Numerical evaluation, convolution and recombination of SANS instrument resolution using real-shape kernels: Application to TOF SANS

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The instrument resolution plays an important role in the correct evaluation and model fitting to Small-Angle Neutron Scattering (SANS) data. Contributions to the resolution function are, for the most part, due to the rather broad wavelength spread, $\delta\lambda$, finite collimation, $\delta\theta$, and detector resolution. Additional smearing can occur due to averaging or regrouping software procedures during data treatment. The most common approach for the treatment of SANS instrument resolution is to approximate these contributions as integration kernels of Gaussian form. This means that the final convolution of all resolution components can also be described by a Gaussian function requiring only the standard deviation, $\sigma_q(q)$, as a parameter allowing rapid smearing for iterative fitting and practical application in analysis software.

Here we demonstrate the use of numerical real-shape kernel weighting functions which accurately describe the resolution components of a typical SANS instrument. We show the practical implementation of such an approach in the data treatment software GRASP and highlight cases where Gaussian shaped distributions do not adequately describe the instrument resolution. This approach is particularly relevant to data from time-of-flight (TOF) SANS instruments such as D33 where $\delta\lambda$ is no longer triangular shaped but is a broad top-hat function and where a particular scattering vector, q, is measured using many wavelengths, at different angles, and therefore different resolutions. The weighted average of the resolution kernels that describe the individual intensity points therefore correctly describe the numerical integration that should be applied for model-smeared fitting to the resultant regrouped data point. This rapid and practical approach allows one to deal with the reduction of TOF SANS data from spallation or reactor neutron sources with an accurate representation of the instrument resolution and ultimately translates to a more accurate model fitting to SANS data.