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THE FIRST OPERATION OF THE MAX IV LABORATORY SYNCHROTRON FACILITIES

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Abstract

On 21st of June 2016 the MAX IV Laboratory was inaugurated in the presence of the officials and has since then welcomed the first external researchers to the new experimental stations. The MAX IV facility is the largest and most ambitious Swedish investment in research infrastructure and designed to be one of the brightest source of X-rays worldwide. The current achievements, progress, collaborations and vision of the facility will be described from the perspective of the control and IT systems.

FIRST OPERATION

MAX IV Laboratory is a synchrotron based research facility which will operate one full energy linear accelerator at 3.2 GeV, two storage ring at 3 GeV and 1.5 GeV, and 14 beamlines (see Fig. 1).

The last 2 years most of the effort was made to bring the storages ring in operation while targeting at least 2 beamlines for user operation. The KITS group, being responsible for all IT infrastructure, information management, control system hardware/software and the scientific software, has supported all subsystem, beamline and accelerator scientists in their projects. The KITS has established a working guideline to balance the constraint of limited resources, in order to achieve this objective and help the stakeholder for their success.

Figure 1: The Machine Status web application accessible for the public, showing all accelerators and beamlines in operation.

Several milestones have been passed since the last report of the MAX IV status [1]. One of the major intermediate milestone happen end of 2015 when the 3 GeV ring could stack for the first time at 4 mA. This event has validated the new design of the 3 GeV ring and especially the optics parameters defined by simulation. As soon as the 3 GeV storage ring reach 50 mA, which is consider as the minimal to start the commissioning of the beamlines, the 3 GeV accelerator entered in operation mode. For the IT system it was the confirmation that the choice of technology, previously deployed for the Linac, could scale for the new accelerators. Some important date of the facility:

- 5 November 2015, the first synchrotron light of the 3 GeV was detected on the diagnostic beamline.
- 31 January 2016, the 3 GeV in operation.
- 9 June 2016, the first protein diffraction detected at Biomax; first light on the sample at Nanomax.
- 21 June 2016, the inauguration of the facility.
- 31 December 2016, the end of the MAXLAB building decommissioning.
- Dec 2016, the first expert users.
- Between March and June 2017, the first user
- June 2017, R1 commissioned.

The facility welcomed the first expert users at the end of 2017. Although 3 beamlines are already in operation not all the first phase beamlines of the original plan are commissioned, especially the 5 Soft X-Ray beamlines of the 1.5 GeV Ring. MAX IV will still continue to expand as well in the next 5 years to 14 beamlines. A project of Soft X-Ray Free Electron Laser, recommended by the Machine Advisory Council in Spring 2017, has now the necessary resource to propose a conceptual design before 2020.

ACCELERATOR STATUS

The commissioning of the 3 GeV have been achieved in 5 months, in spite of few unstable systems, especially the diagnostic. Meanwhile the total user experience of the control system improves quite a lot. Actually the system was made primary for the expert user in order to fine tune it or diagnose the system in details during the installation and subsystem test phases. With the coming operation mode the control system has quickly evolve to reduce the 300 000 parameters and signals of the Machine to a most comprehensive and high level view in order for the operator to quickly identify warning and fault of the equipment and recover as soon as possible for the beam delivery.

1.5 GeV Ring Commissioning

The R1 subsystem test went fast thanks to the experience acquired with the 3 GeV [1]. To reach high current was important to condition the ring. This process is slow and the important parameter is number of hours with beam, i.e.

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time*current. When fully conditioned the stored current should be the same as in the 3 GeV storage ring, i.e. 500 mA. The insertion devices for the beamlines have been installed during the 2017 summer shutdown. And the remaining work to be done concerns mainly the optics to be fine-tuned together with insertion device commissioning with beam.

