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MAX IV LABORATORY'S CONTROL SYSTEM EVOLUTION AND FUTURE STRATEGIES

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Abstract

The MAX IV Laboratory, a 4th generation synchrotron radiation facility located in southern Sweden, has been operational since 2016. With multiple beamlines and experimental stations completed and in steady use, the facility is now approaching the third phase of development, which includes the final two of the 16 planned beamlines in user operation. The focus is on achieving operational excellence by optimizing reliability and performance. Meanwhile, the strategy for the coming years is driven by the need to accommodate a growing user base, exploring the possibility of operating a Soft X-ray Laser (SXL), and achieving the diffraction limit for 10 keV of the 3 GeV storage ring.

The Technical Division is responsible for the control and computing systems of the entire laboratory. This new organization provides a coherent strategy and a clear vision, with the ultimate goal of enabling science. The increasing demand for more precise and efficient control systems has led to significant developments and maintenance efforts. Pushing the limits in remote access, data generation, time-resolved and fly-scan experiments, and beam stability requires the proper alignment of technology in IT infrastructure, electronics, software, data analysis, and management.

This article discusses the motivation behind the updates, emphasizing the expansion of the control system's capabilities and reliability. Lastly, the technological strategy will be presented to keep pace with the rapidly evolving technology landscape, ensuring that MAX IV is prepared for its next major upgrade.

GENERAL STATUS

As of now, the MAX IV Laboratory boasts 15 operational beamlines, with a 16th set to be commissioned by this end of 2023. Discussions regarding the construction of additional beamlines are ongoing with stakeholders, but no firm decisions have been made. Remarkably, the facility's accelerators maintain an impressive availability rate of 98.5% for the 1.5 GeV ring, 98.2% for the 3 GeV and 96.8% for the linear accelerator, although the lab is committed to increase reliability to reach ideally the 99% range.

Accelerators

In a particular effort toward the linear accelerator, the beam diagnostics have received an important upgrade. A Tranverse Deflecting cavity (TDC) [1] conveys a perpendicular oscillation to the particle beam, acting as a diagnostic tool. By converting time differences within a beam pulse into spatial differences, it offers detailed insight into the pulse's temporal structure. Often likened to a "streak camera", the TDC spreads the beam pulse across a spatial dimension for high-resolution examination. Beyond diagnostics, it also manipulates the beam for specific experiments, necessitating precise synchronization with the accelerator's components.

On the other hand, the development related to the Soft X-ray Free Electron Laser (SXFEL) is on-going. The Compact APPLE X undulator is an advanced device tailored for Soft X-ray beamlines. Not only is it more cost-efficient than its predecessor, the APPLE II, but it also boasts the ability to consistently control polarization, maintaining a uniform effective K-value across different polarization states. This feature positions it as the go-to source for the upcoming SXFEL at MAX IV. Furthermore, it can expand the energy spectrum below 2 keV for the FemtoMAX beamline at the Short Pulse Facility (SPF). When benchmarked against the APPLE II undulators at the 3 GeV MAX IV ring, it provides a broader energy range with complete polarization adjustability.

Beamlines

On the Beamlines, a great effort has been made to reach the full capacity of the MAX IV Laboratory within the initial scope of 16 beamlines. Apart from the 2 last beamlines described below, all the beamlines are continuously improving their performance i.e an EXAFS measurement is done now in 3s at Balder, in contract to 30s in 2021.

ForMAX is a new beamline in operation tailored for in-depth research on tree materials. It enables multi-scale structural analysis ranging from nanometers to millimeters by seamlessly integrating tomographic imaging with small- and wide-angle X-ray scattering (SWAXS), as well as scanning SWAXS imaging. Operating between 8-25 keV, the beam size varies from approximately 1 µm to 5mm based on the chosen mode.

MicroMAX, set to launch in the end of 2023, will revolutionize structural biology research. This beamline will facilitate 3D protein studies and their real-time analysis, particularly focusing on the challenging molecules that produce only microcrystals. Operating between 5-25 keV, its beam size varies from around 1 µm to 5mm, boasting a photon flux of 10^{15} photons/s based on the mode selected. An added capability of MicroMAX is its time-resolved mode, offering dynamic insights.

