Break-out session – STORE

Handout for March 2021 canSAS workshop

Current version:

https://manual.nexusformat.org/classes/applications/NXcanSAS.html

- /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
- /entry/data/q/uncertainties
 - Typically, a standard deviation value of the /entry/data/q/data dataset

/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/Qmean

• Mean value of q for the complementary q datapoint

- /entry/instrument/aperture
 - Shape, x & y gaps
- /entry/instrument/collimator
 - Length, distance (to sample)
- /entry/instrument/detector
 - Slit length properties, detector pixel shape & size
- /entry/instrument/source
 - Beam shape, wavelength(s), beam size

/entry/sample

• Thickness (length in grazing incidence)

/entry/process

- Q-binning (re-binning?) information used in processing
- Other information injected after a scan?
- Outside of NXcanSAS remit but to be kept in mind for ANALYSE

STORE discussion questions

- How can we represent the resolution functions and store the data in a manner that can be used for analysis?
- What changes need to be done to accommodate resolution information?