Generic resolution for small angle scattering data

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Objectives

Why should we discuss SAS resolution at the reflectometry meeting…

Underlying description/definition of resolution function is different

However data format may still be similar

Both ORSO and CanSAS data formats are currently under development
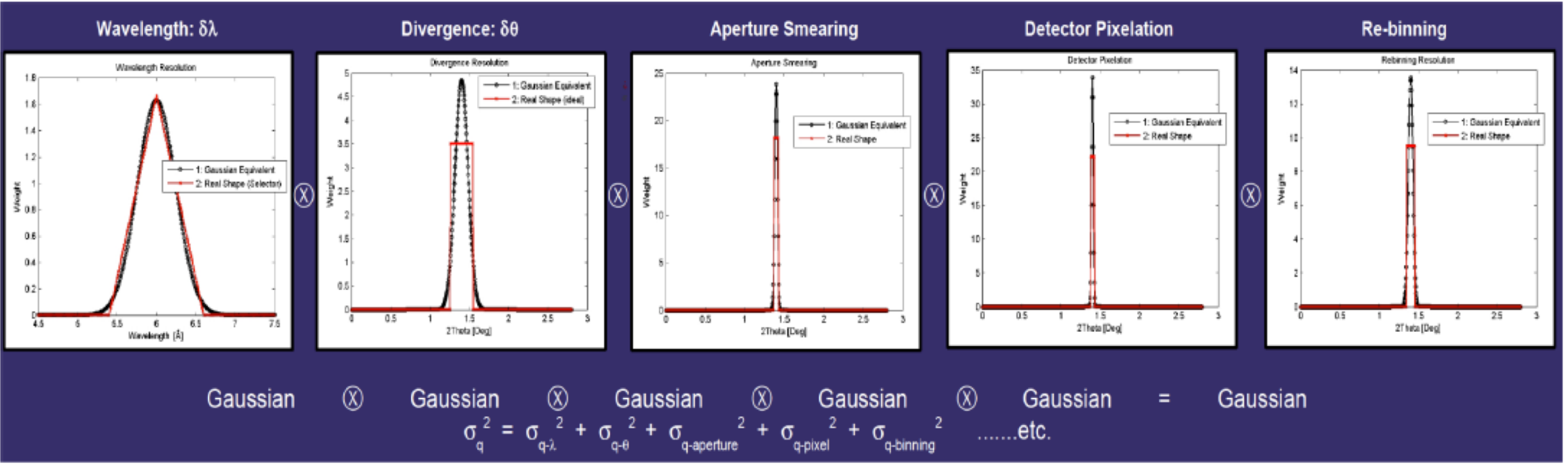
Good opportunity to share experiences/thoughts/ideas

Accurate consideration of the resolution function in data treatment and model fitting is vital to obtain accurate structural parameters

Example: SANS (apologies for X-ray people…)

