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Single crystal neutron diffraction data reduction with OpenHKL

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Data reduction is a crucial prerequisite to data analysis in neutron scattering experiments; in the case of single crystal diffraction, it involves the reduction of a set of detector images at fixed sample rotation increments to a set of miller indices with integrated intensities. However, the only available mature software solutions are either legacy codes, converted from X-ray diffraction, or are closed source.

OpenHKL (formerly NSXTool) is a standalone program with a modern graphical user interface that facilitates the data reduction workflow: locating detector spots on the images, indexing the resulting peaks, predicting an exhaustive set of peaks, refining the instrument states and unit cell to improve the predictions, integrating the peaks, and finally merging the peaks. It is written in C++ for excellent speed, is open source and well-documented, natively handles neutron diffraction experiments with different detector geometries, and has a convenient Python scripting interface.

In this presentation, I will demonstrate the capabilities of OpenHKL, describe the progress of the project, and show the results structural refinement computations using data reduced with OpenHKL.

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