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MARVIN UPDATE – THE ROBOTIC SAMPLE MOUNTING SYSTEM AT THE EMBL-HAMBURG

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Abstract

This article aims at giving an overview about the controls of the robotic sample mounting system MARVIN (MultiAxesRoboticVersatileINstaller) that are installed at EMBL beamlines at the PETRA III synchrotron (DESY, Hamburg, Germany). Currently, two inhouse built systems are in user operation at the beamlines P13 and P14 dedicated to macromolecular crystallography (MX). The different sub-systems and the embedding into BICFROK, the EMBL Hamburg beamline's control framework [1], and especially, new developments to decrease downtimes, as well as system recovery routines, will be described in detail.

INTRODUCTION

Robotic sample mounters are state-of-the-art instrumentation at protein crystallographic beamlines [2]. In general, their function is to mount and dismount sample holders with cryogenically frozen protein crystals onto the head of a diffractometer axis. Samples are stored in liquid nitrogen (LN2) filled dewars and rapidly transferred by the robotic system into a cold gaseous nitrogen stream in order to increase their lifetime in the synchrotron beam. The standardized SPINE sample holders [3], that are used with this instrument and that consist of a cap and a pin with the microscopic crystal attached to its tip, are individually inserted into containers called pucks [4]. In the pucks used for MARVIN and developed by EMBL [5] ten sample holders can be inserted see Fig. 1.

As the robotic systems can considerably improve speed and reliability of the mounting, the EMBL in-house development of a first similar system started already in 2002 and was initially in user operation at a former DORIS synchrotron beamline BW7b at DESY [6]. In 2013, the commissioning of the first new MARVIN system equipped with a Stäubli industry robot TX60L [7] began. The first system is in user operation since 2014 and the second system serving a diffractometer with vertical spindle axis operates since 2016 at the P14 beamline. In 2017, about 30000 samples have been mounted with the two systems.

SUB-SYSTEMS AND INTERFACING

The robot is installed overhead inside a closed cage centred above the LN2 storage dewar. In this dewar 170 SPINE samples in 17 pucks can be stored. The sample storage dewar is equipped with a pneumatically driven lid to open and close the dewar. The LN2 level inside the dewar is maintained by an automatic filling system fed from a central LN2 supply.

Apart from mounting the samples the system has also other functions. After a user has inserted a puck manually on a dedicated loading base, the robotic system distributes it automatically to one of the storage bases. The sample mounting takes always place from the central base. Therefore, a puck has to be shuffled automatically onto the central base before sample mounting.

In order to guarantee a high degree of automation and a high sample throughput as well as a high level of safety, the interaction with several other components is required. Apart from the sub-systems belonging to the core of the MARVIN system like the industry robot, the storage dewar with position sensitive puck switches, the cryogenic system for the dewar refilling, the pneumatic system for the control of lid, robot gripper and a guillotine shutter installed at the robot cage and the safety system, independently controllable instruments have to be interfaced and procedures synchronised. These devices are the diffractometers like the 'MD3' [8], experimental tables, the area detectors mounted on detector translations, cryogenic gasflow sample cooling units, and fluorescence detectors for anomalous phasing experiments.

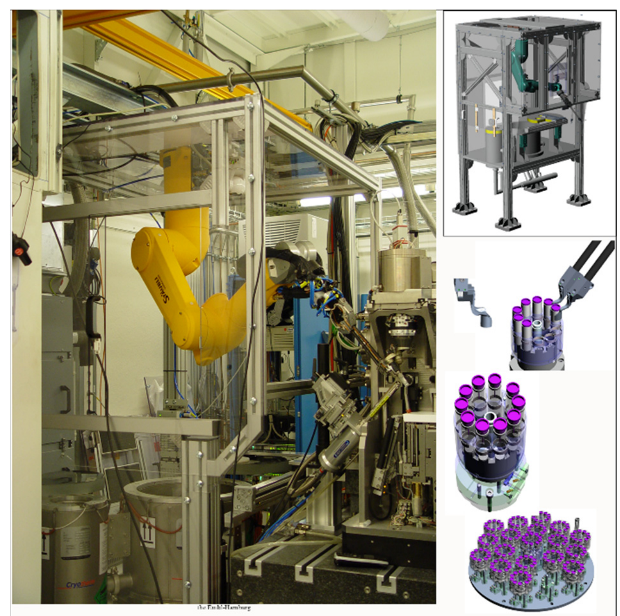

Figure 1: MARVIN mounting a sample on the MD3 Goniometer. And robot gripper, samples Pucks and Puck storage plate on the right.

