

Beamline Scheduling Software: administration software for automatic operation of the RIKEN structural genomics beamlines at SPring-8

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Beamline Scheduling Software (BSS) has been developed for the schedule management and equipment control of the RIKEN Structural Genomics Beamlines I and II (BL26B1 and BL26B2 at SPring-8). The beamline operation is automated with a sample-changer robot and a database system. The experimental schedule is registered to BSS as a list of diffraction measurements for numbers of protein crystals. BSS implements the beamline operation communicating with beamline instruments through the computer network. The RIKEN Structural Genomics Beamline I (BL26B1) opened for users using BSS in October 2002, and the automatic operation was implemented at BL26B2 in October 2003.

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1. Introduction

The RIKEN Structural Genomics Beamlines I and II of SPring-8 have been constructed (Yamamoto *et al.*, 2002; Ueno, Yamamoto *et al.*, 2004) as part of Japan's National Project on Protein Structural and Functional Analysis funded by the Ministry of Education, Sports, Science and Technology (MEXT) of Japan (Protein 3000 project) (Yokoyama *et al.*, 2000; Stevens *et al.*, 2001). The target of the beamline construction is the high-throughput data collection of protein crystals to contribute to structural genomics research, which leads to the accumulation of a large number of protein structures. The beamline is equipped with a sample-changer robot, named SPACE (SPring-8 Precise Automatic Cryo-sample Exchanger), and a sample database system (Ida *et al.*, 2002; Ueno, Hirose *et al.*, 2004) for performing the automated data collections for a large number of protein crystals with maximum efficiency of beam-time use (Abola *et al.*, 2000). For automatic operation of such a beamline, development of administrative software to provide unified control of beamline instruments in accordance with experimental schedule is indispensable (McPhillips *et al.*, 2002; Pohl *et al.*, 2004). Here we describe Beamline Scheduling Software (BSS), which has been developed at the RIKEN Structural Genomics Beamlines to manage the experimental schedules and operate beamline instruments (Ueno *et al.*, 2002).

The graphical user interface (GUI) of BSS offers all-in-one control tools for beamline operation. As well as the schedule editor used for automatic data collection, the GUI consists of tools for manual beamline operation and beamline optics tuning. Users can set up the experimental conditions such as crystal centering, oscillation parameters and others within the BSS GUI.

With automatic operation, the experimental schedule for multiple samples is extracted from the sample database system and is registered to BSS. Beamline instruments are operated by distributed server programs under the client and server architecture. BSS implements the beamline operation by communicating with the device servers through the computer network. BSS successively processes the scheduled data collections by utilizing the centralized control system of the beamline components.

2. Software design

2.1. Client and server architecture

Both RIKEN Structural Genomics Beamlines I and II have identical design, which consists of the SPring-8 standard optics commonly used for the bending-magnet beamlines. The instruments in their end stations, however, are specialized for high-throughput protein crystallography with automated data collection (Fig. 1). In the optics hutch, a fixed-exit Si double-crystal monochromator followed by a cylindrical bending mirror is installed. In the end station, installed on the equipment stage are a kappa goniometer with remote-controllable translation head, a sample-changer robot, and CCD (charged coupled device) and IP (image plate) area detectors. By moving the equipment stage, these area detectors can be switched from one to another to cope with various user choices of measurement conditions.

Beamline instruments are controlled by the software system based on the client and server architecture. In this architecture, BSS functions as the client software to organize beamline devices, where the controls at the lowest level of those devices are distributed to individual server programs. The command protocol and running platform of the server programs vary from server to server because they have been developed and provided by different groups or hardware vendors. The server software and VME control system for standard

