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POSITION-BASED CONTINUOUS ENERGY SCAN STATUS AT MAX IV

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Abstract

The traditional approach of step scanning in X-ray experiments is often inefficient and may increase the risk of sample radiation damage. In order to overcome these challenges, a new position-based continuous energy scanning system has been developed at MAX IV Laboratory. This system enables stable and repeatable measurements by continuously moving the motors during the scan. Triggers are accurately generated by hardware based on the motor encoder positions to ensure precise data acquisition. Prior to the scan, a list of positions is generated, and triggers are produced as each position is reached. The system uses TANGO and Sardana for control and a TriggerGate controller to calculate motor positions and configure the PandABox, which is the equipment in charge of trigger signal generation. The system is capable of scanning a single motor, such as a sample positioner, or a combined motion like a monochromator and undulator. In addition, the system can use the parametric trajectory mode of the IcePAP driver, which enables continuous scans of coupled axes with non-linear paths.

This paper presents the current status of the position-based continuous energy scanning system for BioMAX, FlexPES, and FinEstBeAMS beamlines at MAX IV and discusses its potential to enhance the efficiency and accuracy of data acquisition at beamline endstations.

INTRODUCTION

In the domain of experimental science, the efficiency and speed of data acquisition have always been of extreme importance. A prior MAX IV work [1] tackled the challenges associated with conventional step scans, where in each acquisition process a series of time-consuming steps, including motor movements, detector activation, and data retrieval. Although widely employed, this method has inherent dead time, restricting scan speed to just a few points per second, especially when dealing with millisecond-range measurements.

Building upon the foundation laid in previous research, this subsequent paper delves deeper into our quest for a more streamlined and expedited data collection methodology. The primary focus continues to be on continuous scans, a concept previously explored using a combination of software and hardware solutions. In this work, we further refined the approach, placing a heightened emphasis on hardware-based solutions to optimize motion control and precise trigger pulse generation. Our objective is to significantly enhance the speed and efficiency of data acquisition, ultimately pushing the boundaries of what is attainable in the realm of scientific experimentation.

This paper outlines the ongoing efforts to develop and implement a robust hardware-centric system, shedding light on its novel capabilities, performance enhancements, and applications across various experimental setups.

SYSTEM

The system is based on the TANGO Controls toolkit [2] and Sardana [3] for scan orchestration – Fig. 1 illustrates the implemented system. If necessary, non-linear motions and multi-motor synchronization are effected using parametric trajectories [4] with trapezoidal profile movements (ensuring constant speed while respecting acceleration and deceleration constraints) in IcePAP [5]. Such trajectories can also be applied using any other motor driver with parametric trajectory support. IcePAP features a position closed-loop system with an integral controller for each individual axis. It is imperative to fine-tune this controller to ensure that the motor accurately follows its trajectory over its full range. All interlocks, limit switches, and error stops actuate on all associated axes, ensuring coordinated movements. This setup permits the use of a single motor encoder as a position reference since the driver guarantees synchronization of the other axes.

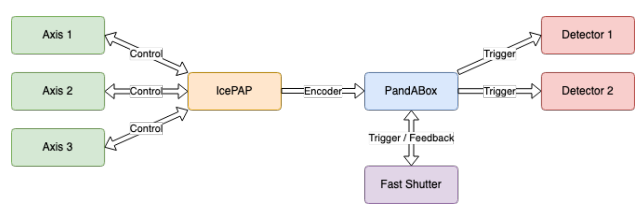

Figure 1: Schematic of the implemented system.

The timing system is based on PandABox [6] and allows the user to choose between position-based or time-based triggering. For position-based, each trigger is determined using the incremental or absolute encoder readings, sampled at 1 MHz by PandABox, and a pre-loaded look-up table. The values in the table are equally spaced in eV, based on the user inputs. For time-based, only the first scan point is determined by the encoder position, afterwards, all remaining pulses are generated with a constant time interval. The system accepts combinations of multiple motors, e.g., undulator, grating and mirror for PGM monochromator, or a single motor used as the master. PandABox supports up to eight encoder inputs. The combination will vary based on the resolution needed for each application. For incremental encoders, the scan routine synchronizes the IcePAP readings with PandABox

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before each execution. It is also possible to integrate other components like a fast shutter for Hard X-ray beamlines, so the opening and closing is synced with PandABox and motion. The PandABox configuration, an depicted in Fig. 2, is versatile and can easily be applied to many systems.

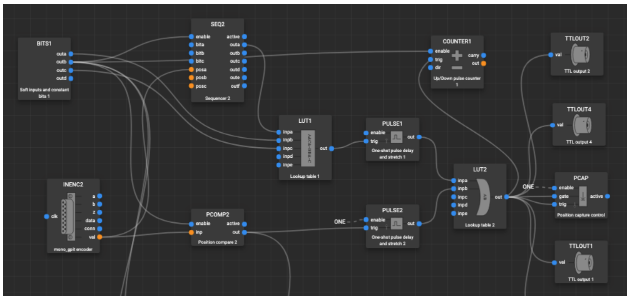

Figure 2: PandABox configuration schema for FinEst-BeAMS beamline.

