SOLEIL II: TOWARDS A MAJOR TRANSFORMATION OF THE FACILITY

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Abstract

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Operational since 2008, SOLEIL provides users with access to a wide range of experimental techniques thanks to its 29 beamlines, covering a broad energy range from THz to hard X-rays. In response to new scientific and societal challenges, SOLEIL is undergoing a major transformation with the ongoing SOLEIL II project. This project includes the design of an ambitious Diffraction Limited Storage Ring (DLSR) to increase performances in terms of brilliance, coherence, and flux, upgrading the beamlines to provide advanced methods, and driving a digital transformation in data- and user- oriented approaches. This paper presents the project organization and technical details studies (TDR) for the ongoing upgrades, with a focus on the digital transformation required to address future scientific challenges. It will depict the computing and data management program with the presentation of the targeted IT architecture to improve automated and data-driven processes for optimizing instrumentation. The optimization program covers the facility reconstruction period as well as future operation, including the use of Artificial Intelligence (AI) techniques for data production management, decisionmaking, complex feedback systems, and data processing. Real-time processes will be applied in the acquisition scanning design, where detectors and robotic systems will be coupled to optimize beam time.

SOLEIL II PROJECT ORGANISATION

The SOLEIL II project [1, 2] was initiated after the Conceptual Design Report (CDR) phase. Since 2021, the project has progressed to the Technical Design Report phase (TDR), which is structured into four distinct programs: one dedicated to beamlines and laboratories (referred to as BL²), another focused on accelerators, a third program dedicated to infrastructure, and an additional program encompassing Information Systems (IS) and data management. The latter program serves as a cross-functional support system for the other programs.

Currently, the project is targeting an 18-month shutdown to occur mid-2028.

The overall project is divided into two five years phases, each. The first one, known as the "Construction" phase encompasses the realization of the accelerators, the necessary adaptations of some beamlines, and the associated infrastructure upgrades. This phase includes the dark period and the commissioning of the new booster and the storage ring.

The second phase, "Towards Full Performance", begins with the continuation of the storage ring commissioning and the initial commissioning of the beamlines The

from this work

upgraded state-of-the-art beamlines will be significantly enhanced by the performance of the new accelerators. These improvements will allow experiments to take full advantage of the photon beams generated by the ultra-low emittance electron beam circulating in bending magnets and innovative insertion devices.

THE SCIENTIFIC CHALLENGE

The scientific motivation behind this upgrade is to provide new tools and techniques to address the societal and technical challenges our society is facing. Based on the CDR findings [3], we have structured four main science use cases, which are listed here with their main benefits:

- 1. Advanced Materials: material engineering, quantum materials, information technologies
- 2. Health and Well-being: new pathogens, antibiotic resistance.
- 3. Sustainable Energy Development: batteries, catalysis, and green chemistry.
- 4. Environment: impact of pollutants and contributing to our understanding of global warming.

These use cases serve as a framework for shaping future instrumentation and methods. By conducting a comprehensive cross-cut review of scientific topics and drawing upon the common methods available across existing beamlines, our goal is to progressively tailor instruments to meet the needs of the scientific community. This entails achieving nanometric resolution scans/positioning, which will become the norm across most beamlines.

Moreover, we are working towards enabling operando analysis at millisecond or sub-millisecond timescales, made possible by enhancements in brilliance, coherence, and flux.

Imaging techniques will benefit highly and naturally from the lower electron emittance. To leverage on this gain, we are designing a multimodal and multi-technique approach to maximize the efficiency and flexibility of the SOLEIL II experimental stations. This strategy includes addressing the challenge of managing the growing data deluge from production to end user analysis, a concern shared and collaboratively addressed by both the computing and scientific teams.

THE ACCELERATORS UPGRADE [4]

To establish this vital instrumental hub, a substantial upgrade of the accelerators is imperative. In this context, the new storage ring will completely replace the current 354meter circumference ring. It will be based on a reference lattice featuring 20 straight sections alternating between 7BA and 4BA Higher-Order Achromat (HOA) cells, all housed in the same tunnel as the current setup. The primary

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objective is to achieve a horizontal emittance of 83 picometer radians at 2.75 GeV while maximizing the intensity of coherent photon flux to ensure the highest possible brilliance and transverse coherence.

