Digital LEAPS League of European Accelerator-based Photon Sources

LEAPS Integrated Platform: final report

Francis Perez[1], Pedro Fernandes Tavares[2], Rainer Wanzenberg[3], Simone Di Mitri[4], Christopher Arrell[5], Linus Pithan[3], Simone M. Liuzzo[6] and Marco Calvi[5]

[1]ALBA Synchrotron Light Source C. de la Llum, 08920 Cerdanyola del Valls, Spain
[2]MAX IV Laboratory, Lund, Sweden
[3]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany
[4]Elettra-Sincrotrone Trieste S.C.p.A., 34149 Basovizza, Trieste, Italy
[5]Center for Photon Science, Paul Scherrer Institute, Villigen PSI, Switzerland
[6]ESRF, CS 40220, 38043 Grenoble CEDEX 9, France
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Executive Summary. The Digital LEAPS project was launched at the start of the pandemic to address the challenges posed by limited mobility and restricted access to facilities. This report focuses on the achievements of the project's third pillar, the LEAPS Integrated Platform (LIP), detailing its seven work packages, outcomes, and deliverables. Since its inception, the project has seen substantial development, with various activities progressing to different stages of completion. Networking activities, particularly those centered on ongoing projects like the development of permanent magnets for diffraction-limited storage rings and harmonic cavities, have been highly successful. These efforts have significantly enhanced collaboration among laboratories and facilitated knowledge exchange through seminar series and workshops. However, the endeavor to create a LEAPS digital twin for research infrastructure has proven more challenging. This initiative required considerable effort and a significant initial investment. The DiTARI proposal, intended to support this goal, failed to secure enough points for a grant, causing a slowdown in progress and necessitating a major redesign. Despite this setback, the LIP has continued to garner interest from related initiatives. Notably, the Python digital twin project has contributed to identifying and preparing future proposals, increasing the visibility of ongoing activities, and providing initial financial support. These efforts are crucial for maintaining momentum and ensuring the continued success of the Digital LEAPS project.

Introduction

The LEAPS Integrated Platform (LIP) is the third pillar of Digital LEAPS, a project initiated in 2021 in response to the emerging COVID-19 crisis. For more information, see its foundational workshop here, https://indico.psi.ch/event/11213/. It was designed to address some urgent issues of our scientific community following a twofold strategy:

from one side it aimed to build of a Digital Twin (DiT) of the Analytical Research Infrastructure (ARI) to enhance the efficiency of our instruments to produce scientific results, on the other it stimulated networking and design activities among LEAPS members to make their facilities more resilient, power efficient and autonomous. If the DiT summarises our knowledge of the ARI and helps us to improve their performance, the hardware defines its limits, thus we strongly support to approach both sides of the problem at once. The DiT shall be designed as much as possible facility independent to allow easy portability among partners to enhance integration and easy deployment of the results. It integrates existing software to allow start to end simulations of beams along the entire facility and allow automatic interactions from and to the control system to act as a fully developed DiT, making use of Machine Learning (ML) to create surrogate models when needed, reconstruct hidden parameters and optimise the output and to efficiently organise the experimental data results. The DiT shall be available as a service on EOSC for easy accessible and to guarantee high standards of data quality and GUI will be designed to enhance the user experience. In summary, we aim to create a new standard benchmark of DiT at ARI and beyond. To fully profit from this new approach, our facilities shall be equipped (and some partially already implemented them) with Androids (WP3.3) to inspect the hardware while operating them, to acquire full knowledge of the status of the infrastructures and counter act in case of failure without the need of human tunnel access, which would require the shutdown of the facility or part of it. Fourth generation storage rings (also referred as Diffraction Limited Storage Rings, DLRS) require a major change in the accelerator lattice (i.e. multi-bends achromats) which could and should be implemented following the example of ESRF-EBS with permanent magnet technology (WP3.1). This novel approach will increase the brightness of our light sources of about two order of magnitude, will reduce the power consumption and the cost of the operation. Finally, the design of the beamlines shall be modified to fully profit from the enhanced supervision offered by the DiT. For this reason a design study involving all members shall be launched to come up with a blue print reference layout to guide the construction over the next decades of a Fully Automated Beamline (WP3.6).