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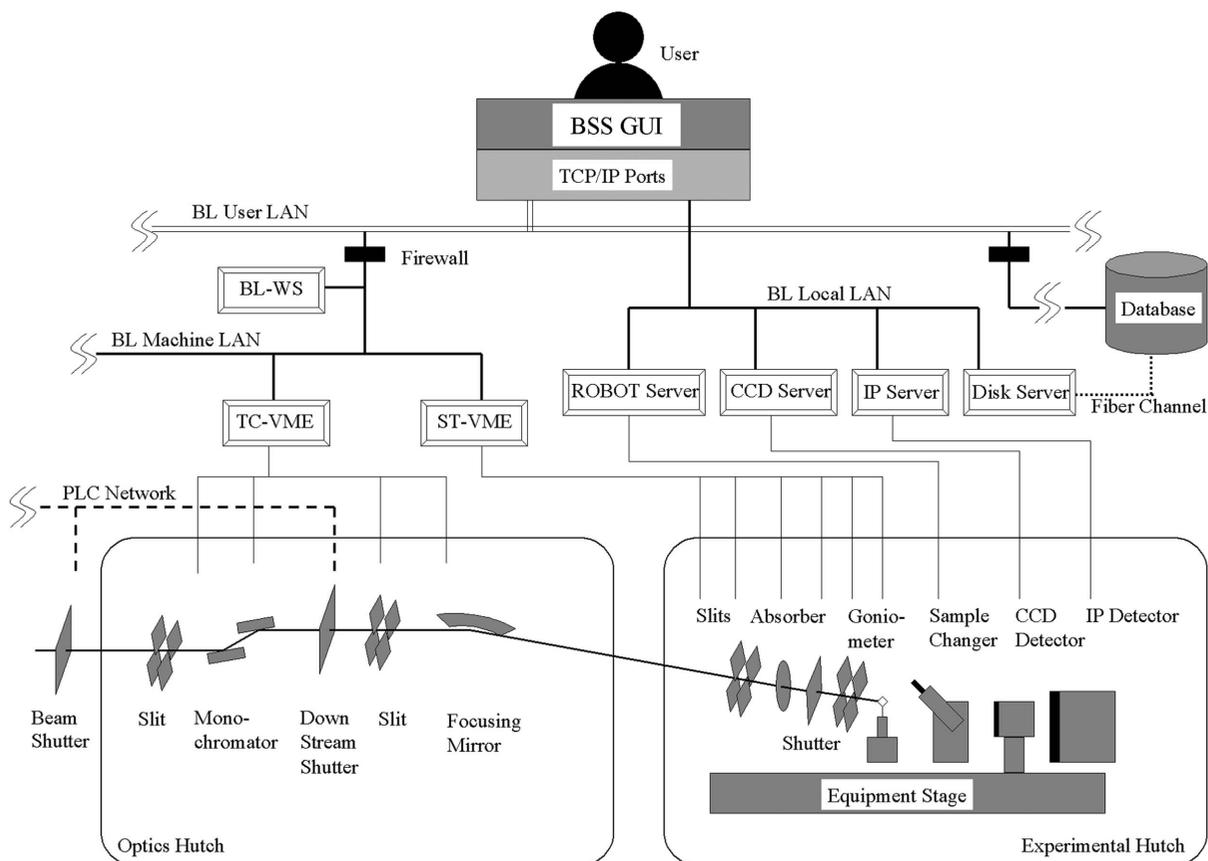


Figure 1
Network and hardware configuration of the RIKEN Structural Genomics Beamlines.

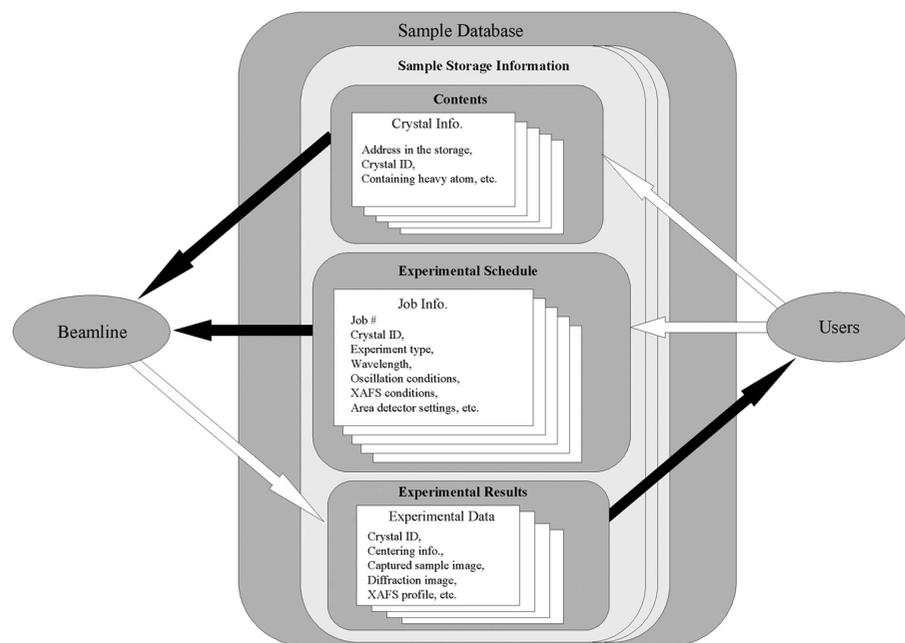


Figure 2
Schematic diagram of the sample database system. White and black arrows in the diagram represent upload and download of the information, respectively.

