



# SANS software update

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# Agenda

1. Data reduction
2. Data analysis
3. Generic resolution
4. Data processing workflow
  
5. Notebook demos (parallel)
6. Scientific projects (parallel)

# Data reduction with scipp

## SANS code in scipp/ess repository

- SANS core code in ess scipp repository
- Demonstrated on experimental data from SANS2D
- Previous version of code cleaned-up and improved
- Improved python and notebook documentation
- Pair-programming with scipp team works very well



🔍 Search the docs ...

### GETTING STARTED

Installation

### INSTRUMENTS

Amor

**Loki**

SANS2D: I(Q) workflow for a single run (sample)

SANS2D: I(Q) for sample and background

## Loki

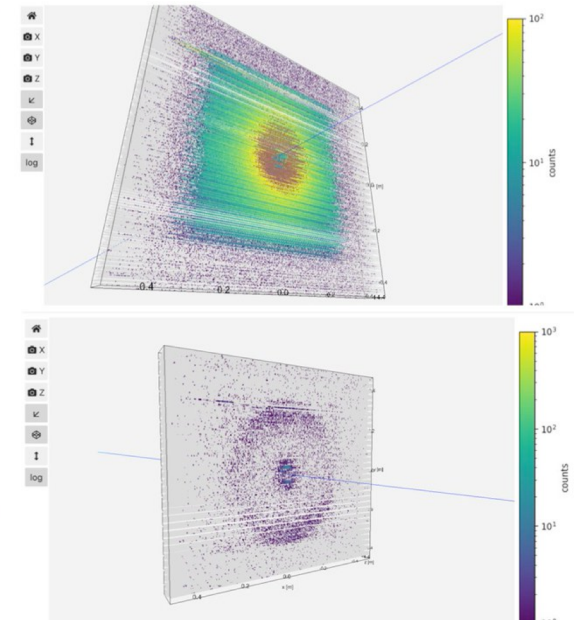
- SANS2D: I(Q) workflow for a single run (sample)
  - Define reduction parameters
  - Loading data files
  - Extract monitors
  - Apply offsets to pixel positions
  - Masking
    - Mask bad pixels
    - Mask Bragg peaks in time-of-flight
  - Coordinate transformation graph
  - Convert the data to wavelength
  - Compute normalization term
    - Transmission fraction
      - Remove background noise and rebin monitors
    - Direct beam function
    - Solid Angle

<https://scipp.github.io/ess/instruments/loki/>

# Data reduction with scipp

## Scipp used at LOKI detector test

- Run locally and on VISA (remote desktop solution)
- Used extensively for debugging
- (Easy) to set up batch scripts for files screening
- Preparing for final data reduction (few corrections needed before files can be fully reduced)
- Generated Nexus files can also be loaded to Mantid



