LEAPS League of European Accelerator-based Photon Sources

LEAPS – WG2 Photon Sources

Marco Calvi

PSI Center for Photon Science

Accelerator Middle Layer Workshop

DESY, Hamburg, 21st June 2024

Overview

- About LEAPS
- LEAPS-INNOV an example of EU project
- Digital-LEAPS the pilot LEAPS Internal project
  - Overview of the LEAPS Integrated Platform as of today
- Conclusion and Outlooks

LEAPS is the largest consortium of analytical facilities world-wide and further expanding its service to an interdisciplinary European user community

19 synchrotrons and FELs - **16** institutions - **10** countries

> 300 operating end stations

> 1.000.000 hours beamtime /year

> 5.000 publications/year

> 15 spin off companies

> 35.000 users from all of EU & beyond

researchers from all research areas

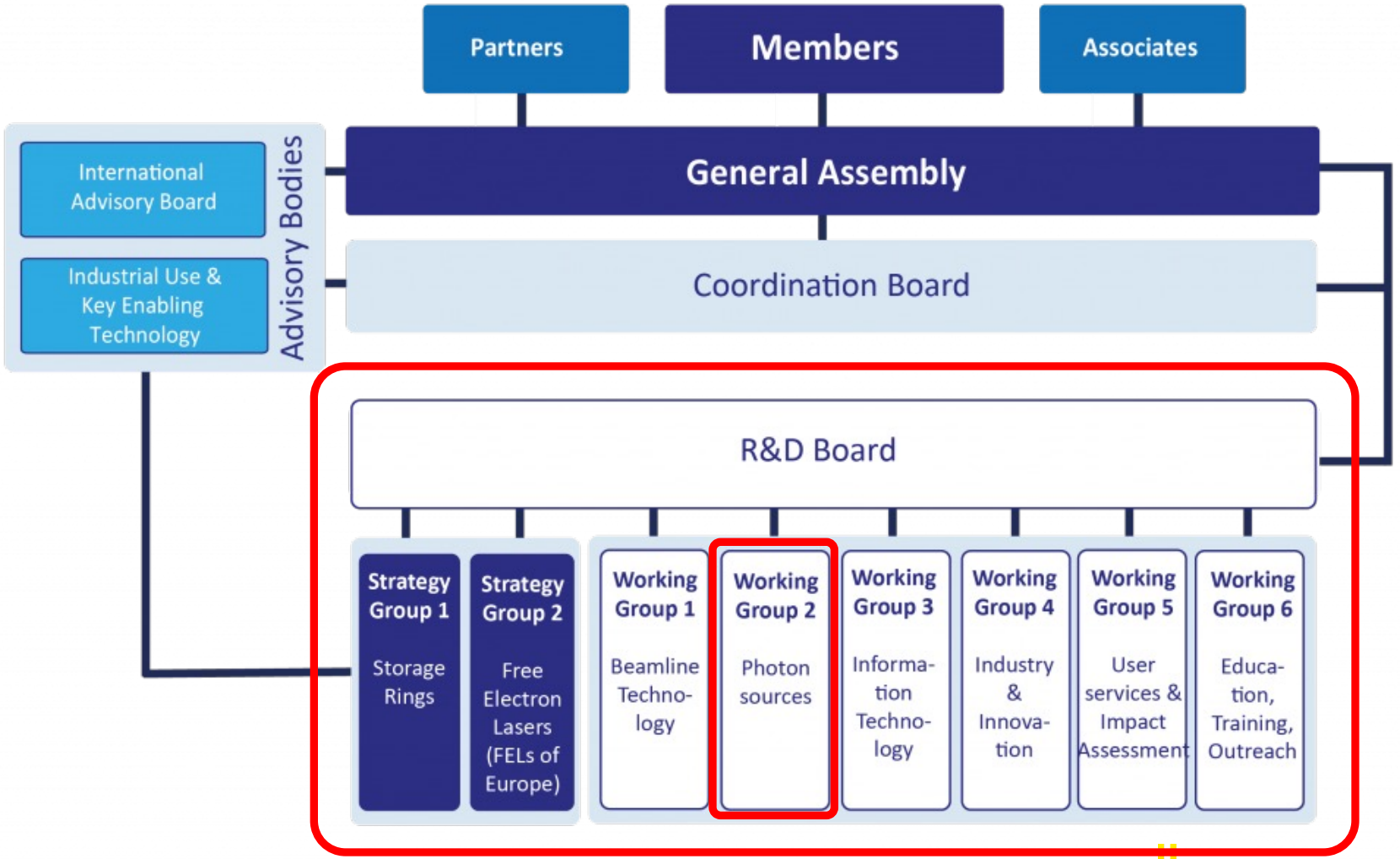
https://leaps-initiative.eu/

https://leaps-initiative.eu/about/leaps-documents/

SESAME LENS Canadian Light Source Centre canadien de rayonnement synchrotron ESUO EUROPEAN SYNCHROTRON AND FEL USER ORGANISATION

Brussels, 13 November 2017

LEAPS Organisation



LEAPS League of European Accelerator-based Photon Sources

LEAPS-INNOV

Open Innovation for accelerator-based light sources in Europe

Six key technology WPs

WP Outreach towards industry

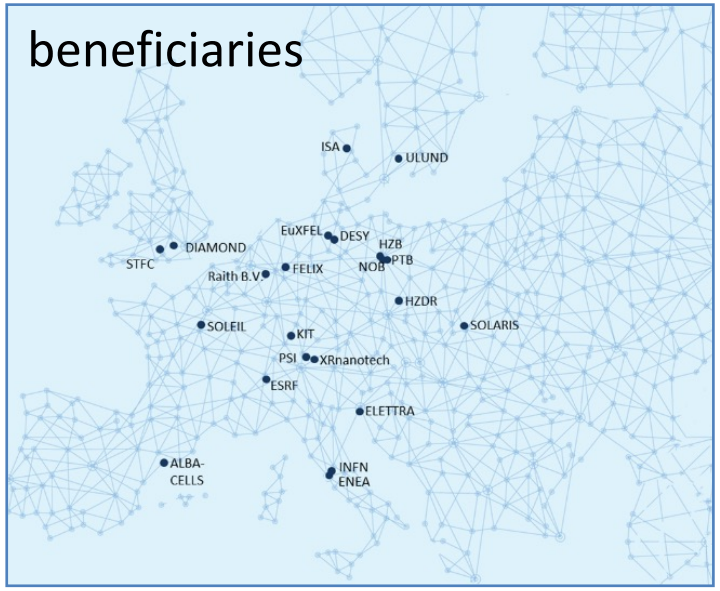
WP Outreach towards user community

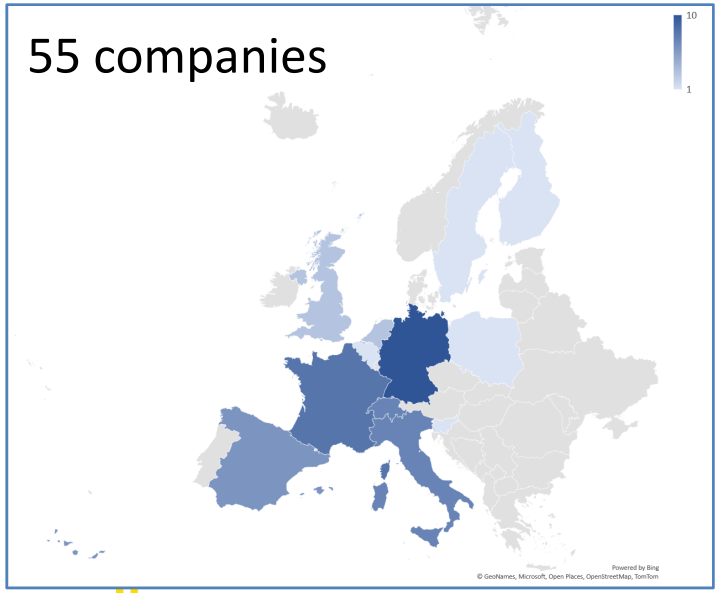
Consortium 24 beneficiaries
all 16 LEAPS members
3 SMEs
3 technology partners
2 users
55 European industrial partners