SPring-8 beamline equipment have been provided by the Beamline Control Group of SPring-8 (Ohata *et al.*, 1998). The beamline monochromator, goniometer, equipment stage and so forth are

controlled by this server, which runs on the workstation (BL-WS). On the other hand, the frame grabber of the CCD and IP detectors run on personal computers, which are provided by hardware vendors. The hardware and server of SPACE have been independently developed at the RIKEN Structural Genomics Beamlines (Ida *et al.*, 2002; Ueno, Hirose *et al.*, 2004). It is one of the essential tasks for BSS to set up a unified environment from the different computer systems involved.

The sample database system consists of SQL-based software and storage area, which can be accessed by web browsers (Fig. 2). The database is used to register the experimental schedules for the automatic beamline operation (see §3). Data-collection parameters for dozens of protein crystals can be uploaded prior to the beam time. Users are able to access the database from their laboratories in order to register the sample information and experimental conditions. The registered schedules are extracted at the beamline through the network. The experimental results including diffraction image files are uploaded to the database and can be referred by users.

BSS has multiple TCP/IP socket ports and can communicate with device servers in respective command protocols. Users can control

computer programs

and monitor all beamline components *via* BSS, and operate the entire beamline by using the BSS GUI window.

2.2. Graphical user interface (GUI)

The GUI of BSS is designed so that users can easily register the experimental schedule and start the automated beamline operation. There are six tab pages, which can be switched by clicking the mouse button. The default active tab is the Schedule tab, which allows a series of experiments for multiple crystals to be set up (Fig. 3). Each row in the list widget represents either diffraction or XAFS (X-ray absorption fine structure) measurement for a given sample. The contents may be edited using control buttons located on the left of the list. The beamline operation can be initiated by pressing the Start button, and BSS can successively execute the measurements registered in the list.

The Mount Sample tab launches a monitor window of the crystal (Fig. 4). Double-clicking on the crystal image invokes the translation of the goniometer head to the optical center. For the centering of crystals, there are several supporting tools such as spindle-axis rotation, backlight insertion and so on. As an option, an automatic loop-centering routine based on the image processing is available.

The XAFS tab is automatically activated during the XAFS measurement, and provides a graphical chart of the data obtained (Fig. 5). A supporting option for users to determine the peak and edge wavelengths by calculating the maximum and minimum derivative of the XAFS profile can be selected.

The Current Status tab (Fig. 6) and the Device tab (Fig. 7) display the status of the storage-ring current and status of other beamline devices, respectively, and the Miscellaneous tab (Fig. 8) displays information such as the program running directory and so on, which are not directly related to user operation.

3. Automatic beamline operation by BSS

Since October 2002, the RIKEN Structural Genomics Beamline I (BL26B1) has been open for users, and the unified environment of BSS has made the beamline easy to use. Once the measurement is

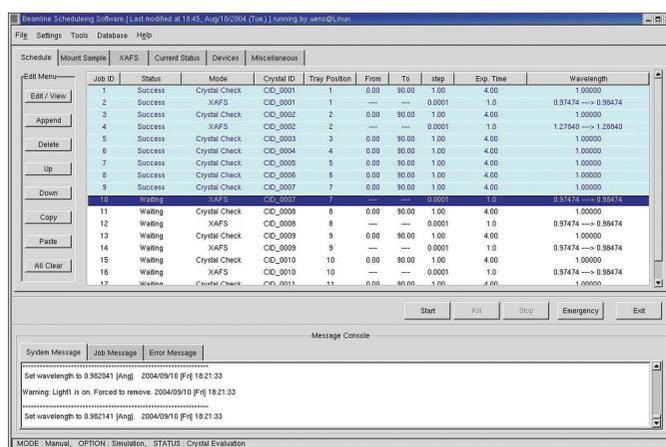


Figure 3
BSS main window (Schedule tab).