TECHNICAL DIVISION

To ensure the sustainability of the technical support, MAX IV has adopted a new organization with the new Technical Division bringing together multiple technical disciplines, including mechanical engineering, electrical engineering,

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software development, vacuum technology, and more. The division includes now the engineering groups, the previous KITS group, and the Central Project Office that were previously under, respectively, the Accelerator Division and the Scientific Division.

A dedicated division ensures that there is proper coordination and expertise available across these domains for ensuring the proper design, installation, maintenance, and optimization of the complexes equipment which the accelerators and the experimental station rely on. The Technical Division ensures that the facility remains operational with minimal downtime with a coherent maintenance and upgrade plan, but it also offers a specialized support to ensure successful experiments. Additionally the Technical Division often leads efforts in research & development, ensuring the facility is equipped with the latest and best tools.

Electronics

After commissioning a larger set of beamlines in the past years and now finalizing the last two, the shift in expectations on a scan of a sample already described in [2–4] have continued in in terms of complexity of the measurements with focus on time resolved measurements and scanning optimization.

The introduction of PandABox [5] at the beamline has been fruitful and now 14 beamlines and 2 internal labs are using 27 PandABoxes for a variety of tasks, often integrated with the EM# electrometer [6] and the IcePAP motion system [7]. All in all, with units soon to be delivered, MAX IV has 40 units. The tasks ranges between synchronization of constant energy scan of mono and insertion device as well as orchestrating timestamped triggering of endstations, often using a position capturing mechanism where a motion is supervised and where preloaded positions creating triggers that are send to other devices. The units also receives multiple status flags and indicators and with Boolean operators sends enable/disable signals or triggers.

Besides motion, it is therefore possible to integrate components like fast shutters, so the opening and closing is synced with PandABox and motion. The PandABox configuration, depicted in Fig. 1, is intuitive and can easily be adopted to many systems. Configurations are saved as files can can be shared or reloaded conveniently thus changing the setup to a new experiment.

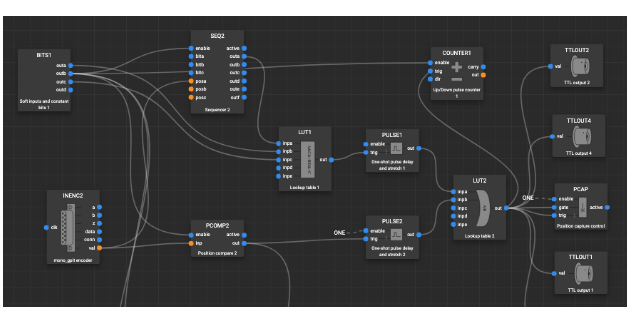

Figure 1: PandABox configuration. This particular one is for FinEstBeAMS beamline.

The scanning optimization have also required a new set of thinking where motions should be synchronized as in [8] where a continuous energy scan routine is described, or as in [9] where trajectories are used to create continuous nonlinear motion through a parameter space, e.g. Rowland circle, while scanning, as motivated in [10].

With a more mature facility, the maintenance to have a facility with high availability and reliability is increasingly important [11] as deployed systems age. The main objective is to find a means to understand and keep track of a facility for which it is hard to have an overview of. Time has been invested to keep drawings and documentation up to date in a manner that can be continuously modified. Further, a maintenance system has been introduced, J5, (a proprietary software developed by j5 International (Part of Hexagon)) and is now being adopted to fill the need of long term documentation, tracking of spare parts, stock records and scheduling of routines and tasks such as greasing and filter replacement. The system is about to be populated with the data from a numerous lists of hardware stored in excel sheets scattered between beamlines and sometimes individuals. The adding of data will be automated to reduce the time and effort. The different equipment types have parents and children with status and identification (Fig. 2), for example a motor having two limit switches as children, or an electrometer identified with serial number and MAC address having the status repair.

