LEAPS League of European Accelerator-based Photon Sources

Report on

LEAPS Integrated Platform

Marco Calvi, Paul Scherrer Institute

PAUL SCHERRER INSTITUT PSI

ICALEPCS 2021: 2nd Data Science and Machine Learning Workshop

15 Oct 2021

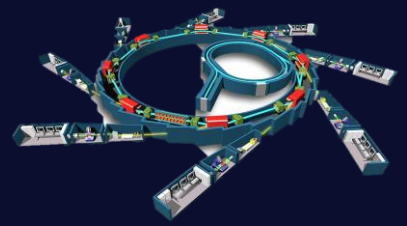
Overview

- Few introductory words about LEAPS
- The Digital LEAPS Initiative
  → **L**EAPS **I**ntegrated **P**latform, **LIP**
- Reporting back from last Spring *"LIP Workshop"*
- HORIZON-INFRA-2021-TECH-01-01:
  an opportunity to support **LIP** over next 4yrs
  → The **DiTARI** Proposal
- Conclusions

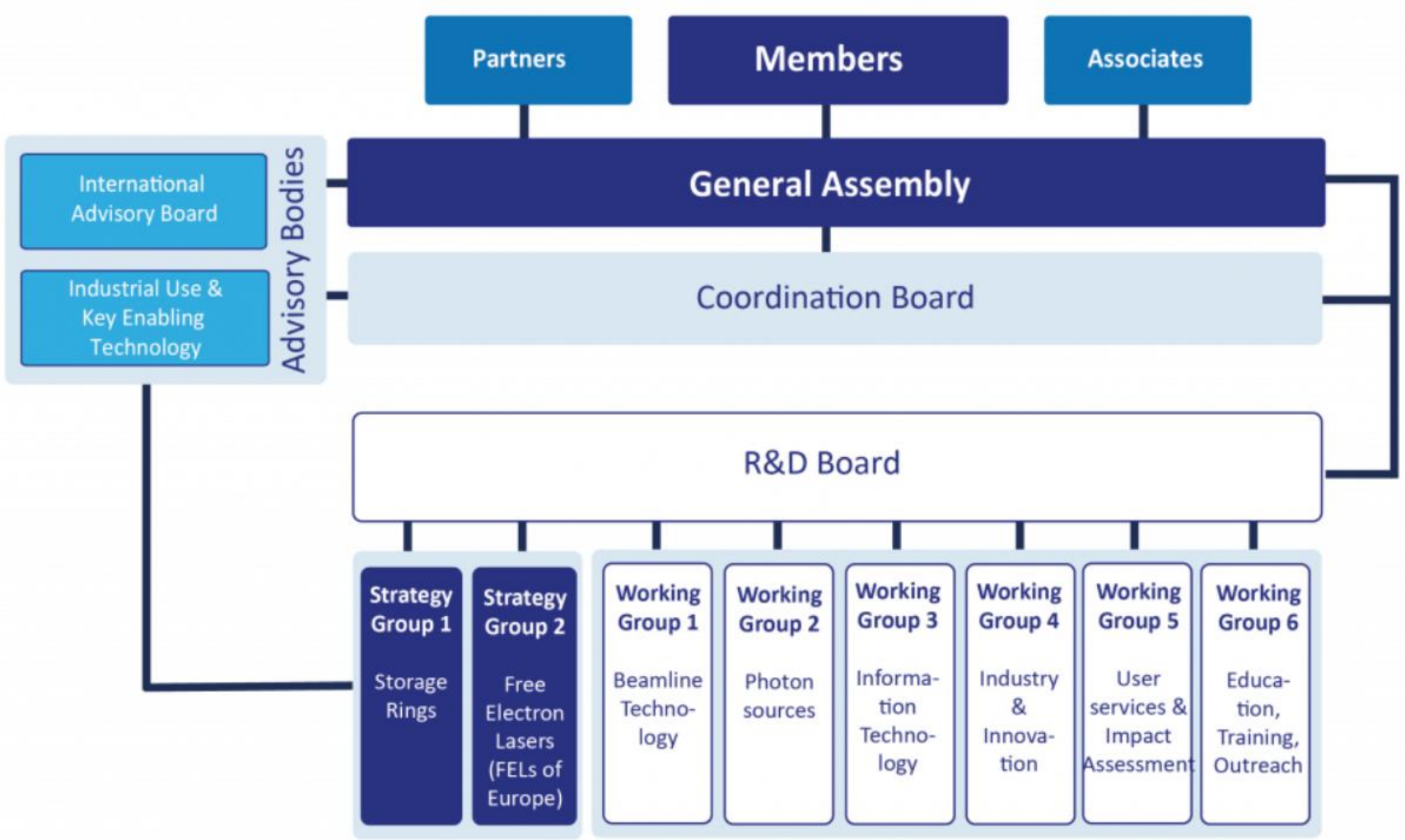
LEAPS League of European Accelerator-based Photon Sources

A new consortium of excellence in Europe devising a transformative level of coordination and integration

