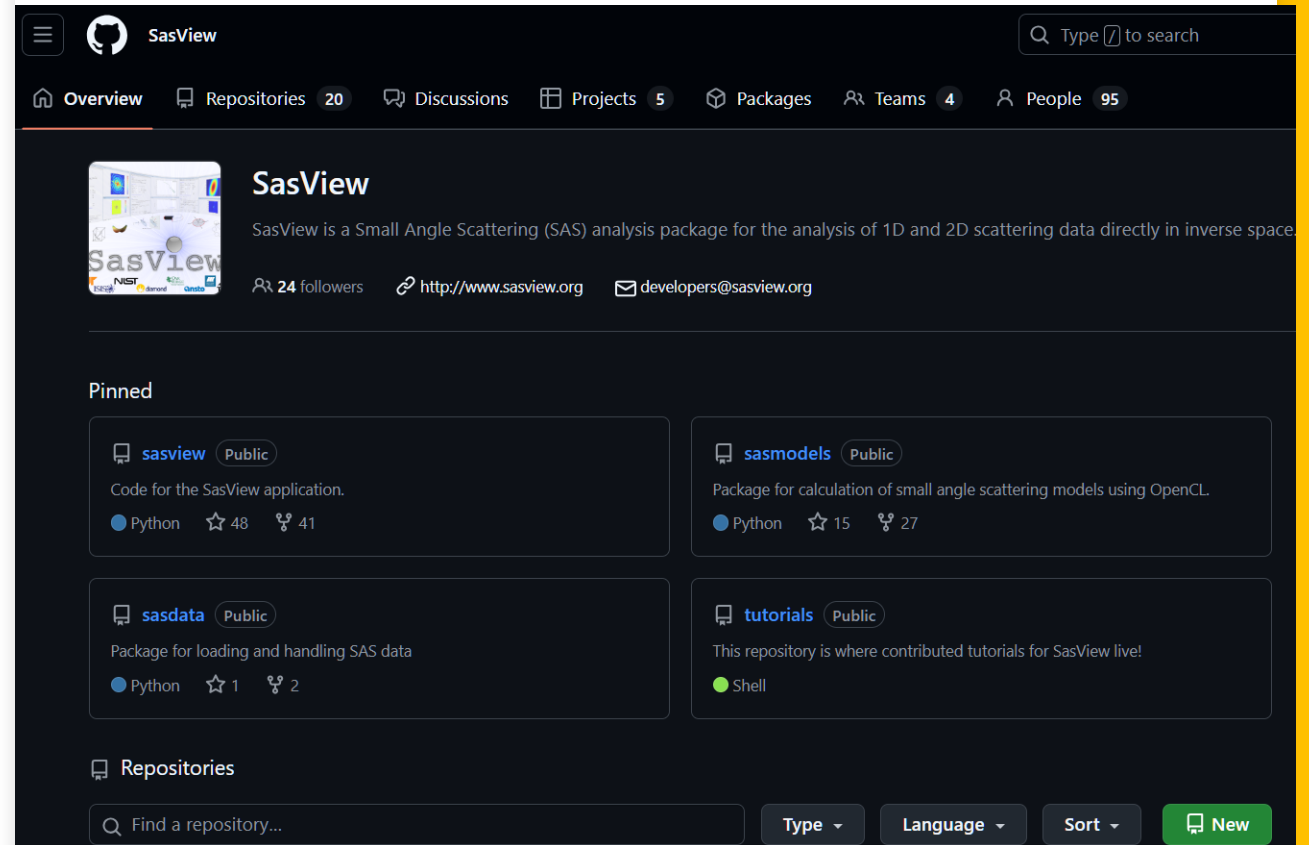
Lessons Learned:

- Global collaboration can be difficult
- “Small” money is a blessing



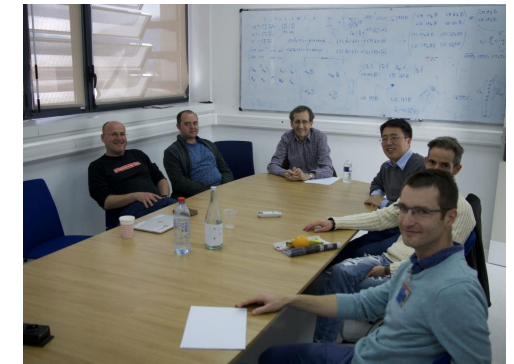
Open, Collaborative, Community Development

- Code Hosting, Issue Tracking, Developer Wikis and CI on Public GitHub repos
- DOI for each final release (Zenodo)
 - Coming soon: every GitHub tag
- Rolling 5-Year roadmap
- Lessons Learned:
 - Establish good practices (release schedule, branch structure, code structure, etc.)
 - Flexibility



Open, Collaborative, Community Development

- Fortnightly Zoom calls
- Recurring `camps` and `hackathons`
- Mailing lists (developers, help, etc.)
- Slack
- Small Leadership Team*
- Lessons Learned
 - Steep learning curve - Orientation Required
 - Actual Collaboration - Response to 'I want this in your software.' Is often 'Great, how can we work together to achieve that goal?'
 - Abilities vary - Sustained Contributions from 'Experts'



