

## **W0042**

**Integration of Data Analysis and Collection at SSRL.** A. Gonzalez, P. Moorhead, S. McPhillips. SSRL, 2575 Sand Hill Rd., Menlo Park CA 94022, N. Sauter. LBNL, 1 Cyclotron Rd., Berkeley, CA 94720.

Recent developments in automation at the SSRL 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. However, the user still plays a vital role in evaluating the quality of the diffraction images and must run data analyzing software to determine optimal data collection parameters including crystal oscillation range, exposure time, and detector distance.

A new software project at SSRL, Web-Ice, intends to integrate data analysis and beamline hardware to the point where only minimal input by the user will be required to carry out a complete experiment. The system is accessible remotely through a web-browser interface, and facilitates the generation of a strategy and browsing of results. Web-Ice currently provides tools to view diffraction images as they are being collected, analyzes the diffraction pattern, and autoindexes and calculates a strategy to maximize data completeness based on two images selected by the user. Future releases of the software will fully integrate data collection strategy with the beamline control software for automated initiation of data collection.