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STABLE OPERATION OF THE MAX IV LABORATORY SYNCHROTRON FACILITY

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Abstract

MAX IV Laboratory, inaugurated in June 2016, has for the last 8 months accepted synchrotron users on three beamlines — NanoMAX, BioMAX and Hippie — while simultaneously pushing towards bringing more beamlines into the commissioning and user phases. As evidence of this, the last call issued addressed 10 beamlines. As of summer 2019, MAX IV has reached a point where 11 beamlines simultaneously have shutters open and are thus receiving light under stable operation. With 16 beamlines funded, the number of beamlines will grow over the coming years. The Controls and IT group has performed numerous beamline system installations such as a sample changer at BioMAX, Dectris detector at Nanomax, and End Station at Hippie. It has additionally developed processes, such as automated IT infrastructure with a view to accepting users. We foresee a focus on end stations and detectors, as well as data storage, data handling and scientific software. As an example, a project entitled “DataStaMP” has been recently funded aiming to increase the data and metadata storage and management system in order to accommodate the ever increasing demand for storage and access.

INTRODUCTION

MAX IV is a fourth generation synchrotron facility with one linear accelerator and two storage rings at 1.5 GeV and 3.0 GeV respectively. The ring lattices are designed as multi bend acromats in order to reach emittances in the ultra-low few hundred pm rad range and hence achieve ultra-high brightness and transverse coherence. Inaugurated in June 2016, the facility has accepted users for three beamlines — Nanomax, BioMAX and Hippie — while design and commissioning for 13 beamlines is ongoing. A milestone was reached in June 2019, when 11 beamlines had their beam shutters open and receiving light simulatneously, Fig. 1.

The facility performance is dependent on the availability and reliability of its accelerators. Without a stable electron beam, the possibility to build state of the art beamlines is very limited. MAX IV is therefore constantly monitoring the availability and reliability of its accelerators, and presents the result to users through a web interface, Fig. 2. For the year to date (mid September, 2019) the up-time and meantime between failures has been 98%, 61 h for the 1.5 GeV ring, 98%, 43 h for 3 GeV ring, and 98%, 42 h for the short pulse facility (located at the end of the linac).

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At MAX IV, the Controls and IT group has the responsibility to find solutions and coordinate the work involving control systems for the machine and beamlines. The group is divided into 5 collaborating subgroups, whose latest activities are summarised in the subsequent sections. As a group, we value taking part in collaborations with other facilities and using open and shared technology and knowledge.

Figure 1: Screenshot of the MAX IV machine status web interface showing 11 open shutters during top-up mode operations of the 1.5 GeV and 3 GeV rings at 250 mA.

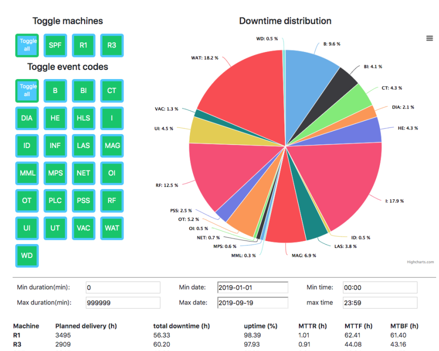

Figure 2: Statistics on the availability and reliability of the accelerators at MAX IV.

INFORMATION MANAGING SYSTEM

The Information Management System (IMS) team has a broad foot-print across MAX IV and strives to find efficient ways to support all the software and tools that falls into the information management and web category. In 2018, a lot of effort was put into making the development and delivery processes more efficient and less error prone with fewer manual intervention. Dockerizing [1] applications and building an automated continuous delivery process were central to this goal. Dockerization in particular has proved

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to be highly successful, as it allows users to take the lead in developing their applications which can be subsequently deployed and maintained within existing infrastructure. It is therefore foreseen that more applications will be migrated to this model.

The IMS team has supported the Digital User Office (DUO) system for user applications with the addition of experiment session management. Through this, the main proposer can manage the co-proposers, select shifts, manage access to the experiment hall, etc. As DUO is synchronised with MAX IV Active Directory, users also gain seamless access to the facility IT infrastructure.

