Contribution ID: **105** Type: **Poster**

Single crystal diffraction data reduction with OpenHKL

Friday 6 December 2024 13:45 (3 hours)

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 crystallography 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.

Primary author: RAZA, Zamaan (Forschungszentrum Jülich)

Co-authors: Dr OSTERMANN, Andreas (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München); WUTTKE, Joachim; SCHRADER, Tobias

Presenter: RAZA, Zamaan (Forschungszentrum Jülich)

Session Classification: Poster Session

Track Classification: Neutron Methods