Q-resolution in SANS

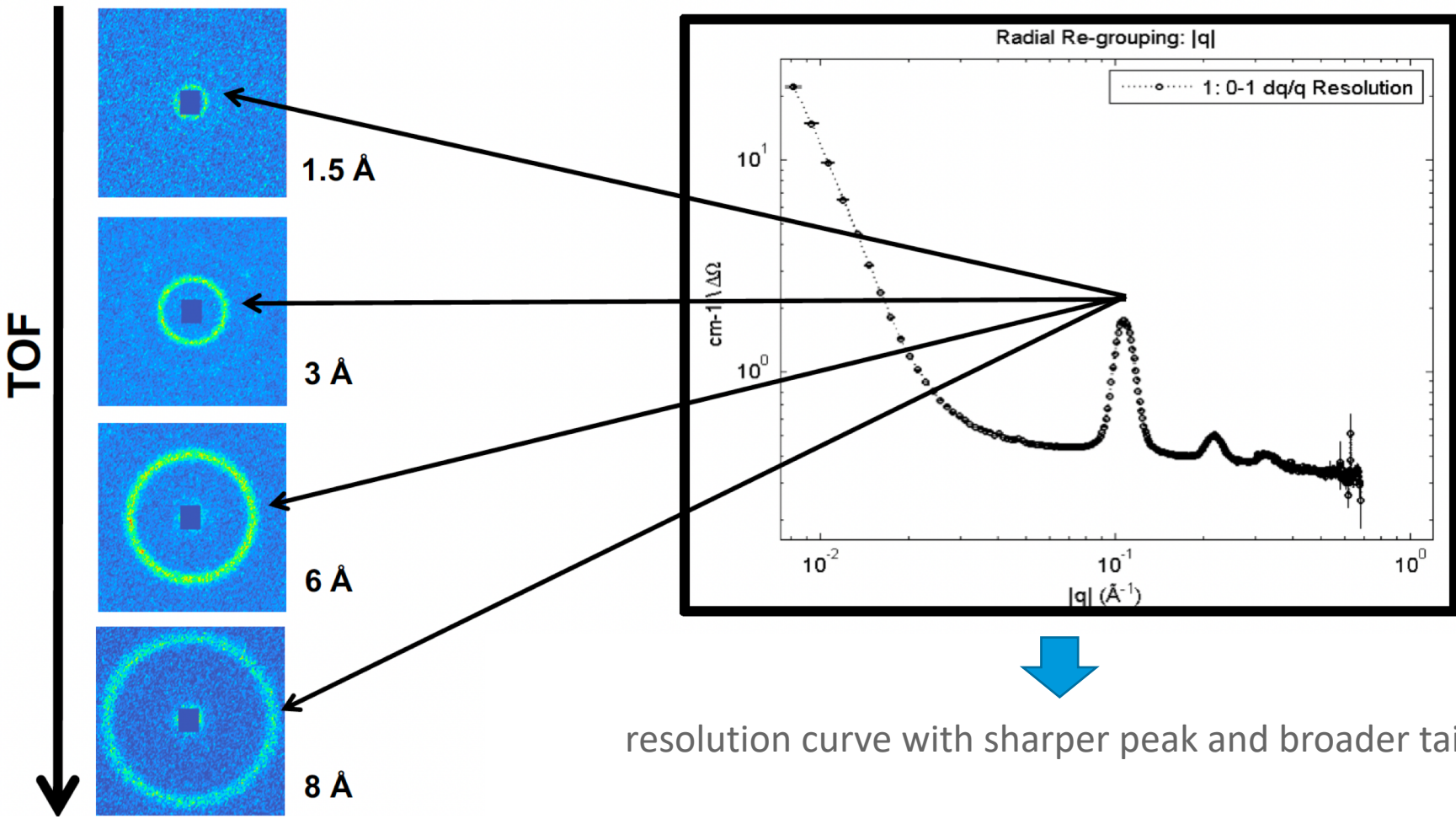## Classic approach assumes resolution components to be Gaussian

Analytical convolution results in Gaussian function that can be easily described

Numerical convolution of "real-shape" kernels gives better estimate but more computationally demanding

Credit: Charles Dewhurst

Q-resolution in TOF-SANS

Particular *q* point is measured with different *dq* resolution

Radial Re-grouping: |q|

TOF

1.5 Å

3 Å

6 Å

8 Å

TOF-SANS combines data from different wavelengths and radii, which may have range of Q resolutions