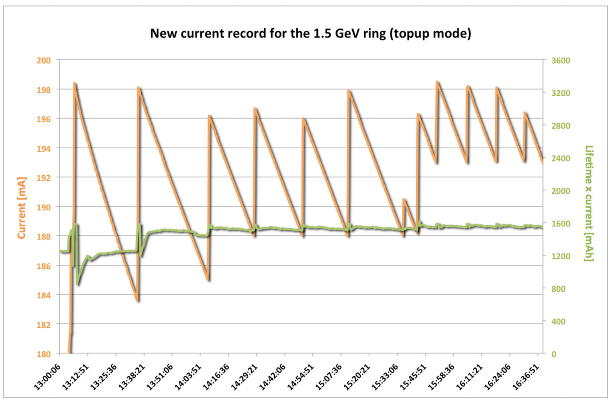

Figure 2: The figure shows top-up operation for a number of hours at the present maximum current. Plotted alongside the current is the product of current and lifetime.

Top-up

Top-up has been used for a year already and it works very well (Figure 2). In present top-up operation we use a single dipole kicker, which disturbs the stored beam for a very short time at each injection. A more sophisticated injection scheme will be soon possible thanks to the Multipole Inection kicker (MIK), a synchrotron SOLEIL collaboration, which should make top-up invisible for the beamlines.

STATUS OF BEAMLINES

The First monochromatic undulator light in experimental hutch was observed 12 May 2016. The User operation has started early in 2017 and will continue in parallel with commissioning activities until 2018.

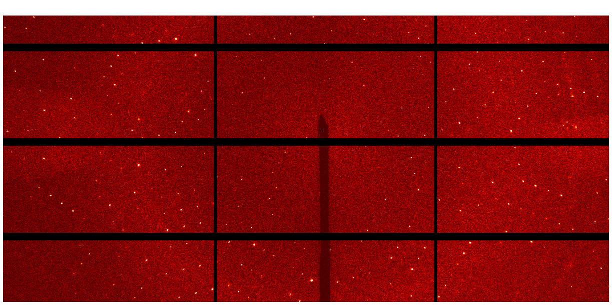

Figure 3: Diffraction patterns from crystals of the protein thaumatin exposed to X-rays produced by the new MAX IV 3 GeV storage ring. Collected with a Eiger XX M.

Biomax is the first X-ray macromolecular crystallography beamline of MAX IV Laboratory, which begins its user operations in December 2017 [2]. It is a state-of-the-art resource accommodating multiple cutting edge experimental possibilities.

In June 2017 the first diffraction experiment with a protein crystal (Figure 3) has been performed at the BioMAX beamline, after 5 years of designing, building and commissioning of MAX IV LABORATORY. This is a very important milestone for the entire MAX IV project as this shows that everything from the source to the detector is working. The instruments that prepare the beam (undulator, monochromator and focusing mirrors) produce a 40 x 20 μm X-ray beam that reaches the protein crystal in the diffractometer producing the diffraction patterns that the detector records. All these parts are not only working but are working together by careful control by the beamline control system.

Earlier weeks the BioMAX and KITS teams could successfully install and start the operation of the Eiger X 16M (Dectris, Switzerland) hybrid pixel X-ray detector. This is a high performance x-ray camera which allows for the collection up to 133 diffraction images consisting of 16 million pixels per images or up to 750 images of 4 million pixels per second. With the hybrid pixel detector technology, the data can be recorded faster and with less noise giving improved data quality. One challenge of this project is the design of the required IT infrastructure, for example the network and the data collection software, which is required to guide the very large and rapidly created data safely to the data evaluation computers.

The whole project is a nice example of the close collaboration between various MAX IV teams, and with the vendor.

NanoMAX the hard X-Ray nanoprobe of MAX IV is designed to take full advantage of MAX IV's exceptionally low emittance and the resulting coherence properties of the X-ray beam.

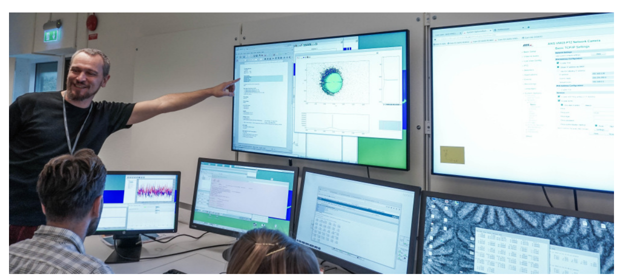

Figure 4: The results are discussed and interpreted in the NanoMAX control room.

