THE CONTROL AND DATA ACQUISITION SYSTEM OF THE NEUTRON INSTRUMENT BIODIFF

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Abstract

The Neutron instrument BIODIFF is a single crystal diffractometer for biological macromolecules that has been built in a cooperation of Forschungszentrum Juelich and the Technical University of Munich. It is located at the research reactor FRM-II in Garching, Germany, and is in its commissioning phase now. The control and data acquisition system of BIODIFF is based on the so-called "Juelich-Munich Standard", a set of standards and technologies commonly accepted at FRM-II, which is based on the TACO control system developed by the ESRF. In future, it is intended to introduce TANGO at the FRM-II. The Neutron Image Plate detector system of BIODIFF is already equipped with a TANGO subsystem that was integrated into the overall TACO instrument control system.

INTRODUCTION

In protein crystallography X-ray diffraction is a successful tool for structure analysis. Neutron diffraction is a complementary method, since it can provide detailed information on hydrogen atom locations [1]. A further advantage is the possibility to differentiate between hydrogen and deuterium atoms. The development of Neutron Image Plate (NIP) detectors was a big advance for neutron protein crystallography leading to the developments of several instruments, e.g. the BIX-3 at the Japan Atomic Energy Research Institute and LADI-III at the Institute Laue-Langevin [2]. Also at the German research reactor FRM-II in Garching a single crystal diffractometer for biological macromolecules called BIODIFF has been developed as a joint project of Forschungszentrum Jülich and Technische Universität München (TUM). BIODIFF is a monochromatic instrument using a cylindrical NIP as its main detector. For adjustment purposes it is equipped with a CCD camera looking at a ZnS:Li scintillator as an auxiliary detector [3]. The complex mechanics of BIODIFF includes about 20 movement axes, mainly equipped with stepper motors. Additional control tasks are related to beam shutter control and sample environment. The control and data acquisition system of BIODIFF is based on the "Juelich-Munich Standard". This is a joint effort of ZEL (Central Institute for Electronics of Forschungszentrum Jülich) and TUM to define a common framework for the electronics and software of neutron instruments that is followed by most instruments at the FRM-II [4]. It is based on the TACO control system developed by the ESRF and the extensive use of industrial type front-end equipment, e.g. PLCs, fieldbus systems or remote I/Os.

OVERVIEW OF THE BIODIFF INSTRUMENT AT FRM-II

According to Fig. 1 the BIODIFF consists of two subsystems, the monochromator with its outer shielding and the detector housing.

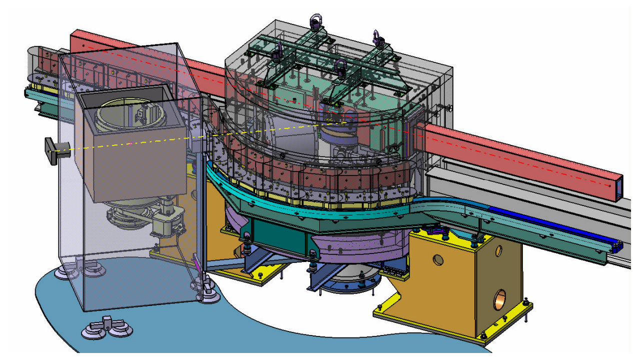

Figure 1: Schematic view of the BIODIFF instrument.

The incoming neutron beam is monochromated by a graphite crystal, which is movable in 6 degrees of freedom. An additional velocity selector from ASTRIUM removes the higher order wavelength contaminations of the monochromatic beam. By movement of graphite crystal, selector and detector housing a neutron wavelength between 2.4 Å and 5.6 Å can be selected. For the interruption of neutron beam and γ-radiation two shutters are foreseen.

The detector housing contains the cylindrical NIP as well as the CCD camera (icon-L series from company ANDOR), which both can be moved in and out by several mechanical axes. The NIP detector system is commercially available from company "Maatel". It contains the PMT-based reading head as well as the erasing system. Control of NIP drum movement, erasing and readout is implemented by Maatel as a self-contained system including an operating PC. On this PC a complete TANGO system is implemented, providing interactive local control as well as remote control via the CORBA-based TANGO protocol.

