IMPLEMENTATION OF CONTINUOUS SCANS USED IN BEAMLINE EXPERIMENTS AT ALBA SYNCHROTRON

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Abstract

Alba[1] is a third generation synchrotron located near Barcelona, Spain. In its first construction phase, accelerators and seven beamlines were designed and built. Commissioning of all of them had successfully finished in 2012 and nowadays all of the seven beamlines host user experiments regularly.

The Alba control system [2] is based on Sardana [3], a software package implemented in Python, built on top of Tango [4] and oriented to beamline and accelerator control and data acquisition. Sardana provides an advanced scan framework, which is commonly used in all the beamlines of Alba as well as other institutes. This framework provides standard macros and comprises various scanning modes: step, hybrid and software-continuous, however no hardware-continuous. The continuous scans speed up the data acquisition, making it a great asset for most experiments and due to time constraints, mandatory for a few of them.

A continuous scan has been developed and installed in three beamlines where it reduced the time overheads of the step scans. Furthermore it could be easily adapted to any other experiment and will be used as a base for extending Sardana scan framework with the generic continuous scan capabilities.

This article describes requirements, plan and implementation of the project as well as its results and possible improvements.

INTRODUCTION

Instruments involved in beamline experiments are normally distributed over several tens of meters (nano focusing beamlines are reaching even hundreds of meters) typically in the following sections: front end, optical and experimental hutches. The insertion devices (ID) are even located in the accelerator's tunnel what could add an extra difficulties in implementation of the experiment control. Their operation, both while preparing an experiment and during the experiment itself, require an extensive user control in many aspects like positioning, data acquisition, storage and synchronization, etc.

Sardana provides comprehensive solutions for building a distributed control system, for not only a synchrotron beamline but, for any other kind of laboratory. Its main strengths are: an easy plug-in solution for the hardware controllers, comprehensive interfaces for the common beamline elements (e.g. motors, experimental channels, pseudo-axes), a python based macro and sequence environment, modern GUI front-ends as well as a generic scan framework (GSF). This framework provides a turnkey solution for applications which require scanning. GSF handles motion, data acquisition and data storage in n-dimensional scans, implemented as Sardana macros, in one of the following modes: step, hybrid and software-continuous.

Most of Alba experiments are based on complex scanning procedures. During commissioning phase as well as early user operation all of these scans had been executed in step scanning mode. A need to reduce the experiment time arose mainly due to the big time overheads of the step scans, related to sequential execution of motion and acquisition parts of the scan, as well as multiple accelerations and decelerations of the moveable axes,.

BEAMLINES AND INSTRUMENTS INVOLVED IN SCANS

BL04 - MSPD [5] is a high energy beamline which operates between 8 keV and 50 keV and ends with two experimental stations. It is devoted to high resolution powder diffraction (HRPD) and high pressure powder diffraction (HPPD) experiments. The main instruments of the HRPD end station are a three circle diffractometer and two X-ray photon detectors. On the outer circle (OC) it resides the MAD26 detector (Alba's in-house design) [6]. On the middle circle a set-up comprising 6 modules of Mythen 1D detector is mounted (foreseen for fast experiments). Most of the HRPD experiments use MAD26 detector. They require scanning of the OC rotational axis on a total range of approximately 40-120 degrees (diffraction angle). Diffraction pattern is gathered with 13 channels of the MAD26 and one monitor channel used for data normalization. Samples are normally exposed to variable environment conditions that needs to be tracked and correlated with the acquired diffraction pattern. This experiment performed as a step scan usually takes approximately 10 h of beam time. The goal was to reduce the experiment duration while maintaining synchronization between the experimental channels and the OC position.

BL22 – CLAESS [7] is a high energy beamline (2.4 - 65 keV) implementing X-ray absorption and emission spectroscopic techniques. Its main instruments are a double crystal monochromator (DCM) and various detectors: ionization chambers, position sensitive and fluorescence detectors located in the experimental hutch. The experiment is based on scanning the beam energy using the DCM while at the same time maintaining the fixed exit offset (beam spot must be focused on the sample during the whole scan at the same point). Normally a subset of the available experimental channels

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is used during one experiment. However it could be required to include channels from absorption and emission techniques together as well as to integrate another devices requested by the users. A demanding requirement is to reduce the scan time to the range of a fraction of a second which could be achieved only by continuous scans.

BL29 - BOREAS [8] is a soft X-ray beamline mainly devoted to magnetic circular and linear dichroism (XMCD/XMLD) measurements. The beamline is equipped with two cutting edge end-stations, a high-field vector magnet (HECTOR) for absorption methods and a UHV reflectometer (MARES) for scattering and reflection approaches. Similar to BL22, experiments are based on scanning the beam energy. They are performed using a variable line spacing plane grating monochromator (VLS-PGM). In contrary to the BL22 the ID must follow the energy change simultaneously to the PGM. This ensures the best photon flux during the whole scan. The ID of the BL22 is a multipole wiggler whose photon flux is relatively uniform on the whole energy range in comparison to the photon flux produced by the undulator being used at BL29. In XMCD absorption method detection is achieved by total electron/fluorescence yield measurements using low current ammeters.