Budget 10 million EUR from EU
with additional own contribution of
8.3 million EUR

Timeline 4 years, started **April, 2021**

Coordinator DESY





LEAPS League of European Accelerator-based Photon Sources

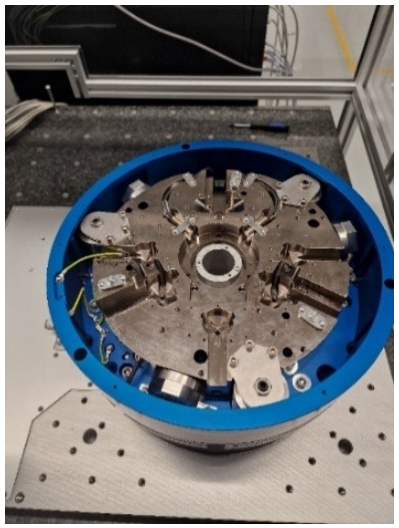
Courtesy of Elke Ploenjes

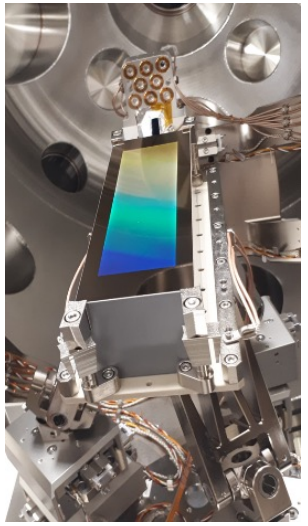
LEAPS-INNOV

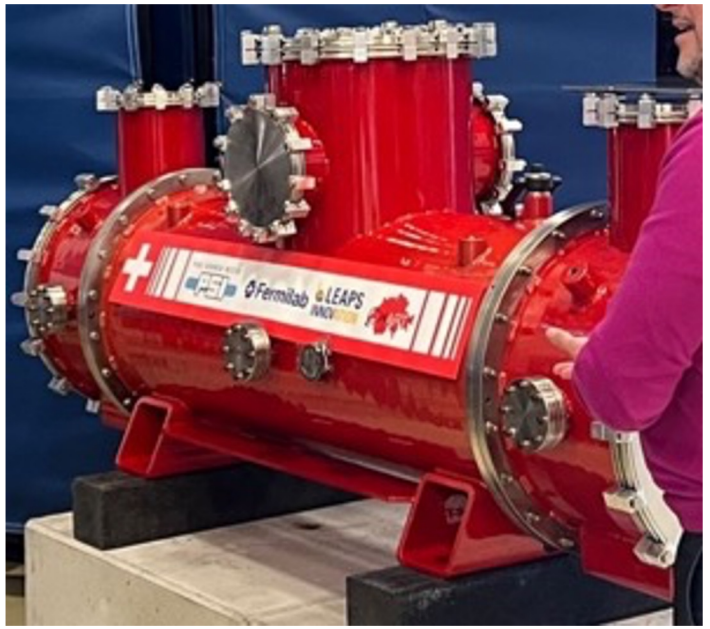
Open Innovation for accelerator-based light sources in Europe

Work Packages

WP1	Project Management and Dissemination
WP2 XAFS-DET	High throughput Germanium X-ray spectroscopy detector
WP3 SuperFlat	Production of high-performance X-ray mirrors, including PCP
WP4 NeXtgrating	e-beam lithography for soft X-ray gratings
WP5 POSIT	New positioning and scanning systems for speed and accuracy
WP6 LIDs	Novel insertion devices
WP7 DATA	Data reduction and compression
WP8 INDUSTRY	Industrial Innovation through Light Sources
WP9 CO-CREATION	Innovation by Co-creation towards Global Challenges







Courtesy of Elke Ploenjes

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Digital-LEAPS

STARS, Enhanced Remote Access for Users:

- Strive for standardized procedures on sample mail-in and remote user access across facilities.
- Provide extensive information on technology tools useful for remote access and digital sample handling.

HR4, Enhanced Digital Platforms for Networking & Training:

- Establish digital collaborative platforms like Innovation Mall for remote and hybrid training.
- Create a smart user network with a strong connection to industry using new tools developed by other pillars.

LIP, LEAPS Integrated Platform:

- Develop a digital interface system for accessing and autonomously operating facilities using AI, machine learning, and virtual diagnostics.
- Design photon instruments for remote access and standards for automated user beamlines.
- Exploit permanent magnets for next-generation diffraction-limited storage rings.

LEAPS League of European Accelerator-based Photon Sources

LEAPS Integrated Platform Workshop

11–12 May 2021
Zoom
Europe/Zurich timezone

Enter your search term

Marco Calvi
marco.calvi@psi.ch

LEAPS Integrated Platform - LIP

This workshop will bring together experts in the field of Digital Twinning (DT), Machine Learning (ML) and Virtual Diagnostic (VD) who apply these methods to the optimisation of accelerator-based light sources (rings/linacs/compact) towards resilient & autonomous operation and address the full facility from source to scientific instruments. The workshop is open to all LEAPS members; colleagues from external laboratories may participate only by invitation.

The objectives of the workshop are :
- set up a detailed survey of the ongoing activities within LEAPS on DT, ML & VD
- draw up a summary document which will constitute the cornerstone of the LIP project.

