ISBN: 978-3-95450-193-9 doi:10.18429/JACoW-ICALEPCS2017-TUMPL08

MAX IV BioMAX BEAMLINE CONTROL SYSTEM: FROM COMMISSIONING INTO USER OPERATION

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Abstract

The BioMAX beamline at MAX IV is devoted to macromolecular crystallography and will achieve a high level of experimental automation when its full potential is reached due to the usage of high end instrumentation and comprehensive software environment. The control system is based on TANGO and Sardana for managing the main elements of the beamline. Data acquisition and experiment control is done through MXCuBE v3 web application, which interfaces with the control layer. Currently, the most critical elements such as the detector and diffractometer are integrated into the control system, whereas the integration of the sample changer has started. BioMAX has received its first users, who successfully collected diffraction data and provided feedback on the general performance of the control system and its usability. The present work describes the main features of the control system and its operation, as well as the next instrument integration plans.

BIOMAX BEAMLINE DESCRIPTION

BioMAX is the first X-ray macromolecular crystallography (MX) beamline of MAX IV Laboratory, which began its user operations in 2017. It is a state-of-the-art resource accommodating multiple cutting edge experimental possibilities. The design goal for BioMAX was to create a stable and reliable beamline that provides a user friendly environment. The beamline experiment set-up is highly automated, in terms of both sample handling hardware and data analysis, including feedback on the data collection. The X-ray beam focus is 20 x 5 μm^2 at the sample position and the operational energy range is 5-25 keV, [1]. Table 1 shows the main characteristics of BioMAX.

Optics

The main optical elements are a liquid-nitrogen cooled double crystal monochromator and two mirrors in Kirkpatrick-Baez geometry (named Vertical and Horizontal Focusing mirrors). The mirrors have three different stripes for different energy ranges, selectable by adjusting the position of several motors. Apart from in-air and in-vacuum motors, there are two piezo actuators for fine adjustment of the second crystal pitch and roll in the case of the monochromator, and additional two for the focusing mirrors' pitch. Before the focusing mirrors there is a slit module, consisting of two identical units, one with horizontal movements and one identical unit with vertical movements. In addition, there are measurements for temperature, flow, pressure, etc.

Several diagnostics modules are distributed along the beam path. The first module includes a fluorescent screen, a fixed Cu mask, a fixed bremsstrahlung mask and a filter unit. The screen switches between two positions by means of a pneumatic actuator and it also includes a CCD camera. The filter unit has two axes that are stepper motor driven. Each axis has five positions including four different filters and one position without filter. This diagnostic module also includes several temperature measurements. The second diagnostic module mainly contains a similar fluorescent screen setup as the previous one.

Table 1: Main Specifications of the BioMAX Beamline at MAX IV

Techniques	MX, MAD, SAD, S-SAD, atomic resolution data collection, large sample ensemble screening, in situ crystal diffraction
Beam Size	20 x 5 μm^2
Energy Range	5-25 keV
Samples	Single crystal (1 - 100 μm)

Experimental Station

This is the area where the most complex elements of the beamline are located. The main components of the experimental station are the beam conditioning unit, the MD3 diffractometer from Maatel/Arinax, the ISARA sample changer (Irelec), the EIGER 16M detector (Dectris) and all the associated motorised support tables (one for the beam conditioning unit and the diffractometer, and another one for the detector). The Figure 1 displays a recent picture of the experimental hutch. The MD3 diffractometer is an evolution from the previous MD2, which is an advantage since the communication API is the same and the MD2 was in use in the old MAX-lab MX beamline, therefore the development has been focused on the addition of the new functionality. Concerning the ISARA sample changer, it can hold up to 400 samples supporting both Unipack and Spine standards and a crystalization plate holder, and it provides a fast sample exchange due to a double gripper mechanism. Together with the state of the art detector, the goal is to provide a fast and highly automated environment for the users, aiming at a sample/crystal processing rate higher than 200 samples per eight hours shift.

