Mario Di Castro, Andres Pazos, Fernando Ridoutt, Uwe Ristau and Stefan Fiedler

EMBL Hamburg, c/o DESY, 22603 Hamburg, GERMANY

A CRYSTAL CENTRING SYSTEM WITH A FPGA BASED POSITION CONTROL APPROACH FOR EMBL BEAMLINES AT PETRA III

Abstract

The EMBL is located at the DESY site in Hamburg and operates 5 beamlines at the DORIS III synchrotron. Additionally the EMBL Hamburg is in charge to build three beamlines at the new PETRA III high-brilliance synchrotron radiation source which will start user operation in 2009.

In this paper, an automatic crystal centring procedure i.e. the automatic positioning of a protein crystal on a diffractometer axis is presented. A reconfigurable FPGA based control solution is evaluated to monitor and analyze in real time beamline parameters for positional feedback. The system is integrated into the TINE control system and can be remotely controlled and configured.

The main elements of the control hardware are motion control electronics by Beckhoff Automation GmbH, piezo motor stages from attocube systems AG for fine adjustments and a National Instrument PXI crate equipped with a real time controller and R-series FPGA. The LabviewRT software to control the system is described as well as the adaptation of the hardware to various applications.

The solution is demonstrated on a test set-up and in the close future it will be transferred to an existing DORIS beamline used as test platform for PETRA III.

Keywords: beamline automation, protein crystallography, crystal recognition.

System Architecture

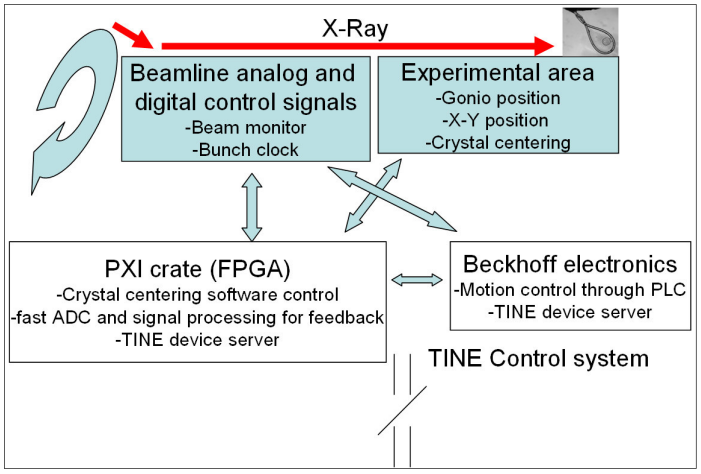


Figure 2: The future architecture of the system at the beamline

Optical System Set Up for crystal centering

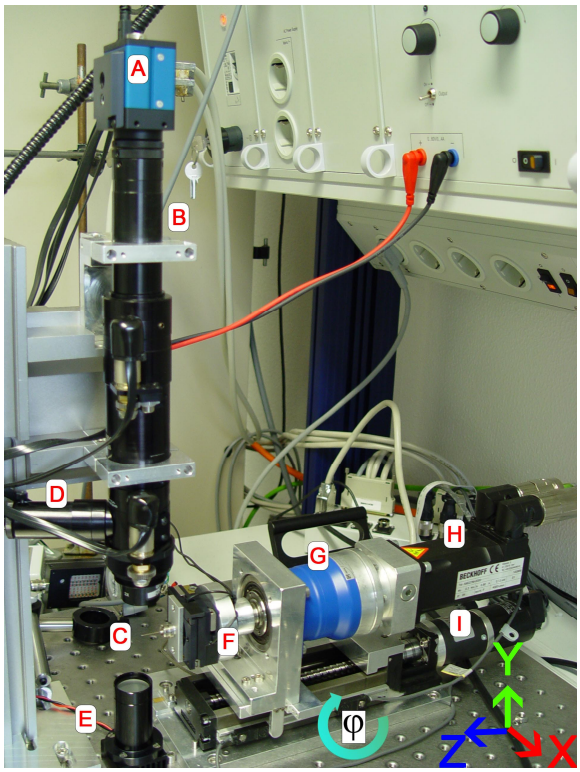


Figure 1: A) MPixel Camera, B) microscope 25:1, C) sample position and holder, D) coaxial light, E) backlight, F) X-Y Attocube piezo motors, G) gearbox, H) DC motor (goniometer), I) stepper motor for gonio translation. The axis orientation is also shown; x is the beam axis.