# Data analysis with SasView

## New release and external collaborations

### SasView 5.0.5

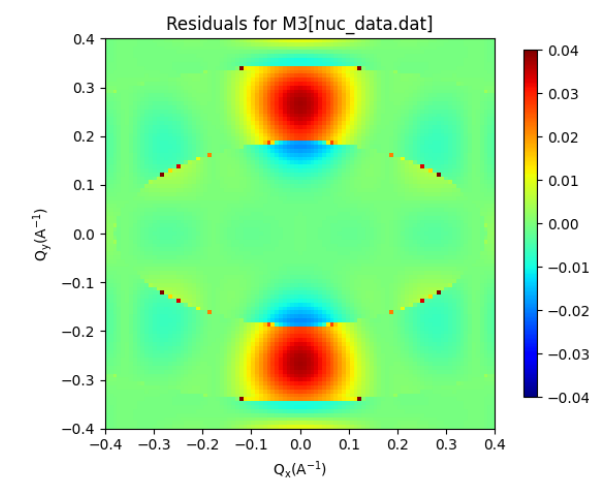
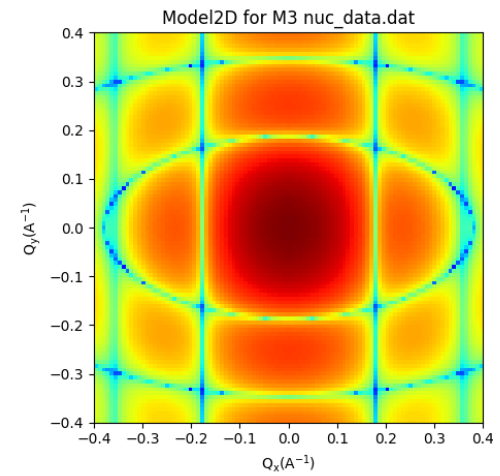
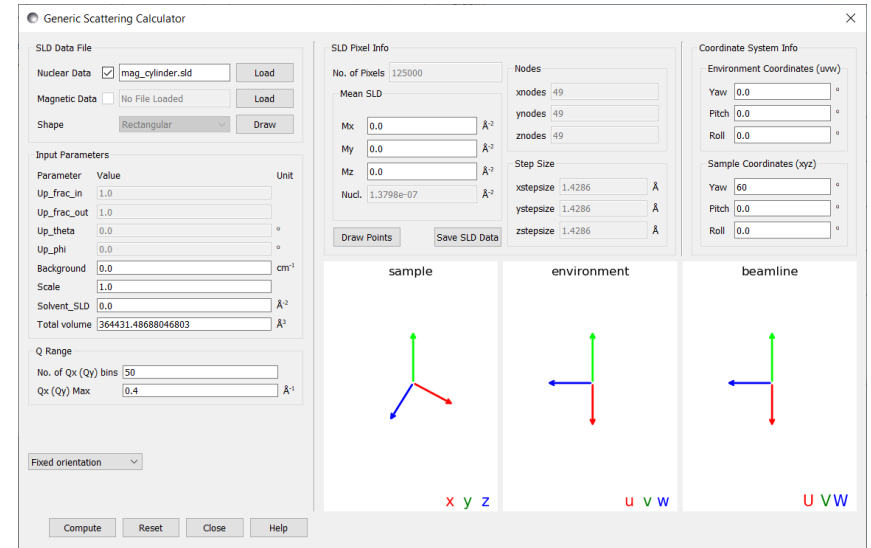
- Generic scattering calculator refactored
- Build system moved to GitHub
- Uncertainties for constrained parameters
- New models added to marketplace
- Bug fixes and documentation updates

External projects: Graphical representation of models (RISE), Polyhedral form factors (Saclay)

Multimodal analysis (developed mostly by ILL)