13 European Synchrotron Radiation and **6** FEL Facilities are joining forces to master the challenges of the next decades



LEAPS Organisation



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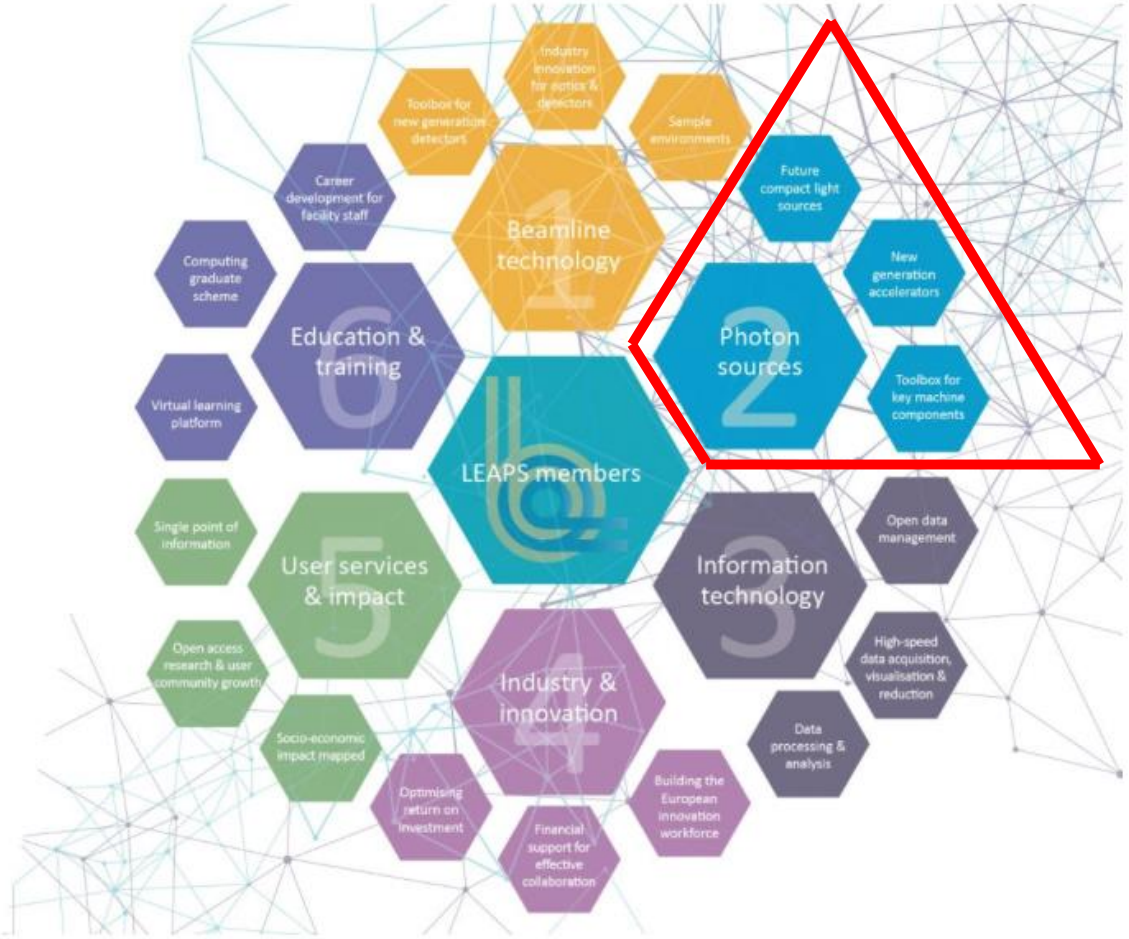

Work Groups & Strategy Groups

WG1, **Beamline Technology**: Heinz Graafsma, DESY; Ray Barrett, ESRF; Klaus Kiefer, HZB

WG2, **Photon Sources**: Marco Calvi, PSI

WG3, **Data Management & Software**: Mark Heron, DLS; Daniel Salvat, ALBA; Steve Aplin, EuXFEL; Darren Spruce, MAX IV

WG4, **Innovation & Industry**: Ed Mitchell, ESRF; Elizabeth Shotton, DLS; Alejandro Sanchez, ALBA

WG5, **User Services & Impact Assessment**: Cecilia Blasetti, Elettra

WG6, **Education & Training**: Franz Hennies, MAX IV

SG1, **Storage Rings**: Amina Taleb, SOLEIL

SG2, **Free Electron Lasers**: Michele Svandrlik, Elettra

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Digital LEAPS

- Within LEAPS steps are taken to strengthen the use of digital methods with the goal to make the operation of the facilities more resilient, efficient and performant
- Starting from WG2 (Sources) a proposal was developed to work towards an integrated platform: **L**EAPS **I**ntegrated **P**latform (**LIP**)
- This includes signals from the accelerators and instruments to optimize the experiments
- This part was augmented by the intention to work towards automated beamline alignment
- As a first step towards formulating concrete activities and deliverables the WG2 considered it important to establish a status what is already done at LEAPS facilities (and beyond).