The First monochromatic undulator light in experimental hutch was observed 12 May 2016. And in the very last days and hours of beam before the inauguration NanoMAX managed to put a sample in the focal position, concluding the same fact about the stability of the photon beam. The beamline has had its first successful user experiment,achieving a full ptychographic reconstruction with a resolution of about 50 nm. Nanomax is design to have 2 End Station (ES1 and ES2). ES1 prototyping is ongoing since 2012 within a SOLEIL-MAX IV collaboration between NanoMAX and

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Nanoscopium. The gained experience is used for an in-house development to realise the instrument (Fig. 4). ES2 is realised almost completely as an internal MAX IV development. All components of the focusing optics and the sample goniometer have been assembled during September-December 2016. Procurement of detectors has been proceed. The installation and test of the XPress3 and Merlin detectors started early 2017. Both came with the Tango [3] LIMA devices implemented. Most of the KITS development was done on the time driven continuous acquisition [4] with the Sardana framework [5].

FemtoMAX makes first time-resolved X-ray diffraction measurement in April 2017. The studied sample is an indium antimonide (InSb) coated with 60 nanometres of gold. This type of structure is called photo-acoustic transducer which is a device that can convert the energy in light to a sound wave. A lot of work still remains before FemtoMAX is a fully up-and-running beamline ready for user experiments. The most important improvement is that the new in-vacuum undulators from Hitachi will be installed in Autumn 2017. These are anticipated to give more than a factor 100 higher flux at this photon energy (5 keV) compared to the present undulator. The performance will also be enhanced by increasing the repetition rate of the electron pulses in the Linear accelerator from 2 Hz to 10 Hz and eventually 100 Hz. In order to accommodate higher repetition rates the data acquisition [6] and storage speed needs to be increased.

KITS VISION

The KITS group requires a well-designed formal communication structure in the organisation, both internally within the different domains of IT expertise and based on the IT requirements of the MAX IV organisation. Communication between KITS and the rest of the organisation is crucial, in order to facilitate efficient communication of requirements which leads to the delivery of appropriate solutions. It is important that the responsibility for choosing the appropriate technical solutions and for the consequences of those choices is shared by the KITS group and others. A number of standards have been adopted which maximise the impact of technical solutions, making them more generally applicable and simplifying their overall complexity. A number of values are applied by the team, resulting in high efficiency and effectiveness and subsequently high motivation and therefore productivity:

Lean Management is an approach used to maximise customer value while minimising waste. The approach needs to be tailored to each organisation and requires continuous refinement. In software development, this overcomes a tendency to over-engineer solutions and anticipate needs that do not turn out to be required. Lean Management also includes automating tasks which take significant time and provide little value or that are so complex as to generate a high risk of human error.

Knowledge Spread is a value which is integrated into the work of the group by promoting a sharing of projects. Over time, the expertise acquired when working on a single project is continuously disseminated to others in the group, to prevent knowledge from being restricted to certain individuals and productivity from being contingent on key individuals.

User Autonomy is a value which focuses on making IT systems more accessible to users. A user can be a KITS member from a different domain, another staff member or a visiting user of MAX IV. This value includes all potential users of any IT system at MAX IV. The aim is to follow the Lean Management principle of minimising waste by reducing the number of key people needed to complete a process. There is a tendency to deliver solutions where the user is dependent on the provider, and cannot maintain or deliver any part of it themselves. We want to make sure that the user is able to participate in development and also have access to troubleshooting in any situation in which they have the capacity to do so. This kind of partnership allows a closer mutual understanding and leads to win-win situations.

Continuous Improvement is a value about analysing current solutions with a view to make improvements. It is a behaviour which can lead to inspiring new ways of doing things, and helps sustain a high level of motivation. All group members are always welcome to propose improvements at any time.