LINXS workshop on magnetic SANS, June 13-14

SasView Hackathon with introduction for new contributors, June 15-17



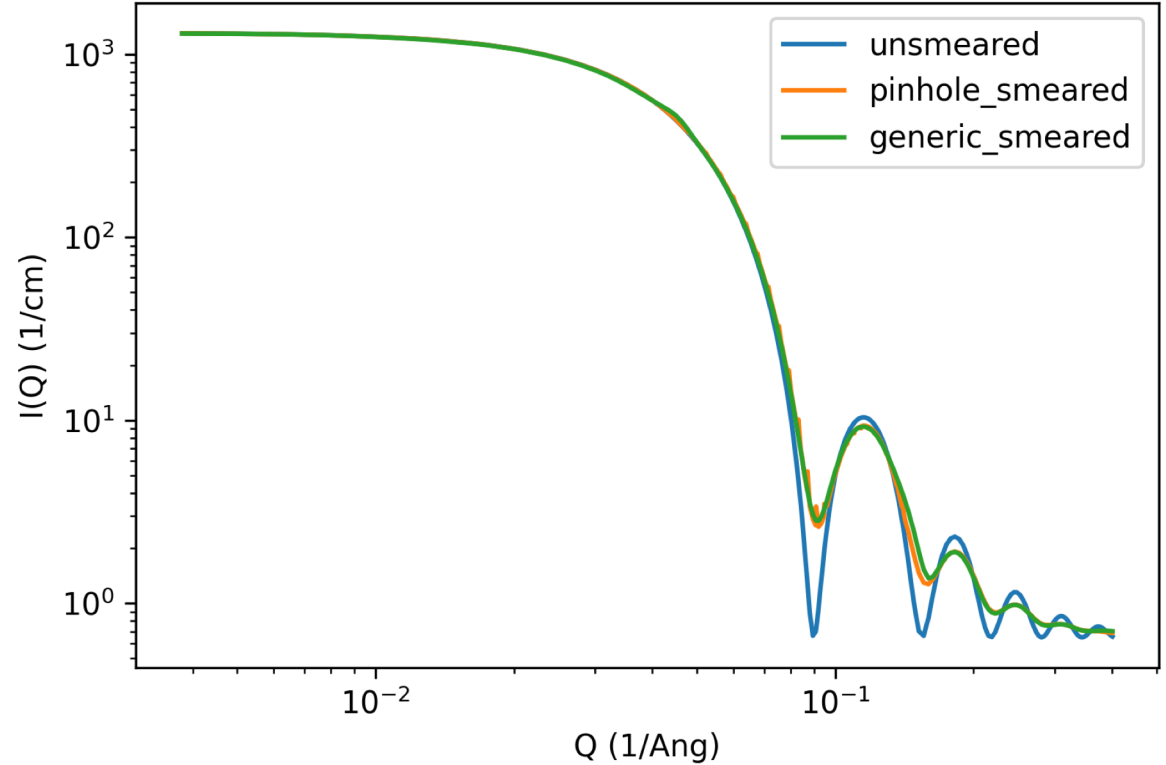


# Generic resolution

## Preliminary results and on-going discussion

Proof of concept in SasView:

- Small working group
- Jupyter notebook available in SasView branch
- Reading in arbitrary resolution function defined for each q point
- Stored in temporary file format
- Compared with Pinhole1D resolution kernel
  
- Extensively discussed at CanSAS workshop in March 2021. Follow-up at SAS2022
- Potentially also interesting for reflectometry (ORSO data format working group)



# Data processing workflows



## Integration with data catalogues (scicat) and databases

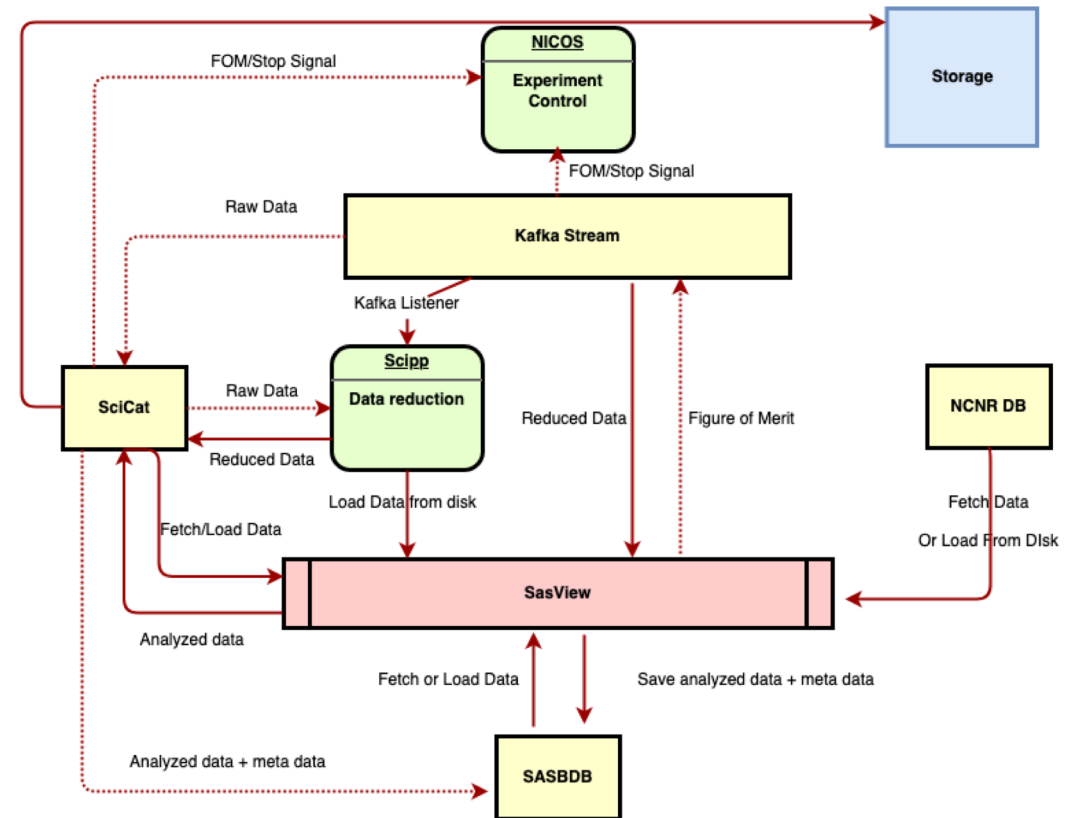
Making sure we can load, store process data from NICOS, scipp and SasView within ESS