→ This was the starting point for last Spring **LIP** workshop on:

Digital **T**winning, **M**achine **L**earning & **V**irtual **D**iagnostic

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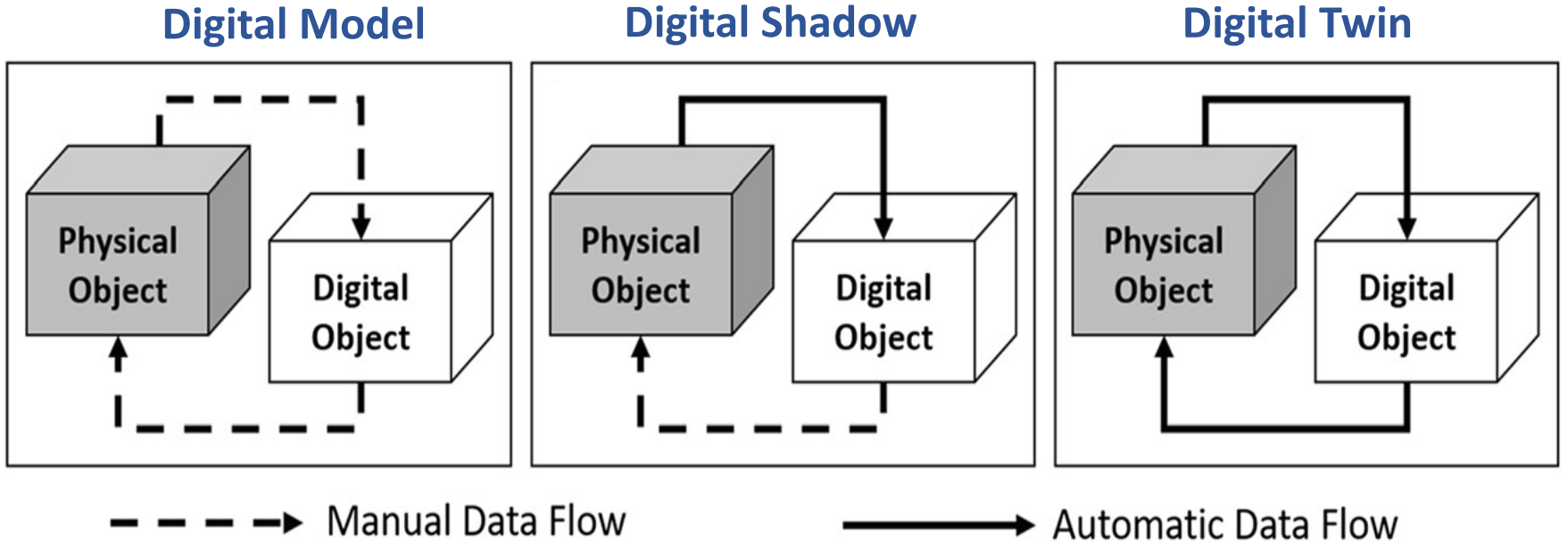
Digital Twinning

From talk by N. Leclercq
ESRF



- Presentations from several facilities reported about existing & operable “DTs”
- Automatic connection wanted!
- Applications for design and/or operation (accelerator, x-ray beam transport…)
- Purpose and implementations vary widely
- Aspects of complex simulation (accuracy) vs. fast feedback (real-time)
- Computing challenges addressed

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Digital Twinning

From talk by S. Liuzzo
ESRF

THE EBS SIMULATOR

Test in progress…. Tested ▯ Tested ▯

User → Control software → hardware → Electron beam

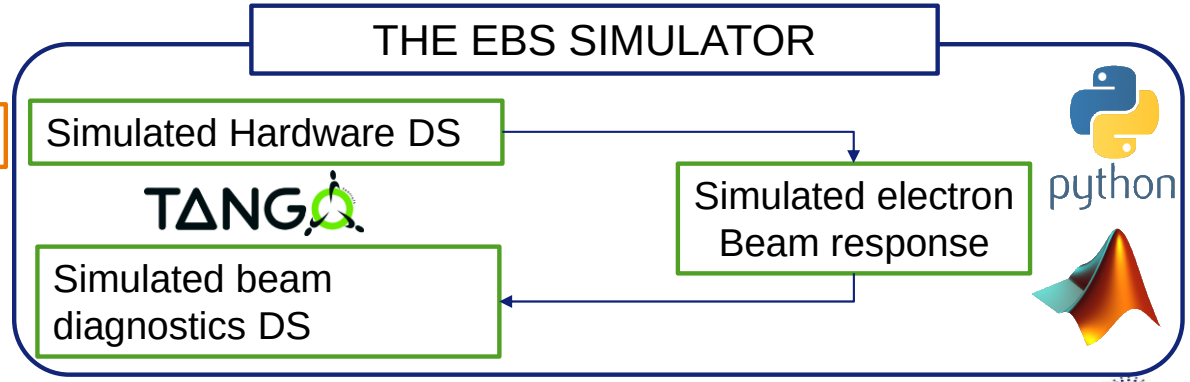
Go to
133 pm!