Open, Collaborative, Community Development

- Everyone Welcome
- Work is done on an as-able basis
- Two basic 'Rules'
 - Pay the piper, choose the tune
 - Do not break existing experiences
- Lessons Learned
 - Social Media Presence
 - Streamline Ways To Contribute

Model Marketplace for Users to share their models

SasView Marketplace

Search

Q

Log In

Categories / All Models

All Models

Name	Description	Category	Upload Date	Author	Score	Verified
correlated_spheres	Definition ----- The 1D scattering intensity of two correlated spherical particles can be written as: $S(q)=F_1^2 + F_2^2 + 2F_1F_2 \cdot \sin(qD)/qD$, where SF_1 and SF_2 are the scattering ...	Sphere	30 Mar 2019	Tianfu	0	<div>Cylinder ✖</div> <div>Ellipsoid</div>
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	0	<div>Lamellae ✖</div> <div>Other</div>
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	0	<div>Paracrystal ✖</div> <div>Parallelepiped</div>
TestModel	Something	Other	12 Oct 2018	tim.snow	0	<div>Shape-Independent ✖</div>
Core Shell Bicelle	Definition This model provides the form factor for an elliptical cylinder with a core-shell scattering length	Cylinder	02 Sep 2018	arm61	0	<div>Sphere</div>

SasView Contributors



EUROPEAN
SPALLATION
SOURCE



Science & Technology Facilities Council
ISIS



NIST

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

How to contribute

Obvious:

Fix Bugs

Add Features

Not so obvious:

Check our math

Check our documentation

Write documentation and tutorials

Video tutorials

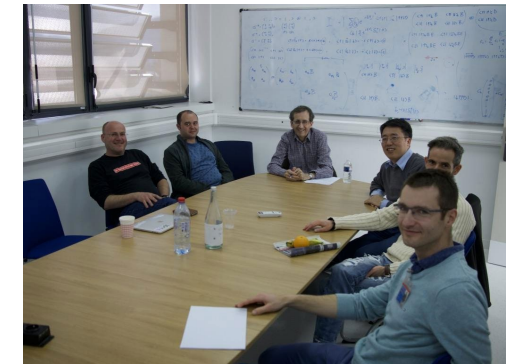
Web pages

Review functionality

Host a student

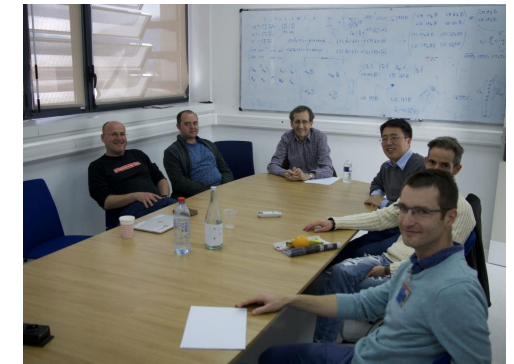
Code Camps

- Active and new developers come together
- Host decided on a rolling basis or need
 - Specific need – we can come to you
- Length
 - 3-4 days too short
 - 8+ days too long
 - Sweet spot: ~5-7 days (Tu – M, Sa rest)
- Frequency
 - Twice per year too often
 - Every other year too little
- Goals
 - Developers come together to work!
 - Establish ongoing collaboration



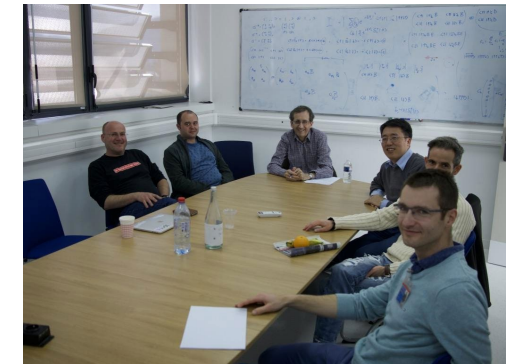
Contributor Camp

- In Person
 - Hosted at a new facility/university/etc.
 - Direct invitees
- Length
 - 7 days
- Frequency – as needed
- Goals
 - Orient new contributors to SasView
 - Immediate contribution and feedback to new members
- Only hosted one so far... but working on scheduling one for ORNL!



Hackathons

- 100% Virtual (COVID...)
- Short, focused, asynchronous efforts
- Established meeting time(s)
- Length
 - 1-3 days
- Frequency
 - As often as necessary (short notice)
- Goals
 - Release
 - PR clean out
 - New features



Ongoing Projects

Generic Scattering Calculator – Calculation Efficiency*, Magnetic structures, analytical model generation** (all in 6.0.0)

MuMag – Unpolarized Magnetic Scattering Analysis Tool (PR)*

Pore Size Distribution Analysis – Beyond well-defined dispersity functions*

Plotting Refactor – Plot consolidation** and plotting across 'meta' data

Sasdata Refactor – Create a better data contract and intelligently use meta data**

Magnetic Scattering – $P(r)$ upgrades (PR)**,
more magnetic modelling, plus more

Web API for remote fitting**

* Contributor Camp

** Student Project