Robust Indexing and Automatic Data Collection at the Advanced Light Source

Nicholas Sauter, John Taylor, Ralf Grosse-Kunstleve, Carl Cork, Thomas Earnest & Paul Adams
Lawrence Berkeley National Laboratory, Physical Biosciences Division
1 Cyclotron Road, Bldg 4R0230, Berkeley, CA 94720-8235

Structural genomics programs and drug discovery efforts that investigate large sets of crystalline samples are placing increased demands on synchrotron beamlines. To facilitate high-throughput work, beamlines 5.0.1, 5.0.2, and 5.0.3 at the ALS have been equipped with robotic arms [*Structure* (2004) **12**:537-545] to transfer cryocooled samples to the goniometer. High-level graphical controls allow the user to conduct experiments with minimal input, while much of the work is performed by underlying software modules. The *AutoScreen* module rapidly evaluates 96 samples, centering each cryoloop on the beam position by analyzing videomicrographs. Two diffraction snapshots are acquired for each crystal, and then the Lawrence Berkeley Indexing Toolbox (*LABELIT)* autoindexes the diffraction pattern and determines the Bravais symmetry. *LABELIT* implements new methods to treat three common failure modes experienced during indexing: 1) non-primitive basis, 2) incorrect beam center, and 3) faulty symmetry. Correcting these problems allows images to be indexed rapidly without the need for interactive visual inspection. An *AutoCollect* module is now under development to deduce and set the optimal data collection parameters, while an *AutoProcess* module will reduce the diffraction data in real time and determine the space group. We anticipate that these tools will increase experimental efficiency for both individual users and large-scale efforts alike.

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