

## W0488

**A Data Processing Software for Neutron (Quasi-)Laue Diffraction.** Z. Ren, Renz Research, Inc., P. O. Box 605, Westmont, IL 60559, USA.

A highly-automated data processing software Precognition™ is developed for neutron (quasi-)Laue diffraction. The software starts from analysis of diffraction images recorded on normal or arbitrarily-included flat detector or cylindrical detector, and results in fully-reduced structure factor amplitude in three steps. Step 1 establishes an accurate geometric model of each diffraction pattern in a dataset, including auto-indexing, refinement of various parameters of crystal and experimental apparatus, and corrections for detector distortion. Step 2 integrates and isolates the intensity of each predicted spot, some easily observable by eye, some not, and some sharing the same detector pixels with each other, known as spatial overlap. Step 3 compares all integrated intensities together in order to reveal therefore to reduce systematic errors, and to identify therefore to reject random noise. The most significant systematic correction is normalization of incident beam intensity at all wavelengths, which process requires no prior measurement of the spectrum of the neutron beam. Crystallographic and structural results from dihydrofolate reductase complex with a drug methotrexate (Bennett et al., *Acta Cryst.* D61, 574-579, 2005) and other testing cases will be presented. This software is being extended to process time-of-flight images.