resolution curve with sharper peak and broader tails

Credit: Charles Dewhurst
Richard Heenan

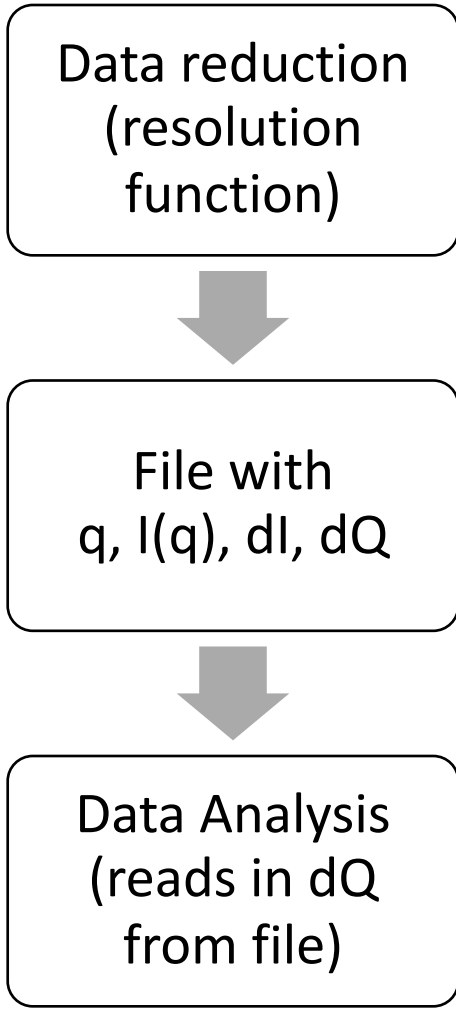# Data processing workflow

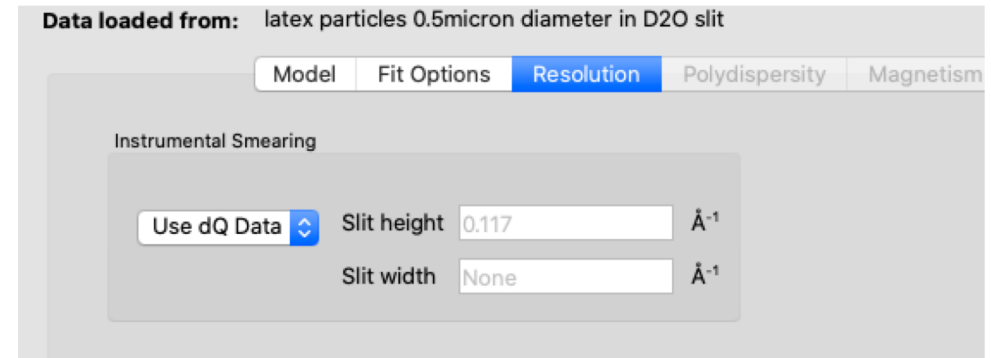Example of what is currently available


```
<Idata>
<Q unit="1/A">0.00714</Q>
<I unit="1/cm">226.539</I>
<Idev unit="1/cm">1.93973</Idev>
<Qdev unit="1/A">0.00144239</Qdev>
</Idata>
```
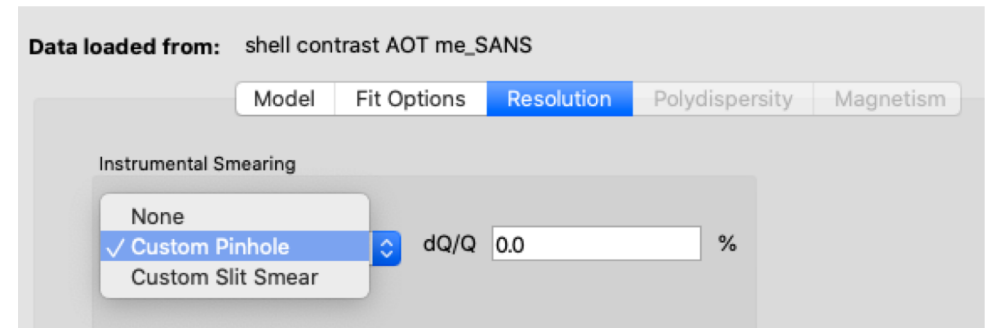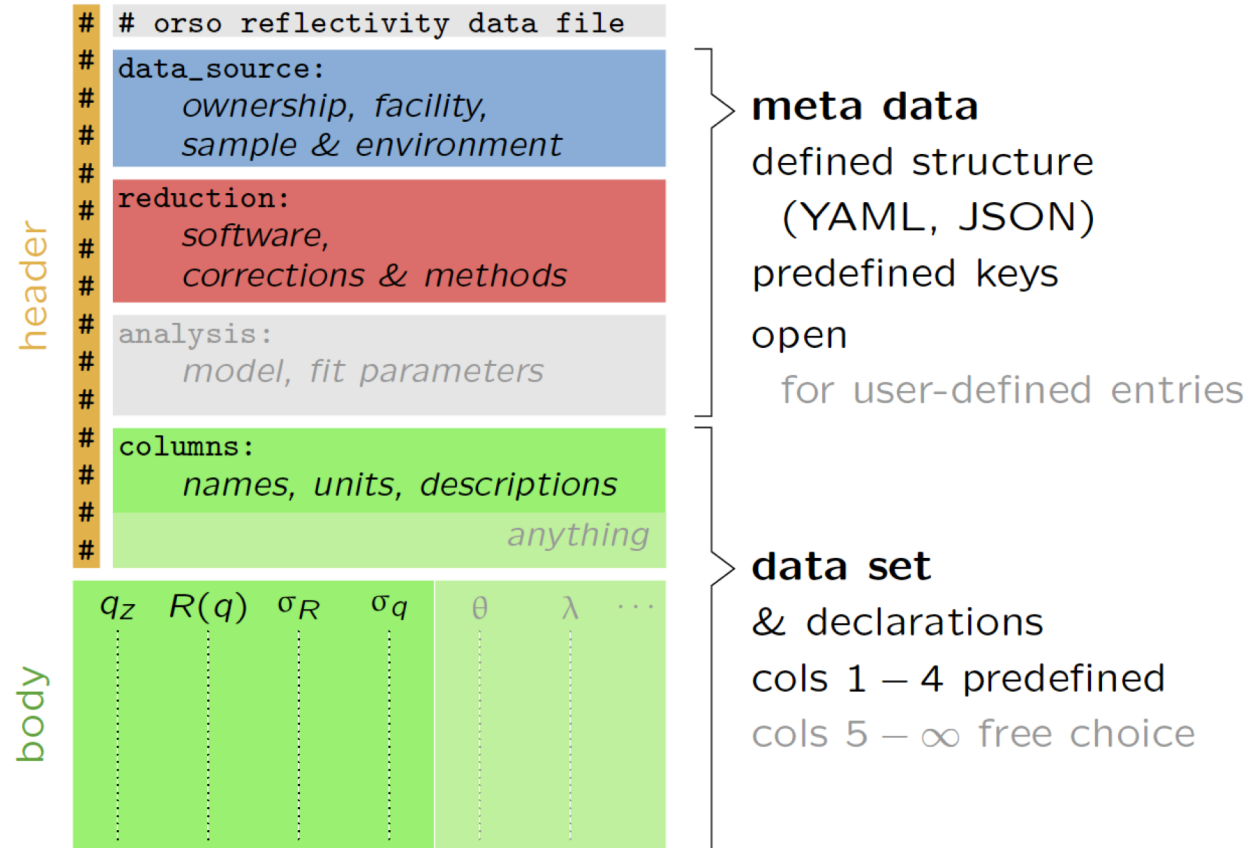
Data reduction
(resolution
function)