The NIP detector provides a solid angle of almost 2π, with the sample in the centre. Sample environments can be mounted on the sample table above the NIP detector, which is movable in three degrees of freedom. Additional fine positioning of the sample can be done with piezo-driven manipulators from company "attocube systems".

THE "JUELICH-MUNICH STANDARD"

The "Jülich-Munich standard" is a framework for the selection of technologies and components at each level of the control system. The definition of this framework was motivated by synergy effects and the reduction of spare parts on the shelf. A guiding principle for the framework was to minimize the development efforts and to acquire as much from the market as possible. A key component of the framework is the consistent use of industrial technologies like PLCs, fieldbus systems or decentral periphery in the front end. Main motivations are:

- low prices induced by mass market,
- inherent robustness
- long term availability and support from manufacturer
- powerful development tools

A control system according to the Jülich-Munich Standard is organized hierarchically into the following levels:

Field level: The field level is the lowest level, at which devices that are not freely programmable reside, like motor controllers, SSI controllers, PID controllers, analogue and digital I/O modules, or measurement equipment. For all industrial type of I/O modules PROFIBUS DP based decentral periphery is recommended. Siemens ET200S is the preferred one. Jülich Centre of Neutron Science (JCNS, Neutron science institute of Forschungszentrum Jülich with outstation at FRM-II) predominantly uses the stepper motor controller 1STEP from Siemens.

Control level: The control level resides on top of the process level. Devices at the control level are freely programmable. They must meet real time requirements and guarantee robust operation in a harsh environment. At the control level Siemens S7 PLCs, mainly from the S7-300 family, are used, because they dominate the European market.

Process communication: Process communication covers the communication of devices at the field and control level with supervisory controllers or computers. For lab equipment GPIB and proprietary RS232/RS485 connections are unavoidable. For industrial automation equipment PROFIBUS DP is the recommended choice. It is the dominating fieldbus in Europe and is naturally supported by S7 PLCs and many other devices. A major reason for its success is the technological and functional scalability based on a common core as well as the programming model, which easily maps to PLC operation.

Experiment Computer: For economical reasons, all experiment computers should be PCs. Linux, being well established in the scientific community, is the only supported operating system. There is no definition of a specific kernel version or distribution. Direct device access should not be implemented on conventional PCs but on CompactPCI systems. CompactPCI allows deploying a variety of existing software in a mechanically more robust platform that fits into 19" racks.

Middleware: Since the framework aims at an inherently distributed system, software support for the transparent distribution of services between systems is required. For this purpose TACO has been selected as the middleware system. TACO is a client-server framework developed for beam line control at the ESRF in Grenoble. In a TACO environment each device or hardware module is controlled by a TACO server. The server offers a set of device-specific functions, which can be accessed by TACO clients via a RPC-based mechanism over a TCP/IP network. To make its functions available to clients, the device server registers itself with the so called "manager" process. The manager operates as a name server, which is consulted by clients to get the actual location of a server. TACO includes a simple database for sharing of configuration data and operational variables between clients and servers.

Application level: On the client side, two variants of application programs are used: Where flexibility is desired and no GUI is needed, the scripting language Python is used. More static GUI applications are implemented in C++, using the "Qt" class library, with TACO access provided by device specific C++ wrapper classes. Recently, due to pressure from instrument scientists a macro language consisting of fixed command words and their corresponding arguments was defined. The idea was to have an extremely simple tool for standard scans without having to deal with the complexity or traps of a full programming language. As a consequence, the macro language has no control structures or variables and instead of loops it provides a "scan" command specific for each instrument. An interpreter for this command language was first implemented in python using the python "cmd" module on the neutron reflectometer MARIA [5].

THE BIODIFF CONTROL AND DATA ACQUISITION SYSTEM

Physical Architecture of the Control System

According to Fig. 2 the control and DAQ system is implemented as a distributed system with a hierarchical architecture. On top of the system resides the so-called control computer with all application software – GUI-based as well as script-based. Via the experiment network the control computer accesses the "server computers", to which all front end systems (detectors, monitors, position encoders, motor controllers, …) are attached. On the "server computers" TACO servers are running, which access the peripheral devices via dedicated device drivers. The only exception is the computer provided by Maatel for the NIP system, where a TANGO server is running.