Crystal centring Steps:

- Background removal
- Automatic coaxial light and backlight adjustment for crystal illumination
- Alarms implemented to detect non standard crystal mounts
- Crystal support centring using the National Instrument Vision software algorithms tools
- XREC crystal detection and centring into the beam axis at high zoom level

Crystal centring highlights:

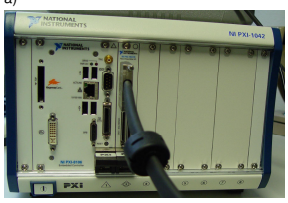
- The system is calibrated to work properly at each level of magnification
- The possibility to centre manually the crystal is also provided
- Auto focus capability
- Barcode reader (for identification of barcodes printed on caps and puck)
- Different images processing functionalities

FPGA Control:

- *40 MHz real time loop*
- *Labview programming language*
- *PID feedback loops*
- *Image acquisition and compression*

NI FPGA PXI-7831R

a)



b)

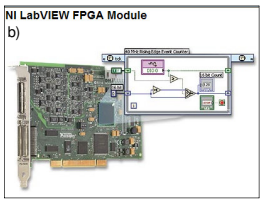


Figure 5: a) The National instrument PXI Real time controller equipped with the PXI-7831R FPGA used for this work, b) the FPGA board running in real time at 40 MHz.

XREC dll running on Labview

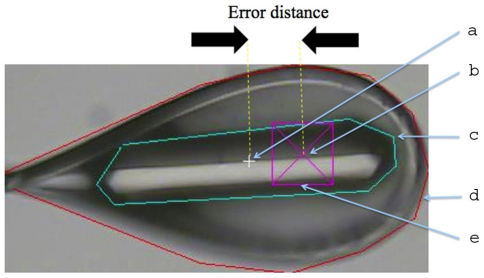


Figure 3: XREC example result on a crystal mounted on a cryo-loop: a) Centre of the crystal polygon, b) detected crystal centre: individual 2D detections are corrected to fit a circular trajectory during rotation, c) crystal polygons, d) loop polygons, e) crystal diameter. In this example the difference between the crystal centre and the detected one is 10 µm.

GUI for system commissioning

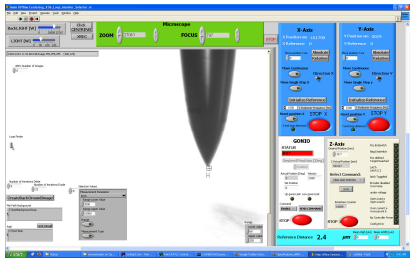


Figure 4: Labview user interface to commission the system. The tiny 5 µm needle used to calibrate the system is also shown.

CONCLUSIONS AND OUTLOOK

The system is in operation since 2 months and produced promising results:

- Automated crystal centring
- Auto focus
- Automatic crystal illumination adjustments

Future improvements will be finding the perfect light conditions for different crystal sizes to improve the efficiency of XREC and to push close to the perfection the crystal support centring and its reliability including the auto-focus option. On axis view has to be foreseen also taking into account the mechanical space restriction at the beamlines. More tests have to be done with the FPGA by analyzing as feedback more signals coming from different beamline monitoring hardware and also different PID feedback loops have to be evaluated increasing the loops speed. At the start in user operation of the DORIS beamline 7B the users will find a fully automated beamline and with a state-of-the-art automated crystal centring.

ACKNOWLEGMENTS

The authors thank Bernd Robrahn and David Watts for their help and support

REFERENCES

[1] Future service: EMBL@PETRA-III Project, http://www.emblhamburg.de/services/petra/index.html.

[2] http://www.embl-hamburg.de/XREC/.

[3] A. Pazos et al., "Embedded Distributed System Based on TINE and Windows CE", WEX04, proceedings of PCaPAC 2008, Ljubljana, Slovenia.

[4] P. Duval, "TINE: An Integrated Control System for HERA", International Conference on Accelerator and Large Experimental Physics Control Systems, 1999, Trieste, Italy, p.526.

[5] U. Ristau et al., "Control of the new sample changer and Goniometer Hardware", WEP019, proceedings of PCaPAC 2008, Ljubljana, Slovenia.

[6] www.ni.com

Contact: mario.dicastro@embl-hamburg.de

EMBL Hamburg, Instrumentation group