TANGO

Replace the electron beam by software!

Applications → High level Device Servers

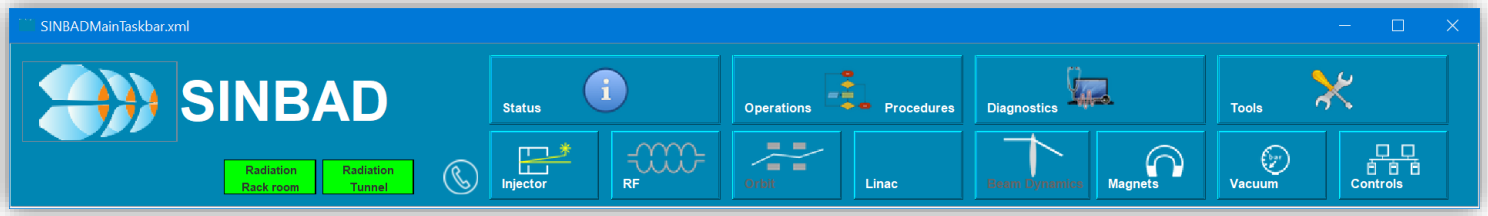
To be tested in the EBS-Simulator
CTRM PRODUCTION SOFTWARE



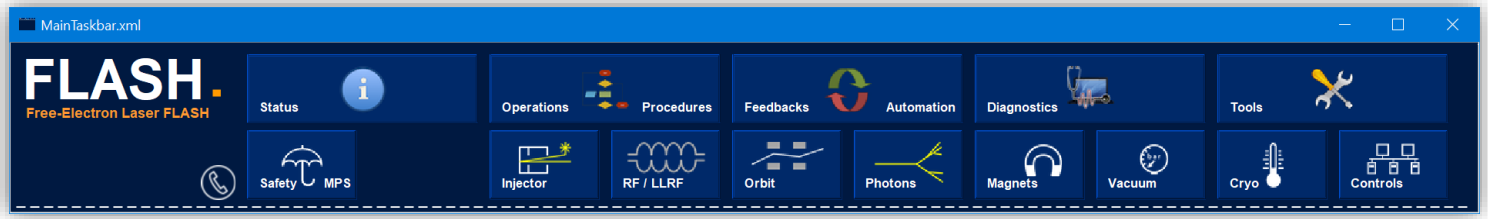
Same DeviceNames/Attributes/Commands as CTRM