To support several of the above activities and in particular the development of the DiT, a proposal named *Digital Twin Platform for Analytical Research Infrastructure Experiments* (DiTARI) was submitted the HORIZON-INFRA-2021-TECH-01. Hereafter we present the abstract, which succinctly outlines the project's scope and underscores its ambitious scientific program:

> *DiTARI provides a sustainable solution for digital twinning of complex scientific experiments performed at Europe's most advanced analytical research infrastructures (ARI). Four types of experiment are addressed that offer paths to significant advances in Material Science, including new energy saving and sustainable cellulose fiber*

> *materials, new fabrication processes for affordable and efficient solar cells, and higher accuracy estimates of safety margins for construction steel. This Digital twinning will make preparation, execution and analysis of such experiments more effective leading to higher success rates in these vital areas of research. DiTARI will enhance robust operation of these technologically demanding ARI facilities, providing higher availability of their probe beams with tailored properties, and support autonomous measurement of hidden parameters, reducing operational effort and increasing performance. Integration of artificial intelligence in DiTARI will allow researchers to swiftly compare observational and simulated data during experiments, increasing understanding of the results in real-time. In providing DiTARI as a service in EOSC via the PaNOSC portal, researchers will use DiTARI beyond the ARIs, greatly enhancing their capabilities for planning experiments or analyzing the results at their home institute. The training and tutorial capability of the DiTARI service forms a vital instrument for inclusion of new communities. This includes expert scientific groups new to ARIs and researchers from less developed areas of Europe, and beyond, with low participation in international research. This DiTARI eco-system aims to become the standard for digital twinning at Europe's ARIs, and will be sustained beyond the project duration through implementation at numerous ARIs and extension to other Material Science applications and science disciplines, reaching all research communities looking to use these facilities and capabilities for virtual experiments.*

The DiTARI proposal, alongside another proposal that garnered an identical score, faced exclusion in the selection process. This compelled us to reassess the program, leading to a realistic reduction in the deliverables. The working packages WP3.1, 3.2, 3.3 were designed within the frame of DiTARI and they need a substantial restructuring since the proposal was not financed. Part of the consortium behind DiTARI applied for a new EU call, focusing on the development of the digital twin of the end stations, that was not funded either. **The following report details the seven work packages that constitute the LIP project. The numbering of these work packages has been updated since the original proposal. The first three packages, which were directly related to DiTARI, have been temporarily suppressed. To maintain simplicity, the numbering has been shifted, making the fourth work package now the first.**

1. WP3.1 - Permanent Magnet LEAPS Internal Collaboration (PerMaLIC)

The PerMaLIC collaboration was set-up in 2021, between the LEAPS members, to interchange information, organize workshops, and stablish joint projects on the development of permanent magnets (PM) for accelerators to be used in future light sources. The first action done was creating a mailing list to coordinate actions and generate open discussions: leaps-permalic@desy.de.

Several coordination meetings have been held in order to stablish the priorities and the actions to be performed. In the first meeting the main challenges that have to be addressed with PM were identified: the tunability of the magnetic field required for accelerators; the possible radiation damage after many years of operation; the drift of the magnetic field with the temperature; and the challenge of accurately measure the characteristics of the magnets with small apertures. To address these issues, two main actions were decided, the organization of remote seminars, and the preparation of workshops. Here after the list of seminars held:

- Permanent Magnets developments at STFC. Achievements and lessons learned. By Ben Shepherd, STFC, Daresbury, on December 3rd, 2021.
- Permanent Magnet Longitudinal Variable Dipole: Design, Construction and Test. By Manuel Dominguez, CIEMAT, Madrid, on March 24th, 2022.
- SIRIUS Superbend: Design, Construction, Instalation and Tests. By James Citadine, SIRIUS, Brazil, on June 9th, 2022.
- Radiation Effects of Permanent Magnets. By Ben Shepherd, STFC, Daresbury, on March 31st. 2023.

and hereafter the list of workshops whihc have been organized:

- 1st PerMaLIC Workshop, September 22nd, 2021. Remote. https://indico.cells.es/event/623/.
- 2nd PerMaLIC Workshop, November 3rd-4th, 2022. ALBA. https://indico.cells.es/event/1229/.
- Low Emmitance Ring – Permanent Magnets Workshop, November 14th-15th, 2023. Trieste. https://indico.cells.es/event/1373/.

This last workshop was organized in collaboration with the iFAST project, and was open to industrial contributions. In conclusion, the PerMaLIC collaboration, supported by Digital LEAPS, has successfully convened a community of scientists, experts, and industry professionals in the field of permanent magnets for accelerators.

2. WP3.2 - Harmonic Cavities LEAPS Internal Project (HarmonLIP)

2.1. Motivation

Fourth-generation storage rings based on multibend achromat (MBA) lattices have, over the past 5 years, completely changed the landscape of synchrotron light sources worldwide. In fact, three such new sources are already in operation and many more are in design or construction in Europe, the Americas and Asia, all profiting by the quantum jump in brightness and coherence provided by their ultralow-emittance electron beams. The need for tight control of the longitudinal phase space distribution of particles in these new rings is a consequence of various distinctive features of MBA lattices as compared to third generation sources: first, the smaller momentum compaction factor lowers coherent collective instability thresholds; second, the smaller emittances and resulting higher bunch charge densities leads to short Touscheck lifetime and third, small angle electron-electron scattering (intrabeam scattering, IBS) may significantly deteriorate the emittance compromising the source performance. All of these challenges can be addressed by lengthening the bunches, i.e., stretching them out longitudinally with the use of harmonic rf systems. Even though harmonic RF systems have been successfully in use at third generation sources since many years, they were often added to those sources as part of upgrade programs while they are part of the baseline design on most fourth generation sources, particularly in the intermediate energy range of a few GeV where IBS is most severe. For future light sources aiming to achieve even lower emittances than the present suite of existing and planned sources, good control of the bunch length will be even more critical and one may envisage the need to achieve considerably larger lengthening ratios than those achieved today (which vary from 2 to 5). Combining different harmonic systems may be a mechanism to provide such extremely long bunches, but its feasibility remains to be demonstrated experimentally. Running with stretched bunches comes with its own set of challenges – The reduction of longitudinal focusing and accompanying increase of incoherent synchrotron frequency spread helps damp coupled bunch coherent modes but at the same time may render bunch-by-bunch feedback systems less effective. Coupling of dipole and quadrupole Robinson modes may also impose limits on how close to “flat potential” conditions (settings for which first and second derivatives of the longitudinal potential are zero) one may run at. Achieving equal lengthening for all bunches in a non-uniform fill pattern may be difficult or impossible due to transient beam loading effects. All of these challenges are currently being analysed as part of design efforts of various ongoing projects and are also relevant for the already running fourth generation rings. Theoretical and experimental work on harmonic systems date back many years. However, the recent renewed interest in the topic is clear from the large number of papers on the topic over the past 5 years. Along with the other initiatives in LEAPS, HarmonLIP will contribute to keeping the European leadership in state of the art light sources. The main purpose of the HarmonLIP Leaps Internal Project is to foster information exchange and joint research efforts amongst the LEAPS members for the further development of harmonic cavity/bunch lengthening systems for present and future ultralow emittance storage rings. There are several already existing collaborations amongst various European Facilities that could profit by running under the LEAPS flag. In addition, further collaboration opportunities could be identified through the closer contact opportunities provided by HarmonLIP. Finally, this internal project activity could evolve into a proposal to a future HORIZON Europe call.

