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DAQ SYSTEM BASED ON TANGO, SARDANA AND PANDABOX FOR MILLISECOND TIME RESOLVED EXPERIMENT AT THE COSAXS BEAMLINE OF MAX IV LABORATORY

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Abstract

CoSAXS is the Coherent and Small Angle X-ray Scattering (SAXS) beamline placed at the diffraction-limited 3 GeV storage ring at MAX IV Laboratory. The beamline can deliver a very high photon flux of 10^{13} ph/s and is equipped with state-of-the-art pixel detectors, suitable for experiments with a high time-resolution to be performed. In this work we present the upgraded beamline data acquisition strategy for a millisecond time-resolved SAXS/WAXS experiment, using laser light to induce temperature jumps or UV-excitation with the consequent structural changes on the system. In general terms, the beamline control system is based on TANGO and built on top of it, Sardana provides an advanced scan framework. In order to synchronize the laser light pulse on the sample, the X-ray fast shutter opening time and the X-ray detectors readout, hardware triggers are used. The implementation is done using PandABox, which generates the pulse train for the laser and for all active experimental channels, such as counters and detectors, in synchronization with the fast shutter opening time. PandABox integration is done with a Sardana Trigger Gate Controller, used to configure the pulses parameters as well to orchestrate the hardware triggers during a scan. This paper describes the experiment orchestration, laser light synchronization with multiple X-ray detectors.

INTRODUCTION

CoSAXS (Coherent and Small Angle X-ray Scattering) beamline [1] is located at the 3 GeV ring of the Swedish 4th generation synchrotron, MAX IV, featuring high photon flux $1 \times 10^{12} - 1 \times 10^{13}$ ph/s and small X-ray spot size . As the state-of-the-art Small Angle X-ray Scattering (SAXS) beamline can deliver high intensity and enable experiments with a high time resolution to be performed.

Time-resolved (TR) SAXS/WAXS (where WAXS stands for Wide Angle X-ray Scattering) experiments require a source of perturbation which might cause a structural change in the sample, while fast data acquisition is performed along the time to monitor the dynamics. Currently, CoSAXS beamline offers lasers for temperature jumps time-resolved studies as one of the sample environments available for the users [2].

Following the MAX IV standard, the beamline control system is based on TANGO [3]. Built on top of TANGO, Sardana [4] it is used for both scan configuration and execution.

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In the present configuration, CoSAXS time-resolved experiment uses either an Infrared (IR) or an Ultraviolet (UV) laser pulse to induce a perturbation in the sample system. The laser pulse duration and the time synchronization for data acquisition of both SAXS and WAXS detectors are controlled by PandABox [5]. PandABox is a FPGA based system and it is integrated in the control system as a TANGO device. On top of it, a Sardana trigger/gate controller is the main interface used for configuration during the scan.

Besides reaching small time-resolutions, avoiding radiation damage is also another challenge faced on this experiment, due to very high beam intensity on the sample. A fast shutter is used to control the sample exposure to radiation in each acquisition window.

EXPERIMENTAL SETUP

The time-resolved sample environment at CoSAXS is primarily developed to study proteins in aqueous solutions. The experimental setup is illustrated in Fig. 1. The sample holder is a temperature-controlled flow cell, consisting of a 1.5 mm inner-diameter quartz capillary and 10 µm wall thickness. The sample delivery is done from a reservoir using a Reglo ICC peristaltic pump.

Two lasers are available for the TR setup: a continuous wave IR laser (1470 nm) and a Q-Switch nanosecond laser with a 532 nm pump laser and an OPO which can tune the wavelength over ca. 700-2000 nm. The laser pulse is delivered to the sample through a fiber physically attached to the flow cell positioned a few millimeters from the capillary wall. The other end of the light guide is coupled to the laser, either IR or UV, and it consists of a 200 mm and 0.22 NA fiber.

Data acquisition is performed by a dual hybrid pixel X-ray detectors system (see Fig. 1). The SAXS detector, positioned inside a vacuum vessel, is a Eiger2 4M and the readout can be performed at 500 Hz. Two WAXS detectors are available at the beamline and can be used, not simultaneously, in TR experiments. The first one is a Mythen2 1K that can be operated at 1 kHz and it is positioned in air, right after the flow cell. The second one is a Pilatus3 2M in an L-shape configuration, positioned in front of Eiger2 in the vacuum vessel, and it can be operated at 250 Hz.

