New Tools to Integrate Data Analysis and Data Collection at SSRL: Web-Ice

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Recent developments in automation at the Stanford Synchrotron Radiation Laboratory Macromolecular Crystallography beamlines have been driven by the needs of the Structural Genomics projects and feedback from the user community. Current capabilities at all beamlines include automated sample mounting and centering; crystal screening; fluorescence scan measurements and analysis; and wavelength changes at side stations with automatic table motion to track the beam. These features are implemented on the beamline control software program Blu-Ice.

The most recent software developments at SSRL aim at integrating data analysis and beamline hardware to the point where only minimal input by the user will be required to carry out a complete experiment. In order to facilitate remote access to the experiment, the software is accessible remotely through a web-browser interface known as Web-Ice. Web-Ice currently provides tools to view diffraction images as they are being collected; analyze the diffraction pattern and display statistics (such as number of spots, shape, diffraction strength, etc.) and autoindex and calculate a strategy to maximize data completeness based on two images selected by the user.

The next Web-Ice release will include a crystal screening interface to analyze and score images from multiple samples. Ultimately, the software will fully integrate data analysis and beamline control software for automated data collection.

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