2.2. The Project

The HarmonLIP LEAPS internal project was initiated following a brainstorming discussion held in a breakout session of Working Group 2 (Sources) during the LEAPs GA meeting in autumn 2021. The resulting HarmonLIP proposal presented to the LEAPS R&D board in February 2022 consisted in the organisation of networking activities to explore the use of Harmonic Cavity Systems in present and future generation light sources. The project was formally presented by the R&D board to the GA and approved in March 2022. A large interest in the topic was quickly identified as many facilities in Europe and around the world are currently involved in upgrades or green-field developments that all include the use of harmonic cavity systems from day one. Research and development topics expected to be covered by the HarmonLIP collaborative activities included among others, beam dynamics simulation tools for stretched bunches, bunch-by-bunch feedback challenges for stretched bunches, harmonic systems for extremely long bunches, Intra-bunch feedback for extremely long bunches, bunch shortening with harmonic systems, experimental characterization of stretched bunches and stretched bunch stability, intra-beam scattering for non-Gaussian bunches, transient beam loading in harmonic systems, engineering design of harmonic cavity systems and the relative advantages and disadvantages of normal conducting versus superconducting and active versus passive systems. The first HarmonLIP workshop (HarmonLIP 2022) was held in October 2022 at MAX IV Laboratory in Lund, https://indico.maxiv.lu.se/event/5098/. With 50 registered participants from 13 Institutions and 10 countries, 25 talks were held in three sessions: Project Status, Beam Dynamics and Engineering and Diagnostics. Amongst the highlights were the first experimental successful results of a normal conducting active harmonic cavity system developed by the ALBA/HZB/DESY collaboration and lively discussions on the relative merits of normal conducting versus superconducting and active versus passive systems as well as critical beam dynamics aspects that become increasingly important in fourth generation sources: Robinson coupling, Mode 1, feedback and tracking tools. HarmonLIP 2022 was a success and the active engagement of the participants in the intense discussions confirmed that Harmonic Cavity Systems are indeed a very hot topic. HCs will be crucial to the current upgrade projects as well as to future generation storage rings.

The second workshop, HarmonLIP 2024, was hosted in Grenoble with the generous local support of ESRF colleagues. During this event, collaborating institutes discussed the possibility of expanding the scope of their collaboration beyond networking activities. More information about the workshop at https://indico.esrf.fr/event/122/.

3. WP3.3 - Androids for Remote Access

During two days (March 23-24th, 2023) scientists and engineers of the LEAPS laboratories met the CERN colleagues in Geneva to start a collaboration within the frame of Digital LEAPS. The subject was about robotics to be deployed in the harsh accelerator environment to improve access and maintainability of the instrumentation. After a welcome from the LEAPS coordinator Marco Calvi and an introduction on the activities of the CERN hosting group (BE-CEM) by Alessandro Masi (slides), the workshop started with a round table where all invited speakers gave a summary of the activities ongoing in their relative institutes, followed by the visit of the CERN laboratories. The program and the presentations can be found in https://indico.psi.ch/event/14358/ while here below the executive summary and conclusions are reported.