Premature sample radiation damage is avoided with CEDRAT fast shutter. The fast shutter takes up to 8 ms to fully open/close and it can be easily controlled with TTL external signals. It also provides a feedback signal reflecting the hardware current state. In the TR experiment setup, the fast

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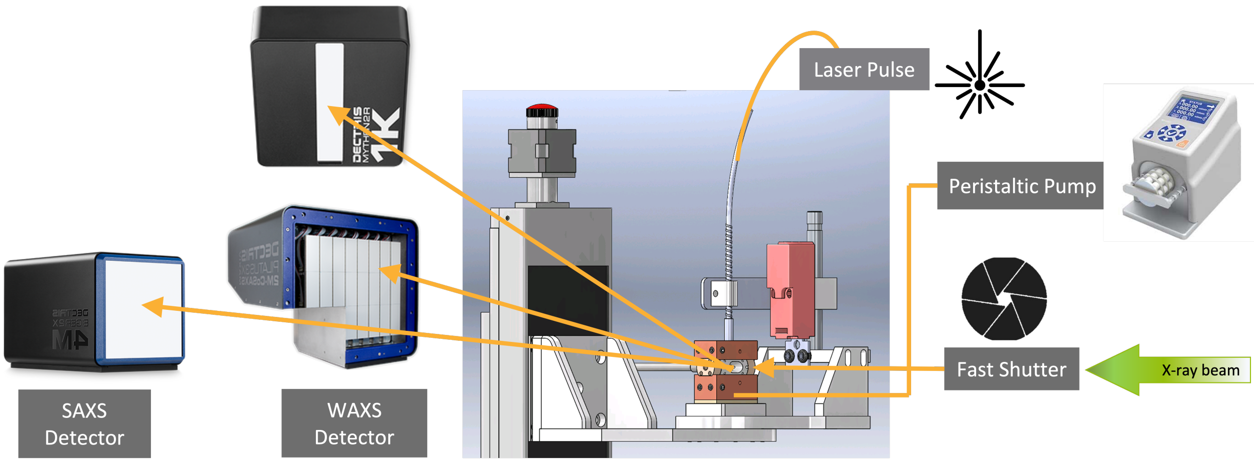

Figure 1: Experimental setup of the time-resolved sample environment.

shutter is used as the master trigger for data acquisition, i.e., triggers for the detectors are sent as soon the feedback signal of the shutter is received.

IMPLEMENTATION

The beamline control system is based on TANGO Controls framework, which provides a distributed architecture for seamless communication between various hardware components and software modules. The experiment and scan orchestration are handled by Sardana, which is built on top of TANGO and provides an advanced scan framework. The synchronization between laser pulse and dual detectors system data acquisition is performed by PandABox. The experiment control system overview is illustrated in Fig. 2.

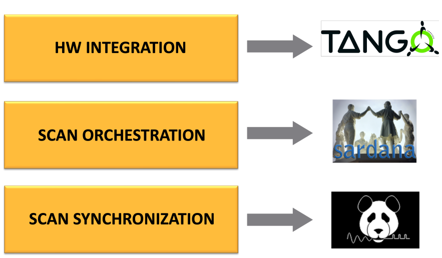

Figure 2: Experiment control system overview.

Hardware Integration

The TR experiment hardware components - SAXS/WAXS detectors, peristaltic pump and PandABox - are integrated in the control system as Tango Devices. Each Tango Device has an associated Tango Device Class, which provides a list of attributes, commands and properties available in each device. A Tango Device Class is responsible for translating each equipment communication protocol into Tango Controls communication.

PandABox PandABox (Position and Acquisition Box) is a FPGA based system and it is the main hardware used at MAX IV for data acquisition synchronization. PandABox provides interface to different types of signals - encoder, trigger, timing - through various connectors installed in both front and rear panels. The main supported I/Os used for the TR experiment are Multi-Channel TTL for synchronous triggering and clocking with high timing resolution, and FMC-ADC slot for receiving analog signal.

