Time-of-Flight Working Group

canSAS XIV – Taipei, November 3rd 2024

Members

About the group

- Working group formed at canSAS-XI in Freising
  - Presentations on challenges of TOF SANS : resolution, inelastic effects, multiple scattering
- TOF resolution workshop held in March 2021 (online)
- Working on any issues that are specific to Time-of-Flight SANS.

Members

- Andrew Jackson (ESS)
- Anna Sokolova (ANSTO)
- Sebastian Jaksch (ESS)
- Judith Houston (ESS)
- Adrian Rennie (Uppsala)
- Wojciech Potrzebowski (SciLifeLab)

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Generic Resolution

Why?

The resolution for a give Q point in TOF SANS results from a weighted combination of data from different wavelengths and detector locations – even across multiple detectors.

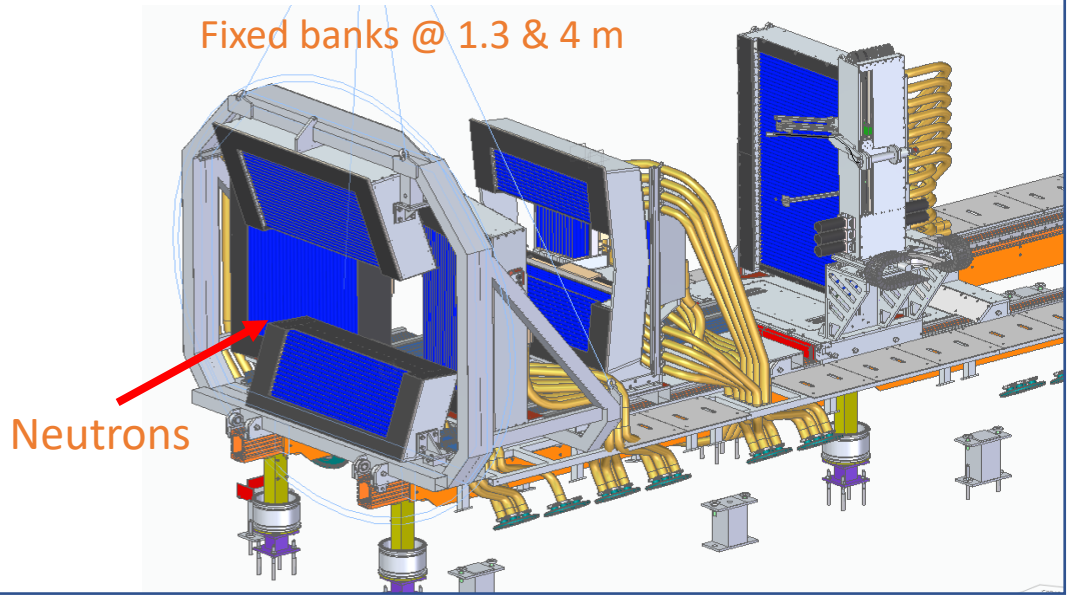
Developing a generalised approach to representing resolution provides for more accurate results from data analysis.

This is not just a simple gaussian and cannot be represented by a single parameter. (Dewhurst SAS2012 Sydney; Nelson & Dewhurst, J. Appl Cryst, 2013; Dewhurst canSAS-VII, Tokai, 2015;)

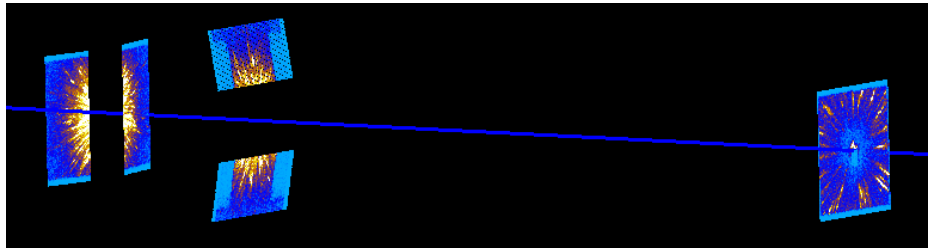
LoKI (ESS)

Covering 0º to 45º in scattering angle and 360º in azimuthal angle

Rear detector moveable between 5 & 10 m



Bilby (ANSTO)