Experimental logging has bene migrated from ELog to ELogy — a web based multi-purpose logbook used by most groups in the facility, including user operations at beamlines Fig. 3. It supports rich text editing and attachments, and each logbook can be configured with a template and custom attributes to increase productivity and facilitate information sharing. Moreover, it exposes a REST API which makes it easy to integrate with other software.

Figure 3: A screenshot of the Elogy logging platform.

We have also been developing WebJive — a web based tool for interacting with a Tango control system enabling devices configuration, command execution and attributes read/write in near-realtime, Fig. 4. Furthermore, it enables users to create custom dashboards with a simple drag and drop interface, to save them for later use, and even share them with others via web links. Currently, it is deployed on six beamlines. MAX IV has recently entered a collaboration to develop WebJive together with SKA (Square Kilometer Array.)

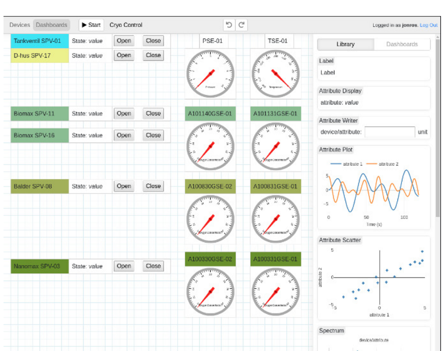

Figure 4: A screenshot of the WebJive platform for web-based visualization of the Tango database.

We are also participating in the development of SciCat — a data catalogue management system in collaboration with PSI and ESS, Fig. 5. SciCat facilitates easy management of data life cycle, from the point of collection of raw data, through data transformation for the purpose of analysis, and finally migration to long term storage. The system helps to link publications to their entire data provenance, manage data ownership and open data requirements.

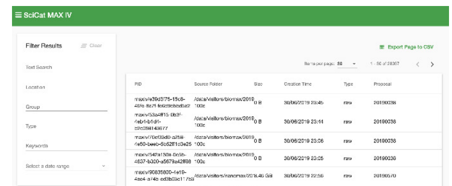

Figure 5: A screenshot of the SciCat tool for data life cycle management.

CONTROL SYSTEM ELECTRONICS HARDWARE

The control system electronics hardware team deals with almost all aspects of motion, detectors, cameras, triggering, timing, data acquisition, counting, etc. Electronics are closely integrated with the control system software, and much of the work revolves around collaborative projects, e.g. the IcePAP motor driver [2] and Em# electrometer [3] [4] to some extent already described in [5] and [6].

Motion System

MAX IV has been part of the IcePAP collaboration since 2013 and is still active in promoting and updating the system. To date, approximately 1300 hybrid two phase stepper motors have been installed at the facility and a further 250 motors will be commissioned in the coming 12 months, mainly at the Softimax, Cosaxs and Danmax beamlines. To increase awareness of the status of the motion system, the Kibana [7] and Grafana [8] frameworks have been used for the development of status grids to present textual and numeric information on the motion control systems, e.g. firmware versions, Fig. 6, logged temperatures, Fig. 7, etc. With these tools in place, alarms conditions such as over temperature or extreme motor configuration can detected and alerts sent out automatically via email or sms.

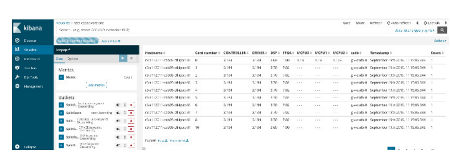

Figure 6: A screenshot of a status grid created using the Kibana framework for facility system monitoring.

To make the tuning of motion faster and more accurate, a tool for plotting motion variables has been developed, Fig. 8, and made available to the synchrotron community through GitHub. Information such as current in the motor

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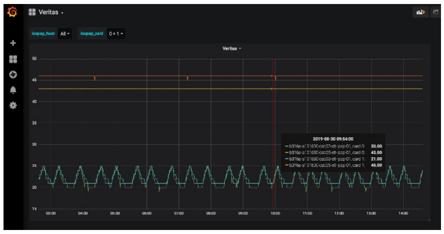

Figure 7: A screenshot of a status grid created using the Grafana framework showing the temperatures of two different IcePAP motor driver cabinets.

wires, encoder position, deviations from expected position in closed loop and status such as motion are layered on top of each other to provide an instant picture of the system.