Workshop organising committee :
Thomas Tschentscher - EUXFEL
Simone Di Mitri - ELETTRA
Marco Calvi - PSI
Eugenio Ferrari - PSI
Jens Osterhoff - DESY
Rainer Wanzenberg - DESY
Pierre Schnizer - HZB
Andreas Jankowiak - HZB
Pedro Fernandes Tavares - MAX IV
Pavel Evtushenko - HZDR
Francis Perez - ALBA

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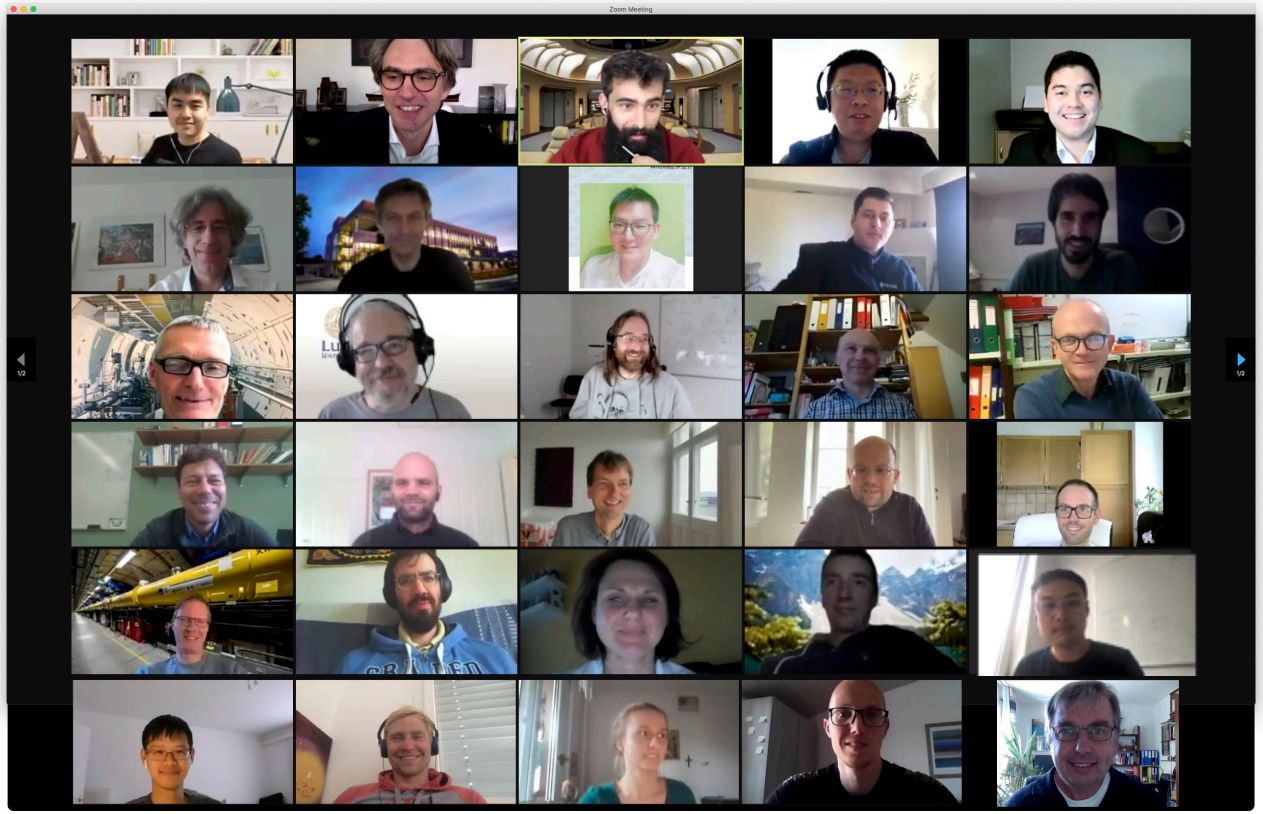
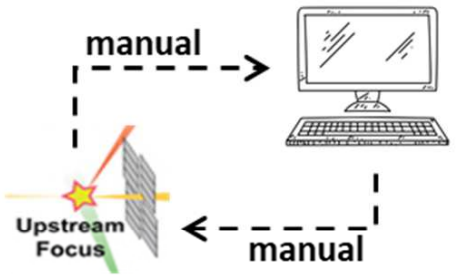
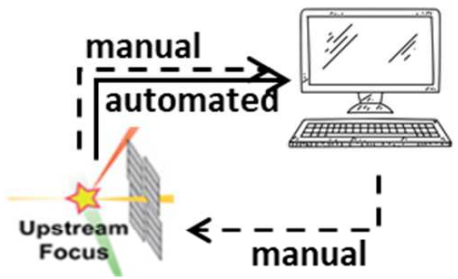
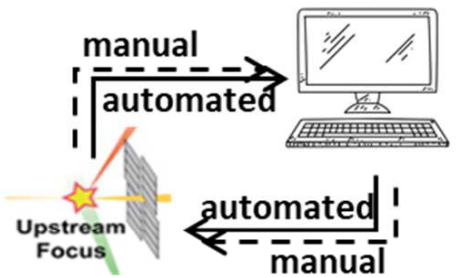
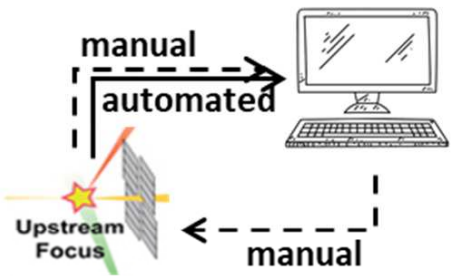


DiTARI Proposal for HORIZON-INFRA-2021-TECH-01

The Technology Platform

shall enable digital twinning to make preparation, execution and analysis of the experiments more effective leading to higher success rates

Preparation	Execution		Analysis
			
Digital modeling Simulation of experiment Probe beam requirements Instrument configuration Sample design	**Digital shadowing** Updating model Comparison of obser-vation & prediction Augmented learning	**Digital twinning** Real-time feedback Optimized parameter selection Automated operation	**Digital shadowing** Data interpretation Re-evaluation of experi-ment parameters Processing data