The LEAPS workshop provided an overview of robotic activities across various laboratories, showcasing advancements in remote handling, telepresence, and maintenance within radiation environments. INFN detailed their development of advanced remote handling procedures at the SPES facility, focusing on exchanging radioactive targets. Automatic procedures and new coupling tools were highlighted, with potential interest for the wider community. They emphasized the importance of developing recovery scenarios for potential intervention issues. ELETTRA invested in robotics for telepresence, enabling automated tool delivery to beamline scientists. They highlighted advancements in navigation through AI and image processing, expressing interest in collaborating with other labs for algorithm testing. ASPERON, in collaboration with DESY, presented MARWIN, a semi-autonomous maintenance robot at the EUXFEL, with ongoing efforts to enhance positioning accuracy. They discussed certification requirements and plans for testing MARWIN in different environments. CERN shared their experience in developing electronics for radiation environments and proposed collaboration with LEAPS laboratories. They introduced a new communication protocol and discussed the potential of 5G technology. MAXIV Laboratories reviewed automated processes, emphasizing the need for a centralized automation service. They discussed developments in robotic hardware and software for precise tasks. DESY, operating multiple light sources, highlighted the need for remote maintenance solutions and explored sharing existing solutions with other labs, seeking support from LEAPS. SOLEIL discussed their use of robotic arms and the potential for sharing APIs with other laboratories. They advocated for a common robotic framework and centralized engineering support. PSI developed robotic solutions for repetitive tasks, optimizing magnetic fields of undulators. They highlighted challenges in electronic implementations and proposed solutions for precise positioning sensors. In conclusion, the workshop facilitated knowledge exchange and identified collaboration opportunities. Plans for LEAPS to become a legal entity are underway, with collaboration agreements to be established. Proposals for future projects, including ”androids for remote access,” are in development, underscoring the importance of collaboration and knowledge sharing in advancing robotic technologies for accelerator facilities.

The measurement, qualification and characterisation of the hardware are of paramount importance for commissioning and operating with beam and it is often a time-consuming process which requires on site personnel. An increasing level of automation can critically improve the execution of these tasks, making those activities more pandemic independent. Indeed, DiTARI can be used to control those instruments and to provide remote access to the laboratories with the possibility to perform basic or advanced operations. As androids can access parts of the facility normally forbidden to people due, e.g., to radiation hazards in accelerator bunkers, they can become the eyes and the hands of a human operator. Examples of readily available androids on the market can be found at Boston Dynamics. Furthermore, robots have been developed at laboratories in collaboration with partners. The procurement of such android and its test in the accelerator environment shall be the starting point of this WP. An assessment of its suitability for application in a radiation environment would be essential for its implementation inside the accelerator bunker. Design changes should be evaluated to improve its compatibility with such environment, preferentially involving the procurement companies. The performances of an android should be compared to less advanced robot. The collaboration with universities and research institutes will complement the business relation with the involved procurement companies. In the last 10 years, CERN invested a lot of resources in this domain of automation and a collaboration between LEAPS members and CERN shall be a strategic goal of this WP. A collaboration framework with CERN shall be defined to simplify the technology transfer to the different LEAPS members. The android can be remotely operated by a human who guides each of its actions using enhanced/virtual reality tools. This could be the initial mode of operating them within our facilities. If this approach would be demonstrated successful, a higher degree of automation could be evaluated. This step requires the implementation of machine learning algorithms for pattern recognition to autonomously identify objects of interest and to act on them accordingly to the specific requirements.

4. WP3.4 - Longitudinal Electron Dynamics (LEDs)

4.1. Description

Exchange of theoretical and experimental know-how on longitudinal electron dynamics for X-ray and THZ coherent light sources. The workshop reviewed the rapidly growing topic of electron beam manipulation for coherent light sources, with emphasis on THz and X-ray FELs. In particular, it was devoted to: review the state-of-the-art of light sources, after a 20-years path of research and developments; point out challenges of design and operation of near-future light sources; identify paths of research and development of coherent light sources. The scientific topics covered by the workshop have been grouped in six sessions:

- CompactLight, lessons learned;
- New FEL sources;
- On the true origin of microbunching;
- Diagnostics of microbunching and beam manipulation;
- Magnetic lattices;
- Suppression of microbunching instability.

4.2. LEDS2023 Workshop

The workshop (https://indico.elettra.eu/event/29/) brought together more than 30 experts of design and operation of coherent light sources, to discuss the state-of-the-art control of particle beam dynamics, and opening up new perspectives in the coherent emission of soft X-rays and multi-THz light pulses. The participants were affiliated to 14 European Institutions, plus two scientists from Tsinghua University in China. The number of oral contributions has been 25. Several informal collaborations were established to carry on simulation studies and experiments at Elettra, PSI, MAX IV, for example. A next edition of the workshop is planned to happen in Autumn 2024.

