robust mechanized experimental hardware, a flexible instrumentation control system with an intuitive user interface [1] and efficient integration of data collection and data analysis.

A key component of the system is the Stanford Auto- Mounter (SAM), which can mount 198 samples without any manual intervention [2]. The robot, in combination with other automated tasks, allow crystallography experiments to be carried out from the researchers' home institutions and other remote locations while retaining complete control over the experiment. Full remote access was implemented in 2005. Currently close to 80% of the user groups collect data totally remotely [3].

Remote access to the SSRL computers is done via the NX client application provided by NoMachine, which provides a response close to that obtained at the beamline when a broadband connection is used. In addition, a web application, Web-Ice, can be used to analyze test diffraction images, calculate data collection strategy and carry out data processing [4].

The latest efforts have focused on developing specialized workflows to fully automate highly iterative experiments (such as fragment-based drug search or mutant comparisons). To achieve this goal, a declarative programming language, RestFlow, has been developed. RestFlow facilitates the integration and sharing of scripts and programs by different workflows. Currently, a workflow automating all the steps from sample screening and selection to model refinement is under development.

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Keywords: automation, remote experiment, macromolecular crystallography

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Automation and remote access at SPring-8 MX beamlines

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Data collection using synchrotron beamline is indispensable for the structure biology research nowadays. At SPring-8, we provide an opportunity to use high intensity synchrotron radiation facility with robust and automated data collection system, which contributes to both high throughput crystallography and a cutting edge research.

The automation is achieved by an integrated beamline control software *BSS* [1] and a sample changer *SPACE* [2]. For the high throughput crystallography, we use two-mode operation which composed of daytime attended crystal screening and night time fully automated data collection. The scheduling function of *BSS* and a screw type special sample pin handled by *SPACE* enables this operation. Mail-in data collection using this two mode operation is routinely conducted since 2005, where database *D-Cha* manages information such as sample information and data collection conditions [3]. For the cutting edge research, which handles small crystals or low-quality crystals in most cases, *BSS* is equipped with tools assisting data collection, such as helical scan to avoid the radiation damage, and grid scan for the centering of microcrystals and screening a well diffracting part of inhomogeneous crystals.

Based on this automation system, we now introduce a remote access data collection system. We did not use a remote desktop, but developed a robust and secure remote system adopting the server/client architecture. A newly developped remote client GUI program installed on the user's PC communicates with *BSS* for the remote operation. The remote access is only allowed for anauthenticated user under the beamline interlock permission. This architecture not only keeps safety and security but also enables users a stress free operation.

We expect that the beamline automation and the remote access increase the borderless use of the beamlines and contribute to the structural biology.

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Automated synchrotron crystallography for drug discovery: The LRL-CAT beamline at the APS

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The Lilly Research Laboratories X-ray beamline, LRL-CAT, sited at Sector 31 of the Advanced Photon Source (APS), is a highly-automated facility supporting rapid acquisition of diffraction data from protein crystals. The facility is designed to operate with minimal human intervention and provide medicinal chemistry teams with timely access to protein co-crystal structure information. All LRL-CAT operations can be controlled remotely, including X-ray beam alignment, wavelength calibration, and crystal mounting, screening, and data collection.

In 2010 the LRL-CAT end station underwent a complete upgrade. New cryogenic crystal mounting robotics, including a custom CATS system with a capacity of 540 samples, were installed to permit long-term unattended operation. The upgrade also included installation of new beam-defining components, a high-speed, air-bearing goniostat, and piezoelectric nano-positioners for precise placement of crystals within X-ray beams of 20-150μm diameter.

All beamline operations are controlled through custom software directly linked to a proprietary Laboratory Information Management System (LIMS) built atop an Oracle® database. Crystal quality and diffraction limit are evaluated automatically from recorded screening images. Samples meeting predefined quality criteria are selected for data collection by database-driven software. The software ensures that collection within a group of duplicate crystals is limited to those that will provide the best data. Data collection and initial processing then proceeds without human intervention. Additional software programs evaluate the scaled data to guarantee its quality prior to transmission from the beamline.

The upgraded LRL-CAT facility now supports screening of up to