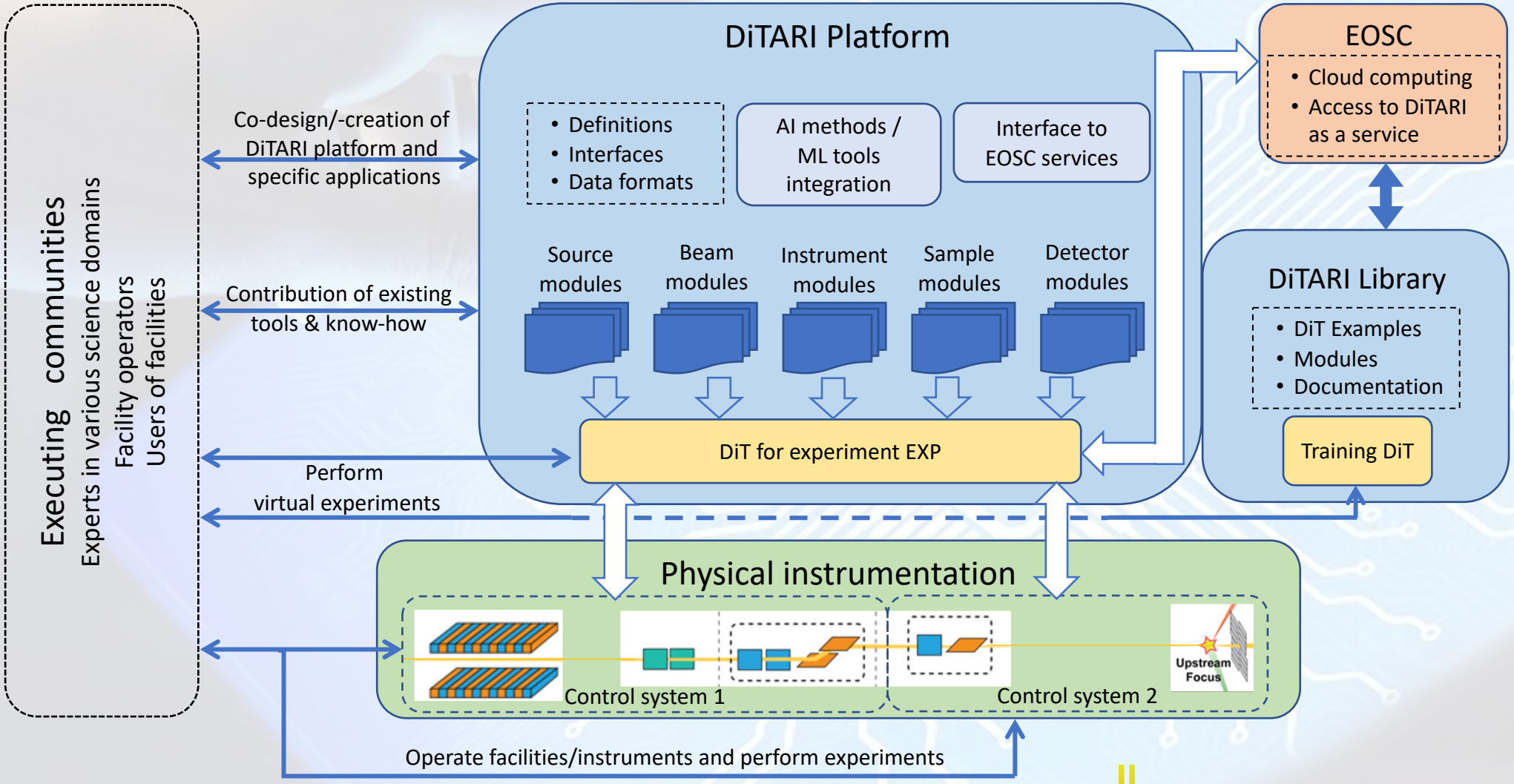
DiTARI Proposal

DiTARI Modules

just a starting point

Area	Available software tool	Application	Location
Source and beams	Genesis 1.3	FEL code	http://genesis.web.psi.ch/index.html
	Ocelot	Multi-physics for Light Sources	https://github.com/ocelot-collab/ocelot
	pyAT	Beam Dynamics	https://github.com/atcollab
	OASYS	X-ray sources and transport, X-ray Optics	https://oasys-kit.github.io/
	WPG	Wave optics	https://wpg.readthedocs.io/en/latest
Instru-ments	McStas	Neutron transport, optics and sample interaction	www.mcstas.org
	SiMEX	X-ray transport, X-ray optics, X-ray matter interaction	simex.readthedocs.io/en/latest/
	OASYS		https://oasys-kit.github.io/
	McXtrace		www.mctrace.org
Sample and sample environ-ments	DCT code	Data processing pipeline for reconstruction of 3D crystal orientation maps from near field X-ray diffraction data. Includes modules for simulation of diffraction images from virtual sample microstructures.	https://sourceforge.net/projects/dct/
	Xraypac	Simulation of dynamics of matter exposed to high-intensity X-rays	https://www.desy.de/~xraypac/index.html
	FEFF	X-ray absorption spectroscopy calculations	http://monalisa.phys.washington.edu/feffproject-feff.html
	Quantum ESPRESSO	*Ab-initio* molecular dynamics, X-ray absorption spectra calculations	https://www.quantum-espresso.org
	LAMMPS	Classical molecular dynamics	https://www.lammps.org

DiTARI Proposal



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PerMaLIC

WP3.1 Permanent Magnets LEAPS Internal Collaboration, PerMaLIC - F. Perez, ALBA

The main goal is to help the transition of our SR based facilities to low consumption DLSR.
Organization of annual face to face workshop and virtual seminars every two months.
Research topics:

- Tunability
- Radiation damage
- Temperature stability
- M-Measurements of small aperture magnets
- **Recycling / Reusing ***

Courtesy of ESRF

*PM Market was USD 20 billion in 2015 expected to grow up to 50 billion in 2024, Report ID: GMI1113, Jan 2017

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PerMaLIC

WP3.1 Permanent Magnets LEAPS Internal Collaboration, PerMaLIC - F. Perez, ALBA

- Kick-off meeting / workshop May 31st 2021 https://indico.cells.es/event/623/
- https://indico.cells.es/event/1229/
- LAST Workshop (with iFAST) on Nov 14th-15th 2023, Trieste, https://indico.cells.es/event/1373/

Courtesy of ESRF

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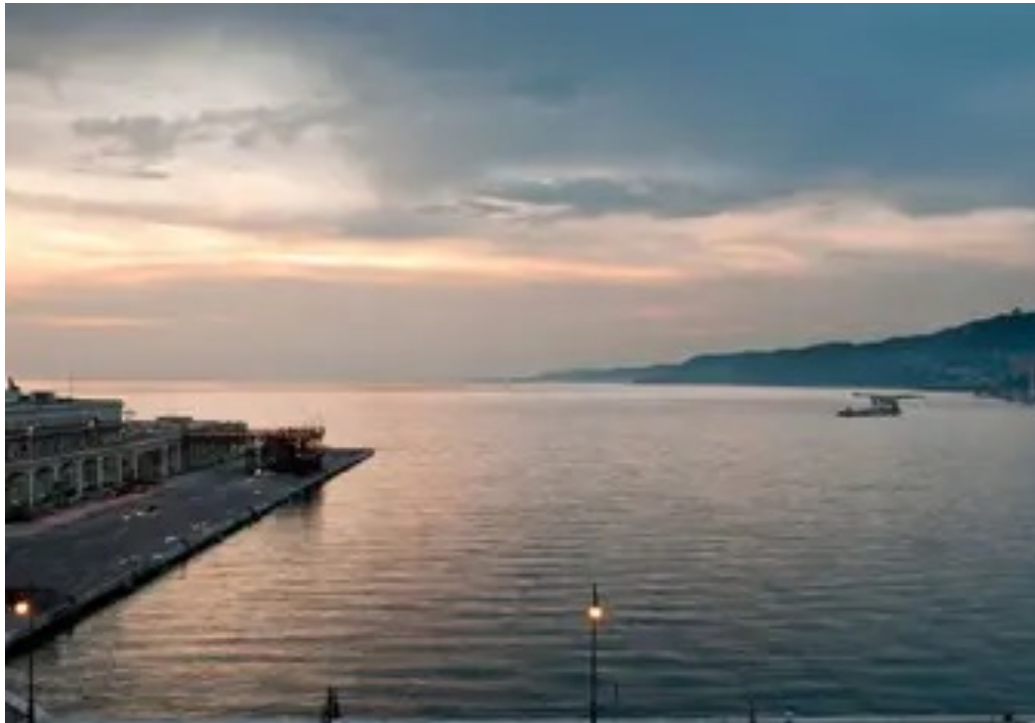
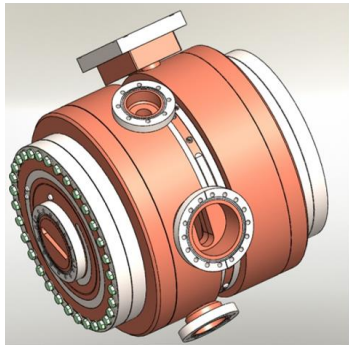
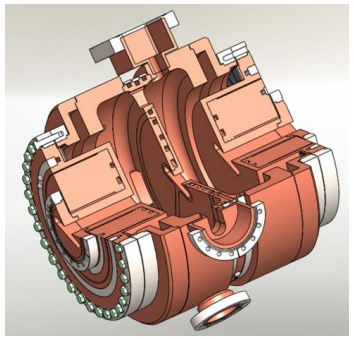