The upgraded facility will be constructed while maintaining the existing infrastructure shielding walls, and most of the beamlines will remain in their current locations. The same spectrum of photons, ranging from to THz to hard Xray energy range, will continue to be available to the scientific community.

These objectives must be attained while preserving stability (with beam sizes held within a 2–3% margin) and maintaining the current level of reliability (achieving 99% beam availability with a 100-hour mean time between failures). Currently, the accelerator program is progressing in parallel with simulations aimed at optimizing the new storage ring and the new booster. Several key components are in the prototype stage, including a high gradient quadrupole with permanent magnets, innovative undulators and a high-performance multipole injection kicker.

Additionally, a girders prototype equipped with dummy loads is under construction to test assembly and alignment methods and to confirm eigenfrequency response. Ongoing testings and validation efforts are being conducted on the existing accelerators, including the development of a new Fast Orbit Feedback system (FOFB) [5] and power supply control using the CERN [6] FGC controller [7, 8].

All of these designs prioritize the creation of a more sustainable facility with a reduced carbon footprint. Choices such as the use of permanent magnets aim to reduce electricity consumption by over 50%, and the new cooling station under commissioning will reduce the water consumption by 80%.

Table 1: Main Paramet	ers for SOLEIL and SOLEIL II
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Parameters	SOLEIL	SOLEIL II
Energy [GeV]	2.75	2.75
Circumference [m]	354.10	353.97
Max beam current [mA]	500	500
Lattice type	DBA	7BA-4BA
Natural emittance [pm.rad]	3,900	83

IT AND DATA MANAGEMENT PROGRAMME

Introduction

In this ambitious project, the next-generation facility aims to address the challenge of data management, which will complement the high-performance capabilities of its accelerators and beamline instruments. It will also play a crucial role in supporting our users in acquiring and leveraging the vast amount of experimental data generated. In this context, the adopted approach to transform the existing IS architecture focuses on enhancing the overall user experience. The upgrade of computing services will benefit all activities at SOLEIL, encompassing the introduction of new collaborative methods and tools, IT infrastructure enhancements, all guided by the implementation of SO-LEIL's data policy. Given the constant evolution of IT technology, the transition from the current state is part of a continuous digital transformation.

Target Architecture

Building upon existing expertise and the outcome of the CDR, the main concept for transforming the IS architecture, has been developed, as illustrated in Fig. 1. The objective of this approach is to improve the automation of experiment, maximize the outcome of the data throughput while carrying out a FAIR (Findable, Accessible, Interoperable, Reusable) data policy.



Figure 1: Target architecture for the SOLEILII IT system.

An integrated, cross-functional architecture is being implemented to unite all IT stakeholders, with a primary focus on creating a modular foundation that allows for agile, long-term evolution. This paradigm will be technically realized through service-oriented technologies, such as API management. The design will incorporate new technologies, including cloud-native and big data infrastructure. Existing services will be enhanced, and new ones will be developed to effectively store, expose, and retrieve valuable information, data, or metadata through intelligent processes. The envisioned digital transformation will also emphasize automation improvements to integrate smart systems, advanced processing, and the use of artificial intelligence for control, operational maintenance, and data processing.

This conceptual architecture has been designed to provide technical, scientific, and organizational added value. The current phase of the Technical Detail Report (TDR) aims to select, evaluate, and validate the tools, methods, and organizational structures that will be implemented during the construction phase. The TDR has been structured into work packages detailed below in Fig. 2.

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Figure 2: IT and Data management program organisation with the work package description.

Work Packages (WPs) Organization

The IT and Data Management Program is an integral part of the organization of SOLEIL II, providing support for accelerators, infrastructure, and the BL² program. It is structured into six work packages, each led by a pair of leaders to foster a cross-disciplinary approach that includes accelerators, scientific, and computing teams. These work packages, as summarized in Fig. 2, are further divided into 32 sub-tasks. They encompass various aspects, including organizational improvements, control architecture, future operational tools, data acquisition integration, user experience enhancements, and the implementation of new data processing techniques, including artificial intelligence.