Digital Twinning

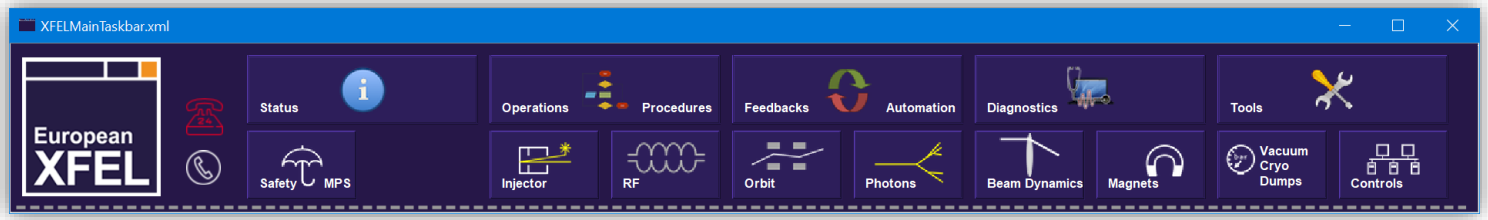
From talk by L.Fröhlich
Europen XFEL



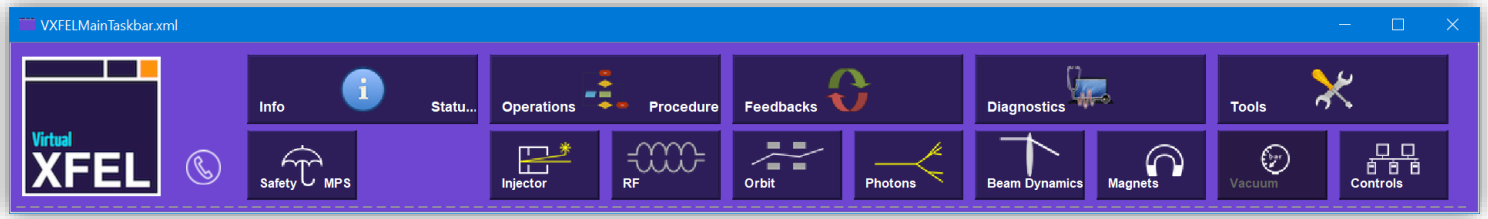
SINBAD–ARES
Linear Accelerator



FLASH
Free-Electron Laser



European XFEL
Free-Electron Laser



Virtual XFEL
"Digital Twin" of European XFEL

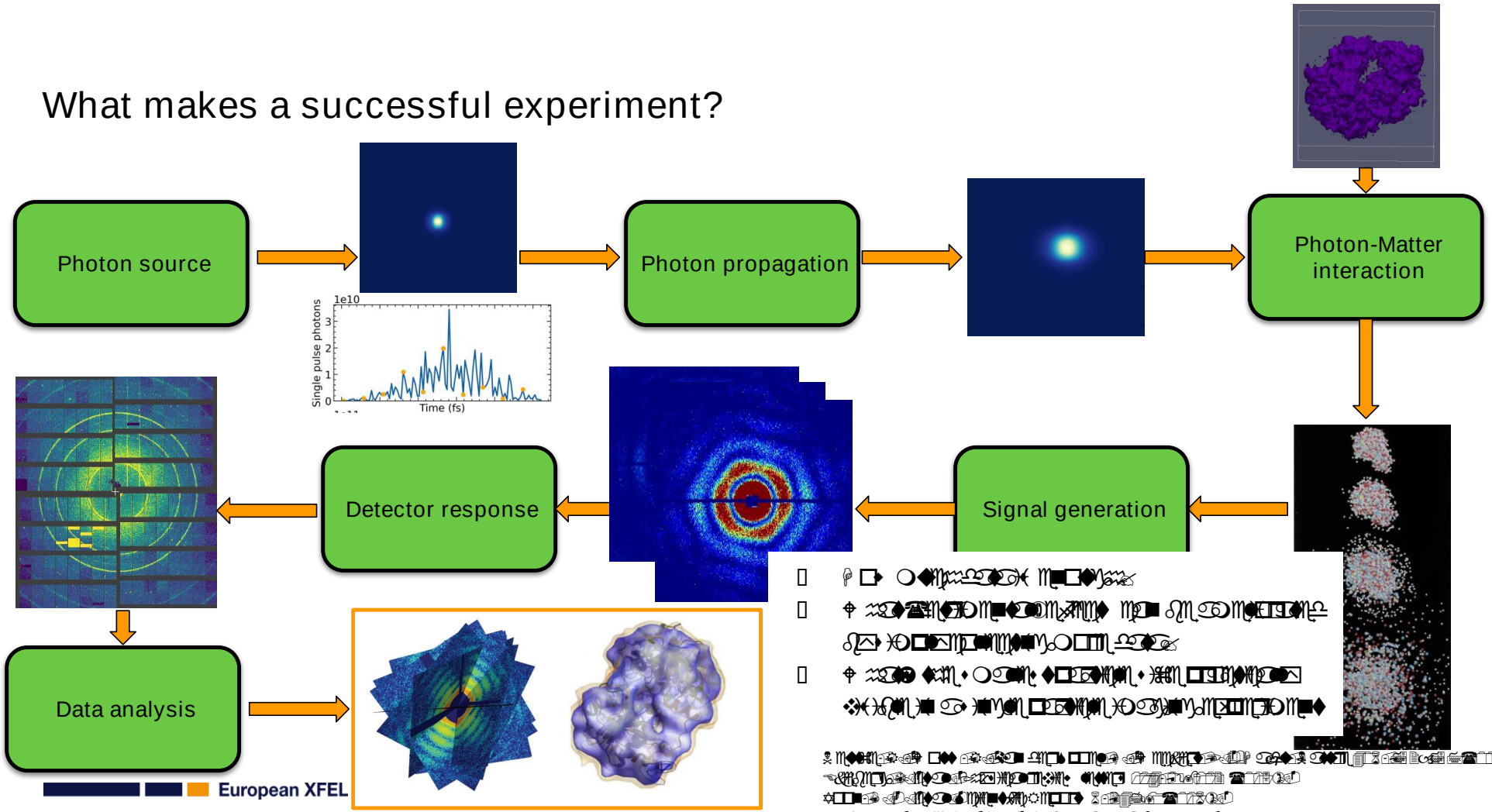
League of European
Accelerator-based
Photon Sources

Digital Twinning

SiMEX

From talk by E Juncheng
European XFEL

What makes a successful experiment?