Redundant signals and sensor cross-checks have been added in order to improve the reliability of the system. Examples are a vial detection switch at the robot grippers, gripper temperature control to avoid icing of the robot grippers, detection of the opening state of the grippers, tool changer detection signal and a crash protection state signal. While in the first sample changer system no detection of samples and pucks was present redundant sensors check in the current system the positioning accuracy to avoid sample losses and deformations of the grippers and potential damaging of the other instruments involved in the process.

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As an example, two independent sensors detect in the LN2 environment the presence of a puck on the central base. Hardware signals are used in general for the handshakes between the robot controller and the devices to be interfaced. The only exception is implemented for the change between two distinct mounting positions on the P14 diffractometer (toggling between two optical setups) for which a software handshake is in place.

The MARVIN system comprises also a personnel safety module. An important part is to ensure that the sample changing takes place only if all users have left the experimental area and the hutch to this area is interlocked. This precaution has been taken in particular to avoid crushing hazards with the heavy duty detector stage that is moved during the sample changing process. It is guaranteed in the standard mode for external users by electrical safety switches that are integrated into the door interlock of the experimental hutch. However, during the loading of the pucks onto the storage bases users have to be present inside the experimental hutch. For this process, only movements of the robot inside the safety cage are carried out with the door of the cage closed and interlocked. There exists also a password protected maintenance mode in which samples can be mounted with open experimental hutch door.

SYSTEM CONTROL

The instrument control of the instruments at the EMBL beamlines is performed by a modular control software package BICFROK and by standardized control electronics as a Master Electronic Unit installation for each major component like the robotic sample changer.

Controller for the TX60L robot is the Stäubli CS8C. The Stäubli Robotics Suite offers VAL3 as API to program the robot trajectories and to all DAQ signals to operate the robot. Both, the CS8C and the Master Electronic Unit have a Profibus fieldbus interface card to enable communication between them. The fieldbus protocol of the Master Electronic Unit is EtherCAT. There are about 50 electrical signals digital and analogous in use to run the MARVIN sample changer.

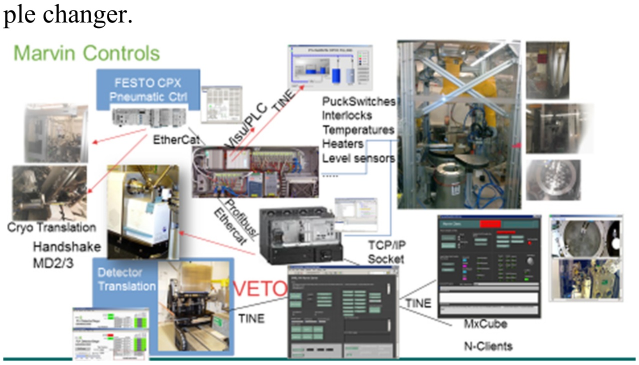

Figure 2: Sketch of the control devices and Server and Client Graphical User Interfaces.

Tasks of the Master Electronic Unit see Fig. 2 are the control of the automated nitrogen filling system for the cryogenic dewar, the robot cage access control and the alarming in case of low oxygen level inside the enclosed robot cage. An alarm can be active only if a user access request to the Robot cage is requested. In case of a too low oxygen level inside the robot cage visible and acoustical alarms are produced.

In the following the electrical handshake signals between robot and MD3 are described. On command to the robot Server to mount or dismount a sample the request signal is set as an electrical high signal to the MD3 controller.

Next the MD3 controller sets all its involved axis to predefined positions called transfer position and replies after finishing that the device is ready for the sample transfer. The CS8C Robot server program changes a robot idle digital signal to busy and the robot starts a motion to mount or dismount a sample depending on which request has been send. As soon as the mount/dismount process has finished the signal of the CS8C controller is set back to the idle state and the mount or dismount request is erased.

As an additional important diagnostic, a sample detection signal is implemented on the MD2/3 which proofs that the robot mount or dismount process has been successful. In case of unsuccessful motions, the motion will be repeated by the robot. If there is still no success the experimental user has the chance to correct the situation by manual interaction.

Inside the dewar position sensitive switches are in place to detect that pucks inside the dewar are proper placed. Malfunction of these switches can lead to robot motion errors or crashes of the robot. In case of inconsistence between software state and hardware state a warning or error message is raised by the robot server and a user interaction is demanded.