↓

File with
q, I(q), dI, dQ

↓

Data Analysis
(reads in dQ
from file)

File with dQ

Data loaded from: latex particles 0.5micron diameter in D2O slit

Model | Fit Options | Resolution | Polydispersity | Magnetism

Instrumental Smearing

Use dQ Data | Slit height 0.117 | Å^{-1}
Slit width None | Å^{-1}

File without dQ

Data loaded from: shell contrast AOT me_SANS

Model | Fit Options | Resolution | Polydispersity | Magnetism

Instrumental Smearing

None
✓ Custom Pinhole | dQ/Q 0.0 | %
Custom Slit Smear

https://www.sasview.org/

ORSO format

Credit: Jochen Stahn

Q resolution in SANS

Limitations of current approach

Gaussian approximation is quite handy and usually good enough

However there are cases where it is not sufficient

More accurate (than single dQ parameter) description is required

CanSAS workshop in March 2021

Can we do better than "single" number description

CANSAS Resolution Workshop

📅 25 Mar 2021, 13:00 → 26 Mar 2021, 18:30 Europe/Stockholm

📍 Zoom ()

Description In order to maximise the information extracted from SAS data, it is important to have a well characterized resolution function for the instrument and measurement conditions used. The combination of geometric (collimation, detection element size) and wavelength components in quadrature to produce a gaussian representation of the resolution at each Q value is well known, and widely used. However, there are a number of areas that have emerged where this representation does not adequately describe the measured data.