Flexibility is a value about adapting to people's needs, while maintaining a high standard of delivering effective solutions and staying efficient. Standards can be bypassed or changed, as long as it doesn't compromise the overall efficiency of the group.

CONTROL SYSTEM/SOFTWARE

The software development of the control system has progressively shifted from the accelerators to the beamlines experimental station, especially on the data collection [7]. The experience with the Sardana Framework started to ramp up with the continuous acquisition system [4].

Meanwhile the maintenance of the existing system received lot of attention i.e upgrade to Tango 9 and CentOS 7. To improve and deploy every where the new standard is considered part of the refactoring phase of our agile development. The current major campaign concerns the migration of 80 % of our python 2.7 Tango devices to python 3.4 since Red Hat announced its deprecation for the next CentOS 8. In these cases our configuration management was a key player. Defined 5 years ago [8] it becomes a indispensable tool in our process. Thanks to Ansible in particular, the development time take advantage of the low workload maintenance by keeping coherent and standard the systems. This time is invested to increase the part of the web development continue, mainly for the general services. One of the direct benefit helps to increase the user friendliness of the control

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system. Today tens of web application are part of our port folio [9]. Our project management continue with the Agile

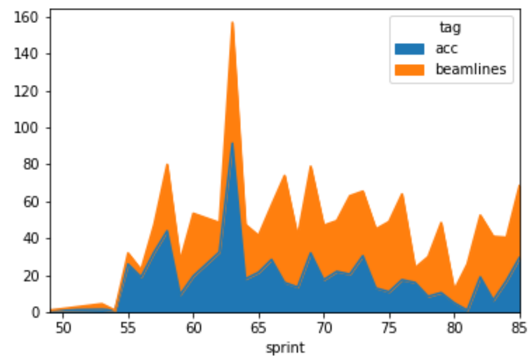

Figure 5: Workload of the control software along the different Scrum sprint, based on the initial estimation of the task complexity.

method and the Lean Management [1] as they current works very well. The expected outcome are pretty stable along the Scrum sprints. Time to time the tasks accumulate at the validation step by lack of stakeholders' time; the pic on the Figure 5 alarms us to keep contact with them.

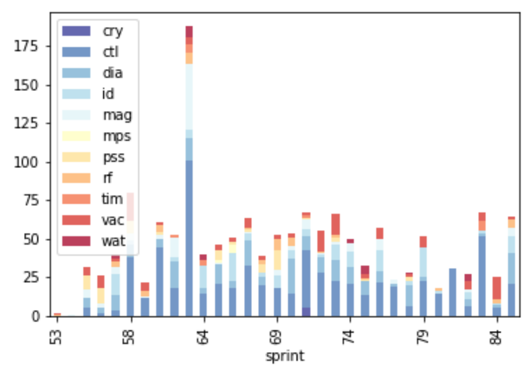

Figure 6: Workload of the control software along the different Scrum sprint, based on the initial estimation of the task complexity.

The priority given by the Beamline Office and the Accelerators deputy keep a good balance of distribution over the different subsystem last year (Figure 6):

- About 30 to 50% covers the control system regarding archiving, operators UI, data acquisition, high level computation and own infrastructure.
- about 20 to 30% for the diagnostic (BPM issues and beamline detectors) and the control of the insertion devices.
- about 5 to 10% for the vacuum including PLC upgrades.

As seen today the control system is not yet a bottleneck in the global project management. The model is not fully tested with the beamlines and partially unknown for the new beamline staff. Changes can be foreseen when the focus will be more and more on the user experience of the MAX IV Users.

Automatic Machine

The automatic machine project aims to have self driving accelerators during the beamlines operation. One of the idea is to streamline the transition between the different state of the machine e.g 3 GeV to SPF injection mode. In order to understand the feasibility of the project a special advisory council has been hold end of 2016. The robustness and the development resources were the main controversy in connection to the control system. An audit has been proceed regarding the current resource and the main show-stoppers. In this context the role of the machine operators and the control system became more than relevant. How to identify repetitive action? How accurate and reliable the metrics for the diagnostic are? How to replace human decision making by computer?