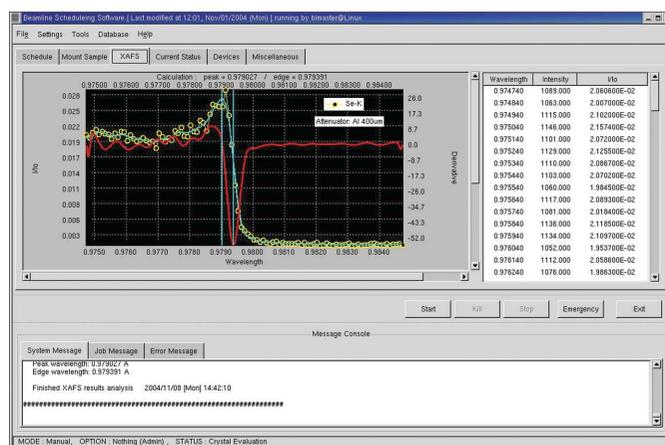


Figure 5
XAFS tab. A graphical plot of XAFS measurements is displayed. The results of profile analysis, *i.e.* peak, edge (maximum, minimum derivative) wavelengths and derivative plot are superimposed.

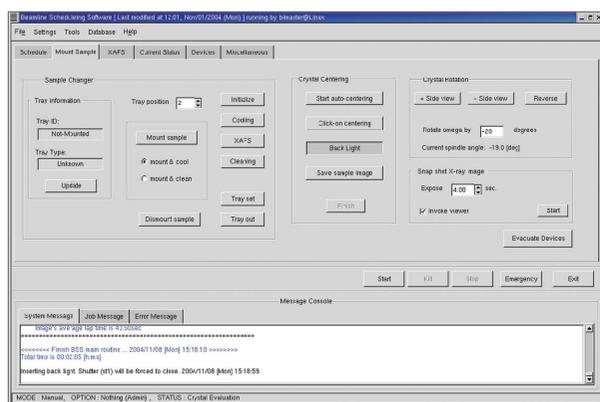


Figure 4
Mount Sample tab and the crystal monitor window.

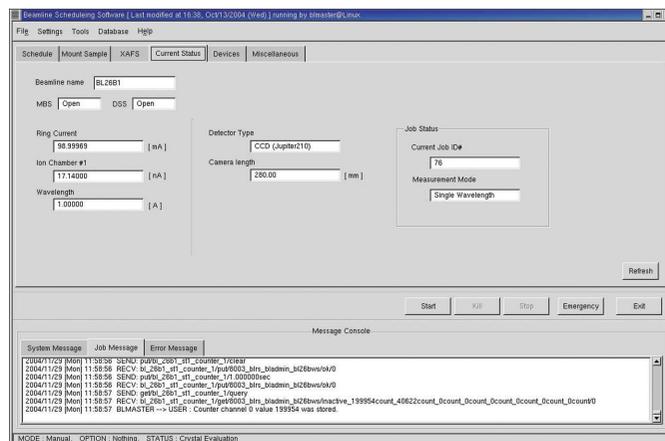


Figure 6
Current Status tab. Status of the storage ring, the beam shutters, X-ray intensity *etc.* are displayed.

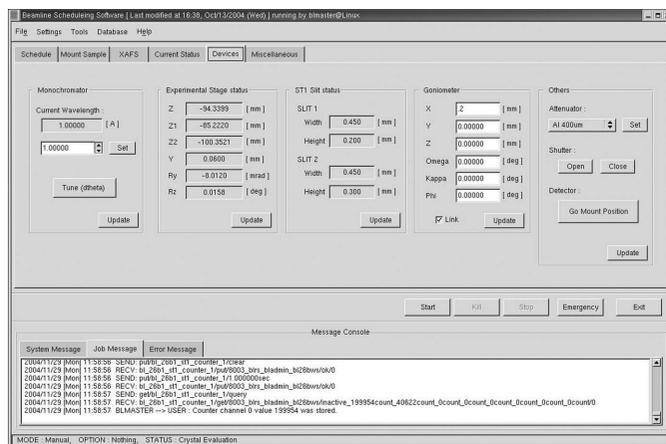


Figure 7
Devices tab. Allows setting the wavelength, the goniometer, the attenuator *etc.* by manual operation.

