PROTEIN CRYSTALLOGRAPHY BEAMLINE SIMULATION

E. Zimoch

The requirement of high availability of the protein crystallography beamlines at the Swiss Light Source (SLS) conflicts with the requirement of software development and debugging at the same beamline. A solution could be implemented with an EPICS 3.14 IOC running on a Linux PC. One can test graphical user interfaces and high level applications using Soft Records to simulate beamline hardware.

INTRODUCTION

Protein crystallography uses synchrotron radiation to determine the three-dimensional structure of macromolecules. Knowledge of these structures provides information on the functions and processes on the atomic level of biology, which is needed for advanced medical research.

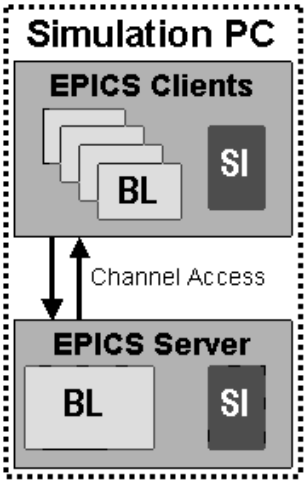
There are two protein crystallography beamlines at the SLS: PXI is working on a very tight schedule, PXII is currently under construction. Both beamlines are controlled by a distributed EPICS database, running mainly on VME computers, and Channel Access Clients running on Linux PCs.

At PXI the tight schedule leaves only one day per week to maintain the beamline, install new hard- and software, as well as for testing and debugging. The users demand a flawless and comfortable control system that must not fail.

The problems at the PXII are different but nevertheless come up to the same point. As long as the beamline is under construction, there is no hardware available for software tests. On the other hand, the beamline will be made available for users as soon as possible and therefore the control system has to be easy to use and stable immediately after the installation of the hardware.

THE SIMULATION

In order to prepare the control system software before installing it to the beamlines, an EPICS 3.14.6 server (IOC) was set up on a Linux PC. So the server and the clients of EPICS are on the same computer.



To be able to use the same database at the beamline and for the simulation PC some additional work was needed to simulate the behaviour of the hardware. In the figure this additional work is labelled "SI" in contrast to the parts that could be used in the simulation as well as at the beamline, which are labelled "BL".

For example, to simulate a diagnostic device like an X-ray beam position monitor, some graphical user interface is needed to set position values and intensity. On the EPICS server, some extensions of the database are needed to calculate the "input" signals from those set positions. This could be used to set the beam position to values, which may never occur in reality. Such a check can provide information about the stability of the used algorithms.

There are several advantages of the simulation: it is available all the time, it reboots in seconds, and there is no fear of breaking hardware accidentally. Furthermore, hardware errors like wrong cabling will not interfere with software debugging. In addition, some error conditions can be simulated safely and extreme values can be tested.

As the simulation uses the same configuration for the EPICS database as the beamline, most bugs can be found and fixed prior to the installation at the beamline.

The PC is not a dedicated computer but can be used for other software development as well. Therefore this solution comes with no additional costs.

RESULTS

The first result of the simulation was the control of the CVD X-ray beam position monitors at the PXI beamline. Cabling differences of several monitors could be detected, because the correct functioning of the software was tested before.

Almost all software developed for the new PXII beamline was tested prior to installing it to the beamline. This assures the functionality of the beamline just immediately after the installation of the hardware.

FUTURE PROSPECTS

The simulation of the protein crystallography beamlines has been proven to be very useful for control system software development and debugging. In addition it simplifies the design and test of graphical user interfaces.

The next step will be the simulation of the X-ray beam. This includes the interaction of the beamline hardware and requires some physics to be included into the simulation.

This full simulation may be useful for training of the users and the beamline scientists. Beside the correct operation of the beamline, even severe errors may be simulated to train the proper reactions and develop emergency plans.