All components are exposed with their own TANGO devices, allowing monitoring of each component's state during scans. Diagnostic tools have also been incorporated to provide rapid feedback to users. As illustrated in Fig. 3, a live view of the energy difference per scan point, at FinEst beamline, while moving the monochromator is available. The system resolution is influenced by factors such as cabling noise, mechanical stability [7], encoders, and other components [8]. Additionally, the system supports gated signals as trigger outputs, where the pulse length equals the integration time of the requested scan.

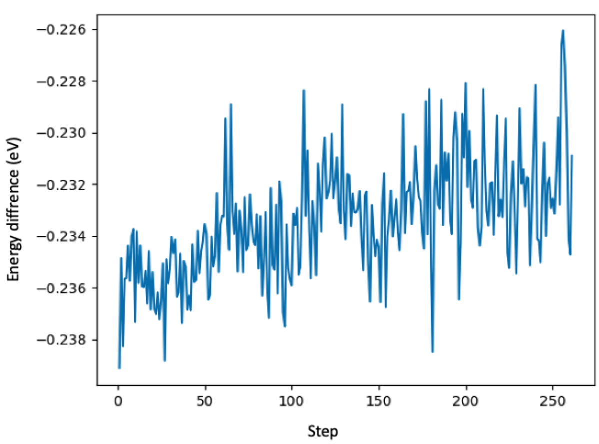

Figure 3: Energy difference in eV per scan point for the monochromator during a scan. Ideally the curve should be a constant line.

The scan script is written in Python in the form of a Sardana macro and can easily be integrated in different user experimental interfaces such as MXCuBE [9], as represented in Fig. 4. The scan sequence takes the user parameters, validates them, calculates positioning tables, pre-start and post-final positions, configures motion setup (trajectories if needed), arms detectors and PandABox and finally starts the motion, the data recording is done in parallel with the ongoing triggers. During execution the user is notified about progress and general system monitoring. The system and scripts, can also be applied for general continuous scanning using complex motion trajectories such as tomography.

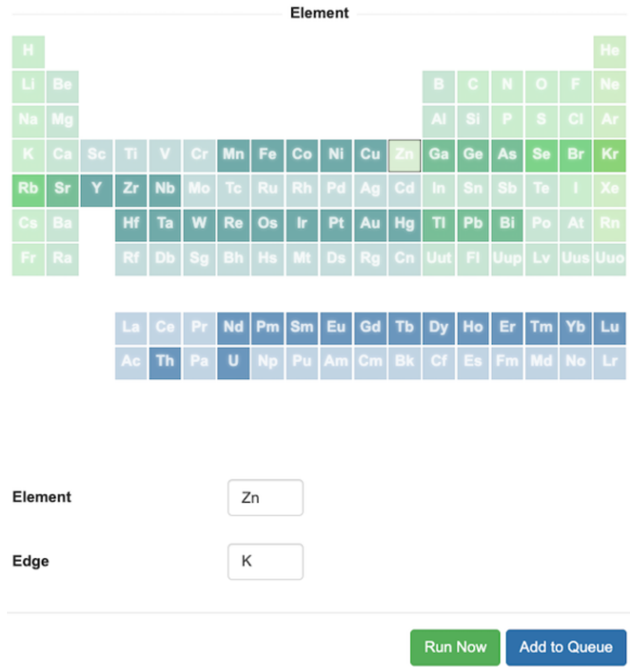

Figure 4: BioMAX MXCuBE continuous energy scan integration.

APPLICATIONS

FlexPES

FlexPES [10] is a Soft X-ray beamline at MAX IV's 1.5 GeV ring. The system achieves synchronization between the gap motion of the planar undulator and a PGM monochromator (grating and mirror). The undulator operates within its linear range, while the monochromator utilizes a non-linear parametric trajectory using IcePAP. In the monochromator trajectory it is possible to configure several parameters such as line density, diffraction order, etc. The undulator tapper and harmonic does not change during the scan and the required resolution is 10 meV for the full energy range. The detectors involved are Xspress 3 Mini (Quantum Detectors, UK) for photon counter and ALBA electrometers for photodiode readings. Figure 5 illustrates the similarity of the step-scan and the continuous scan. However, the continuous scan took just 46 seconds to complete, compared to 494 seconds for the step scan. More than an order of magnitude faster. While not visible in the graph, the spacing in the energy dimension is also much more consistent for the continuous scan.

BioMAX

BioMAX [11] is a macromolecular crystallography hard X-ray beamline at MAX IV 3 GeV ring. The system is synchronizing the gap motion of the in-vacuum undulator, the

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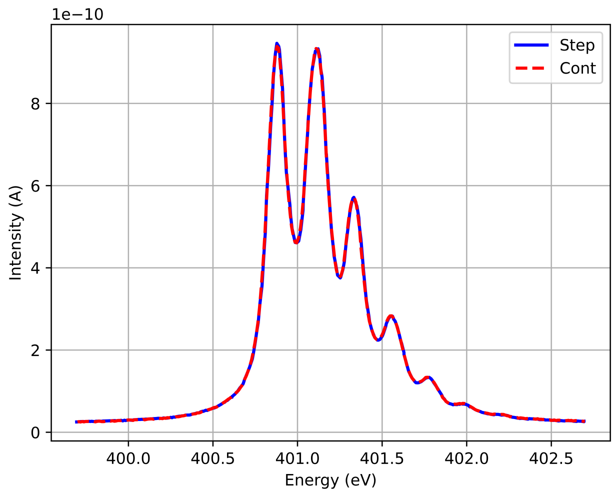

Figure 5: FlexPES nitrogen K-edge absorption scan compared between standard step scan, in solid blue, and continuous scan in dashed red line.