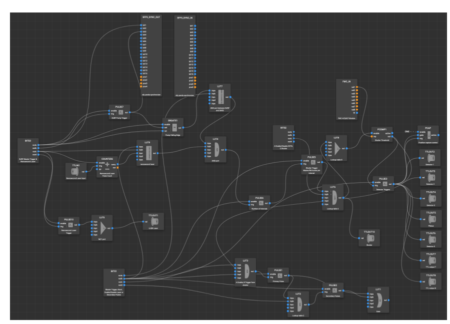

Figure 3: PandABox functional blocks on web GUI.

The experiment logical synchronization is performed via PandABox web GUI, which provides a visualisation and possibility to change wiring of the FPGA Functional Blocks, as illustrated in Fig. 3. The main Functional Block used for the implementation is the Pulse Generator block, which produces pulse trains with configurable width and delays. For the TR experiment, both Laser and Fast Shutter are controlled exclusively by PandABox.

The software communication with PandABox is implemented with PandABlocks-server [6] for the TCP/IP protocol, which provides an interface to the FPGA firmware controlling Panda. The access to PandABox Functional Blocks, fields and attributes is provided by PandABlocks-client [7], a pure Python library. On top of it, PandABox is integrated in the control system as a Tango Device, from

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where the generated pulse trains can be easily configured, as well the start and stop of the triggers generation commands can be executed.

Detectors For TR setup, both SAXS and WAXS detectors share the same Tango Device Class API. As the Tango Device Class provides an abstraction of the hardware interface, similar equipment can share the same list of attributes and commands, although the underlying communication protocol is not exactly the same.

The detectors Tango Devices main functionalities include the capability of configuring both Eiger2 and WAXS detector (Pilatus3/Mythen2) for a scan with multiple points, as well choosing between software trigger or external hardware triggers for the data acquisition synchronization. Besides configuration, the detector (Eiger2 and Pilatus3/Mythen2) can be armed with the command Arm and triggered either with the software command SoftwareTrigger or by PandABox generated external pulse trains. Moreover, the Tango Device of each detector is also responsible for recording the data in a HDF5 file format in a specified directory.

Peristaltic Pump The Reglo ICC peristaltic pump hardware communication is based on RS232 serial protocol and the access through the network is implemented with a serial-to-Ethernet converter. Therefore, a Python [8] communication library implements the pump main functions via socket communication. On top of it, the Reglo ICC is integrated in the control system as a Tango Device.

Time-Resolved Experiment Orchestration

Integration in Sardana The time-resolved experiment is performed and orchestrated by Sardana. Every hardware required for the scan execution, requires a controller (a piece of software) capable of translating the hardware Tango Device Class API to a Sardana controller specific API. Sardana supports many different types of controllers Class; some of them are designed for specific type of hardware.

The SAXS and WAXS detectors Tango Devices are integrated in Sardana with the controller class *TwoDController*, which is designed to support experimental channels that generate 2d data type. PandABox controller inherits from *TriggerGateController* class, which is designed to support hardware used to synchronize the experimental channels by the digital trigger and/or gate generation. Regarding hardware not involved directly with the experiment data acquisition, as the peristaltic pump, a Sardana controller is not required. On this case, the pump Tango Device is controlled directly with a Sardana macro.

Scan Overview The TR experiment scan consists of scanning the laser state, alternating between *laser on* and *laser off*, while multiple frames are acquired by the detectors in each step. The TR scan overview is illustrated in Fig. 4. The experiment time resolution is given by the current detectors system in use, the slowest one will determine the minimum time between two successive frames as the same pulse train is send to all the detectors. The dual system composed by Eiger2-Mythen2 can operate in 500 Hz, successive frames can be acquired with 1.9 ms exposure time and 100 µs for readout time. The dual system composed by Eiger2-Pilatus3 is limited by 250 Hz, successive frames can be acquired with 3 ms exposure time and 0.95 ms for readout time.