At this occasion an internal audit on the control software was done end of 2016 while the 3 GeV ring where in commissioning, using a categorisation following ISO 9126 [10]. The audit reveals that the infrastructure is ready for automation. The control system covers all the active equipment necessary for sensing and actuating, see Table 1. And there is no risk to scale the system with the new installation in term of global performance (Scalability in Table 3). Nevertheless the system is still basic and complex. Only the expert of the system with good knowledge can steer the machine. Meaning that the system lack of high level functionalities (Table 2). In term of performance (Table 3) the system should be able to work in closed-loop for the slow correction in the order of tens of hertz by software. Even if some class of hardware are saturated in bandwidth it's mainly due to the polling strategy. An event strategy should free the necessary bandwidth. Anyhow a specific effort should be made in order to study the long term metrics from the archiving system, in particular. The limited efficiency in time-stamping can be a

Table 1: Functionality

Attributes	**Pro**	**Cons**
Suitability	300 000 channels R/W @HW and Computation level	Lack Feedback, Correction, Compensation and diagnostic
Accurateness	Functions always validated and reviewed	Not enough test coverage
Interoperability	Between accelerators, Tango binding and MML	Has to be interface with Tango
Security	not required	-
Compliance	not required	-

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Table 2: Usability

Attributes	**Pro**	**Cons**
Human factor		Some general services are not intuitive
Documentation		Expert and Experienced People only
Consistency	Standard Naming and behaviour (ALARM vs FAULT state)	
Responsiveness	polling model	low

show stopper to identify post-mortem a failing equipment and launch a automatic procedure of disaster recovery.

Table 3: Performance

Attributes	**Pro**	**Cons**
Speed	dependent on the hardware but enough for 100 Hz fast diagnostic. Real time on the hardware	
Efficiency	The network latency is the order of hundreds of µs	Time stamping in review, Not enough for archiving, snapshot and alarms
Resource consumption	Overall below 80%	Some HW bandwidth are consumed (ITest)
Throughput	Should handle camera at 50 Hz. Network 1 GBs and 10 GBs, 40GBs on premise	
Capacity	40 CPU and 300 GB for archiving	Tied for the 1.5 GeV installation
Scalability	Tango system	Limited on general service (mysql, polling system)

Table 4: Reliability

Attributes	**Pro**	**Cons**
Availability	MTTF in improvement (PSS Watchdog)	MTTF issue with Delta Powersupply, Libera, Basler camera... Known software issue (Radiation Monitor,...) Known software issue (Radiation Monitor,...)
Failure Extent	VM fail over, monitoring of the servers	no metrics apart from day oncall support
Stability	overall the system is predictable	
Accuracy	In continuous improvement	Frequency vs Severity not available apart from the ticket system

The robustness of the system was one of the main concern. The study showed that the system is quite predictable and not the more demanding regarding the MTTF of beam operation. Even so few known issues are counter productive i.e requiring a physical reboot a regarding the start up of the linac (camera Basler not responding) or to cycle the magnet (delta power supply network disconnection). But one of the critical equipment in instance can affect directly the beam operation (BPM). These items have been identified as a top priority to resolve before to start any automation development (Table 4).

At last the automatic machine project need to rely on a proper maintenance and evolution (see Table 5) in order to implement the functionality. Even if the KITS group works with very short iteration a constant presence during the operation is mandatory to define the requirements face to the complexity. In such case the organisation of KITS based on share of resource would only delays the implementation. On the other side it's important to develop the operation sequences as soon as possible in order to increase the knowledge database.

Since this audit several actions have been taken. The most important was to reduce a number of critical issue. A strong effort was made to identify the different issues of the BPM which a recent firmware could resolved.

