New development for neutron total scattering data reduction and analysis

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A generic workflow for calibrating time-of-flight (TOF) instruments has been developed. Three major steps are involved in the workflow - automatic grouping of pixels, cross correlation, and calibration. At the stage of grouping, an unsupervised machine learning based clustering algorithm is introduced to group pixels 'next to' each other, in terms of peak properties. By grouping those similar pixels, the following cross correlation can be conducted more reliably, through which the statistics could be accumulated to further guarantee a reliable calibration against the nominal peak positions of standard sample (e.g., diamond). The calibration workflow has been successfully applied to NOMAD and POWGEN diffractometers at Spallation Neutron Source, Oak Ridge National Laboratory. It is worth noting that by applying this calibration workflow to replace the initially used pixel-by-pixel calibration routine on POWGEN diffractometer, the measurement time needed for diamond calibrant could be successfully reduced from ~10 hrs to ~3 hrs. Such a generic calibration workflow is expected to be generally applicable to TOF instruments which are seeking for the proper TOF-to-d transformation. On data analysis side, total scattering data modeling with RMCProfile package will be focused on and specifically, the implementation of arbitrary Bragg peak profile in a tabulated manner and the correction for finite instrument resolution effect going beyond the conventional Gaussian assumption will be discussed. Typically, the implementation of resolution correction enables the modelling to an otherwise-unreachable super-large length scale, e.g., 100 Å, following the supercell approach.

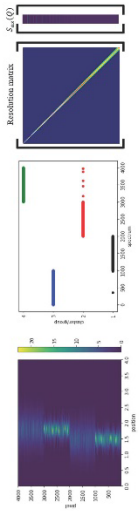

Figure 1