HarmonLIP

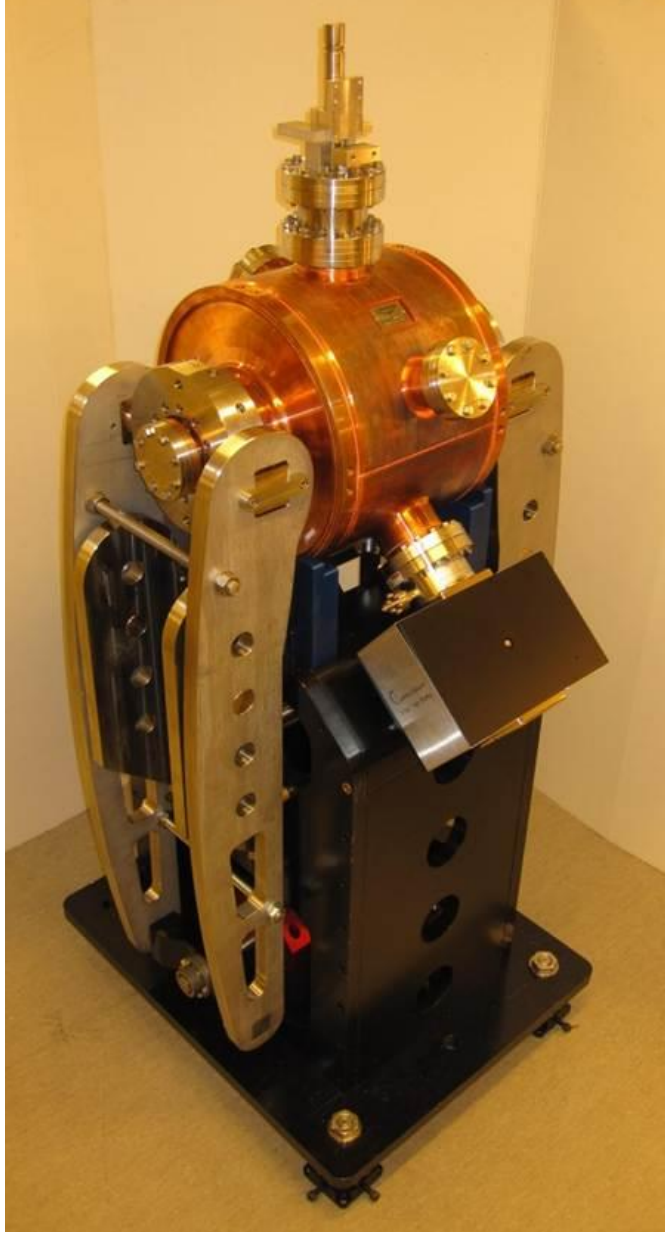
WP3.2 Harmonic Cavities LEAPS Internal Project

- HCs are used since many years in third generation sources to lengthen the electron bunches in order to
  - Improve the beam lifetime
  - Improve stability





- Main topics of the collaboration:
  - Beam dynamics simulation tools for stretched bunches
  - Bunch-by-bunch feedback challenges for stretched bunches
  - Harmonic systems for extremely long bunches
  - Experimental Characterization of stretched bunches and stretched bunch stability
  - Intra-beam scattering for non-Gaussian bunches – theory and experiment.
  - Transient beam loading in harmonic systems



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HarmonLIP

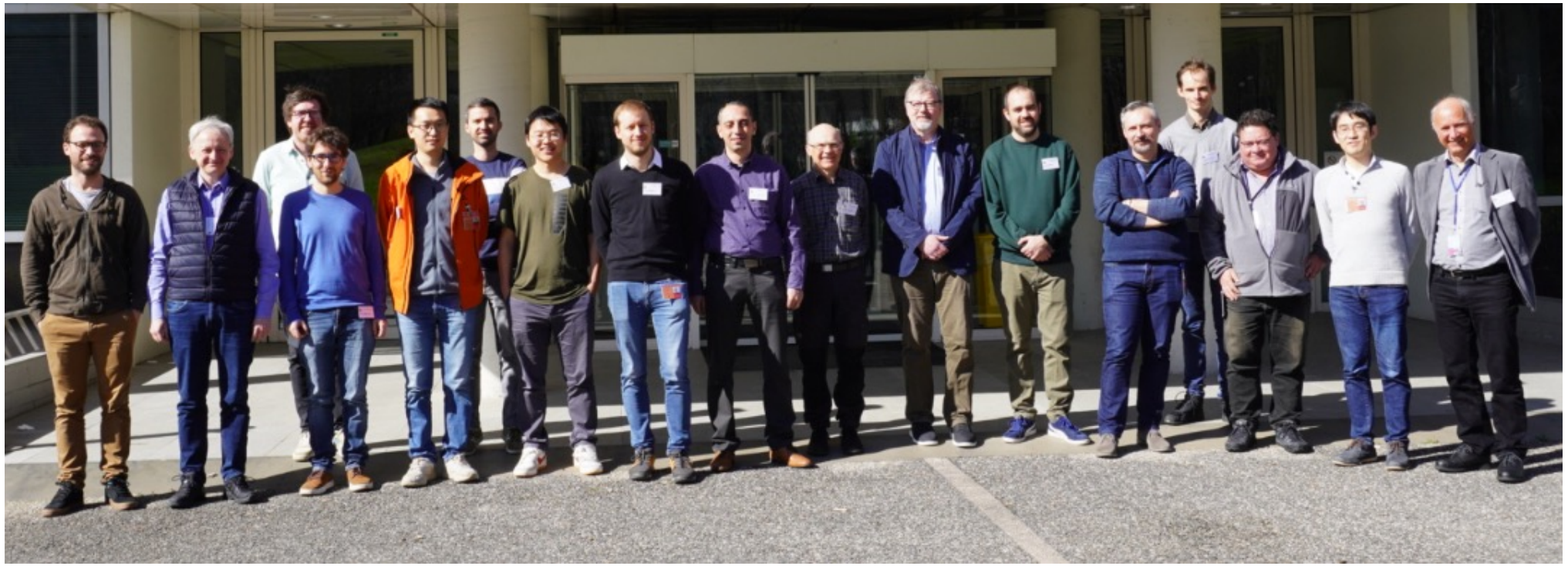
WP3.2 Harmonic Cavities LEAPS Internal Project – P. Tavares, MAX IV

- Kick-off meeting / workshop @MAX IV on Oct 10th-12th 2022, Lund
  https://indico.maxiv.lu.se/event/5098/

HarmonLIP

WP3.2 Harmonic Cavities LEAPS Internal Project – P. Tavares, MAX IV

- Kick-off meeting / workshop @MAX IV on Oct 10th-12th 2022, Lund https://indico.maxiv.lu.se/event/5098/
- Workshop @ESRF on March 19th-20th 2024, Grenoble: https://indico.esrf.fr/event/122/



