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BART: DEVELOPMENT OF A SAMPLE EXCHANGE SYSTEM FOR MX BEAMLINES

J. D. O'Hea, M. Burt, S. Fisher, K. M. J. Jones, K. E. McAuley, G. Preece, M. A. Williams,
Diamond Light Source, Oxfordshire, United Kingdom

Abstract

Automation plays a key role in the macromolecular crystallography (MX) beamlines at Diamond Light Source (DLS). This is particularly evident with sample exchange; where fast, reliable, and accurate handling is required to ensure high quality and high throughput data collection. This paper looks at the design, build, and integration of an in-house robot control system. The system was designed to improve reliability and exchange times, provide high sample storage capacity, and accommodate easy upgrade paths, whilst gaining and maintaining in-house robotics knowledge. The paper also highlights how peripheral components were brought under the control of a Programmable Logic Controller (PLC) based integration unit, including a vision system.

INTRODUCTION

Data collection on Diamond's [1] Macromolecular Crystallography beamlines [2] involves working through hundreds of crystallised macromolecules mounted on small sample holders and stored in liquid nitrogen. Each sample needs to be mounted on a rotatable stage before being exposed to the X-ray beam. The data collected are the diffraction patterns created by the beam passing through the mounted crystal. [3]

Robotic arms are ideal for the mundane process of exchanging samples: moving them from inside a storage dewar of liquid nitrogen to the mounting point and back again. Their motions are precise and repeatable even at high speeds, they can operate in the controlled radiation area of the experiment hutch and the gripper tools can be engineered to operate with liquid nitrogen. They also offer great flexibility; very useful on beamlines where equipment and configurations can change and develop frequently.

The DLS MX beamlines have been using robots for sample exchange since 2007, employing either Rigaku ACTOR robotic systems [4] or IRELEC CATS robotic systems [5]. Diamond's data acquisition software (GDA) [6] communicated with the Rigaku or IRELEC control software directly to trigger robot actions. Three beamlines used Rigaku ACTOR robots which used a Mitsubishi RV-6S robot arm and two beamlines used the CATS robots, which utilised a Staubli TX60 arm.

These systems worked well but over time, as beamline technology developed and data collections became quicker, both systems required significant upgrades to increase sample capacity and reduce sample exchange times.

A project was created with the goals of fully integrating a robot system into the beamline control system, to upgrade and optimise peripheral devices to improve performance and reliability and, through this process, to gain and maintain in-house automation knowledge allowing for better local support including faster problem resolution. The decision was made to develop a single robotic system, based around a Mitsubishi RV-6SL arm that could be installed on all of the MX beamlines with only minor customisation required.

This would be achieved by moving software device support to EPICS [7], creating our own integration unit built around a PLC, and the redesign of supporting components and peripherals to maximise performance and cater for future upgrade paths. (See Fig. 1)

INTEGRATION UNIT

The complete system consists of many components, each requiring a software interface and their own control requirements. The role of the integration unit is to connect all these separate peripherals to a common interface with which the software can communicate, whilst also providing low level logic and feedback control. The decision was made to build the unit around an Omron CJ2M CPU33 Ethernet PLC [8]. This model is used extensively at DLS for all the machine protection systems and so was already familiar to our engineers, with proven performance, reliability and versatility, and with established EPICS software support. It can also be supported by stock parts, removing the cost and overhead of maintaining an independent spares set.

The unit controls the robot's gripper, drier, beacon, computer vision system, liquid nitrogen fill control, and dewar heaters. In addition, by passing all of the robot's input and output channels through the integration unit, it allows these signals to be overridden by the PLC, either pulled high or pulled low. This is incredibly useful for testing and debugging, or simulating an input from a failed or missing component on the beamline.

DEWAR AND LIQUID NITROGEN SYSTEM

Sample storage dewars for MX beamlines need to have high capacity, reliable autofill systems and should be designed to minimise ice build-up in or around the dewar. The dewar used in the BART system is based on a design developed by the P11 beamline at PETRA [9] and manufactured by CryoTherm [10]. Up to 592 samples can be accommodated within the dewar.