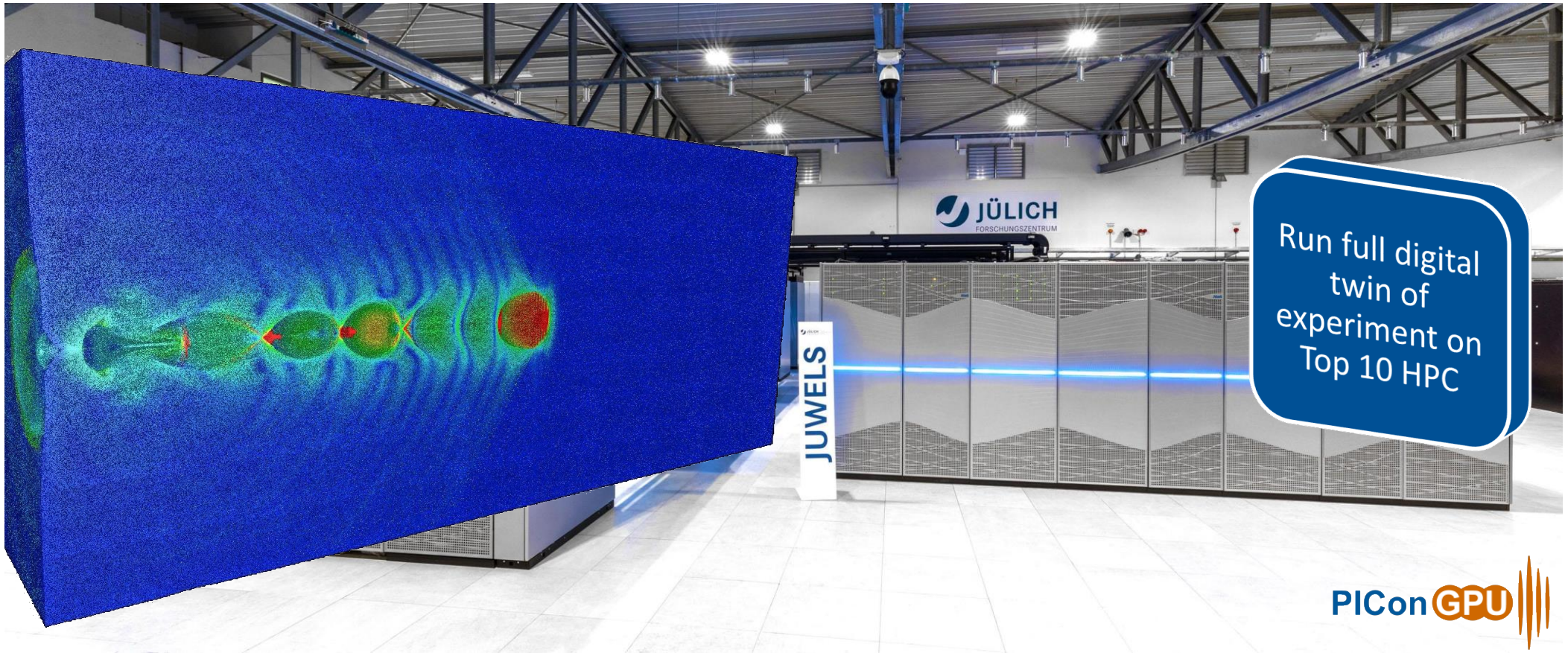


Digital Twinning

From talk by M.Bussmann
CASUS

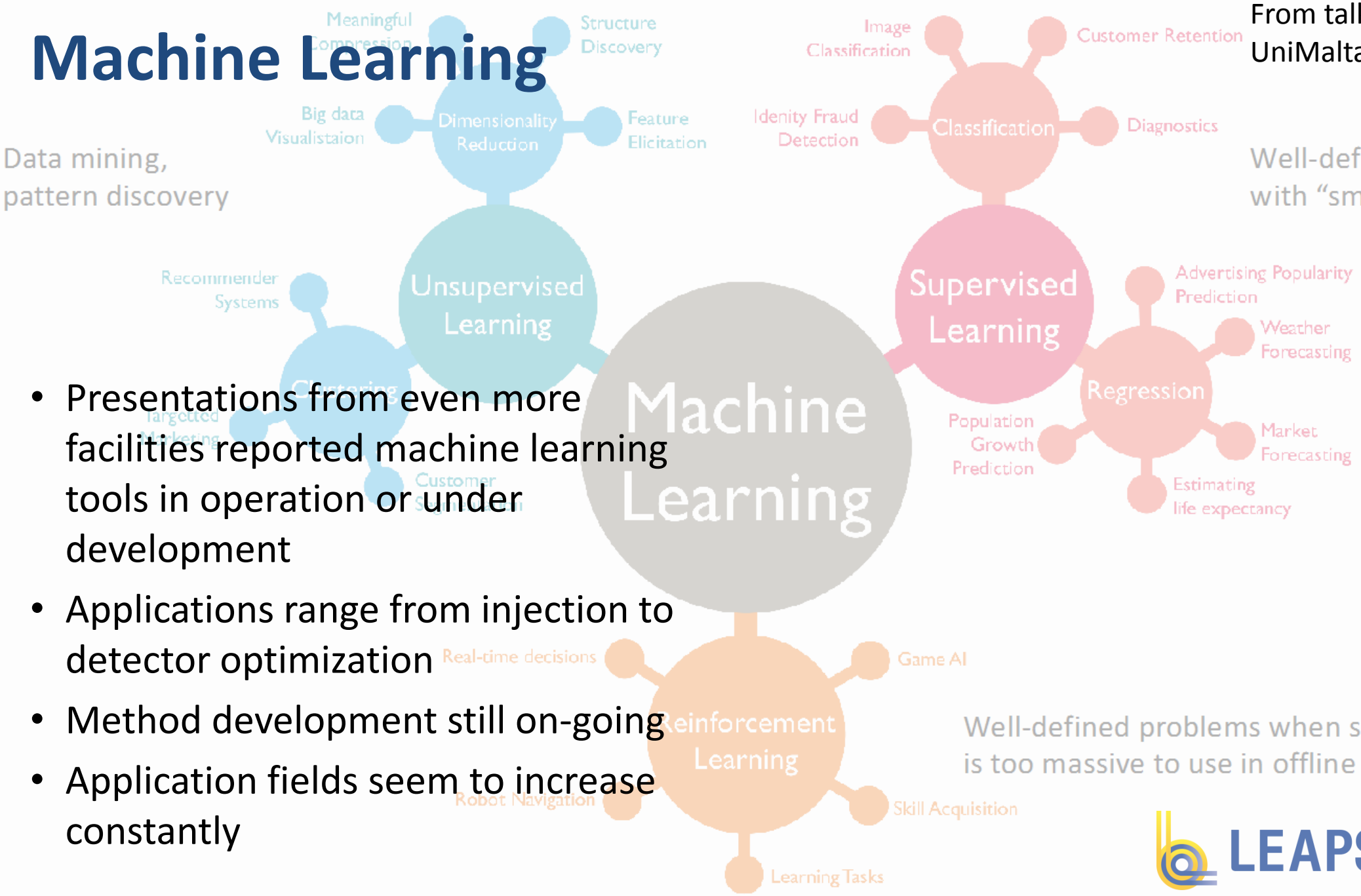
Digital Twins of Plasma Accelerators for Electron Beams