In addition to those main components, further elements are the Beamline Conditioning Unit, which encloses several motorised devices such as two piezo actuator driven slits, an attenuator device consisting of three wheels, an

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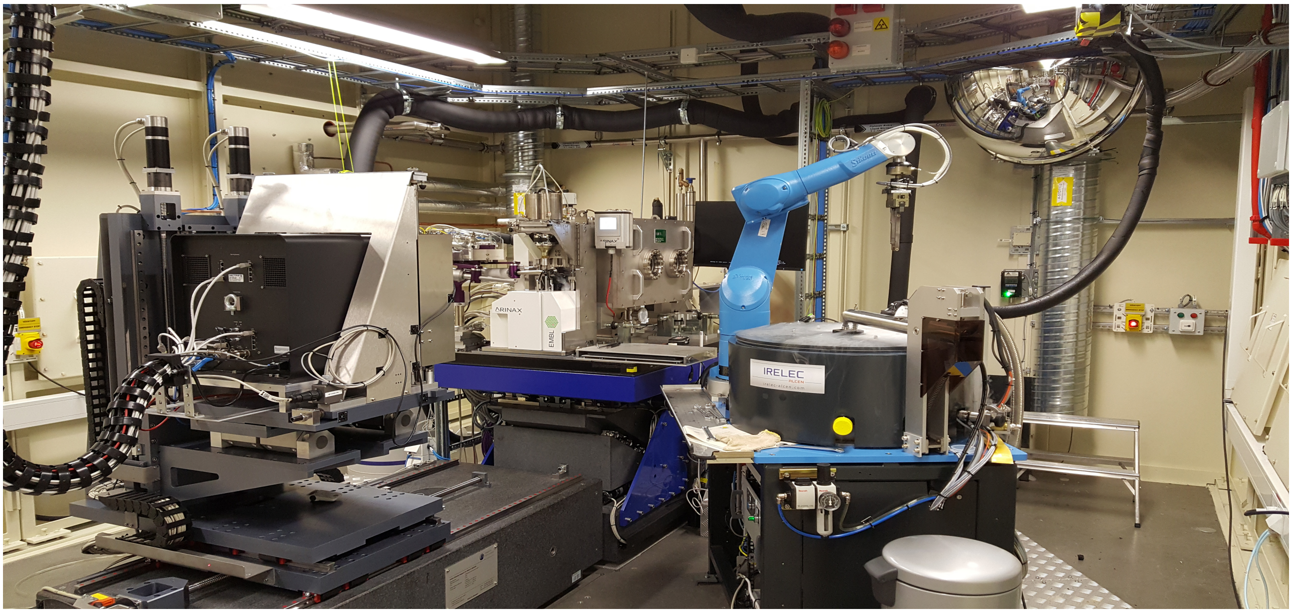

Figure 1: BioMAX experimental station; from left to right: EIGER 16M detector and its support table, MD3 diffractometer and the Beam Conditioning Unit (BCU) on their table, ISARA Sample Changer.

intensity monitor and several diamond XBPMs. Also, the Rapid Nozzle Exchanger (REX) is a remote controlled nozzle exchanger used to quickly switch between the cryogenic flow and the crystal dehydration nozzle (HC-Lab Humidity Controller).

CONTROL SYSTEM DESCRIPTION

In order to simplify the control system design, implementation and maintenance, the MAX IV controls and IT group (KITS) have defined a set of procedures, tools and devices as standard. As a principle, KITS team pursues the user autonomy, a value that focuses on making control and IT systems more accessible to users, so it is easier for them to contribute. A user can be a KITS member from a different domain, another staff member or a visiting user of MAX IV. The control system development has to ensure that the user is able to participate in the development and also have access to troubleshooting in any situation in which they have the capacity to do so. Together with an Agile development process, the development team is able to provide solutions quickly and react to changing specifications earlier in the process, [2, 3].

Therefore, from the initial beamline design, the control system group has been tightly involved in the design process and provided support as needed. Moreover, the advanced necessities regarding experiment automation and the important needs on software development has made this beamline an interesting model of the integration of highly complex elements following the MAX IV standards.

Table 2 shows some reference numbers with the aim of describing the size of the control system, although the complexity of such cannot be represented so easily. Most of the pseudo-motors are straightforward mathematical calculations, such as slits or bragg-energy conversion. The movables mostly consist of motor axis, but there are several piezo actuators as well. Regarding the vacuum, there are sixteen ion pumps together with a variety of vacuum gauges and valves. In addition, a few hundreds of analog and digital signals are acquired; limit switches, sensors (temperature, flow, etc.), beam position, etc. Most of those signals are available through the corresponding TANGO device.