GUI and command line interfaces

Special needs for Live Data Analysis considered

Integration with external databases (SASBDB).  
Workshop in May 12-13.

Collaboration with other ESS groups (ECDC and DRAM) and external collaborators (NIST and ISIS)





# Parallel session

2022-04-26

# LINXS magnetic SANS workshop



<https://www.linxs.se/events/2022/6/13/linxs-workshop-magnetic-sans-data-analysis-and-software-prospects>

- 2 day workshop
- The goal is to develop a series of prioritized items that the community would like to see added to SasView
- Identify people/resources who could help implement those priorities.

The screenshot shows the LINXS website with a navigation menu (HOME, THEMES, GOING ON, PEOPLE, EDUCATIONAL, APPLY, RESOURCES, CONTACT) and a search bar. The event title is "LINXS Workshop - Magnetic SANS – Data Analysis and Software Prospects", scheduled for Monday, June 13, 2022, 09:00 CET to Tuesday, June 14, 2022, 17:00 CET. The event features three SasView software interface panels displaying SANS data analysis. A "REGISTER HERE" button is visible. At the bottom, the following details are provided:

**Title:** Magnetic SANS – Data Analysis and Software Prospects  
**When:** 13th-14th June 2022  
**Where:** LINXS office, IDEON Delta 5, Scheelevägen 19, 5th floor  
**Registration deadline:** 30th April



# SasView hackathon

<https://indico.esss.lu.se/event/3009/>

- 3 day event
- Hybrid format:
  - in person in Lund
  - Online
- Follow-up to magnetic SANS workshop but with wider scope
- Introduction for new contributors

## SasView Hackathon

15 Jun 2022, 09:00 → 17 Jun 2022, 18:00 Europe/Stockholm

ESS

**Description** A SasView hackathon will be held in hybrid mode, with people working at both the ESS office and on-line all over the world. The hackathon will follow the [LINXS workshop on magnetic SANS](#) with the intention to continue work initiated at that workshop, however, the overall scope of the hackathon will be wider. There will be a few sessions aimed at newcomers to the SasView Collaboration with more experienced developers and contributors available throughout the event to offer advice and guidance. There will also be an opportunity to visit the ESS construction site on Day 1 of the hackathon, and proceedings will conclude with the traditional discussions over pizza :).

The following agenda is tentative and maybe subject of change.

