JBluIce-EPICS: a fast and flexible open-source beamline control system for macromolecular crystallography

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Abstract. This paper overviews recent advances in the JBluIce-EPICS open-source control system designed at the macromolecular crystallography beamlines of the National Institute of General Medical Sciences and National Cancer Institute at the Advanced Photon Source (GM/CA@APS). We discuss some technical highlights of this system distinguishing it from the competition, such as reduction of software layers to only two, possibility to operate JBluIce in parallel with other beamline controls, plugin-enabled architecture where the plugins can be written in any programming language, and utilization of the whole power of the Java integrated development environment in the Graphical User Interface. Then, we demonstrate how these highlights help to make JBluIce fast, easily adaptable to new beamline developments, and intuitive for users. In particular, we discuss several recent additions to the system including a bridge between crystal rastering and data collection, automatic detection of raster polygons from optical crystal centering, background data processing, and a pathway to a fully automated pipeline from crystal screening to solving crystal structure.

1. Introduction

JBluIce-EPICS (Java Beam Line Universal Integrated Configuration Environment - Experimental Physics and Industrial Control System) is a control system designed at the macromolecular crystallography beamlines of the National Institute of General Medical Sciences and National Cancer Institute at the Advanced Photon Source (GM/CA@APS). While the general architecture of the system and implementation of some functionalities were described in [1-3], JBluIce is in rapid development and many new features have been implemented since then. This paper reports on some of these new features and discusses how the JBluIce architecture helped to bring them to life rapidly.

2. Why another control system?

JBluIce was specifically designed for relatively independent beamline support teams such as the Collaborative Access Teams at the Advanced Photon Source and groups at the majority of synchrotron sources in the US. A major difference between beamline management at European and US
Synchrotrons strongly affects the trends in designing beamline controls. In Europe the tendency to have centralized management has resulted in generic wide-applicability beamline control systems such as OpenGDA (Diamond Light Source) and the BLISS Framework (ESRF). While the concentration of developing resources helps to come up with some brilliant software solutions, achieve higher unification of user interfaces, enforce common standards on data management, etc., it has certain drawbacks too. First, the generic systems need an abstraction layer between the graphical user interface (GUI) and the hardware servers, which helps the generic systems to hide beamline hardware differences from the GUI and thus maintain their wide applicability. This layer makes the system heavier and complicates access to non-common advanced hardware capabilities. Second, contributing new code to complex systems often requires software knowledge beyond the training of beamline scientists, which may slow development of new features at facilities where scientists serve as customers who must request new features instead of experimenting and developing on their own.

Several technical solutions were incorporated into JBlulce to address the above issues and make it fast and easily adaptable to new beamline developments. First, JBlulce-EPICS has only two software layers, the EPICS backend for robust control of distributed beamline hardware and the multiple graphical user interface (GUI) clients written in Java. This provides the GUI with direct access to any advanced hardware features, such as on-the-fly scanning capabilities of motion controllers, and simplifies addition of new features. Second, JBlulce-EPICS deploys multiple plugins (or "helpers") that can be written in any programming language, thus involving more staff in development of new features. In addition, the GUI mimics the look and feel of the successful SSRL BluIce [4-5], which helps most users to become proficient with beamline controls within minutes. From the user's perspective, this is the same simplicity as switching between different beamlines controlled by e.g. OpenGDA. Finally, JBlulce clients are designed to operate in parallel with other beamline controls, thus streamlining beamline preparation and maintenance, operations auditing and user assistance. Since the expert staff tools do not need the same level of user friendliness as user controls, it is another area where the JBlulce architecture allows for reduced development effort.

The "helpers"-enabled architecture has worked very efficiently while porting JBlulce to the Australian Light Source. Helpers are standalone programs, for example a fluorescence scan, or beamline intensity feedback system, or a script to realign the beamline to a changed energy. They can run on their own and as such, can be written in any language. Integration of helpers into JBlulce consists of adding a respective call to JBlulce and agreeing on message exchange ("handshaking") between the two programs via EPICS process variables. In the GM/CA@APS implementation all helpers were either written in EPICS state notation language or as Perl scripts using EPICS libraries for Perl. At the Australian Light Source, the state notation programs were modified according to the local hardware while all Perl scripts were rewritten in Python, as the local staff scientists had expertise in Python. This helped to involve the scientists in the development and made possible the conversion of fully operational beamlines to JBlulce controls within a short period of time and with limited resources.

3. JBlulce architecture helps rapid development of new automation features

In [2,3] we demonstrated how the streamlined architecture of JBlulce helped the rapid development of new beamline automations such diffractive and fluorescent crystal rastering over polygon areas and adaptive energy scans. The past year brought a number of new developments, which were possible due to close involvement of beamline staff in the software design. In particular:

- In the JBlulce Raster tab, a feature was implemented to automate polygon generation from loop contours detected by an optical autocentering helper that interfaces with XREC [6].
- A raster-to-collect feature was implemented. In the JBlulce Raster tab, the locations of well diffracting sites on samples can be passed to the Collect tab. This required a re-design of the Collect tab to include "raster mode", i.e. the controls for moving between crystal spots during data collection. This new feature generalizes the vector data collection previously implemented in JBlulce [3].
• In the JBlulce Raster tab, a feature has been implemented for users to subtract erroneous "Bragg" spots and specify resolution limits, which improved the reliability of raster image analysis for poor-quality samples.

• In the JBlulce Collect tab, a new dropdown menu "XDSProc" was implemented for automated processing with XDS [7]. The menu has options None, Native, and Anomalous, which produces Bijvoet-pair data. After a data set is collected, the XDS processing is started in the background on the least-loaded workstation selected by Oracle Grid Engine. XDS is automatically restarted with revised parameters if the initial run fails. The results of data processing are displayed in the new Analysis tab (figure 1).

• In the JBlulce Collect tab, the strategy calculations were substantially extended. All possible space groups in the LABELIT [8] solution are displayed in the strategy window. By default data are processed in all space groups of the highest symmetry solution, and the strategy output is displayed according to this selection. The user can choose a lower symmetry solution and JBlulce will process and display a strategy for it. Multiple space groups are processed in parallel to increase the speed. Strategy can be reported for native or anomalous data; for the latter, the results can be displayed for continuous or inverse beam modes. All strategy results are now kept and can be reviewed as needed. An option is provided to use either BEST [9] or MOSFLM [10] for strategy calculations.

• In the JBlulce Hutch tab, beam alignment scans were integrated. Previously these scans, which are carried by a helper script, were displayed in separate popup windows.

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**Figure 1. New JBlulce Analysis tab**

[Image of JBlulce-EPICS: Beamline ID-D Version 2012.2 Build 4803 interface with analysis data and graphs showing energy vs resolution and iSigma vs resolution.]
At the time of writing this paper, the list of planned new automations within JBluIce consists of almost 200 items. This list is continuously replenished due to active feedback of beamline users and the ideas of beamline scientists. Despite the impressive length, the list has been gradually shortening as the implementation pace is high due to the efficient JBluIce architecture. Among the developments planned for this year is addition of rastering to the list of crystal centering techniques on the Screening tab. In combination with the recently implemented raster-to-collect feature and background data processing, this will create the basis for a fully automated pipeline from crystal mounting and screening to solving structures.

The JBluIce source code and video manuals are available at http://www.gmca.anl.gov.

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