The Data Formats Working Group of canSAS is holding a workshop via video conference on the 25th and 26th March, 2021 to discuss SAXS/SANS resolution and in particular address the following points:

- Resolution close to Q=0 / close to the beamstop
- Effect on resolution of non-gaussian beam shapes / structure in the beam profile
- Non-infinite slit geometries – e.g. VSANS

The workshop will address the questions by breaking them down into four areas:

1. CALCULATE : Can we calculate these effects? First principles, approximations, simulations.
2. MEASURE : How can we measure the resolution functions? Standard samples, measurement strategies.
3. ANALYSE : How do we apply these resolution effects into our data analysis? What information is needed by analysis software? How do we determine what is appropriate usage of these effects?
4. STORE : How can we represent the resolution functions and store the data in a manner that can be used for analysis?

https://indico.esss.lu.se/event/2506/

CanSAS data format

Current format can accommodate more descriptive resolution functions

/entry/data/Qdev

- Estimated q resolution, usually a standard deviation

/entry/data/dQw

- Q resolution along the axis of scanning, primarily for slit-smearing instruments such as Bonse-Hart instruments

/entry/data/dQI

- Q resolution perpendicular to the axis of scanning, complements dQw

/entry/data/q/resolutions

- Dataset name corresponding to Q resolution data

- Multiple entries allowed for 2D slit-smearing geometries (dQw, dQI, etc.)

/entry/data/q/resolutions_description

- Can be a simple description (i.e. Gaussian) or metadata on Q resolution data

Credit: Tim Snow

Data format

We will presume that a **CanSAS** hdf format file is going to be used. The normal historic "Gaussian equivalent" standard deviation provided by an instrument Qdev(Q) should always be provided

	ResName	ResData
Analytic Gaussian	GaussFn	Qdev
General, equally spaced	CurveEq	Ndata, V0, V1,V2, ..., Vmid, ... Vend
General, arbitrary spacing	CurveGen	X0, V0, X1, V1, X2, ..., Xj, Vj, ..., Xend, Vend
User supplied	UserRes	FnName, FnData

Generic resolution in SasView

Proof of concept for generic curve (CurveGen)

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

> **<q> <I> <dq> <dI> <ResName> <[ResData]>**
>
> 0.003797 4006.05896074137 0.00109
> 160.350516888371 CurveGen [(0.003797, 366.002),

- Compared with Gaussian resolution kernel
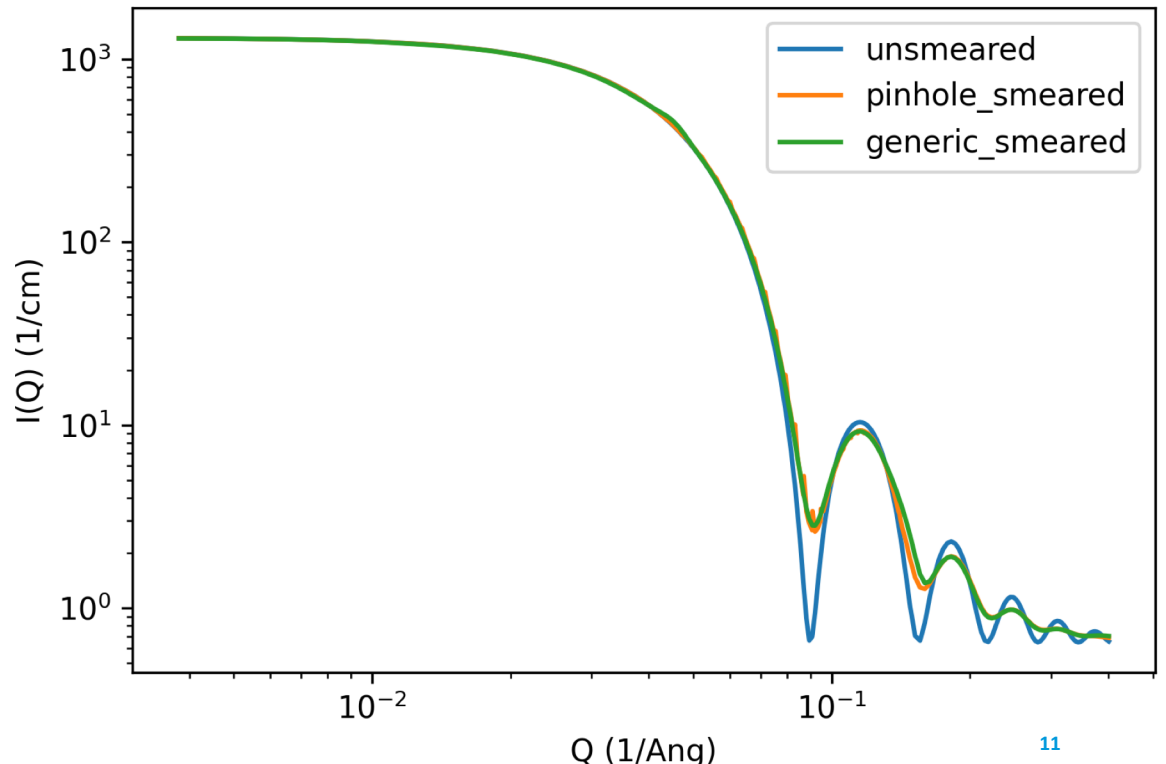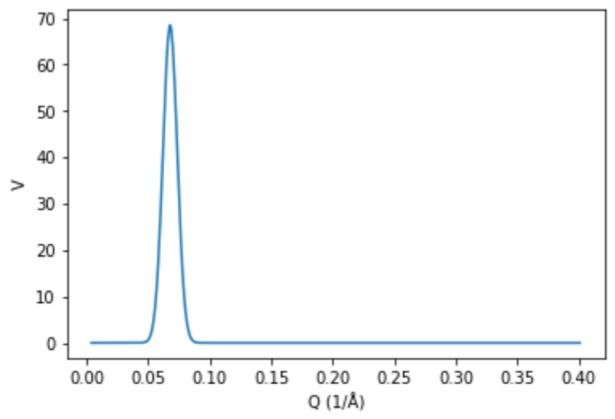
SasView notebooks demonstration