**Registration** You are registered for this event.

### WEDNESDAY, 15 JUNE

09:00 → 10:00	ESS site tour	
10:00 → 11:00	Morning Session: Play with SasView. Helicopter overview, IDE	
11:00 → 12:00	New Contributors Session: GitHub workflows: issues, pull request actions	
	Q&A session for those new to SasView	
12:00 → 13:00	Lunch	
13:00 → 15:00	Afternoon Session: Create own issues. Attempt "good first issue". Create Pull Request	
15:00 → 16:00	New Contributors Session: Code structure and where to start	
	Q&A session for those new to SasView	
16:00 → 18:00	Afternoon Session: Dive into the code	

### THURSDAY, 16 JUNE



# Scipp notebooks demonstration

<https://scipp.github.io/ess/instruments/loki/loki.html>

## SANS2D: I(Q) workflow for a single run (sample)

This notebook describes in detail the steps that are undertaken in the `sans.to_I_of_Q` workflow.

It assumes the detector data has been recorded in event mode, while the monitor data has been histogrammed.

The data used in this notebook has been published in [Manasi et al. \(2021\)](#), and we kindly thank the authors for allowing us to use their data.

**Note:** It uses sample run for simplicity and it is not intended to describe complete data reduction pipeline. The complete pipeline is described in [SANS2D reduction](#).

### Outline:

- We will begin by loading the data files containing the sample and the direct (empty sample holder) measurements.
- We will then apply some corrections to beamline components specific to the SANS2D beamline.
- This will be followed by some masking of some saturated or defect detector pixels
- Both sample and direct measurement, as well as their monitors, will then be converted to wavelength
- From the direct run, and the direct beam function, the normalization term will be computed
- Both sample measurement and normalization term will be converted to  $Q$
- Finally, the sample counts (as a function of  $Q$ ) will be divided by the normalization term (as a function of  $Q$ )



# SasView notebooks demonstration

[https://github.com/SasView/sasview/tree/generic\\_resolution](https://github.com/SasView/sasview/tree/generic_resolution)

## Generic Resolution Function (Proof of concept)

In time-of-flight SANS the resolution curves from all the wavelengths contributing to a particular Q value are averaged together, weighted by the number of neutrons detected at each wavelength. Since the resolution width is inversely proportional to wavelength this often gives a curve that is noticeably sharper in the peak and broader in the tails than a simple Gaussian.

The purpose of this notebook is to provide a proof concept for extending SasView with generic resolution function. In the first approximation it has been demonstrated with resolution function described by Gaussian curve, which allows for easy comparison with already existing implementation into sasview.

The notebook goes through following steps:

1. Load CanSAS file using SasView loader
2. Generate Gaussian curves based on dQ values from the file
3. Store generated curves to file (custom format that can be used for testing - not CanSAS yet)
4. Modifies sasmodels resolution functions to use generic resolution
5. Compares generated  $I(q)$  obtained with Pinhole1D function and generic resolution

```
from sas.sascalculator.loader import Loader
import matplotlib.pyplot as plt
import scipy.stats as stats
import numpy as np

from scipy.special import erf # type: ignore
```