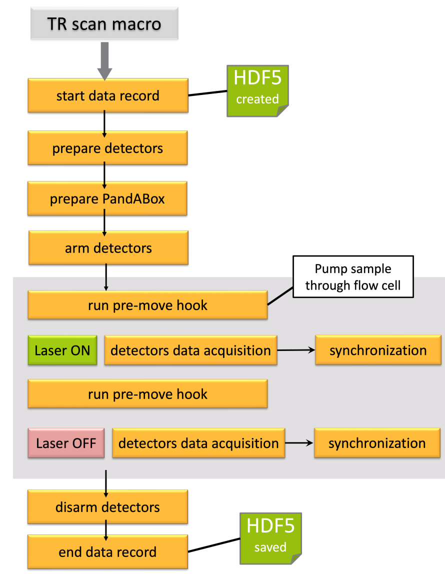

Figure 4: Scan overview.

The data record is managed by a Sardana Recorder class, responsible for creating the scan file and recording every data point acquired during the scan. Regarding SAXS and WAXS detectors, the related scan data is linked into the scan file in the end of the acquisition, as these equipment have specific service to record and save the data in a separated file from the Tango Device.

In each scan step, the sample is pumped through the flow cell, as the high intensity X-ray beam might damage the sample during the acquisition window, requiring a refresh of the sample before another long exposure to X-rays and data acquisition. A Sardana *pre-move hook macro* is used to control the peristaltic pump between each step of the scan and to start the sample pumping in the flow cell.

The involved experimental channels - detectors and trigger/gate - are configured with the scan parameters through the Sardana controllers API. The detectors are set to the expected number of triggers and exposure time of each frame. The trigger/gate (PandABox) is configured to generate the desired number of triggers, and each pulse is configured to have a width equal exposure time and step size equal exposure time plus detectors readout time.

Besides preparing and configuring the experimental channels, Sardana also manages the start of the data acquisition. The detectors are armed and trigger/gate is started, through the controllers API. Then, the data acquisition is fully synchronized by external hardware triggers (PandABox - more details in the next section), while Sardana monitors the State and Status attributes of the involved experimental channels.

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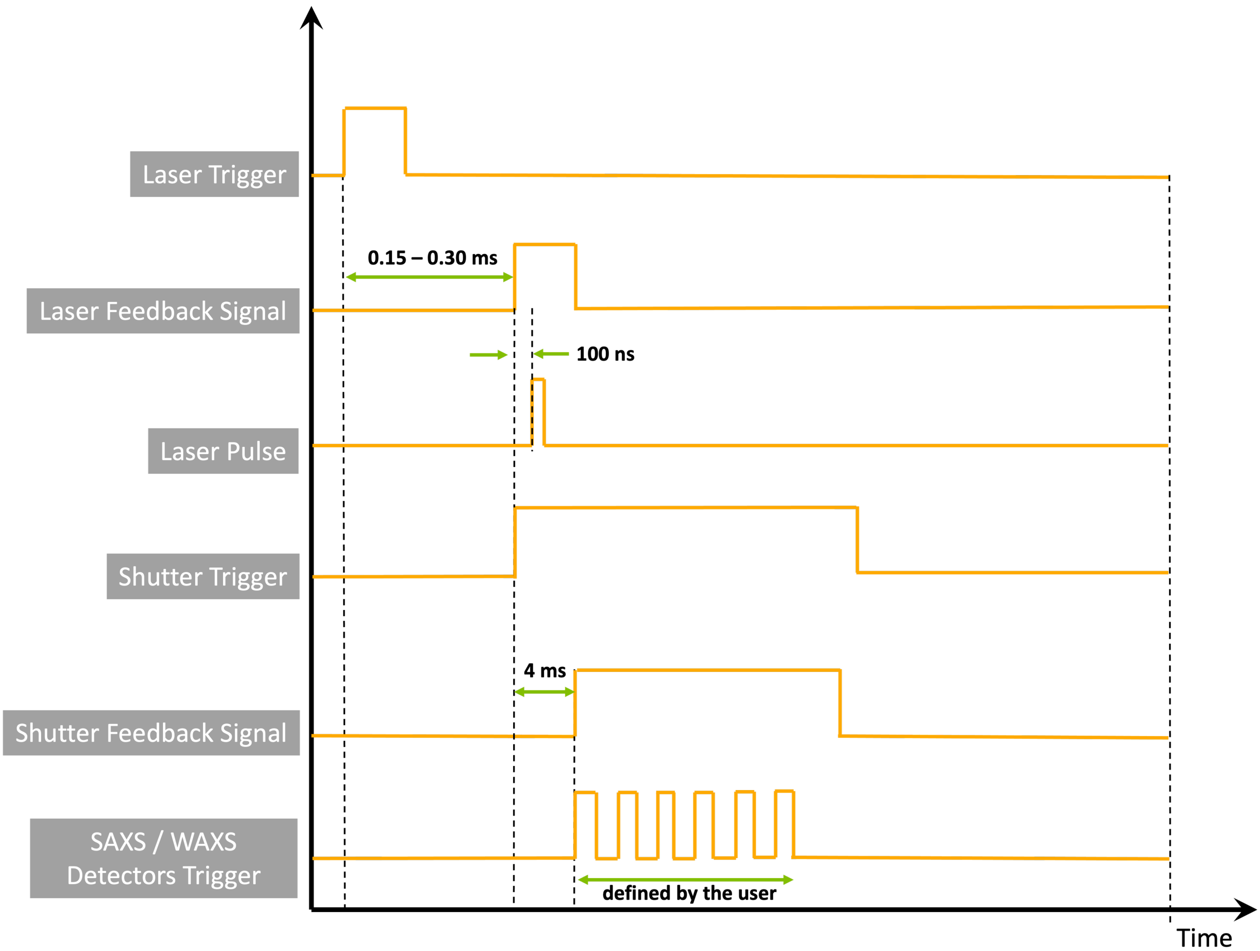