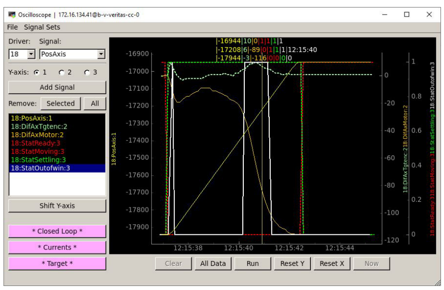

Figure 8: A screenshot of the IcePAP oscilloscope tool used for motion configuration and tuning.

Electrometer

The Em# has become a de facto standard electrometer at MAX IV, with 37 low voltage and 21 high voltage units in operation at the facility. Developed at ALBA, this four channel picoampere meter is present at almost every beamline as it is fully integrated into the Tango, [9], and Sardana, [10] environment. The electrometer is also located in the Front Ends for the 3.0 GeV ring where each Front End has two x-ray beam position monitor (XBPM) stations for diagnostics of the photon beam. The photon beam position data is stored in long term archive and complements the data for the electron beam positions.

Integrated Data Collection, Encoder Reading and Triggering

In the near future we see another long term collaboration emerging in the form of PandABox [11] — an integrated data collection, time stamping, position readout and triggering tool. MAX IV has one unit that has passed the testing phase and is now in operation at the Balder beamline. Further units for the NanoMAX and SofitiMAX beamlies have been ordered, and other beamlines are also considering their use.

DATASTAMP

The rising adoption of high-data rate detectors and the resulting ever-increasing generated data volumes is driving demand for storage capacity and performance at all synchrotrons and free electron lasers worldwide. Similarly, the open science movement and the desire to make all valuable experimental digital assets available and accessible to the science community, puts high requirements on the stewardship and data management services provided by a facility.

To address these issues and meet the most immediate needs of the science community, the Knut Alice Wallenberg foundation (KAW) has decided to fund a project called DataSTaMP (Data Storage and Management Project) [12] at the MAX IV laboratory. The project has a budget of 75 MSek and a time line that stretches from July 2019 to December 2023. DataSTaMP is a cross-functional effort between the teams in Controls and IT group (KITS) at MAX IV, and is estimated to occupy 14 full time equivalents at its peak. The overall mission is to improve the value of the data generated at the facility in terms of the benefit to research, in the spirit of the European Open Science Cloud [13] and the FAIR data principles [14].

The implementation of DataSTaMP is split into four work packages, Fig. 9, each covering a different aspect of the improvement of storage and the management of experiments. The project will be an evolution of the Scientific Data Management [15] developed at MAX IV.

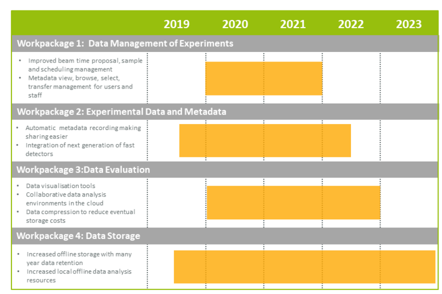

Figure 9: The four key workpackages of the DataSTaMP project: Data Management of Experiments, Experimental Data and Metadata, Data Evaluation and Data Storage.

The work package of *Data Management of Experiments* covers both optimization of the user office system and a portal to access experimental data and services such as visual browsing, analysis of data and data downloading. The aim is to make all experimental data and other digital assets related to a proposal accessible for users.

Experimental Data and Metadata collection includes the development of a data acquisition framework that will be capable of handling high the data rates predicted in the next few years [16]. The framework will support the separation of control from data flow and has a unified way of handling the harvesting of data from all the detectors at MAX IV. Experimental data will be made more valuable to researchers by automatically recording metadata at an experiment in a data catalogue.

Data Evaluation encompasses the implementation of a collaborative analysis platforms. *JupyterHub* will serve as the basis for the multi-user environment and will allow re-

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mote data processing and sharing of analysis workflows. The current MAX IV JupyerHub was implemented in a collaboration with the Niels Bohr Institute at Copenhagen University and utilises containerization with support for *swarm* and *dockerspawner* [17].

Data Storage aims to provide a user-friendly storage service and expand the offline storage to include warm storage for offline processing and cold storage for non-active data. The goal is to offer experimental data generated at the MAX IV laboratory a permanent home.