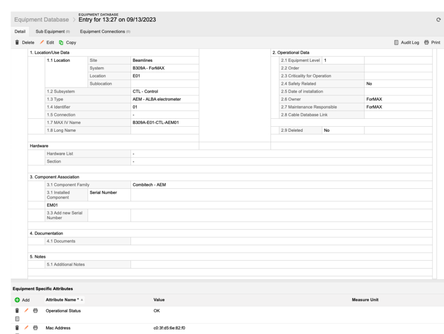

Figure 2: In the maintenence system, an electrometer is registered as a stock item and is thus available for deployment in another system according to its operational status.

Scientific Data

The detectors at the beamline end stations are the starting point for the data acquisition (DAQ) and can be the single most complex pieces of equipment to be integrated into the control system. The main challenge are the two-dimensional imaging detectors, the performance of which can be the limiting factor in diffraction, imaging or tomographic techniques at a fourth generation light source. It was recognised several years ago that dedicated effort was needed for efficient operation of these detectors, and this approach has evolved such that today detector integration and support is concentrated within the Scientific Data group.

In the last year the main effort has been to unify the DAQ

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from all two-dimensional detectors into a common streaming standard. This now covers ten Dectris Eiger detectors, three Dectris Pilatus, one custom X-Spectrum Lambda and numerous sCMOS cameras from various manufacturers, distributed across eight beamlines. In all cases the approach is to stream the data from the corresponding detector control server, which interfaces with the detector hardware in a vendor specific way, with ZMQ over 40 Gb/s links to a central DAQ cluster. The DAQ cluster is now managed entirely under kubernetes, and DAQ receiver "pods" can be brought up as needed for any detector. These "stream-receivers" handle the file writing over native gpfs to the storage, and is now a single common application written in Python that can handle the streams for all of the above detector types, the streams themselves adhering to a shared albeit loose standard. Combined with the kubernetes management, this has been a major simplification of the system from an operation and deployment point of view. The beamline user need not interact with any kubernetes tools, or even be aware of the container system, since the Tango device provides a control interface to restart the receiver (ie the pod) if needed and check its status.

The stream receivers running in the DAQ cluster also provide images at a reduced bandwidth that can be requested by a live-viewer application back in the control room. A simple liveviewer based on SILX [12] has also be standardised for all two-dimensional detectors. Moreover, the stream receivers can republish data at full rate as the starting point for any analysis pipeline. Commonly used for many beamlines and techniques is an azimuthal integration step [13], which is implemented in Python as *azint* [14] to run parallelised also in kubernetes in the same DAQ cluster. The output of that pipeline step is another hdf5 file of the integrated images saved to disk in a directory for processed data parallel to the raw frames. As detectors become faster and data rates grow we foresee a greater need for this type of online processing, which has motivated combining the DAQ and scientific data processing activities in the new Scientific Data group. The two topics are likely to become increasingly intertwined, with more application specific pipelines developed to run directly from the detectors, for example for tomography.

Software

As noted above, the focus in developments for the beamlines has shifted from baseline functionality to providing better performance in terms of faster scans, more complex measurement scenarios with a wide range of sample environments, and increased reliability for the end users.

To achieve faster scans we are concentrating our efforts in the continuous domain. 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 [2] and is now in use at three beamlines, BioMAX, FlexPES, and FinEst, with a roll out planned for several more during 2024.

At the beamline CoSAXS, an upgraded beamline data acquisition strategy for a millisecond time-resolved SAXS/WAXS experiment has been implemented, using laser light to induce temperature jumps or UV-excitation with the consequent structural changes on the system [15]. 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 state-of-the-art pixel detectors, in synchronization with the fast shutter opening time. PandABox integration is done with a Sardana Trigger Gate Controller [16], used to configure the pulse parameters as well to orchestrate the hardware triggers during a scan.

To better support the large number of Sardana installations in the facility, MAX IV has contributed to the implementation of a new Sardana feature - the "config tool". It is inspired by tools like Ansible, which define an entire configuration. The config tool is centered around a YAML file format which describes an entire Sardana system. The format is designed to be human read/writable, easy to generate programmaticaly and friendly to version control (e.g. git). The tool can set up a new Sardana system from such a YAML file, as well as creating a file from an existing system. This will allow a way to discover manual changes, as well as a way to restore a system to an earlier state. In general MAX IV is endeavouring to make a stronger contribution to the Sardana collaboration by participating in the developments outlined in the Sardana road map presented in [17].