Androids for Remote Access

WP3.3 Androids for Remote Access

- 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
- Assessment of a commercially available androids within the accelerator environment
- The performance of androids should be compared to less advanced robots

Example of commercially available androids from Boston Dynamics

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Courtesy of André Dehne

Androids for Remote Access

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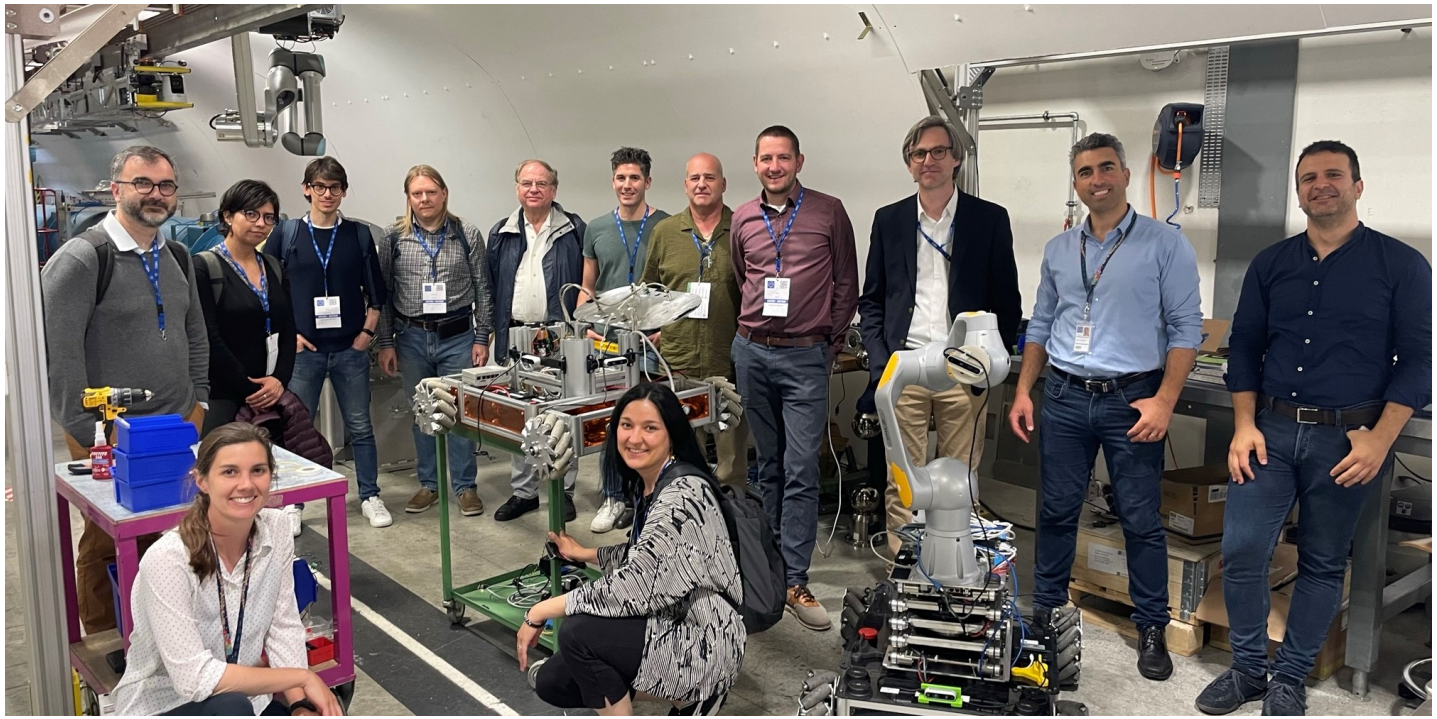
- Assessment of a commercially available androids within the accelerator environment
- The performance of androids should be compared to less advanced robots

Courtesy of M. Di Castro, CERN

Androids for Remote Access

- Androids for Remote Access (**ARA**) - R. Wanzenberg, DESY
  - Kick-off meeting / workshop @CERN on May 23rd-24th 2023, https://indico.psi.ch/event/14358/
  - MoU in preparation between DESY & CERN (to be extended to LEAPS)



Longitudinal Electron beam Dynamics (LEDs)

WP3.4 S.Di Mitri, HZDR-Elettra

– Kick-off meeting / workshop @ENEA on Oct 3rd-5th 2023, Frascati
https://indico.elettra.eu/event/29/

"The workshop aims at collecting the most recent advancements in the controlled generation of high brightness electron beams from photo-injectors for coherent light sources. Open routes of research in the manipulation of modulated electron beams will be investigated. Future experiments, supported by specific technological developments, and their comparison with accurate massive simulations, will be proposed and discussed."

Longitudinal Electron beam Dynamics (LEDs)

WP3.4 S.Di Mitri, HZDR-Elettra

- The workshop will run from September 17th to 19th in Bern, Switzerland, and will be a talk by invitation-only, in-person event: https://indico.psi.ch/event/15973/

"The workshop aims to collect the most recent advancements in high brightness electron sources: this year's event will focus particularly on ***scattering, instabilities, and other collective effects*** *that impact brightness in FELs and storage rings."*

Overview
Timetable
Contribution List
Registration
Registration and Payment Information
Participant List
Venue and Travel Information
Lodging Information

Contact
thomas.lucas@psi.ch
shawn.bell@psi.ch

The second annual workshop on Longit
will be run by the **Paul Scherrer Institut**
brightness electron sources. This year's
collective effects that impact brightnes
September 17th to 19th in **Bern, Switze**
the **20th of September**, we will have a v
exchange of ideas, and we will leave an
participate in the workshop please cont
Simone Di Mitri (simone.dimitri@elettra

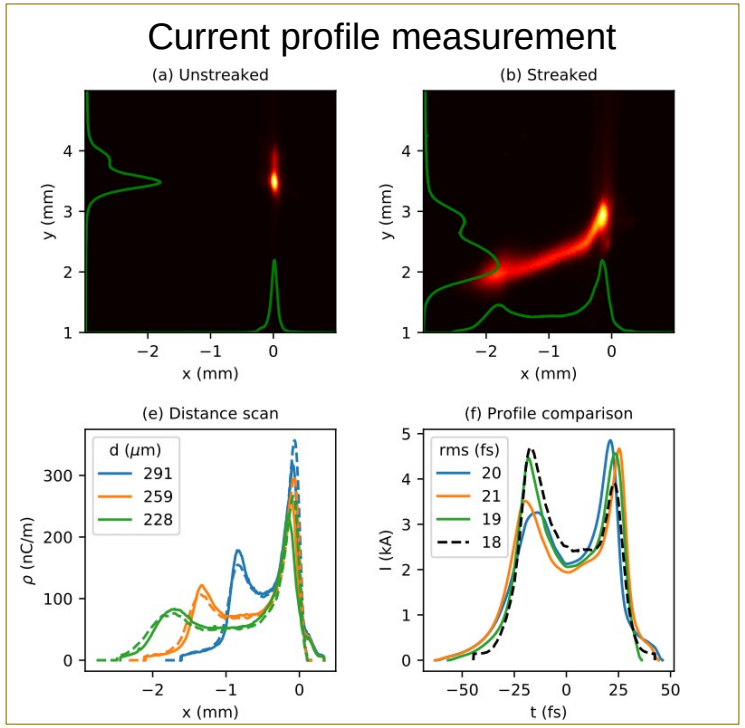
Starts 17 Sept 2024, 07:00
Ends 20 Sept 2024, 14:30
Europe/Zurich