Use Europe's largest Supercomputers



Machine Learning

From talk by G. Valentino
UniMalta



- Presentations from even more facilities reported machine learning tools in operation or under development
- Applications range from injection to detector optimization
- Method development still on-going
- Application fields seem to increase constantly

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Machine Learning

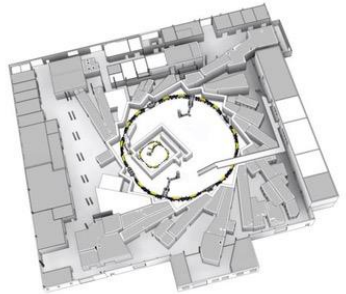
From talk by A. Santamaría García
KIT

Talk Outline

Machine Learning Activities

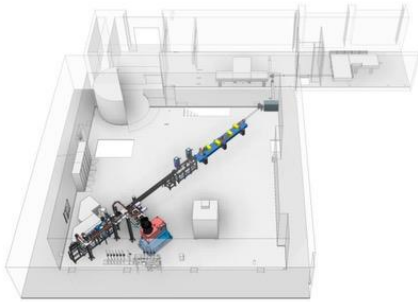
- Real-Time Control of the **Micro-Bunching Instability** with **Reinforcement Learning**
- **Bayesian Optimization** of the **Injection Efficiency**

Test Facilities @KIT



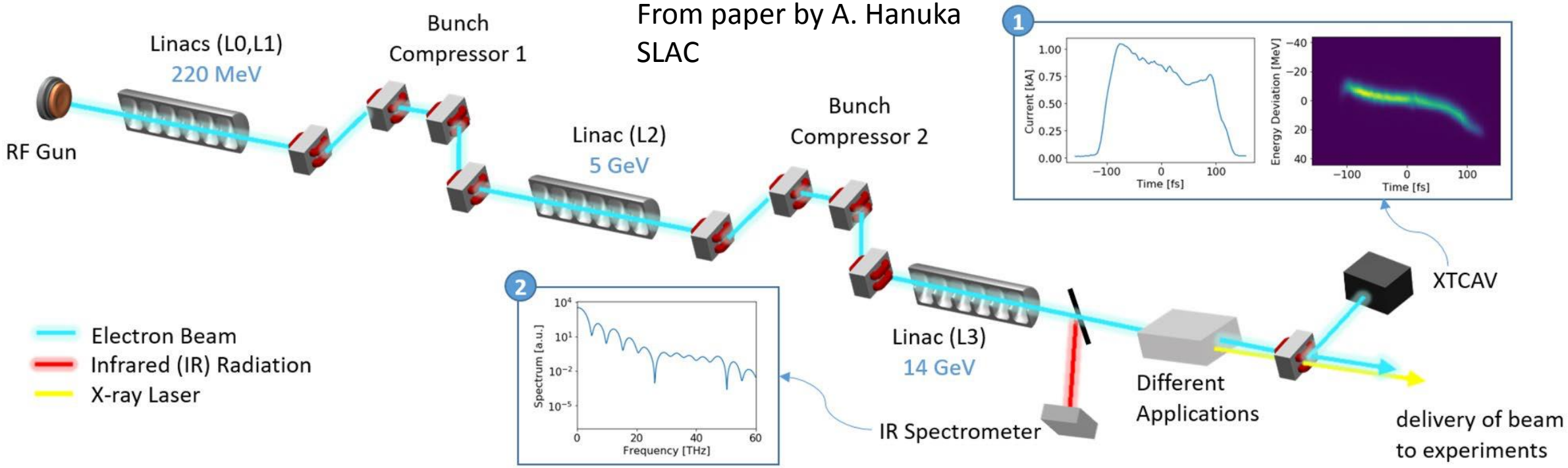
KARA
Synchrotron light source
2.5 GeV

- Machine Learning Towards Autonomous Accelerators: Control of the **Bunch Profile** with **Reinforcement Learning**