There are a high number TANGO devices running on twelve different hosts. Some of those devices contain a few attributes, for example a thermocouple measurement is exposed as a single TANGO device consisting of a temperature attribute and additional ten attributes (alarms, status). On the other hand, a complex device like the sample changer contains a few hundred attributes and commands.

Table 2: Control System Size

Section	Movables	Pseudomotors
Front end	14	3
Optics	28	14
Experimental	22	4
TANGO hosts	12	
TANGO devices	471 in 53 servers	

The following subsections are devoted to the software and hardware part of the control system.

Software Elements

The MAX IV control system is based on TANGO, [4], a free open-source distributed control system in use and in active development in most of the European synchrotrons.

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In BioMAX, most of the devices are integrated into TANGO, at least with their main functionality implemented. Some of them are based on existing developments, others are developed from scratch using Python TANGO bindings, [5]. Ideally, all the control system elements should have their corresponding TANGO device. Currently, the main device not integrated in TANGO is the diffractometer, although it is possible and supported by the manufacturer, the existing code we used for the data collection forced the usage of a custom TCP based communication protocol.

The control system functionalities are exposed to the user by several elements. On top of TANGO there is Sardana [6], a software environment that provides the user with tools to be able to steer motors, to define and act on pseudo-motors (or virtual motors composed of real axis) and to run macros. Typically, the command line interface named Spock is used for those tasks, and mostly by the beamline staff. At BioMAX we do not expect the end-users to deal directly with the Sardana environment, neither for data collection or for acting of moveables.

At BioMAX, as in some other MX beamlines in Europe, the data collection and experiment control is provided by MXCuBE, [7]. It is a software platform that provides users of beamlines at synchrotrons an easy to use graphical environment. From one side it hides the complexity of the beamline hardware, facilitating normal operation, while on the other side provides routines for automated complex data collection strategies. The third evolution of this software is under development as part of the MXCuBE collaboration, on this conference [8]. A pre-release version has already been used in user experiments at BioMAX, see Figure 2. The main evolution compared to the previous versions is the transition to a web based environment, which is expected to facilitate remote data collection and on-line data analysis, among other things.

In addition, at BioMAX there are several user interfaces based on the Qt based Taurus SCADA framework [9]. The composition and the layout of the panels can be easily changed by the users and beamline staff. It displays a raw list of motor positions, temperatures, flows and pressures split by section. For complex data display and/or operation BioMAX rely on MXCuBE as described above. Also, the beamline synoptic enables an intuitive way of interaction with a control system, by displaying a graphical representation of the physical beamline structure, and allowing various information and interactions to be tied in to this representation. The user can interact by panning/zooming and clicking elements to bring up informations or launch more specific panels, see Figure 3. This application is widely used in MAX IV for beamlines as well as for the machine control systems, the underlying library is the same and the only difference is the svg file used for the drawing.

Apart from the above mentioned standards, a facility like a synchrotron usually needs to adapt to software elements which do not fall within the facility's standards. This is also the case of BioMAX, where the cryogenic control system is supplied as a black box from the manufacturer and the only interface to it is based on an EPICS IOC. In this case, a TANGO/EPICS gateway device server is used to expose in TANGO the most important EPICS PVs of the cryogenic system. Also, the NanoBPM diagnostics comes with a LabVIEW application which was modified in order to export the measurements to TANGO. For that purpose, a DataSocket device server was configured.

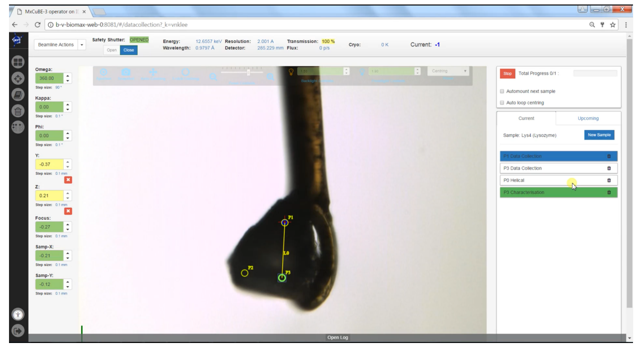

Figure 2: MXCuBE v3 user interface displaying a crystal and a successful data collection and another one just started.