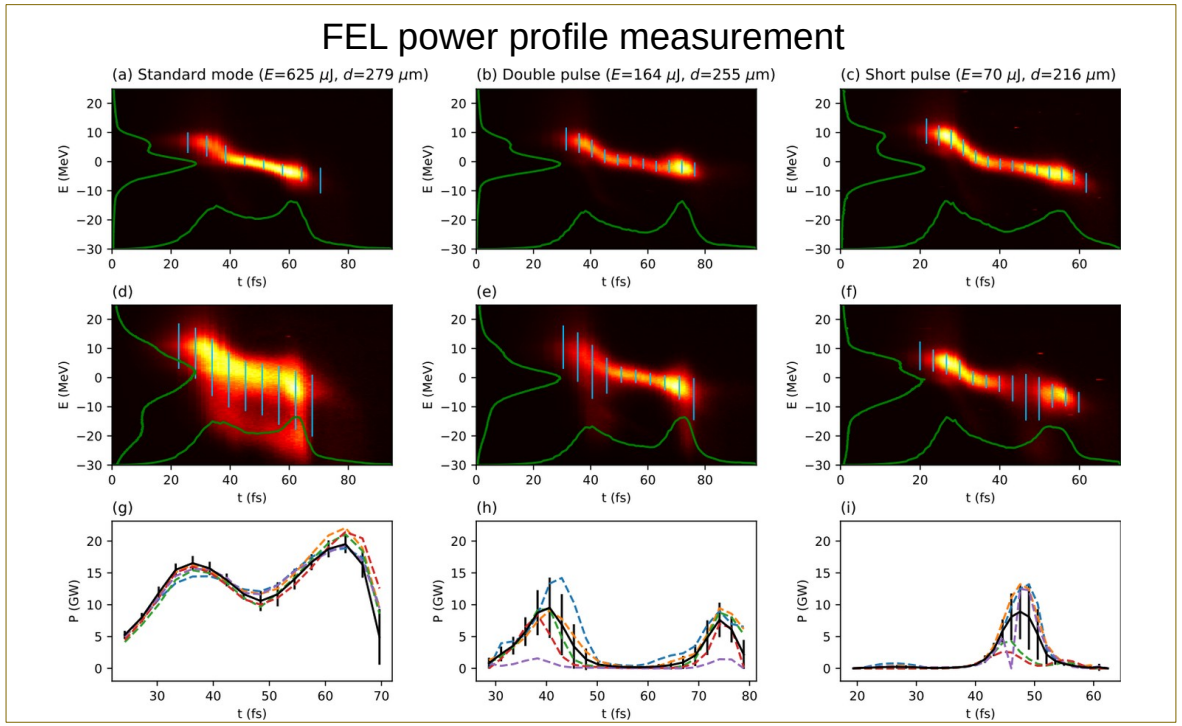
Thomas Geoffrey Lucas

Virtual (Longitudinal) Diagnostic

WP3.5 Virtual Diagnostic (VD) - C. Arrell, PSI

- kick-off meeting @DESY on Sep 28th-29th 2023, Hamburg





Courtesy of P.Dijkstal, PSI

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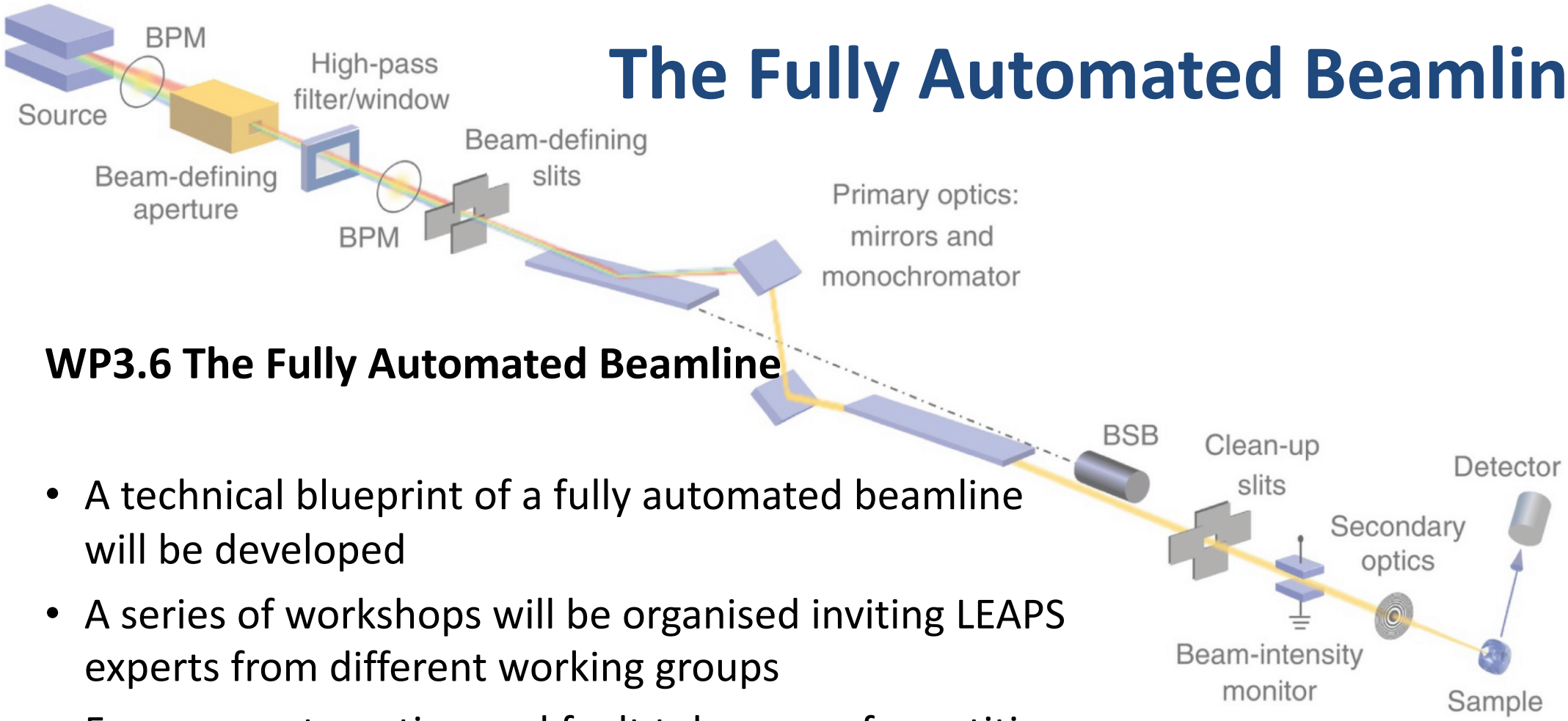
The Fully Automated Beamline