The accelerator control system is also receiving improvements to increase the reliability and robustness of the system. A Model Predictive Control(MPC) approach for the beam orbit has been proposed to address issues on the slow orbit feedback(SOFB) system related to saturation of corrector magnets [18]. The controller uses iterative optimisation based on beam position measurement, ring representation models and system constraints to calculate changes in control signal.

To achieve high temporal resolution for longitudinal beam characterization, a transverse deflecting cavity (TDC) system has been developed and installed in a dedicated electron beamline downstream of the LINAC [19]. A control system with scanning routines has been implemented in Tango and Sardana, to facilitate systematic data acquisition for comprehensive beam analysis.

Taranta, developed jointly by MAX IV Laboratory and SKA Observatory, is a web based no-code interface for remote control of instruments at accelerators and other scientific facilities. In the last year, performance analysis, refactoring and improvements of the Taranta dashboards, as well as optimization of the communication with the backend TangoGQL, has led to Taranta becoming an attractive option for several other facilities [20].

The implementation of SciCat at MAX IV represents an advancement in the field of scientific metadata management. Over the past two years, MAX IV has dedicated substantial resources to provide a solution for automatically and effi-

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ciently collecting, storing, and accessing metadata for a wide range of scientific experiments from different orchestration systems. MAX IV has successfully tested the backend after migration from Loopback to NestJS and will continue the effort for future developments, including automated data processing and analysis pipelines linked to SciCat [21].

PyTango continues to be a popular interface the Tango Controls ecosystem, and MAX IV is dedicated to maintaining it. The number of contributors to the project has grown, and the team is now committed to at least two updates per year. The most notable changes are dropping support for older Python versions, including 2.7, and trivial installation (binary wheels are now available for the most common platforms). The API's consistency, and usability has been improved, there were fixes for rare crashes and memory leaks, and the documentation and continuous integration tooling was refined. More details about the project status are available in the Tango status paper [22].

MAX IV has been using Ansible [23] to manage and deploy its full control system, both software and infrastructure, for many years with great success. We have now adopted conda as our primary packaging tool instead of the Red Hat Package Manager (RPM). Contributing to the public conda-forge channel has benefited the Tango Controls and scientific software community. In the last two years, we improved our Ansible workflow with an easier way to define Tango Device Servers in our inventory [24]. A new role ensures necessary applications are restarted automatically during deployment. When tagging a repository, a GitLab CI job automatically creates a merge request to update the Ansible inventory. It's even possible to setup continuous deployment so that this change is merged and the application automatically deployed. This is for specific use cases only but helps increase user autonomy. For the control system, we put in place a regular deployment process that helped us keep the inventory clean and the beamlines up-to-date. On the monitoring side, we developed tooling to provide us with an accurate picture of what is deployed where. Ansible has served us well — we expect this to continue, and that our processes will continue to improve.

ROAD MAP 2023-2030

The recently established Technical Division will play an essential roles in enabling MAX IV Laboratory to solidify its place among the world leading synchrotron facilities beyond 2030. To fulfill its ambition, the Technical Division road map is spearheading initiatives towards two key objectives: to enable the transition to operational excellence while simultaneously enabling world-leading technology.

In alignment with these ambitions, the Technical Division is defining within the governance structure a so-called "Program" to uphold these objectives, leveraging the new competence portfolio and the experience acquired previously.

In particular the establishment of the ICT (Information and Communication Technologies) program will manifest these two keys objectives by five specific lines of development (so-called "streams") along the short, mid, and long term of the road map as described below:

New Operational Readiness and Reliability

The path towards the Operational Excellence required a change in the way of working, previously optimised for the building of the facility. A study based on the support log provided by the on-call organisation so-called KITOS [25] in 2022 has revealed the necessity of improving the reliability of the Experiment Control System and the diagnostic process of KITOS. The Experiment Control System is the main ICT system used by the Users at the beamlines which represented 30A task force project was launched in May 2023 focusing on 2 experimental stations at the time to investigate and solve the critical reliability issues, as well as spreading the good practice.