The program is overseen by a steering committee, which reports directly to the SOLEIL Board of Directors.

WORK IN PROGRESS

Organisational WP (SPT1)

This work package, based on our experience, focuses primarily on defining methods and tools to establish common practices early in the construction phase. Our current top priority is to achieve the identified deliverables. It includes the definition of a baseline nomenclature that will used everywhere for control as well as CMMS or PLM up to the purchasing office. Our goal is to prepare for the integration of new hardware systems into lifecycle management tools and promote a shared understanding across teams. We adopt the same approach to manage software (SW) lifecycle upgrade with implementation of CI/CD tools [9] and training teams to the use of Gitlab. The final major ongoing work is the way we share knowledge. Among the tools Atlassian's JIRA [10] and Confluence software are mainly adopted to facilitate collaborative work.

Architecture Baseline WP (SPT2)

The work currently in progress within this work package aims to provide all the building blocks required to interconnect the SOLEIL services developed by various teams. This approach seeks to leverage and maximize the use of data at the facility level rather than in isolated silos. A project known as PLUSS (see details [11]), illustrated in Fig. 3, stands for the Platform for Urbanization at Synchrotron SOLEIL. Technically, we have chosen to implement an Apache Kafka broker and WSO 2 API manager. A TUMBCM021 Kafka broker setup has already been established and is operational for test development purposes. The API manager is already in use for exchanging data between our CMMS and JIRA software. The sample tracking application under development will be the first one using Kafka.



Figure 3: PLUSS architecture.

Among the basis foundation, the control system will continue to rely on TANGO which will be one of the systems connected to PLUSS. In the process of consolidating multiple applications, an essential component is Identity Access Management (IAM) services. Within the existing IT infrastructure, several solutions have been implemented, leading to complexity in maintaining and evolving these applications. An initial assessment of the existing IAM landscape has been conducted, and ongoing work involves cleaning up the Active Directory and transitioning to a unified solution. This initiative encompasses best practices in cybersecurity.

Another planned development within this work package is the enhancement of the control architecture, with the aim of providing a collaborative, flexible, and agile approach to contribute to and utilize services for controlling the accelerators and beamlines. This work includes two primary aspects. Firstly, there are studies to design processes for the continuous integration and automated deployment of software or firmware (FPGA, microcontroller) provided by multiple teams, while ensuring the quality and security of control, acquisition, and processing services. Secondly, plans are underway to offer SOLEIL staff and users an ondemand service approach for driving experiments, maintenance, or other operational activities related to accelerators, beamlines, or laboratories. The potential implementation of cloud-based technologies is being considered, and a scheduled Kubernetes training will provide further insights into the details of this approach.

Enhanced Tools for Operation WP (SPT3)

The performance of the new facility will rely heavily on the implementation of more automated processes in various areas, including control, maintenance, and data processing. The leaders of this work package have decided to initially prioritize beam alignment processes for accelerators and beamlines, as well as sample alignment for experiments. In these fields, the strategy includes the ongoing deployment of robotic arms for tasks such as sample pickand-place applications. A system is already operational at the CRISTAL beamline for powder diffraction [12], and another is scheduled for commissioning in October 2023 at the SWING beamline, where it will be used for pipetting liquid solutions in BioSAXS experiments. Robotic solutions for manipulating X-ray detectors have also been installed at the NANOSCOPIUM beamline for Bragg CDI experiments. Initial results are promising, and commissioning is underway. This automation is not limited to beamlines; it is also being considered for test benches, such as the automated measurement of magnet modules for the new insertion devices of SOLEIL II [13, 14].

Following the lockdown during the COVID-19 pandemic, remote access has been established using the NoMachine solution. This mode of operation will be further enhanced and optimized during the upgrade to provide greater flexibility and make the most efficient use of beam time.