Hardware Elements

A dedicated PLC is used for most of the input output signals, as well as for the vacuum and the machine safety systems. In addition, an independent PLC manages all the safety system which several connections between both PLCs to allow the operation of the most critical elements from a safety point of view, e.g. beam shutters. A TANGO device talks to these PLCs and exposes the relevant parameters as TANGO attributes. On top of this device there are TANGO devices for temperatures, vacuum pumps, etc.

Regarding motorisation, Icepap was chosen as the standard motion equipment for MAX IV, [10]. All the beamline motors are steered through this controller (in addition to the hundreds of axes in the whole MAX IV facility). It is very easily integrated into TANGO/Sardana by means of existing libraries. It can also execute synchronous multi-axis movements and a single Icepap driver can manage up to 128 axes, which is below the requirements of BioMAX.

An industrial PC serving as Standard Input Output Controller (IOC) have been installed to read several digital and analog input signals. The IOC is based on Adlink IPC and National Instrument acquisition card (NI-6602). This equipment is intended to be used as a General Purpose Input Output acquisition system on the experimental station of the beamlines in scenarios when the standard PLC acquisition system does not meet the requirements.

For the monitorization of the photon beam several XBPMs are controlled by a new electrometer developed in collaboration with the ALBA synchrotron, [11]. It consists of 4 current amplifiers in a single chassis, controlled and synchronised through a backplane managed by an FPGA. This will allow synchronised measurement and the possibility to embed custom algorithms for a control loop to steer, for

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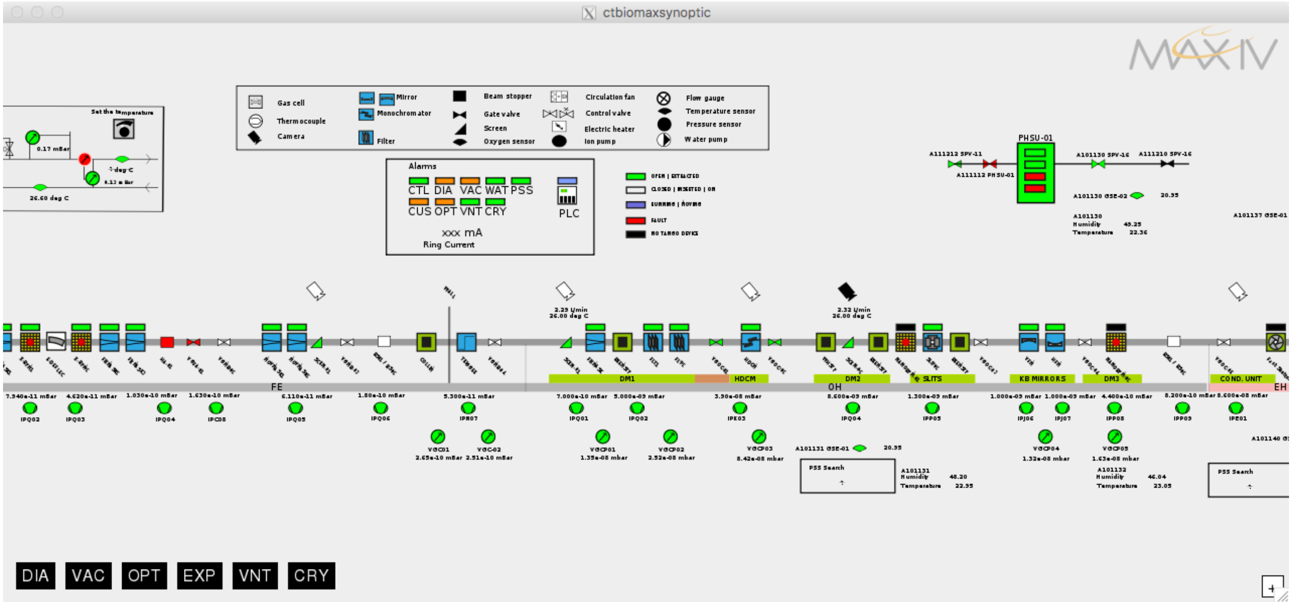

Figure 3: BioMAX beamline synoptic, a graphical interface describing the status of the main devices of the beamline. Users can hover and click on elements and the corresponding device panel is displayed.

example, a piezo fine tuning based on current and quickly adapt the beam to changing operating conditions.

