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Monte Carlo Multiple Scattering Corrections In Neutron Scattering Experiments

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A Monte Carlo integration method has been developed in the Mantid data reduction package that calculates the multiple scattering intensity for a given structure factor, sample shape and instrument definition. The calculation works for both elastic and inelastic instruments (both Direct and Indirect geometries).

The calculation is based on the Fortan DISCUS program that was previously developed by Mike Johnson and Spencer Howells at ISIS, initially in the 1970s.

The calculation doesn't require an assumption that the scattering is isotropic and can explicitly calculate all scattering orders without an assumption that the ratio between the orders is constant. The calculation uses the Mantid sample geometry engine which is able to calculate track intersections for arbitrary shape types described using CSG or mesh geometries.

Some results of the calculation on real\synthetic samples will be shared and work on how this calculation can be formulated into a correction process will be presented. Some of the software engineering challenges around performance and the process for porting a valuable legacy Fortran program into a modern data reduction platform will also be discussed.

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