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Publication Date

2008-05-06

ARGONNE USERS WEEK 2008

Workshop on Software for challenging cases in macromolecular crystallography

Web-Ice and Labelit: Tools for Convenient Diffraction Analysis at the Beamline

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Data collection often requires the examination of numerous crystal samples. Typical beamline applications include the determination of the best growth and cryocooling conditions, and the screening of large compound libraries. The Berkeley Center for Structural Biology and the Stanford Synchrotron Radiation Laboratory are collaborating on software to make the crystal screening process as efficient as possible. Web-Ice is an application server that executes established crystallographic programs, delivering an immediate analysis of the diffraction from each new crystal. The user uploads a spreadsheet identifying each sample, and then views the emerging table of results within the beamline GUI, or on a remotely accessible Web page. A Web-based image browser permits inspection of the autoindexing solution. Once the best candidate crystal is chosen, a data collection strategy is recommended, and run parameters are sent to the beamline controls. Since the control environments are different at each facility, Web-Ice exposes standard software interfaces to achieve portability. Other institutions can experiment with the package by consulting the manual and developers' wiki at <http://smb.slac.stanford.edu/research/developments/webice>. Labelit, the underlying spot analysis and indexing engine, can process most diffraction images without recourse to user input from a graphical interface. Since large complexes (viruses and ribosomes) are increasingly targeted by crystallography, recent work has focused on optimizing Labelit for large unit cells. Additional heuristics have been added, e.g., to distinguish between elongated Bragg spots (acceptable), and overlapping spots that must be excluded from the initial autoindexing calculation. New procedures can recognize unusual diffraction phenomena. Pseudocentering (non-crystallographic translation that approximates exact crystallographic centering) produces a sublattice of weakly diffracting Bragg spots. Although the weak pattern can be undetectable prior to indexing, the problem is amenable to a targeted search after the main lattice is indexed. Labelit can be downloaded from <http://cci.lbl.gov/labelit>.

This work was supported in part by DOE contract No. DE-AC02-05CH11231 and by NIH/NIGMS funding under grant number 1R01GM77071.