All controls related to air pressure are driven by an FESTO [9] control island with EtherCAT fieldbus. The actuator control and the position detection are part of the system. The functionalities of lifting of the dewar lid, opening the robot gripper, actuation of a pneumatic actuated translation and a control of a proportional valve to control the air pressure are beside others part of this control unit.

CONTROL SOFTWARE

The control concept at the EMBL Petra beamlines is based on the described approach of a hierarchical structured server architecture. Heart of the controls is the TINE [10] control system. In the layered control structure the CS8C robot server is the front end controller device server.

Servers are written in Val3 for the robots and in G-Code using LabVIEW [11] for the MARVIN TINE Server. The Marvin controls as part of the beamline control software is visualized in Fig. 3. The MARVIN server is part of the framework of the EMBL instrumentation framework BICFROK. Clients programmed with LabVIEW, the PLC programming of the Beckhoff [12] fieldbus system is implemented with the 'structured text' language.

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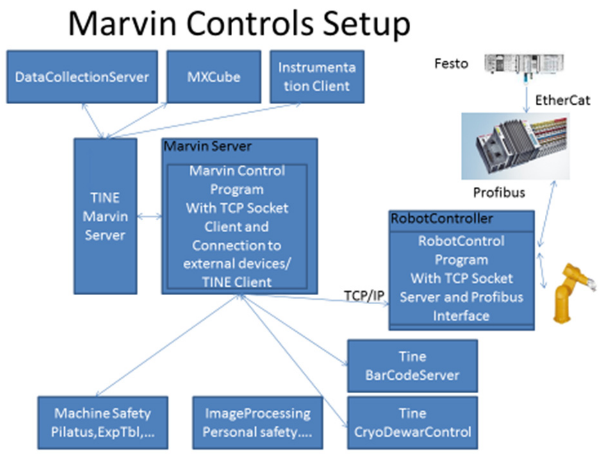

Figure 3: The MARVIN controls integrated in the beamline controls.

Server

The MARVIN TINE server is acting as a sequencer which coordinates the I/O signals and provides the sequencing of the commands called on the CS8 controller. The low-level device server of the robot is executed on the robot controller itself. The code splits the process in tasks of defined priority where each of the tasks can execute n programs.

The implemented tasks are the communication task, the status task, the state machine task and the exception task. The function blocks called programs are the mirror of the functionality offered by the robot. Examples are the open gripper or the mount sample program.

A TCP/IP Socket server is chosen to communicate remotely with other devices. The server uses a string communication to communicate with the TINE Robot server which is in the control hierarchy one level above the Robot Server.

The TINE Robot server communicates with low level Stäubli server and coordinates the interfacing devices. All functionalities are exported as TINE properties. The Server logs all possible statuses and commands and exports system statuses, warnings, error messages and task progress of the system.

Figure 4: MARVIN Clients as part of the BICFROK project and the User Client as part of a software called MXCube.

Clients

The asynchronous programmed event driven TINE clients Fig. 4 provided by the system are G-Code LabVIEW programmed GUIs. N-Clients can connect to the server. A TINE access control makes sure that only defined user have the right to control the system. The LabVIEW Clients can be exported as web clients for remote monitoring or password protected also as a web control application as part of the EMBL Hamburg BICFROK framework. Beside the main client for the MARVIN operation a LabVIEW web browser client is in place which displays two camera perspectives to monitor the robot actions.

Monitoring and Debugging

The Robot controller is connected via Profibus to the Master Electronic Unit DIOs. All commands send to the robot are logged. For easier debugging of system errors and tracking of mal functions there are two cameras for each of the systems available. Sequences of robot motions can be optionally saved.

All relevant signals of the detector translation, of the MD3 and of the communication handshakes are stored by the TINE archiving system. The TINE Archive Viewer synchronizes all signal and software states and allows to correlate them to each other.

After each of the user groups has finished its experiments an experiment debriefing takes place to track potential errors and to identify and correct them.

SUMMARY & OUTLOOK

Both EMBL MARVIN sample changer at the PETRA III beamline are in daily user operation. Plans for further improvements of the sample changer are the increase of the sample through put due to requests for shorter cycle times and the integration of new pin standards like the mini SPINE standard.

Optional the integration of a robotic plate screening which is available as a prototype presented for the MD2 at Beamline P13 are possible System extensions.

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