In the maintenance domain, there is a significant increase in the amount of data and parameters, with expectations of handling ten times more data (and ten times faster) for the accelerator. In line with this, an upgrade of the archiving system is in progress, involving the transition from the existing Oracle database to a timeseries-based PostgreSQL database with TimescaleDB. New tools, such as Grafana, are being implemented to provide web-based solutions with dashboards for data visualization and analysis. Additionally, new methods of analysis will be evaluated with the aim of implementing predictive maintenance. This approach will closely align with the ongoing work on AI technology in the Data Valorization WP (SPT6), which is depicted below. Other databases are required early in the construction phase to manage the configuration of systems at each stage of assembly, measurement, and calibration of new parts or systems for the upgrade. These methods and tools will be tested on existing *facility*, with the goal of managing the full lifecycle of hardware and software systems. This includes the ability to automatically reload saved configurations at runtime when a system needs to be replace or initialized after a major failure.

Integrated Data Acquisition WP (SPT4)

In recent years, significant improvements in data collection techniques, particularly the development of on-the-fly services [15], have greatly enhanced data acquisition (DaQ) on beamlines. As a result, the availability of data processing tools has also expanded significantly. Looking ahead to SOLEIL II, our goal is to establish a fully integrated architecture as illustrated in Fig. 4. This architecture will support automated online data processing and visualization, enabling quick and responsive adjustments to DaQ to ensure the highest data quality for rapid scientific result publication.

To facilitate easy access to data processing services, we are in the process of installing and testing the Virtual Infrastructure for Scientific Analysis (VISA) [16] platform, which allows applications to be launched remotely on demand.

The connection between data collection and processing will be facilitated using technical components selected from PLUSS. This architecture will undergo testing on existing beamlines during the construction phase.

Naturally, as we aim to combine the performance of the new accelerators with the fastest data collection methods, we must adapt our storage strategy. SOLEIL has devised a strategy for managing data just produced locally at the facility, while data produced earlier will be curated at General

national data centers. We are currently prototyping this solution in the FITS project [17] project and making data remotely accessible using the GLOBUS tool [18].

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Figure 4: Functional block for the data architecture in the IT integration.

User Experience WP (SPT5)

As previously mentioned in the introduction, our strategy is centered on improving the user experience. The objective of this WP is to enhance the tools used throughout the entire experimental project lifecycle: from project launch and progress tracking to sample management, data analysis, and publication.

Work is currently underway to specify improvements to the user office tools and project lifecycle monitoring. Additionally, we are actively developing a Minimum Viable Product for a sample tracking application (Fig. 5). This application will collect essential metadata related to the samples. Integrating the logbook and taking into account the BAG (Block Allocation Group) access mode are key considerations in its design, although specific solutions have not yet been identified. Regarding the Logbook, testing is ongoing with ElabFTW [19] and Scilog [20].

work may be used under the terms of the CC BY 4.0 licence (© 2023). Finally, when it comes to data publication, SOLEIL is in the process of installing the SciCat data catalog [21], aligning with its data policy that adheres to the open science principles defined in the European standard.



Figure 5: Sample tracking architecture.

Data valorisation WP (SPT6)

In pursuit of increasing the throughput of scientific content, there is a clear need for fast and automated data processing. Currently, the primary software expected by the user communities for data reduction and scientific data

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analysis has been packaged and will be made avaiable through the VISA web interface as Data as a Service (DAaaS). The utilization of Artificial Intelligence (AI) is becoming increasingly important in experimental data processing. Within this domain, scientific techniques such as tomography can benefit from the dynamic research and development activities focused on creating AI-based algorithms and models.

Additionally, this WP explores new approaches in IoT and Big Data architecture and technology as well as Digital Twin. We have initiated log analysis using Elasticsearch [22] as a first step towards improving Machine and Beamlines operations. Initially applied to TANGO logs, this approach will be extended to other sources of data. Currently, this WP is in its early stages of research and the establishment of dedicated expert task forces for AI or IoT is still in progress.

CONCLUSION

SOLEIL II is an ambitious project that encompasses ongoing technical innovation in the design of new accelerator components, new beamlines instrumentation and enhanced data management. Across this digital transformation, Cybersecurity is a collective concern. It is considered in each work packages.

This upgrade also presents a human challenge as we transition teams involved in current operations towards the new engineering challenges required to design state-of-theart facilities.

We approach this project collaboratively, dynamically across SOLEIL teams, contributing to national and European projects, and forming partnerships with other facilities and industries. This project serves as an opportunity to harness and develop the human capital within SOLEIL organization.

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