

Software for data acquisition and processing with area detectors

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A device-independent software package for processing detector images from single crystal x-ray diffraction experiments is being developed for Rigaku R-Axis imaging plate systems and the ANL Structural Biology Center CAT at the APS. The software is written in the language C++ with a modern object-oriented programming style. We have developed a code that encapsulates the various objects in diffraction experiments, such as crystals, sources, detectors, goniometers, images and reflections.

Modules have been designed for detector calibration, image collection, peak picking, autoindexing, cell reduction, Bravais lattice determination, refinement of crystal, detector and source properties, predicting reflections, data collection strategy, integration with profile fitting, scaling and merging of reflections. A graphical user interface will guide users through experiment setup, data collection and data evaluation with results presented in concise graphs. Novice and power users alike will be able to take advantage of a complete "blackbox" approach with minimal input that does not preclude a more "hands on" style.

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