Figure 5: TR experiment timing diagram.

A scan is finished after all expected triggers are generated and all detectors finish the data readout and recording.

Scan Synchronization The scan data acquisition synchronization is managed by PandABox. In the TR setup, Panda is responsible for generating the pulse trains for the detectors, as well to control both fast shutter and laser pulse. The timing diagram describing the implemented synchronization when performing experiment with UV laser is illustrated in Fig. 5. As soon PandABox is started by Sardana, a TTL signal is sent to the UV laser. In an interval of 150-300 µs after the **Laser Trigger** (see Fig. 5) rising edge is sent, the laser has the capability of sending a digital feedback signal 100 ns before the actual laser pulse be fired.

As soon the **Laser Feedback Signal** rising edge is received, a TTL signal is sent to the X-ray fast shutter. The shutter takes up to 8 ms to be completely opened, but as the aperture is much bigger than the beam size, 4 ms is enough to have full beam at the sample. The **Shutter Feedback Signal** can be configured to return high digital signal for specified conditions, and in this case is related with the minimum opening time to have full beam intensity.

The pulse trains to the SAXS/WAXS detectors are sent as soon the fast shutter feedback signal rising edge is received. The first data frame is acquired 5.9 ms after the laser pulse being fired, considering the shutter opening time and the minimum exposure time of 1.9 ms (Eiger2-Mythen2 system). The choice of opening the shutter after the laser has been fired is correlated with the sample dynamics and radiation damage. For the current setup, the users had previous knowledge that the first 6 ms after the laser pulse is fired, no important dynamics were expected to happen. Besides, as the sample is sensitive to radiation, it is preferable to expose the sample to X-rays when the data acquisition is ready to start than to take the risk of damaging the sample on the preparation or laser firing phase.

FUTURE DEVELOPMENTS

- For the current implementation, a single trigger was sent to the laser every time a pulse was required. This resulted to instabilities of the lasing power. A better approach would be to run the laser at its natural frequency of 10 Hz, and extract a single pulse with the use of a fast shutter or the manual trigger input.

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- Implementation of a scan capable of scanning both laser states - on and off - as well the delay time to start data acquisition after the laser is fired.
- An easy way to integrate different excitation sources, eventually provided by the user, should be implemented.
- To expand the beamline experimental capabilities, we are working to use the gate mode of the Eiger2 detector. In such configuration microsecond time resolved experiments will be possible. The development will also include an upgrade of the hardware synchronization on such time resolution (us)."

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