Bragg angle of horizontal double crystal monochromator (HDCM) and the fast shutter. The undulator tapper and harmonic does not change during the scan and they are operated in the linear region. The system is applied for experimental phasing using the SAD or MAD techniques [12]. The resolution is 1 eV at full range and only the Bragg motor for HDCM is used as trigger source. The detectors involved are Xspress 3 Mini (Quantum Detectors, UK) and ALBA electrometers. Figure 6 illustrate the difference between the step-scan and the continuous scan.

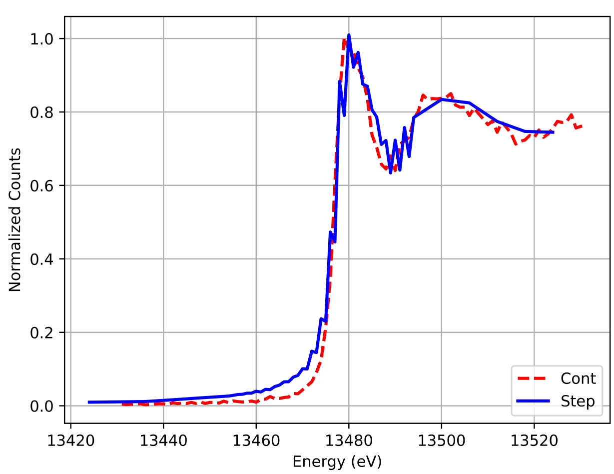

Figure 6: BioMAX Br K-edge absorption scan compared between standard step scan, in solid blue, and continuous scan, red line.

FinEstBeAMS

FinEstBeAMS [13] is a Soft X-ray beamline at MAX IV's 1.5 GeV ring. The system was synchronizing the gap motion of the APPLE-II undulator and the PGM monochromator (grating and mirror). The undulator is operated in linear range, same harmonic and polarization during the scan. The current system only supports inclined polarization at a fixed phase. The resolution varies according to the energy range and experiment type (20 meV maximum resolution). The monochromator parametric trajectory is the same as implemented for FlexPES. The system is used for photoluminescence excitation and XANES. The detectors involved are ALBA electrometers. Figure 7 illustrates the similarity of the step-scan and the continuous scan.

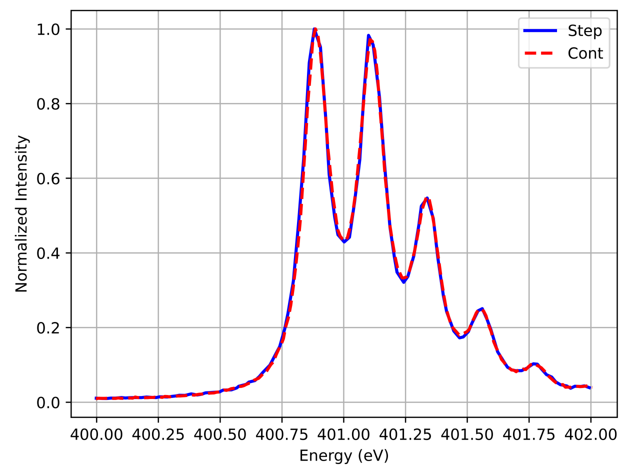

Figure 7: FinEstBeAMS nitrogen K-edge absorption scan compared between standard step scan, in solid blue, and continuous scan in dashed red line.

FUTURE DEVELOPMENTS

The system will be expanded for NanoMAX, HIPPIE, and SPECIES beamlines. FinEstBeAMS will be upgraded with non-linear parametric trajectories for its APPLE-II type undulator, at lower energies for photo-luminescence measurements, that includes advanced control over gap and polarization (circular and inclined).

CONCLUSION

Conducting continuous scans offers a clear advantage in terms of significantly enhancing scan speed. This enables the more efficient utilization of X-ray beams in storage ring facilities, especially when the signal strength allows for high-quality measurements to be achieved with brief exposure time. The heightened scanning speed also brings an additional benefit by minimizing the radiation dose to which the sample is subjected during each scan. This aspect holds particular significance for sensitive biological samples that are susceptible to damage from radiation exposure during scanning procedures.

The adaptability and scalability of this system make it readily transferable to other beamlines with minimal need for bespoke adjustments or modifications. Its inherent flexibility allows for straightforward integration into diverse experimental setups, rendering it a versatile and cost-effective

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solution for a wide range of research facilities, improving user experience and enabling more science.

All software developed by MAX IV are open source and available to everyone interested.

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