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 demonstarted with resolution fuction described by Gaussian curve, which allows for easy comparison with already existing implementation into sasview.

The notebooks 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

```python
from sas.sascalc.dataloader.loader import Loader
import matplotlib.pyplot as plt
import scipy.stats as stats
import numpy as np

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

SASBDB – Small Angle Scattering Data Bank

https://www.sasbdb.org/

Nearly 3000 data sets deposited

Mostly proteins

Planned extension for other types of molecules

Q resolution currently not available

Planned in future release (as a single number)

Conclusions

And next steps

Proof-of-concepts for format and treatment in the analysis software

Facilities to routinely provide the full resolution curves

Approximate curves (generated e.g. by stand alone code) may still better than the single dQ

We haven't really touched 2D data yet…

CanSAS meeting at SAS2022

Action items from CanSAS workshop (for reference only)

CALCULATE

1. Explore possibility of loading resolution kernel provided by GRASP/Charles into SasView. Explore implementation of bumps optimizer to treat full resolution curve

2. 2D function for slit geometry. Identify if 2D case is relevant for it (take a strip)

3. Description instruments resolution (breakdown chart). What covered in NEXUS?

4. Explore possibility of the student project to implement GRASP functionality into SasView

5. Explore possibilities of using neutron simulations (e.g. McStas) for X-ray instrument upgrades

6. Consider gravity calculations

MEASURE

1. Contact Adrian Rennie if you are interested in joining this group

2. Try to ensure we have representatives from all the facilities

3. Standard samples should include monodisperse sphere AND gratings. Suggestion to collect together essential and desirable qualities first

4. Working group should reach out to institutes and research groups to help. e.g. groups dedicated to colloid synthesis or groups specialising in nanotemplating, e.g. mesoporous silica

5. Initiate another round robins type activity, ensuring this time we ask that the facilities provide sigma/resolution curves along with there data.

STORE

1. Identify a working group to come up with workflow of where data should be stored and why?

2. Create reference implementation examples and recommendations

3. Improving the manual/documentation of the NXCanSAS on NeXuS website, with examples. Needs to be more accessible.

4. Update the NXCanSAS examples on the websites (github and CanSAS website) with the current version, including examples from all the institutes

5. Github CI to check examples

ANALYZE

1. Ask SasView community to take the lead to work on testing implementations, keep the work of taking instrument parameters into the resolution in a way that is instrument agnostic- put the onus on the instrument maker.

2. Maybe start with demonstration projects as above before asking the NXcanSAS data formats to look at definitions - How to ensure input from large group of data producers and data consumers to make sure solution is not to parochial

3. Would be good to develop recipes for handling resolution including when is too much - can somebody produce a paper a la Brian Pauw for SAXS reduction

4. Need to include commercial lab SAXS makers to provide the resolution as well. Need to keep in mind their need to balance work vs profit.

5. Use SasView at least as demonstration before approaching other data consumers - but other volunteers would be welcome

6. Collect bibliography of resolution including examples of where it was important to use.