ENEA-Frascati has offered for free the seminar room and the secretary room. Elettra Sincrotrone Trieste has supported the organization with personnel for administrative activity and information technology. The cost of the workshop was €6850, of which €2500 from EU funds managed by Elettra, and €1680 directly reimbursed to Elettra by Digital LEAPS.

The date and venue for the upcoming *LEDS2024* workshop in Bern, Switzerland, have been confirmed, and registration is now open. Registration can be completed through the following link: https://indico.psi.ch/event/15973/.

5. WP3.5 - Virtual Diagnostic (VD)

One key application of Digital Twins in facilities is virtual diagnostics. These tools significantly enhance the effectiveness of beam diagnostic devices such as beam position monitors, screens, and spectrometers. By training neural networks to derive critical quantities that are often not directly available from measured data, these systems can provide deeper insights and more accurate diagnostics. The next step involves implementing these methods in hardware using field-programmable gate array (FPGA) technology, which can reduce processing time to below a microsecond, enabling ultra-fast feedback.

This project involves developing a comprehensive machine-learning-based model for electron accelerators and free-electron laser (FEL) processes. The goal is to provide rapid photon pulses and electron beam properties simulations. Predictive machine learning uses inputs from online electron and photon diagnostics to determine photon pulse properties, such as pulse duration. This approach requires a high-fidelity training set of data for accurate predictions.

To enhance the quality of diagnostic data, both machine learning and other deterministic algorithms are used for fidelity augmentation. This improvement is crucial for obtaining high-repetition-rate photo-electron spectra of photon pulse spectra.

Additionally, the project focuses on advancing electron energy loss measurements and spectral diagnostics. Improvements to data analysis from passive and active electron streaking cavity data aim to accurately measure single-shot X-ray power profiles. Pipelines are being developed to facilitate the online use of this data, enabling real-time diagnostics and analysis.

The results of the first Virtual Diagnostics workshop, held in 2023 at DESY in Hamburg, are presented here https://drive.switch.ch/index.php/s/uGU8u4OumtKhpgT.

5.1. *Summary of the first workshop*

Participants expressed their satisfaction for the valuable exchange of information it facilitated. There was a consensus among representatives from PSI, DESY, and EuXFEL to pursue demonstrative virtual diagnostics, machine learning projects, and combined systems. It was proposed to rename the initiative *Virtual Longitudinal Diagnostics* for better alignment with its goals. Initial virtual diagnostics projects will identify priority areas for upgrades and additions to physical electron and photon diagnostics. The participants committed to building a joint body of work within the next year, aiming to use it as a basis for future grant applications. They emphasized the need for dedicated control and software support at the facility level to develop and support usable virtual diagnostic tools. Key themes emerged, highlighting common areas of interest among the institutions. These included integrating existing FEL models with machine learning for a comprehensive FEL model, fully implementing virtual diagnostics into machine data flow, and enhancing the fidelity of spectral and electron beam LPS measurements. Several test projects were outlined to be completed within the next 6-12 months, including using a surrogate model to predict X-ray pulse properties and reconstructing the phase and temporal profile of photon beams. It was agreed that these projects could be implemented with currently available resources, and support would be provided through members of the working group offering commissioning beamtimes at each other's facilities. Looking ahead, participants acknowledged the need to form work package ideas for future funding calls by early 2024. Plans were made to distribute a summary document and for smaller groups to continue working on the outlined projects, with periodic reports to be shared among the larger group. The next full group meeting was scheduled for early 2024, following the availability of information regarding future grants.