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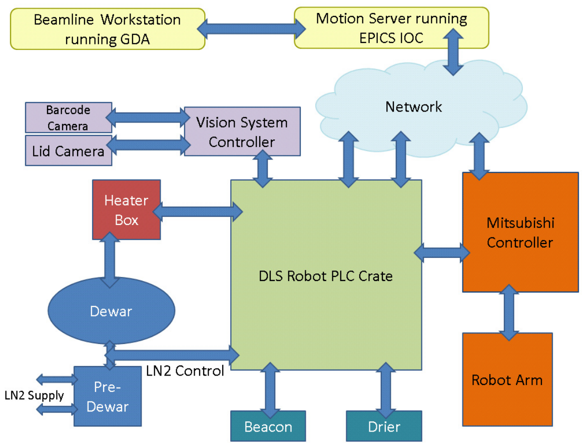

Figure 1: Block diagram of system.

To avoid icing, the rim of the new dewar (which is in contact with the lid) is packed with 12 heating elements divided into two banks of six and monitored by a thermocouple. The PLC regulates the heating system and provides two temperature setpoints: one for when the dewar is being filled with liquid nitrogen and another for when the liquid nitrogen level is stable. Under normal operation only six elements are enabled. When the autofill mode is active, all 12 are enabled.

Originally a separate 3rd party liquid nitrogen fill control system was used to maintain the dewar liquid level. With the introduction of the in-house integration system it was recognised that this control could also be handled by the PLC unit. A level probe consisting of five temperature sensors was mounted at different depths within the dewar. This allows five level heights to be distinguished. The PLC closes the feedback loop between the probe and the fill valve to maintain the liquid nitrogen level at a defined height. If the level drops below a setpoint for 60 seconds, a refill is triggered. This refill process consists of cycles of one minute of filling, three minutes of settling time, until either the desired level or a timeout limit is reached.

COMPUTER VISION SYSTEM

One of the identified development needs of the system was a better way of avoiding collisions between the robot arm and peripheral equipment on the beamline. Computer vision systems are routinely used for industrial robots and are becoming more widely used for MX sample changing robots [9, 11]. For the P11 beamline, the vision system is able to identify the opening in the dewar lid and track its position. This position can then be fed back to the robot.

We adopted the same approach using an Omron FZ-SC2M camera [12] and FZ5-L355 vision system [13]. These models were chosen as they integrated into the chosen Omron PLC of the integration unit.

The system looks for a circle of a given dimension within a coloured square of defined size to identify the opening. It calculates the centre point of this circle and checks that it is located within the internal diameter of the dewar. If it is, the position is reported to EPICS to be passed on to the robot controller. If not, an error is raised and the robot will not attempt to enter the dewar.

The vision system can support up to four cameras, and so a second camera was also used to read sample barcodes. 2D Data Matrix barcodes are located on the underside of SPINE [14] sample holders and are used to link sample information to a particular sample holder. The barcode is read during the sample exchange process. (See Fig. 2)

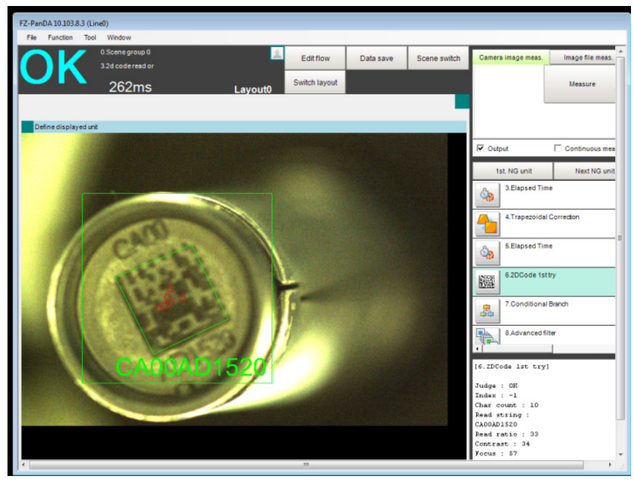

Figure 2: Screenshot of vision system reading a Data Matrix barcode.

DRIER

A drier is used to heat up the robot gripper after it has been in liquid nitrogen to avoid ice restricting its movement and to prevent contamination of samples with ice crystals. A drier has been designed that couples a funnel shaped nozzle, of similar diameter to the gripper, with a system moving compressed air across a heating element to completely envelop the gripper in hot, fast moving air. The drier remains on until the gripper's internal thermocouple reaches 310K, after which the compressed air supply remains on for a further 30 seconds without heat to cool the drier itself. This design was found to be very effective, completing a dry routine in 30 seconds.