Recognising the need for perpetual evolution of the experimental setups, this line of development integrates also the Technology Readiness Level (ISO 16290:2013) approach to evaluating the maturity of a new deliverable or asset against the required reliability before its usage by our Users (visiting researcher). This methodology aims at establishing the correct process that will safeguard the facility against releasing User systems prematurely and will optimise the development trajectory.

Secured Operation Support

Acting as the operational safeguard, KITOS [25] is an internal organisation within the ICT groups to respond quickly to any disruption of operation and to monitor pro-actively the ICT infrastructure. The new operation support strategy will champion the stability and security of the MAX IV functions all along the the next seven years. It targets the importance of minimization of operational disruption, increasing availability with self recovery feature, smart diagnostic feature and a delivery of efficient technical support. The efficient technical support will be achieved by building the expertise on critical experimental components such as detectors by building a strong center of knowledge.

The diagnostic process relies on the information reported by the beamline staff to investigate the issue. A user-friendly issue report of the beamlines would help to accurately target the root cause. Several improvements can reduce the Mean Time To Repair(MTTR): better diagnostic software, alarm, logging and test system. This should lead to a more accurate Continuous Improvement process i.e closer follow up action to improve the reliability of the system.

Experimental Measurement at MACH4

Fourth-generation synchrotrons produce extremely bright and intense X-ray beams and this enhanced brightness means that samples can be illuminated with a much higher flux, allowing for rapid data collection. Fast measurement systems are essential to match the potential speed of such new light source. For example, Time-Resolved experiment [15] on dynamic processes in materials allows scientists to observe

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phenomena that were previously too quick to measure. Other techniques like coherent diffraction imaging, nano-probing, and fast tomography require also rapid data acquisition systems which are incompatible with the latency of traditional scanning software.

Another significant advantage of a fast acquisition is to reduced the exposition of the sample to the intense radiation which is especially important for biological sample that can be damaged by prolonged exposure. And or course, overall less time is required for each measurement, which reduces the beamtime required and increases the overall efficiency in the use of the beam delivery.

Faster measurement will automatically impact in a larger extent the research experience. In experiments where adjustments are needed based on intermediate results (e.g., in iterative reconstruction or optimization processes), fast measurements can provide almost real-time feedback, allowing researchers to make timely changes to the experiment parameters. Real-time of data analysis will become necessary to make the most of fast measurements. For an increasing number of experiments, the complexity and volume of data will require more sophisticated analytical techniques, such as machine learning and AI.

User Experience

The User Experience stream aims to prioritise the development of intuitive user interface from the proposal submission to the data retrieval. Since MAX IV Laboratory is a user oriented facility, enhancing the overall experience for the researcher is critical. A streamlined experience can significantly impact the efficiency of the research activities.

With the additional beamlines the capacity and the panel of research will increase although the existing beamlines can also develop their potential to utilise the beam as much as possible. Comprehensive tools will become necessary to guide the research to reach their experiments goals during the experiment.

Technology development

The key objective of this fifth stream is to enable Technology to adapt to the future needs of experimental research. The overarching theme is about integrating AI/ML into the operations and research of a scientific facility, with an emphasis on data management, experiment optimization, and technological advancements. These goals are essential for modern research facilities aiming to stay at the cutting edge of science and technology.

For MAX IV, leveraging AI and ML can help in maintaining its leading edge as a top-tier research facility. However, to fully understand the strategic significance of AI/ML for MAX IV specifically, one would need to delve into their current operational challenges. For this reason a internal forum has been set up to act as a dedicated platform for sharing of best practices, ideas, and tools that can target our AI/ML projects. The aim is define a cross-functional collaborative development of AI/ML pilots between the ICT groups, accelerator physicists and beamline scientists, with the addition of external collaboration with universities, research facilities and R&D department of private companies.

CONCLUSION

MAX IV Laboratory has entered now in a steady state of operation with a particular focus on increasing the reliability of experiments conducted at the facility. With a solid foundation in its new Technical Division organisation supporting the scientific division, MAX IV is now in position to carefully shape its future for the next seven years.

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