WP3.6 The Fully Automated Beamline

- A technical blueprint of a fully automated beamline will be developed
- A series of workshops will be organised inviting LEAPS experts from different working groups
- Focus on automation and fault tolerance of repetitive tasks like:
  - beamline alignment, focus, sample alignment, fault tolerance, maintaining safe operation
  - detector calibration, software configuration, parameter selection

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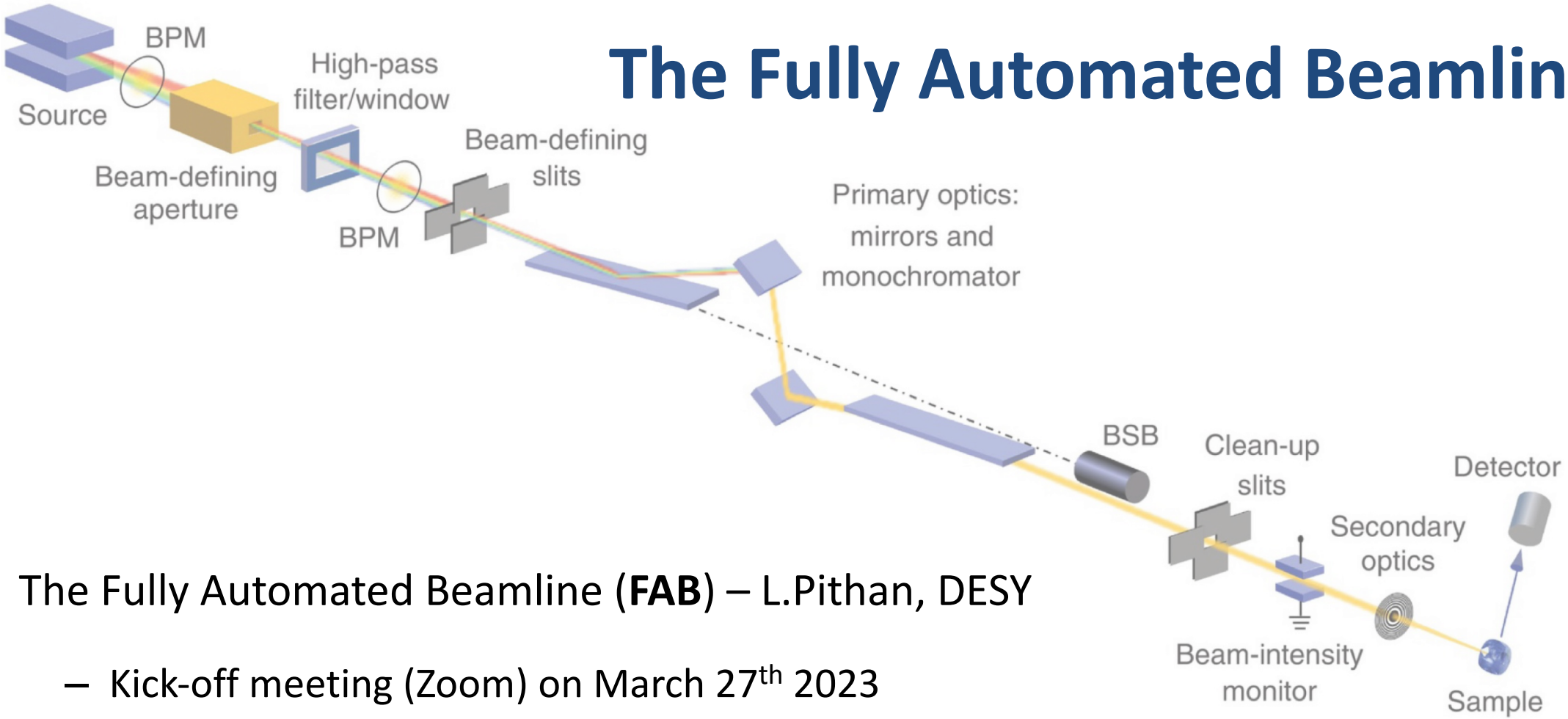
The Fully Automated Beamline



The Fully Automated Beamline (**FAB**) – L.Pithan, DESY

- Kick-off meeting (Zoom) on March 27th 2023
- The leadership of this WP is now shared with individuals responsible for the ROCK-IT project: https://www.rock-it-project.de
- with the aim to establish a broader, international platform for this endeavour with ROCK-IT as seed.

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Py-DiT

WP3.7 – S.M.Liuzzo

The python digital twin would provide a long term solution in an open source license free environment:

- Simplified collaborative development,
- integrate modern CI/CD approach
- Clean and simple installation procedure
- Easy to interface with others recent developments using modern techniques such as advanced correction algorithms (pySC) or AI/ML optimizers (Badger/Xopt) and HPC implementation of pyAT (MPI/GPU)
- Clear automatically generated documentation
- Works for any accelerator (ring, linac, transfer lines) and control systems

Courtesy of Simon White, ESRF

SUMMARY

1. Permanent Magnet LEAPS Internal Collaboration (**PerMaLIC**) - F. Perez, ALBA
   https://indico.cells.es/event/623/ https://indico.cells.es/event/1229/ https://indico.cells.es/event/1373/
2. Harmonic Cavities LEAPS Internal Project (**HarmonLIP**) - P. Tavarez, MAXIV
   https://indico.maxiv.lu.se/event/5098/ https://indico.esrf.fr/event/122/
3. Androids for Remote Access (**ARA**) - R. Wanzenberg, DESY
   https://indico.psi.ch/event/14358/
4. Longitudinal Electron Dynamics (**LEDs**) - S.Di Mitri, HZDR-Elettra
   https://indico.elettra.eu/event/29/ https://indico.psi.ch/event/15973/
5. Virtual Diagnostic (**VD**) - C. Arrell, PSI-EUXFEL
   https://drive.switch.ch/index.php/s/uGU8u4OumtKhpgT
6. The Fully Automated Beamline (**FAB**) - L. Pithan, DESY
   https://www.rock-it-project.de
7. Python Accelerator Digital Twin (**Py-DiT**) - S. M. Liuzzo, ESRF
   https://indico.desy.de/event/43233/

SUMMARY

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   https://indico.maxiv.lu.se/event/5098/ https://indico.esrf.fr
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7. Python Accelerator Digital Twin (**Py-DiT**) - S. M.
   https://indico.desy.de/event/43233/

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]

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[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
June 17th 2024

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:

Conclusion and outlook

- LEAPS is a strategic consortium created in 2017 by our directors, *"whose primary goal is to actively and constructively promote and ensure the quality and impact of fundamental, applied and industrial research carried out at their facilities."*
- LEAPS supports applications to EU calls:
  - directly as it is the case for LEAPS-INNOV and OptiBEAM and
  - indirectly, as for DiTARI, EU-MAHTS etc.
- LEAPS promotes internal projects and Digital-LEAPS is its pilot
- After 8 years from its foundation, LEAPS will transform in 2025 into an AISBL: (*Association Internationale Sans But Lucratif*)
  - to Increase its visibility in Brussels
  - to establish a new and more effective way to finance R&D via a BLOCK-GRANT
- LEAPS organises conferences:
  - LEAPS meets Quantum Technology (ELBA, 2022)
  - LEAPS meets Life Science (ELBA, 2023)
  - NEXT about "Advanced Materials for Energy" (Gdańsk, Poland, 2025)