CONTROL SYSTEM SOFTWARE

Since the previous status report [18], the focus of the control system software team at MAX IV has been directed more and more towards data acquisition. A dedicated time has been allocated to follow up the development of detectors since it is a critical component for synchrotrons. The Control System Software group has also developed a unified data acquisition platform [16], running in a dedicated data acquisition cluster connected to all beamlines, using ZMQ as a data transfer protocol, and gRPC for the inter-process communication.

Regarding the project management, the process is in a very mature state using Agile and Lean management [19].

Accelerators and Beamlines

A generic Tango Feedback Device [20] has been developed to run the Slow Orbit FeedBack (SOFB) which tunes feedback in the storage rings, the trajectory feedback in the linac and the monochromator stability on the beamlines. The device is fully configurable for Single/Multiple Input/Output applications and requires only that the sensor and actuator are available as TANGO attributes. For multiple input-output applications, the device handles the inversion of the response matrix using using Singular Value Decomposition.

At the Nanomax beamline, the previously presented [21] flyscanning motion and trigger scheme has been in user operation throughout 2017 and 2018. This system allows time-based triggers to be sent to Dectris Pilatus, Quantum Detectors Merlin, and Xspress3 detectors synchronised to measurement of the sample position over a 1D linear scan. Over teh course of 2019, the system has been redeveloped, with the replacement of the original Physik Instrumente (PI) piezo stage with an NPoint model capable of supporting a heavier sample environment, Fig. 10. A new Tango device written in C++ and communicating over USB has been developed to communicate with the NPoint piezo controller. As in the original scheme, the linear motion is based on a programmable waveform motion, with a time duration over the linear region to match the requested number of trigger cycles. A Stanford Delay generator operating in burst mode is used to send the time based triggers, initiated by an output trigger signal from the NPoint. This new system will enter user operation in October 2019.

Hdb++ Cassandra has been chosen as the long term archiving database in order to achieve performance in heavy

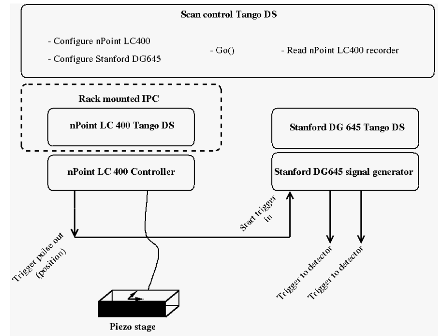

Figure 10: Design of the new Nanomax sample environment.

read/write operations. Its distributive nature provides high available and horizontal scalability. Only one cluster is shared by the accelerators and the beamlines. This system has been migrated to a physically new dedicated cluster based on Cassandra. The decommissioning of the previous nodes, based on virtual machines, took longer than expected as the migration involved much more data than originally anticipated. A recurrent repair job which frees storage by removing redundant data has now been added to mitigate this. Cassandra Reaper has been installed as a new tool for Cassandra database maintenance, and has enabled excellent stability since the last virtual node was decommissioned. Currently, 60,000 event records are stored per minute which results approximately in 1 TB data increase per month in data storage.

At the Balder beamline [22], a linear energy quick scan has been implemented to perform fast experiments when moving the monochromator. The signal timing is coordinated by a PandAbox [11] unit which reads the motor encoder position and generates gate pulses with a controlled high time. This makes it possible to acquire fluorescence (Xspress3 detector) and transmission (Em#, [3]) data synchronously. The setup is fully integrated in Sardana, [10].

The ICE (Ions in Coincidence with Electrons) endstation at Balder uses a RoentDEK HexAnode Delay Line Detector to obtain complete kinematic information on specific dissociation channels in a reaction. The electron bunch triggers up to 22 ADC cards connected to two detectors. The hardware vendor provides capture drivers which have been modified to push the data stream to a DAQ cluster [16]. Here a sorting algorithm distinguishes the digital traces and serializes electron and ion hits on the detector. The raw and sorted data are stored in the MAX IV online data storage in Nexus-compliant HDF5 files. Post-processing produces histogram plots of time-of-flight information which provide insight into the chemical reactions taking place in the sample. The raw data can also be re-analyzed with changed experimental parameters to achieve a more complete view of the physical processes.