# Determining structure of Hepatitis B virus



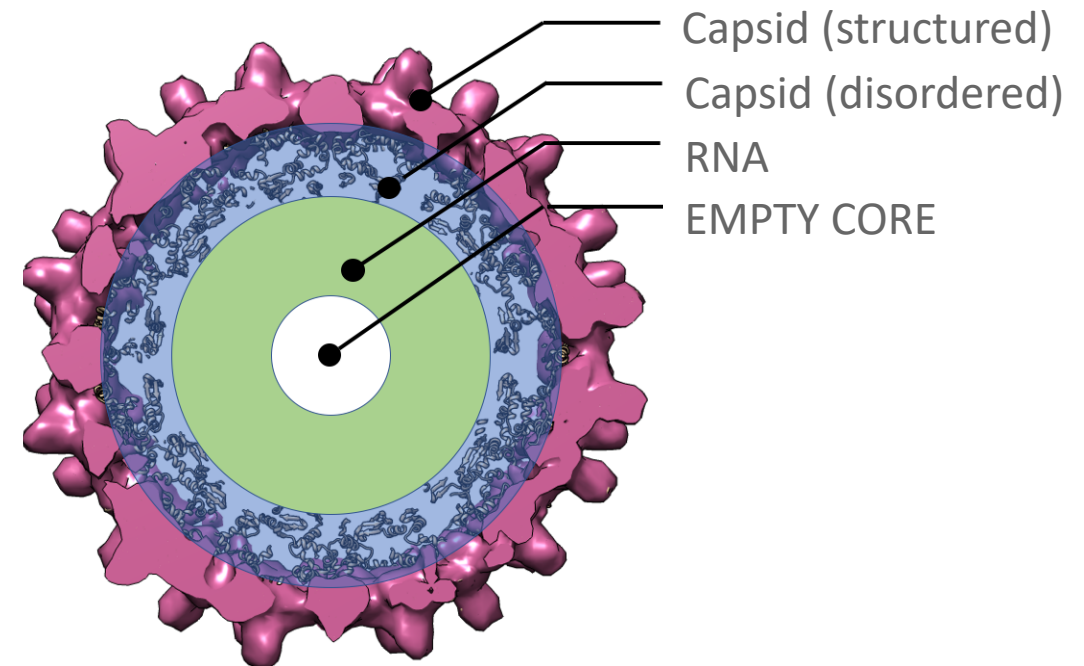
In collaboration with LU and ISIS

Developed method for decomposing contrast variation data to basis spectra (protein and RNA)

Using cryo-electron microscopy data to guide fitting in SasView (scripting)

Biological questions addressed:

- Where is RNA located?
- How does it bind to the protein (extended vs compact)?
- How is overall capsid assembly affected by RNA?

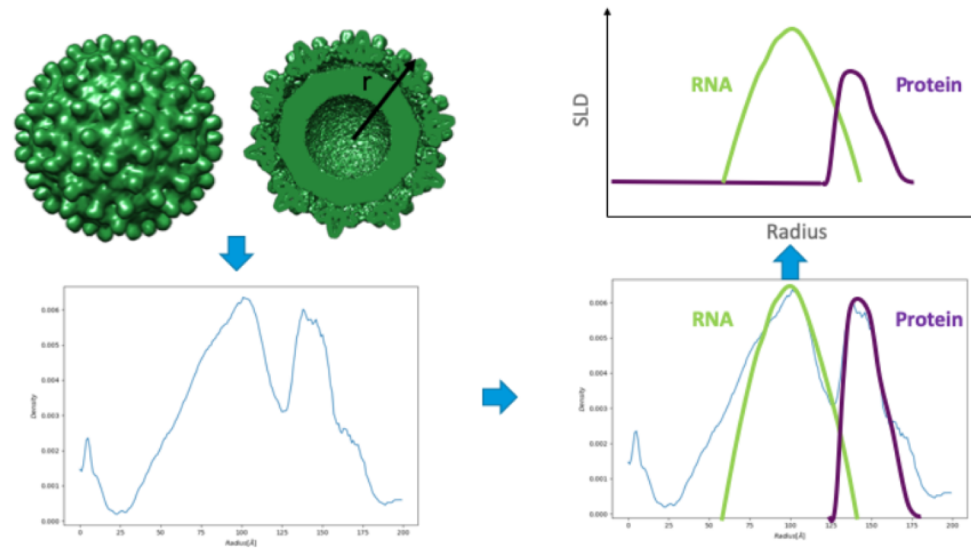


# SasView notebooks demonstration

## Additional notebook from Hepatitis B virus project (optional)

### Spherical SLD models fitted to BULCH profiles

This notebook demonstrates how Cryo-EM data can be used to guide modeling of SANS data using SasView.



Radial profile is calculated from electron density and is subsequently used to generate corresponding SLD profile, which is then applied to construct spherical SLD models in SasView.

#### Outline:

- Load data
- Set up models
- (Plot SLD profile)
- Fitting