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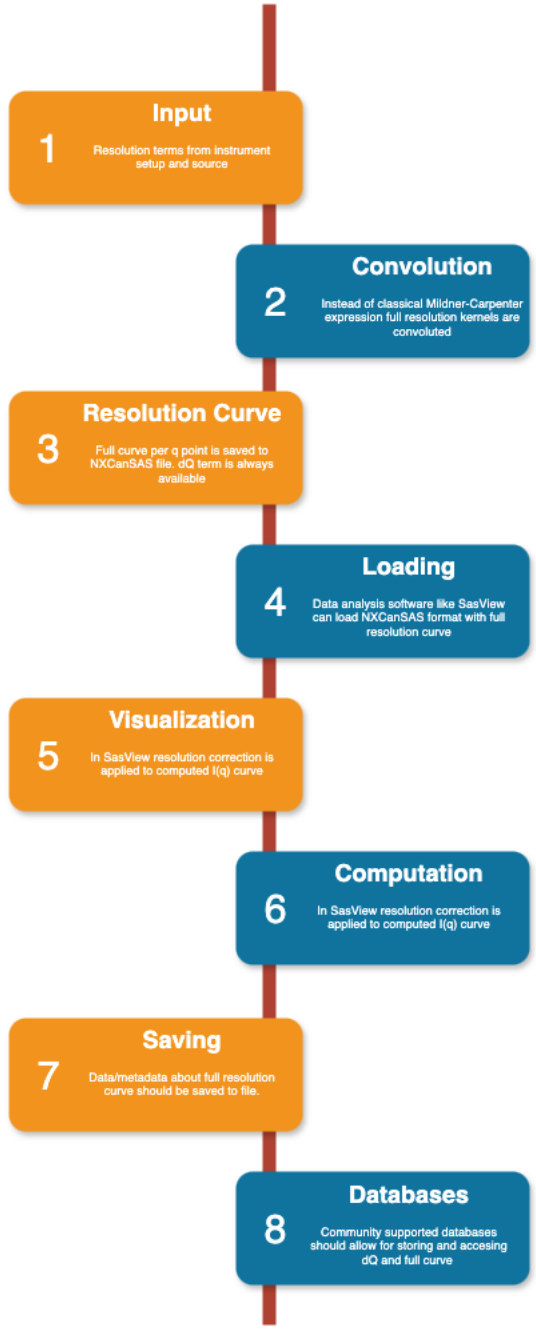
Generic Resolution

Generic resolution function

A workflow for utilizing the full resolution curve is shown in figure 1.

In order to avoid repetitions and keep the message coherent, bellow I provided mostly the collection of relevant links and current status (March 2024).

- **Input** data consists of instrumental parameters and shapes of corresponding terms contributing to the resolution function. Please check https://github.com/scipp/esssans/issues/111 for more details
- **Convolution.** Following developments in GRASP individual resolution kernels are convoluted rather than collapsed to a single number (as classically has been done with Milldner-Carpenter equation). Please review Jupyter notebook on how this can be potentially done https://github.com/scipp/esssans/files/14509637/checkbox-convolution.ipynb.zip
- **Resolution curve.** The full-resolution curves (defined per q points) are saved to NXCanSAS file. Anticipates entries are /entry/data/q/resolutions and /entry/data/q/resolutions_descriptions. dQ as a single number should always be provided.
- **Loading.** NXCanSAS files with resolution functions need to be loaded by the analysis software. It will require development in SasView.
- **Visualization.** Majority of users will probably apply resolution as it is. It may however be useful to be able to plot individual resolution curves and for example, compare it with Gaussian estimates. There may also be some option for changing sampling. This part needs to be defined and developed.
- **Computation.** Proof-of-concept of applying full resolution curve has been demonstrated using SasView: https://github.com/SasView/sasview/blob/generic_resolution/notebooks/GenericResolutionPOC.ipynb. (Also https://github.com/SasView/sasview/issues/1497)
- **Saving.** The information about the full resolution curve should be carried on as metadata or the report. It needs to be established
- **Databases.** It would also be useful if community supported databases can consume this information (both dQ and full description).



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To Do / Open Questions …

- Method of resolution storage – curve per Q point, or parameterised function?
  - Required precision of resolution description (how many points in curve, point spacing, linear or logarithmic spacing)?
  - Required precision of integrations (is trapezoidal method good enough)?
- Q resolution for nD data sets
  - 2D Q maps (SANS)
  - 3D Q maps (GISANS)
- Visualisation?
  - Is it needed?
  - If so, how do we show it? Just give standard deviation of the resolution curve?
- Implementation into NXcanSAS
  - Use the /entry/data/q/resolutions and /entry/data/q/resolutions_descriptions fields, but needs detailing
- Implementation into data analysis software (proof-of-principle exists for SasView
- Multiple scattering (overlap with RRWG):
  - Use TOF information / wavelength dependent information to detect/correct for multiple scattering
- Inelastic effects (overlap with RRWG) – well known and a number of papers are published. Need a modern, systematic, data set to complement previous work
  - Needs standard samples
  - Needs a measurement campaign – beamtime? (JEH and AJJ planning to use LoKI commissioning time if nothing else)