Sardana [10] — a software suite for supervision, control and data acquisition — is used extensively at MAX IV. Such a critical system needs a modern way of logging and monitoring the different events that happen behind the scenes, in

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order to better understand and maintain the software available at each beamline. Elastic Stack has been selected to performs this role at MAX IV, and uses Beats [23] to monitor the existing log files generated by Sardana generates and and push the log entries to an Elasticsearch [24] instance. Finally, Kibana provides a simple means to access and analyze the registered logs via web interface. An individual Kibana dashboard has been created for each beamline, allowing its users to monitor the logs from a browser.

Webjive is an easy and quick-to-use web interface with the aim of supporting interaction with the control system. The Devices view exposes the configuration of all the devices in an interactive treelike hierarchy. The Dashboard view allows the users to create their own interfaces [25]. The frontend is developed using React, Redux and Typescript whereas the backend includes a GraphQL based API which exposes Tango, a Mongo Database for persistence and JWT based authentication. A prototype of the SVG Synoptic [26] has been migrated to a similar Webjive technology stack.

Software Infrastructure

An automatic Continuous Integration and Continuous Delivery process has been implemented, integrating several tools such as GitLab CI [27] and Ansible AWX [28], Fig. 11. In just one commit, the packages are built, published to our internal repository, and — for some projects — deployed to our production machines. We also use periodic routines to diagnose, notify and deploy packages.

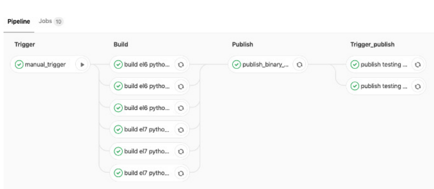

Figure 11: An example of Gitlab pipeline for a python module.

Ansible AWX is a web application for remote configuration of the accelerators and beamline control systems. The main functionality provided by Ansible [29] is the provision of version control of the control system configuration. A daily cron job checks any important modification of the system, but also reports any possible updates to be applied. The Continuous Delivery pipeline uses this application in order to apply weekly software and system updates. In the future, it is envisaged that the machine and beamline staff will be able to manage the version of their software through this portal.

The aforementioned containerization of the various development environments at MAX IV has brought several advantages. Docker allows a stable and repeatable operating system to be quickly set up so that multiple developers and testers can be assured of a homogeneous environment. Furthermore, Docker lets developers have different and distinct system configurations so as to best match the eventual runtime environment. One use-case is a Docker stack in which a device server, client and data stream simulator were run. In another case, Docker enabled 32 simultaneous instances of a stress test to be quickly launched in an attempt to isolate an infrequent bug. In yet another case, Ansible deployment logic was efficiently tested within a Docker image.

PLC2Tango is a new web application used to decrease the lead time of Programmable Logic Controller (PLC) configuration in the control system, Fig. 12. The tool has been deployed to Species, FlexPES and other beamlines , and has proven to be faster to work with than the previous tools. The PLC group also produces more complete and stable configurations due to the PLCe2Tango validation features. It brings more autonomy and faster feedback since the control group no longer needs to be directly involved.

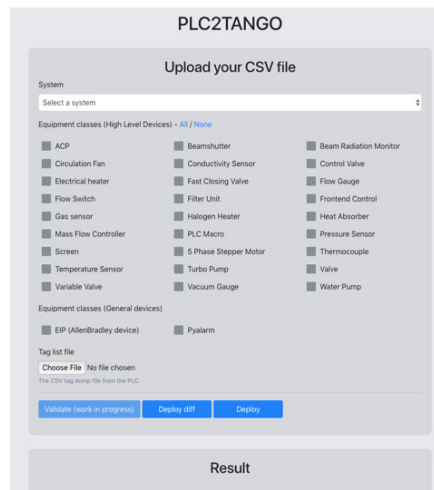

Figure 12: A screenshot of the PLC2Tango web application for configuration of Tango devices communicating with PLCs.

CONCLUSION

MAX IV is well on its way to transcending from a commissioning state to a operational state, where stable accelerators deliver beams to a number of beamlines that in turn accepts users. MAX IV has adopted the strategy of having one group, Controls and IT System (KITS in Swedish) to solve the challenges associated with mcahine/beamline control system integration, user account management, and machine/experimental data handling. From a facility point of view, the synergy from having few competing systems and all staff dedicated to supporting them, have payed off due work load sharing and knowledge spread.

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