Present operation is heavily facilitated by a state machine software which provides automation for running the three accelerators in a coordinated manner. Nowadays the state machine automatically handles the switching between delivery to the Short Pulse Facility (SPF) at the end of the linear accelerator and the top-up of both the 1.5 GeV and the

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Table 5: Supportability

Attributes	Pro	Cons
Testability	Unit test on most of the Tango device, Maintenance smoked test, Incremental validation	less and less available time due to operation, obsolescence to manage
Flexibility	modularity of Tango, within scope > real time, management of the configuration	Archiving, Snapshot . . .
Speed	Min 2 weeks iteration	real time for critical operation
Install-ability	Accessible from dedicated local and remote computer	
Capacity	possibility to increase the inventory	
Scalability	Tango system	Limited on general service (mysql, polling system)

3.0 GeV storage rings. In order to implement an automatic machine the operators started to write down their actual process but quickly they managed to program their own python application [11]. This strategy is totally compatible with our User Autonomy. In the mean time KITS started to converge the development to an architecture based on a State Machine. The proof of concept allows the operators to describe a state machine for each accelerator in DOT format (way to describe a directed graph) and generate a live version in the Tango control system.

HDB++ and Event Paradigm

Following scalability issues observed with the existing archiving system we have almost completed the migration to the new HDB++ archiving system [12]. HDB++ is event-based, using so-called EventSubscriber devices to subscribe to archive events. A distributed Cassandra cluster is used as database. The system reflects the inherent scaling capability of Tango, since any number of the EventSubscriber devices can be deployed.

Since not all Tango devices push archive events from the code, the challenge has been to migrate a large fraction of the control system to an event-based model. The polling periods must be carefully study per class or device specific depending on the hardware performance and the needs of the clients. For example, power supplies that are used in the cycling of the magnets must refresh their state in approximately 100 ms, so the polling rate must be set accordingly. At the same time, the polling of all attributes must respect the response time of the hardware, ensuring that not more than 80% of the bandwidth is used. In addition to the update frequencies, the relative or absolute change thresholds for the archive events must also be configured.

A set of scripts have been written to configure the HDB++ Archiving Manager device and set the change thresholds and polling, if required, on the attributes themselves. We plan to integrate these scripts to a Web UI to create a tool that will continually update the archiving system configuration to match the latest state of the devices in the Tango database.

High Level and Automation

There are currently many applications implemented in the Matlab Middle Layer (MML) [13] used in the accelerator control room which would benefit from being migrated to Tango. One example is the Slow Orbit Feedback (SOFB) for the storage rings, an algorithm that continually updates the settings of the corrector magnet power supplies based on deviations of the beam from the target orbit as measured by the BPMs. The Matlab implementation, based on polling of the beam positions in the Libera devices, is constrained to run at less than 1 Hz. Reimplementing this in Tango could allow the corrections to be applied at the full 10 Hz rate of the acquisition data from the Liberas. In addition, as a Tango device the SOFB could be integrated to the foreseen State Machine. Technically, the SOFB Tango device could also be used to run the trajectory feedback in the linac which is also currently implemented in Matlab.

CONTROL SYSTEM/HARDWARE

The strategic decisions taken over the last years have so far proven to hold the test of time. One of them was to join the IcePAP collaboration and up to date we have more than 1300 stepper motors driven by IcePAP and only a handful exceptions. We see this number continuously increase with the number of beamlines growing and we have additional 700 drivers in stock, which allow us about 7 more beamlines before we build yet another set of drivers. It is not just the optical elements and the end stations that are included in the IcePAP beamline systems, but also the front end and the insertion devices. Due to the insertion devices weight and magnetic forces, most of them are driven by servo motors and hence servo drivers or five phase steppers and their drivers, but we are controlling those drivers with step and direction signals from IcePAP drivers. The choice to use IcePAP as a driver also for those motors makes the integration into the control system smooth and tools are reused. Another advantage is the ease which the beamline can set the desired energy on a pseudomotor and control monochromator and insertion device as well as other elements such as the first mirror.