LASER SCANNER

A Keyence safety laser scanner, model SZ-04M [15], was added to form part of the personnel safety system of the robot, monitoring for the approach of a person to the robot. It has two defined zones: a warning zone from a distance of 2m to 1m, in which the sensor will beep loudly but the robot motion is unhindered; and a danger zone from a distance of 1m, in which the sensor will beep loudly and the robot motion will be disabled.

ROBOT PROGRAMS

All actions of the robot are written in Mitsubishi's MELFA BASIC language and are stored and run on the robot controller. They are written as functional blocks to

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limit repeated code and aid development. The functionality is provided across 51 programs. EPICS only provides triggers to initiate six 'top level' routines which in turn trigger any sub-programs. EPICS monitors a Program Running status provided by the controller to determine when a routine has finished.

Figure 3: Complete system: Base table housing Mitsubishi controller, PLC integration unit, with laser scanner mounted on left hand side and a camera gantry and dewar with heating elements on top.

BASE TABLE

A support table was needed to accommodate all the components. The table top accommodates the robot arm, the sample storage dewar and reservoir, the drier unit and camera system gantries. The robot controller, PLC integration unit, computer vision controller and peripheral cabling is housed underneath. The whole table is mounted on wheels to allow it to be easily moved into place on a beamline before being bolted to the floor. All internal units and wiring are mounted upon a drawer mechanism allowing easy access for maintenance and upgrades. (See Fig. 3) All external connections are brought to a patch panel on the rear of the table.

EPICS SOFTWARE

Communication to the robot controller by EPICS is made via the streamDevice support module [16]. This allows the sending and receiving of strings to pass data between EPICS and the hardware. The supported command set and their expected replies are defined within a protocol file and it is this file which EPICS interacts with. The connection is over TCP/IP established with the asyn support module [17]. An associated user GUI is available (See Fig. 4).

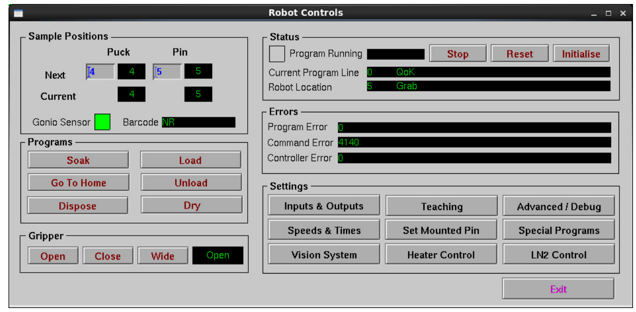

Figure 4: The EPICS GUI.

Communication with Omron PLCs is made over the Factory Interface Network Service protocol (FINS). The FINS and dlsPLC support modules were used to read and write to PLC registers from EPICS.

The genSub support module [18] was used to allow C programs to be incorporated into the EPICS driver for tasks such as error and location code lookup, operation logging, and barcode string conversion from bytes to ACSCII characters.

GDA remains the end user interface but instead of talking directly with the robot controllers it now interacts with the EPICS driver via process variables (PVs). This matches the way that GDA interacts with all other devices on the beamlines.

RESULTS

The first completed BART system was installed on DLS MX beamline I03 in early 2015, and since then, more than 60,000 samples have been loaded by the I03 robot. A further three BART systems were deployed on the MX beamlines I04, I04-1, and I24, and all of the robot systems are fully operational.

The rate of sample exchange on the beamlines has been increased by utilising several time-saving approaches. Firstly, the close integration between the control of the robot arm and the beamline hardware means that both robot movements and movements of equipment in the sample environment can be optimised. Secondly, moving the device software to EPICS gave us greater control of operations, speeding up command response times and allowing us to leave the robot arm servo motors energised. Thirdly, customisation of the drier brought significant time-saving to a regularly used peripheral. Finally, tighter integration of the beamline status into the robot's I/O allowed us to parallelise robot and beamline component movements.

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One of the aims of this development project was to produce a robot system that could be customised for different beamlines and this aim has been realised by adapting the BART system for the small molecule single crystal diffraction (I19) beamline [19] and the in-situ crystallography beamline, VMXi [20].

CONCLUSION

The project successfully improved the performance and reliability of the robot system and its peripheral components, with full integration into the beamline control system at both the hardware and software levels. In-house knowledge was expanded considerably and amongst a wider pool of people. The system was able to be adapted to work on a plate handling beamline and has proved flexible enough to support some additional peripheral projects.

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