6. WP3.6 - The Fully Automated Beamline (FAB)

Current initiatives understandably look at ways how to make existing facilities, accelerators and beamlines more automatic and resilient. This WP focuses on studying common aspects of highly automated beamlines optimized for remote operation. This could include self-aligning and self-calibrating of the beamline, robotic sample handling or advances measurement scheduling for remote and autonomous operation. Connected engineering questions are:

– Which diagnostics is needed where along the beam path?
– How should the beamline components be designed and constructed?
– How should detectors be constructed so they can auto-calibrate?
– How to adopt standards for sample holders and to implement automated sample change systems ?
– How to achieve increased resilience by through increased experiment stability (compensation of ne-beam-instabilities or of vibrations of optical components)?

Further with respect to software support the analysis could include the following aspects:

– Remote Connection & Cyber Security
– User interfaces including web interface for beamline controls and electronic logbooks
– Standardized interfaces for online data analysis and feedback into beamline controls to steer data driven, autonomous experiments

Since each beamline is different, a rather high level of abstraction is needed per component. The experience of the pandemic induced travel restrictions and restrictions regarding on-site personnel have added significant push towards increased beamline automation. Already, Macromolecular Crystallography (MX) beamlines have a high degree of automation because they perform high throughput standard measurements and can offer mail-in and near-intervention free operation. Meanwhile, other experiments are more highly variable and require more manual intervention. Nevertheless, key components are common between beamlines and can be automated so as to improve efficiency and resilience in the face of personnel limitations. What is missing is the automation of control, and the automation of key intervention steps such as sample changing and ensuring safe operation in the hutches. For example, alignment and focus optimization may be suited to automation. Indeed, all beamlines are currently automated to some extent as key components are motorized due to radiation protection requirements. The purpose of this WP is to identify, develop and share automation of key beamline components to improve resilience and reduce the reliance on human intervention. Similarly, recovery from software faults can be automated so that measurements can continue without human intervention. This requires an investment in high-grade, fault-tolerant controls engineering and interface design. The development of divergent solutions at different facilities is a hindrance. In this WP, the aim is to develop common top-level interfaces and feedback loops that can be implemented on underlying infrastructure at multiple LEAPS facilities. The initial focus will necessarily be on instruments performing near-routine measurements, such as MX, tomography, Small-Angle X-ray Scattering (SAXS), and common beamline components. A third pillar of automation is including remote experimenters in the loop. This involves providing remote data analysis and remote feedback so that decisions about what to do next can be made in collaboration between remote and on-site users. Data analysis pipelines need to be remotely usable and better integrated with the data taking; electronic logbooks need to be integrated into the facility so that remote and on-site users can collaborate and coordinate when not in the same location. An obvious example: paper logbooks are useless when the experiment teams are distributed between those on-site and participating remotely.

Following an initial exploration of various LEAPS facilities, the ROCK-IT (Remote, Operando Controlled, Knowledge-driven, and IT-based) project, funded by the Helmholtz Association (Helmholtz-Gemeinschaft Deutscher Forschungszentren) and accessible at https://www.rock-it-project.de, emerged as a national initiative addressing similar challenges. Consequently, a decision was made to consolidate efforts and establish a broader, international platform for this endeavor with *rock-it* as seed. Multiple joint meetings have since been organized, and leadership of the work package (WP) is now shared with individuals responsible for the ROCK-IT project. This collaboration aims to streamline implementation, minimise duplication, and fully leverage the support offered by the entire LEAPS consortium, while reciprocally benefiting from their expertise.

