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Single crystal 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 images at fixed sample rotation increments to a set of Miller indices and detector coordinates. However, the available mature software solutions for this problem are either legacy codes, converted from X-ray diffraction, or are closed-source.

OpenHKL is a standalone program, currently under development, with a modern graphical user interface that facilitates the data reduction workflow. 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. It has been successful in the reduction of macromolecular crystallog-raphy data from the BioDiff instrument, and is being extended to work with other instruments.

This poster will present the latest updates in the development of OpenHKL.

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