CONTINUOUS SCAN DEVELOPMENT

Implementation of any continuous scan is a challenging project, especially if a certain generalization level is targeted. Usually the biggest difficulties come with design of the data collection and buffering system. The other major challenges are: abstraction of the time/position trigger and/or timestamps as well as support of the transparency between scanning modes [9].

This project started from a deep requirement analysis, which lead to the conclusion that many of the requirements coming from the beamlines were common, mainly due to the hardware solutions used in these set-ups. Baseline analysis of the GSF showed that concepts already implemented for step and hybrid scans could be easily adapted to the continuous scans. Software design started from building the activity diagrams followed by forming the classes of main scan “actors”. After that, the sequence diagrams of main activities were prepared. Implementation process followed an iterative method trying to deliver a working version of the continuous scan at the end of each iteration.

Hardware Solutions

Motion. Only in case of BL04, the scanning variable is a direct rotation of OC (standalone moveable axis). In the rest of the cases (BL22 and BL29) scans are performed on a non-linear function - the X-ray energy. Furthermore, to meet extra requirements, scans must involve motion of multiple axes. Energy scan of BL22 requires maintaining a fixed exit offset during the whole scan. This was achieved by constantly changing the crystal separation distance while varying the bragg angle. This combined movement of bragg and perpendicular axes is implemented as a motion program inside of the Turbo Pmac2 controller. Energy scan of BL29 is even more complicated. While changing the PGM's energy, the ID's energy must follow this move with a certain accuracy. This scan requires motion of 7 physical axes: grating rotational axis and 6 moveable axes, vertical and horizontal translations, of the ID. This could be achieved only by programming motion trajectories for all the 7 axes inside of the motion controllers. Relaxation of this requirement was achieved by limitation of the energy range per one scan, what is acceptable for most of the cases.

Data acquisition. In case of BL04, each of the 14 channels (13 detection + 1 monitor) of the acquisition chain: MAD26 + Cyberstar X2000 Pulse Processing Unit (PPU) provides a high rate of digital pulses, each of them representing an X-ray photon. National Instruments counting cards (NI6602 - PCI), with internal clock of 80 MHz and 32 bits counters (8 per one card) are used to count the digital edges.

BL22 and BL29 experiments require low current measurements. Depending on the required resolution and sampling frequency, two options were provided: 12 bits and 16 bits. Both options use the Alba Electrometer (AlbaEM) [10] for the current amplification. For measurements where sampling frequency of 1 kHz and 12 bits digitalization are enough, an internal ADC of the AlbaEM is available. For more demanding measurements an option of digitalization of the output voltage signal, proportional to the input current of the AlbaEM, with an external ADC card exists. For this purpose the Adlink2005 - PCI 16-bits ADC card, implementing 500kS/s sampling rate (simultaneous for all the 4 input channels) was used. All the above mentioned devices are configurable to start acquisition (or latch register values in case of NI6602) on a hardware trigger.

Synchronization. In order to achieve synchronization between the experimental channels and the position of the scanning variable, the approach of using time driven hardware trigger was chosen. Range of motion where constant velocity is assumed forms an effective scan region, where acquisition could be performed on equidistant time intervals. In this approach, positions of master axes are latched at the same time as the experimental channels start the acquisition process. In case of BL22 a master axis is a bragg angle brushless DC motor. Its encoded position gets captured on each hardware trigger and gets stored in the internal memory of the Turbo Pmac 2 controller in a plain buffer capable to store 4000 positions. In case of BL04 and BL29 examples, master axes are encoded stepper motors driven by Icepap motion controller, OC and PG respectively. Quadrature signals of their encoders are read by NI6602 position measurement application and are latched on hardware triggers as well.

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All the referred scans implements their triggering channels using the pulse train generation application of NI6602 card. One card allows generation of up to 4 pulse train sequences parametrizable in: number of pulses; high, low and initial delay times; idle state. BL04 example requires synchronization of 14 counting channels + position measurement channel, where the RTSI bus was used to propagate the triggering signal between channels from 3 Ni6602 cards.

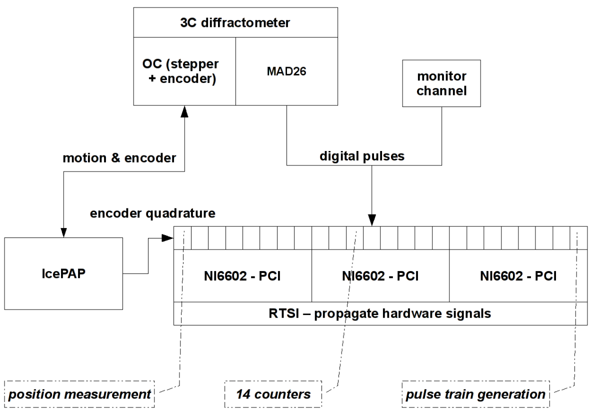

Figure 1: BL04 (MSPD) HRPD experiment. Application schema with involved instruments and controls hardware.