7. WP3.7 - Python Accelerator Digital Twin (Py-DiT)

Presently, the Matlab Middle Layer (MML) software is used by most synchrotron light source laboratories to link the beam dynamics simulations with commissioning and operation activities. It acts as a digital twin. All required high-level software (from magnet calibration to storage ring optics tuning (LOCO algorithm)) is developed based on beam dynamics simulations in the Accelerator Toolbox (AT). The same code (including user interfaces) is used directly with the real beam by simply switching a global flag (”physics”/”machine” or “simulator/online”). This tool has tremendous advantages for the development of new storage rings and for their commissioning and operation. Moreover, the tools developed in one laboratory within MML are immediately usable by all other laboratories using MML, thus fostering the exchanges between accelerator physicists. However, the Matlab Middle Layer, developed in the 90’s, is becoming difficult to maintain in a collaborative way. Choosing Python to replace MML allows reaching a much wider audience, simplifies interfaces to many other codes used by our community, and will help in the future developments critical for the new fourth-generation light sources. Available python packages allow integrating modern computing techniques such as heavy parallelization (CPU/GPU) or to interface for modern scientific libraries involving advanced data analysis, optimization algorithms or machine learning algorithms that are now a critical aspect of accelerator design and operation. The newly designed Python Accelerator Digital Twin will then be a common work among all involved EU and non-EU institutes, to put together the existing tools and create the missing components (such as graphical interfaces and GPU support). The common project of a Python Accelerator Digital Twin (Py-DiT ‡) would profit from all these recent developments and include all the features of the *MML* software:

- Control system agnostic
- Accelerator agnostic
- Works for transfer-lines, linacs, ramped accelerators
- Digital twin: allows to test tuning tools in real life conditions without need of expensive and rare beam time

It would also, thanks to existing python packages and features:

- remain a fully open source code, but will include a licence (to be defined) to allow integration in the main code production streams (`github`, `conda`, `pip`, etc..)
- include the possibility to be used on large computing clusters for automated commissioning simulations,
- profit from recent beam dynamics developments to be faster and more precise than the existing *MML* (GPU, analytic Jacobians) using state-of-the-art programming techniques and state-of-the-art accelerator-oriented libraries,
- enable seamless connection to our facilities’ control system (EPICS, TANGO, DOOCS, and so on),
- make use of most modern OPENDATA and OPENSCIENCE and FAIR (Findable, Accessible, Interoperable, Reusable) principles. Provide data labeled for Machine

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‡ the collaboration will likely change the name and acronym

learning and Artificial intelligence algorithms include off-line digital twin for tuning tools development and on-line digital shadow for monitoring of indirect observables.

- enable straightforward implementation of available python based Artificial Intelligence and Machine Learning tools (e.g.: `pytorch`, `Badger/Xopt`)
- Enforce thorough documentation and easier/shared maintenance (`github`)
- The operation of accelerators will strongly benefit from such modern numerical tools. The collaboration has just started and it has an high level of participation and commitment from all participants.
- A view of the present preliminary declared involvement for the next 4 years is included in the brainstorming document, but not all laboratories have declared their intentions at the moment.

The action taken toward the creation of *Py-DiT* May 2024 are the following:

- Collaboration start during workshop in October 2023, ESRF (https://indico.esrf.fr/event/93/)
- Meeting in December 2023 (https://indico.esrf.fr/event/119/) to start the realization of a brainstorming document
- Meeting in February 2023 (https://indico.esrf.fr/event/123/) + mini–remote-workshop on Matlab middle layer, Bluesky, Functional Mockups
- Conclusion of the redaction of a brainstorming document (about 20 pages) including all features requested by all laboratories. The document includes:
  - a main overview of the project objectives,
  - the status of the existing tools,
  - a time line for the development in short, medium and long term,
  - schematics of the project developed tools,
  - a table of software packages to be developed and tested in real SR,
  - a table of present resources and names of participants to each task,
  - a possible task subdivision for future application to EU projects,
  - first draft definition of the involved resources by each laboratory.

The next workshop will be held 19-21st June 2024 in DESY (https://indico.desy.de/event/43233/). Start of activities for *Py-DiT* are based on best effort actions. A pre-study project aimed at Linear Optics from Closed Orbit (LOCO) based on existing codes `pyTAC` and `bluesky` is being pursued and hints to a possible overhead introduced by `blueksy`, while `pyTAC` seems a rather good starting point in order to build the whole *Py-DiT* project. The results will be presented at the next workshop.