The "slow control" peripherals are indirectly connected to the "server computers" via a PROFIBUS segment with the main S7-300 PLC. Stepper motor controllers and SSI modules as well as digital and analogue I/Os reside in ET200 decentral periphery systems, which are connected to the PLC via an additional subordinate PROFIBUS segment. The safety PLC (ET200S F-CPU), the adapter modules for encoders with NDAT interface as well as a touch panel for local operation of the PLC are connected to the same subordinate PROFIBUS segment.

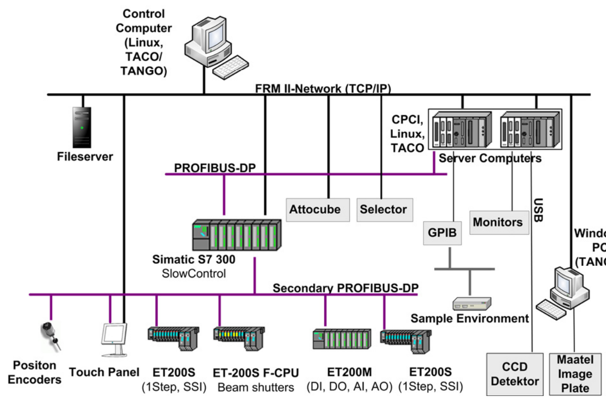

Figure 2: Physical architecture of the BIODIFF control and data acquisition system.

The CCD camera is connected to a server computer via USB. Selector and the controller for the attocube positioners are connected to a server computer via Ethernet.

Software Architecture

As shown in Fig. 3, the implemented software is distributed between three levels of the system hierarchy. All software below the lower dashed line runs on PLCs in the front end. The software modules shown between the dashed lines are running on the server computers. This comprises TACO servers and device drivers for dedicated HW modules, e.g. detector electronics, counter/timer board, PROFIBUS controller or GPIB controller. The TACO middleware is the glue that connects the server computers to the control computer, where the client application programs as well as the TACO manager and database (all above the upper dashed line) are running. Since TACO is location-transparent, the application programs could run on any Linux-based system.

A thin abstraction-layer implemented in Phython above the generic TACO-Python binding hides many details from the user, e.g. it allows the use of symbolic names and provides the conversion between device units and physical units. This abstraction layer provides a comfortable script access to all spectrometer features. On top of this abstraction layer the above-mentioned macro language has been implemented, which is the standard tool to do measurements with the Instrument. Measurement data are stored in the NeXus format. It is intended to implement a GUI-based measurement program in future, but its functionality has not been defined yet. Up to now only one GUI-based program has been implemented, which visualizes the mechanical setup of the instrument and allows interactive control of each axis, in order to support service by technical personnel.

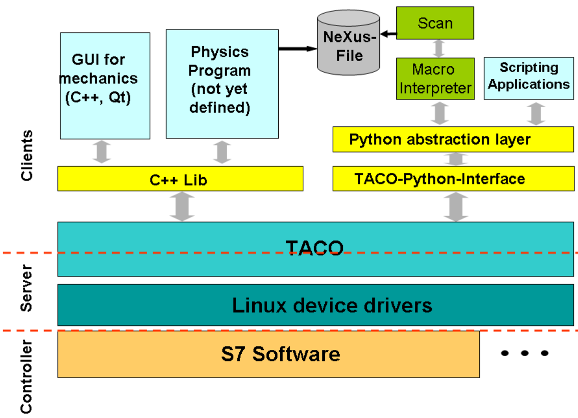

Figure 3: BIODIFF Software structure.

CONCLUSION AND OUTLOOK

Since the "Juelich-Munich Standard" is the common, powerful toolbox used in all JCNS instruments, the implementation of the control and data acquisition system was straight-forward. Especially the integration of the TANGO subsystem controlling the NIP was without any problems, due to the generic TANGO/python binding and because of the similarities between TACO and TANGO. The BIODIFF started commissioning in October 2010, when it saw first neutrons. Due to a one year shutdown of FRM-II the commissioning had to be interrupted and is expected to continue in October 2011.

Currently the introduction of TANGO for the neutron instruments at FRM-II is discussed, since TANGO is the natural successor of TACO. As a consequence, in future the BIODIFF control and data acquisition system may switch from TACO to TANGO

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