Additional beam positioning devices are the NanoBPMs, which is a device that encloses a thin screen in the beam path that scatters X-rays that are captured by an X-ray camera. A dedicated FPGA performs the calculations and exposes the relevant data.

Linking All Together

Once the main components of the control system have been described, it is worth to explain how they are related. Figure 4 depicts the interfaces between the most relevant elements. Since BioMAX heavily rely on MXCuBE as its main user interface for the experiment control and data acquisition, it needs to interface to all the motors, pseudo-motors and data acquisition devices such as the detector. As opposed to other beamlines where sardana macros and controllers are in charge of the experiment sequence (configuration of the experiment, triggering acquisition, data collection, etc.), at BioMAX, MXCuBE performs such tasks together with the diffractometer. Therefore, the Sardana layer has a reduced number of responsibilities, limited to motorisation and beamline optimisation macros and such.

The subsystems not mentioned like the vacuum, ventilation or the cooling systems are also interfaced through TANGO.

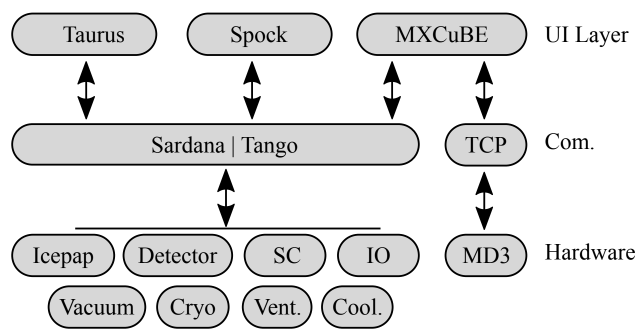

Figure 4: Simplified structure of the control system describing how the different elements are related.

INITIAL USER EXPERIENCE

The first successful experiment ever performed at BioMAX happened in June 2016. After that, the user operation began at the end of 2016 and finished in summer 2017. During those months the user operation was limited to one or two days a week, while the rest of the time was devoted to beamline and ring commissioning, software development, maintenance and to the installation and testing of new equipment such as the sample changer. The general consensus among the users was very positive. They were able to perform data collections in a variety of scenarios. They were impressed by the speed of the data collections, by the ease of use of the software, and the general stability of the control system. The users were also kind to understand some situations were the control system did not behave properly, mainly in the beginning of the operation. Twelve extended user groups have made experiments at the beamline, and they were able to start operating the equipment on their own after a short introduction of less than an hour.

The next user operation is expected before the end of year, and all the involved actors are confident that BioMAX control system will work smoothly and with increased capabilities. Those additional features are in some cases beyond the scope of the control system of a single beamline and involve more teams at the MAX IV facility, for example the data management and processing.

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CONCLUSION AND FUTURE WORK

The main conclusion of the present work is that the control systems group, together with the specifications and descriptions by the beamline staff, was able to provide a functional control system able to perform data collections in a very complex and demanding environment.

There is still equipment that needs a proper integration, as for example the sample changer. It was recently developed and integrated, however it has not been properly tested to be considered as finished. In addition, the usage of the sample changer will increase dramatically the usage of all the components as well as the amount of acquired data and, therefore the reliability of all the elements must be guaranteed.

In addition, the main user interface, i.e. MXCuBE, is still under development but the first release of the version 3.0 is expected for mid-october. Therefore, some adaptation time will be needed in order to fine tune its functionalities as well as bug fixing, although the development version has been tested at the beamline quite frequently.

ACKNOWLEDGEMENTS

The authors are very grateful to the rest of the MAX IV teams for their help and support during design, commissioning and operation stages. They also express their gratitude to the MXCuBE collaboration for the joint development of the latest version of the software.

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