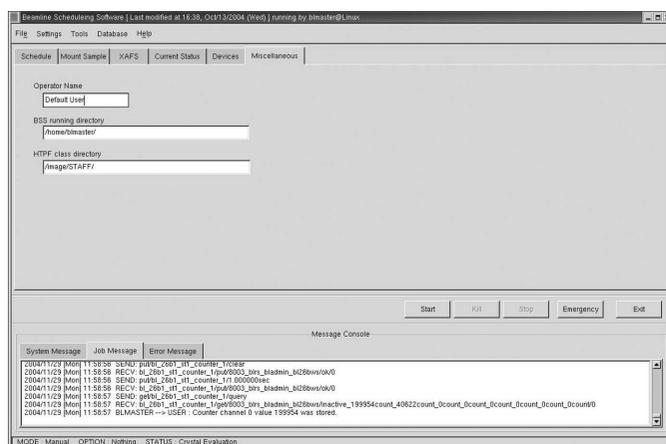


Figure 8
Miscellaneous tab. Informs the operator name, BSS running directory *etc.*

initiated from the GUI of BSS, the X-ray wavelength is automatically set to the specified value, and the area detector (CCD/IP) is moved to the experimental position. BSS automatically optimizes the X-ray intensity at the sample position by the automatic tuning sequence. Each time the X-ray wavelength is changed, the beam intensity at the end station is checked by an ionization chamber located upstream from the sample on the equipment stage. Then the Bragg-angle correction axis of the first crystal of the monochromator is tuned in order to maximize the ionization chamber signal. Switching the area detectors or changing the camera length to a large extent can cause misalignment of the crystal position owing to the mechanical stage movement. In this case, BSS automatically corrects the sample position by adjusting the equipment stage height at which the ionization chamber signal is maximized.

Automatic beamline operation started at BL26B2 using BSS with the sample changer SPACE in October 2003. Once a day, dozens of protein crystals are delivered to the beamline, and are set in the sample storage of SPACE. With the sample changer in automatic operation, a day of the beamline is separated wherein two different experimental modes are carried out sequentially (Ueno, Hirose *et al.*, 2004). The first mode is crystal evaluation, performed by beamline operators. Users can preliminarily store the evaluation schedule in the sample database, and the operators extract it through the

network. During the evaluation mode, operators center the crystals, which are sequentially exchanged by SPACE. According to the schedule, preliminary diffraction images and XAFS profiles for MAD (multiwavelength anomalous dispersion) samples are measured. After the evaluation measurement, the sample is placed in storage.

The sample changer SPACE has adopted a specially designed sample pin equipped with screw threads which is attached to the goniometer. The pin ensures that the position of the crystal is reproducible under multiple mount and dismount actions. Therefore, once the first centering is completed, the record of the necessary motions of the goniometer head is registered to the database, and re-used later for automatic centering. This centering information, together with the diffraction images and XAFS profile data, are uploaded to the database.

The second mode of the beamline experiment is dedicated to automatic data collections for samples which were qualified during the evaluation mode. Judgement of crystals and preparation of experimental schedule are performed by users according to the evaluation data stored in the database. For individual samples, users determine the appropriate oscillation conditions. From XAFS profiles, the users can easily determine the peak, edge and remote wavelengths for MAD data collection. The desired schedule of the data collection is uploaded to the database and extracted at the beamline. In the data-collection mode, BSS applies the goniometer translation records, which were stored during the evaluation mode, for each crystal centering. BSS successively carries out the data collections by exchanging crystals, centering crystals, setting the wavelength, switching the detectors and taking diffraction images. In case of storage-ring problems, BSS automatically pauses for a while, and continues the measurement when the problem has been sorted out and X-rays are ready. Under the BSS administration, the beamline can be uninterruptedly operated without any attendant until all loaded samples are measured.

4. Platform, language and availability

BSS has been developed to run on the Linux operation system, and the source code is written in the language C. The GUI is coded using a GTK+ and Glade interface builder. BSS forbids the running of multiple instances in order to avoid interference between multiple users. During the execution of each experimental sequence, the BSS GUI is locked and does not accept any request of device operation.

BSS is currently customized to operate protein crystallography beamlines at SPring-8. Now, BSS has also been adopted at the Macromolecular Crystallography Beamline (BL38B1), the Pharmaceutical Industry Beamline (BL32B2) and Structural Biology Beamline I (BL41XU), in addition to the RIKEN Structural Genomics Beamlines. Furthermore, installations at some other beamlines at SPring-8 are in progress. Beamline-specific configurations such as the IP address and socket port number of the server programs, the product information of the detectors and so forth can be easily changed by editing the text-based BSS configuration file. This allows BSS to be kept compatible with these beamlines within SPring-8. The possibility of adaptation for other facilities should be consulted with the authors.

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