Software Solutions

Motion. Continuous scan receives the start and end position as the input parameters, which should correspond to the start and end of the constant velocity region. Selection of the proper motion parameters: acceleration times, deceleration times and velocities of all the physical axes, was implemented by the top-down inspection of the hierarchy of the all involved moveable axes. The slowest accelerating and decelerating motor is used as a reference for the rest. The velocities are calculated for each of the displacements separately. Initial and final positions of each displacement are calculated. By starting motion at the same time it is assumed that all of the motors reach the constant velocity, as well as stop the motion, at the same time. Post movement action of correcting the overshoot takes place at the end of the scan.

Data acquisition. In the referred examples, the standard measurement groups contain only experimental channels that produce one scalar value per one scan point. The early version of the scan was implemented so that all the data were stored in the hardware buffers and were extracted only at the end of the scan. This approach was not optimal due to hardware buffer limitations.

The most recent version collects and stores data from the very beginning of the scan. In this way, advanced features of the hardware, like half-buffering (Adlink2005), could be fully explored. Furthermore notification of the experiment progress could be provided. Collection of the new data was implemented using a polling thread interrogating all the hardware controllers for new data. Whenever new data is available, it gets transferred to the data recorders for storage or notification and finally experiment progress can be reported (Figure 2).

Synchronization. In the referred examples time driven hardware triggering was chosen. Generalization of all the possible synchronization approaches was not achieved in the current version. Time driven trigger class was equipped with the following member variables: high time, low time, delay time, idle state, number of triggers and basic methods for starting, stopping and getting the state. Its role limits to backup, configuration (prior to the scan execution) and final restore of the trigger device parameters. Furthermore it allows aborting the trigger generation (if necessary).

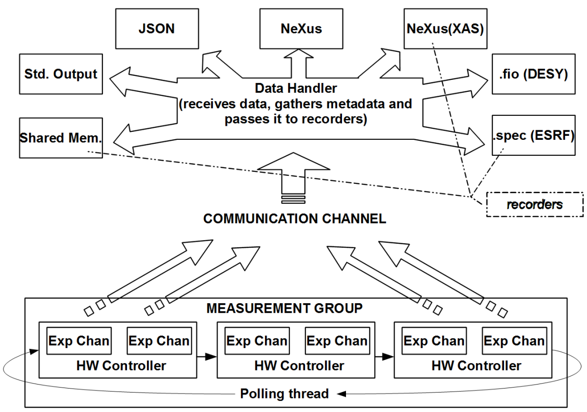

Figure 2: Data collection mechanism during the scan execution.

PERFORMANCE AND RESULTS

A continuous scan has been developed and installed in three Alba beamlines. Referred scans were compared, in terms of the execution times, to their step scan equivalents and these results are presented in Table 1. Prior to using continuous scans, BL22 and BL29 had optimized their experiments by implementing variable step size and integration time region step scans. In this way their experiments were shorten in time to ~40 min in case of BL22 and to ~10 min in case of BL29.

Table 1: Achieved Improvement in the Experiment Duration in Comparison to the Step Scan

Set-up	Step scan time	Continuous scan time
BL04 angular range: 100° integ. time: 0.025s nr of points: 100 000	~ 9h 26min	~ 42min
BL22 energy range: 1keV (8969keV - 9969keV) integ. time: 0.0291s nr of points: 4000	~ 1h 3min	~ 3min
BL29 energy range: 65eV (755eV - 820eV) integ. time: 0.0124s nr of points: 4000	~ 1h 25min	~ 3min

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BL04 HRPD experiments are now performed in less than one hour where step scans could take even 10 hours. BL22 QEXAFS is now possible in just a few minutes while EXAFS in region step scanning mode takes approximately 40 minutes. BL29 XMCD experiment is possible in few minutes, comparing to 10 minutes in region step scanning mode. Furthermore the continuous scan developed in this project could be easily adapted to any other experiment, and will be used as a base for extending Sardana scan framework with the generic continuous scan capabilities.

FUTURE DEVELOPMENT

Current state of the continuous scan described in this paper is just an intermediate version, which ideally would become a major part of the GSF of Sardana. It is far from fulfilling all the requirements of the generic continuous scan. Aspects listed below will be treated with high priority in the future development iterations.

Flexibility of selection of the experimental channels implementing various triggering modes: hardware triggering and/or gating as well as software triggering must be provided. Correlation of the data, produced by the channels of different nature, should be also implemented. This would facilitate interpretation of the results to the end user.

The 1D and the 2D experimental channels are very common in the experimental set-ups. Normally they generate much more data than 0D experimental channels. GSF should be able to handle experimental channels producing data at the high rate and of considerable size.

Various approaches for implementing hardware triggering in the continuous scans exists. The most common are position driven and time driven. Generalization and transparency in implementation and usage should be achieved.

An approach of using software/hardware synchronized timestamps, redistributed to all the participant devices, seems to be the future standard of the continuous scans. Each data acquired during the scan would have a timestamp and higher software layers could then manage this data to be easily interpreted by the end user [9].

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