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Another strategic decision taken is to join a collaboration with ALBA about an electrometer called EM # [14] after evaluating the first model at Species beamline [15]. Cells have made the design and we are contributing to the Sardana/Tango integration. Up to now, we have produced and handed over 25 units of the low voltage version to different beamlines, where they already have been involved in commissioning and science. Also, 25 more low voltage versions and 25 high voltage versions are under manufacturing and will arrive during autumn 2017. The high voltage versions will, amongst other places, be used in the XBPMs in the beamline frontends in the 3GeV ring. To further increase the electrometer capabilities, a multiplexer is built to expand the 4 channels of the electrometer to 32 channels [16].

By selecting a few multipurpose DAQ cards [17] (ADLINK 2005, ADLINK 9114, National Instruments 6602) and a rack mounted industrial PC to host them a few years back and continue to build and refine the software support for them, together with patch panels, have proven to be both cost and time effective. Its more a question of integrating than inventing when a need is identified and, with a number of cards and patch panels in stock, the time between a request to a first setup is within days or weeks instead of months. This has enabled the implementation of continuous scans both in the Nanomax beamline [18,19] where a sample positioned on a piezo is scanned in one dimension while taking spectrum and Balder beamline where a continuous energy scan is implemented.

Timing System

A MAX IV timing system [20,21] commissioning process was finished together with the construction of MAX IV:

- Linac: 2014
- Short Pulse Facility (SPF): December 2014
- Storage Ring 3 GeV (SR3): September 2015 + top-up
- Storage Ring 1 GeV (SR1): September 2016 + top-up

The hardware structure is based on Micro Research Finland cards: cPCI 300 family and Instrumentation Technologies platforms: Libera Single Pass Electron and Libera Brilliance Plus.

The system synchronizes the following:

- Diagnostics: beam position monitors, acquisition cards
- Beam injection: kicker/pinger magnets, photocathode and thermionic gun
- RF synchronization: laser oscillators, phase shifters
- MAX IV operation modes with 4 different working schemes [20] with the photocathode or thermionic gun

Apart the timing capabilities, a fast machine protection system (FMPS) was embedded into the existing timing electronics protecting fast closing valves at beamline front ends with a response time below 3 ms.

General fast orbit feedback (FOFB) works started at the end of 2016 - its optical installation was finished together with the timing schedule. Still, power supplies for fast corrector magnets are missing but a public procurement will be released in 2018/2019. Beam stability works (for SR1 and SR3) are ongoing in parallel, a FOFB measured input (global orbit data) will be used to evaluate oscillations and improve the electron beam quality.

A beamline timing installation for Veritas, SR1&SR3 Diagnostic, Nanomax was completed in 2017 and will deliver the machine synchronization for detectors/acquisition cards and eventual choppers/shutters, plus a top-up operation. In 2018, the installation will be extended with new beamlines (Flexpes at the moment).

INFORMATION MANAGEMENT

Information management has the last couple of years installed, developed and refined the necessary systems using mainly Open Source software. The first call for proposal went out March 2017, marking a milestone in the development of the digital user office DUO (PSI). DUO has been heavily modified to fit our needs, mainly of being able to cope with proposals with multiple beamline, creating a strong REST API and a new single username/password schema for the scientific data management [22]. We are currently involved in a number of collaborations to harmonise and ease the user experience i.e ISPyB which is currently being deployed at the BioMAX beamline but also a new meta-data catalogue which will be a single page application where all user experiments will be catalogued and searchable.

LESSONS LEARNED

The progress made with the initial phase of the MAX IV 3 GeV ring operation and the first experimentation with the Users of 2 beamlines gives us increased confidence that the standard choose by the Control System and the IT infrastructure suits the fast evolution of MAX IV. Much is still to be done to extend the facility by 12 beamlines.

Most difficulties are related to the technical subsystems that need time for maturing. Additionally the development are shifting more and more on the experimental set up, particular to each beamline. Our standard prove to be flexible but later a faster adaptation will be required thus evolving the standard inventory.

We will still rely on the integration of solution by collaborating with the other facilities or from the open source industry.

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