FLUTE
Linac-based THz source
41 MeV

Virtual Diagnostic



- Machine-learning based diagnostics
- Improve accelerator or more general beam diagnostics by using scalars or spectra to retrieve beam properties non-destructively and with higher resolution
- Once trained such a system allows for quasi real-time feedback much faster than a re-construction of real data.

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Conclusions of the LIP workshop

- There were 109 registered participants
- Typical attendance varied from 60 to 100 people
- A total of 25 speakers
- Presentations available at https://indico.psi.ch/e/11213
- Executive conclusions:

  There are a lot of activities ongoing which merit more support and enhanced integration, HORIZON-INFRA-2021-TECH-01-01 is a great opportunity (10M€)

→ **DiTARI*** proposal submitted (23 Sep 2021)

*__Di__gital __T__win Platform for __A__nalytical __R__esearch __I__nfrastructure Experiments
ditari [latin] = enrich (engl.), bereichern (dts.)

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The DiTARI Proposal

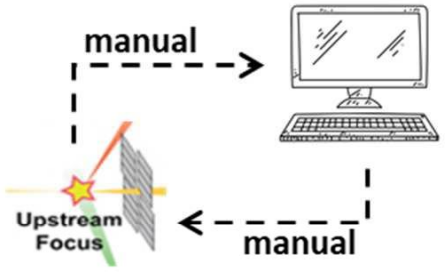
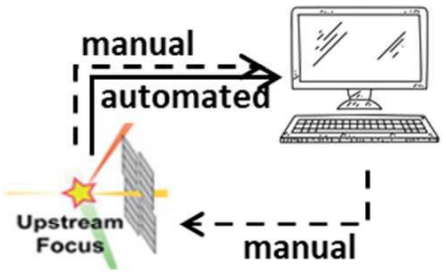
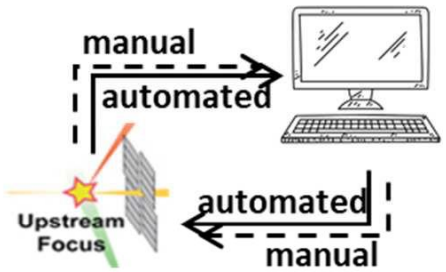
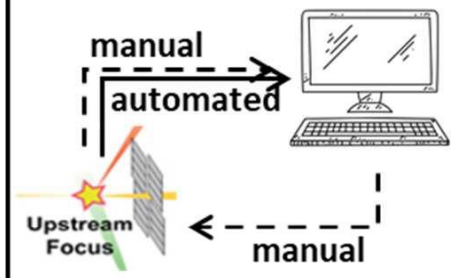
- **The problem**: ARIs offer highly performant facilities & instruments allowing complex experiments by multi-disciplinary communities to solve important questions of societal relevance. Preparation, execution and analysis of experiments is complex and takes long. This hinders early science success and creates an entry threshold for new communities.
- **The proposal**: Provide a digital twinning platform to make preparation, execution and analysis of such experiments more effective leading to higher success rates. Enhance robust operation of ARI facilities. Integrate AI to allow swift comparison of observational and simulated data during experiments, increasing understanding of the results in real-time. Establish DiTARI as a service in EOSC. Address and include new communities (expert & learning) by DiTARI training and tutorial capability.
- **The ambition**: Become the standard for digital twinning at Europe's ARIs, sustained through implementation at numerous ARIs. Extend to other Material Science applications and science disciplines. Reach all research communities looking to use these facilities and capabilities for virtual experiments.

DiTARI Consortium

Participant No. *	Participant organisation name	Country
1 (Coordinator)	European X-Ray Free-Electron Laser Facility GmbH – EuXFEL	Germany
2	European Synchrotron Radiation Facility – ESRF	France
3	Stiftung Deutsches Elektronen Synchrotron – DESY	Germany
4	Paul Scherrer Institute – PSI (associate partner)	Switzerland
5	Institut Max von Laue – Paul Langevin – ILL	France
6	European Spallation Source – ESS	Sweden
7	Forschungszentrum Jülich GMBH – FZJ	Germany
8	Helmholtz-Zentrum Berlin für Materialien und Energie GmbH – HZB	Germany
9	United Kingdom Research and Innovation – UKRI	UK
10	Centre Nationale de Recherche Scientifique – CNRS	France
11	Association pour la Recherche et le Developpement des Methodes et Processus Industriels – ARMINES	France
12	Kungliga Tekniska Högskolan – KTH	Sweden
13	Technische Universität München – TUM	Germany

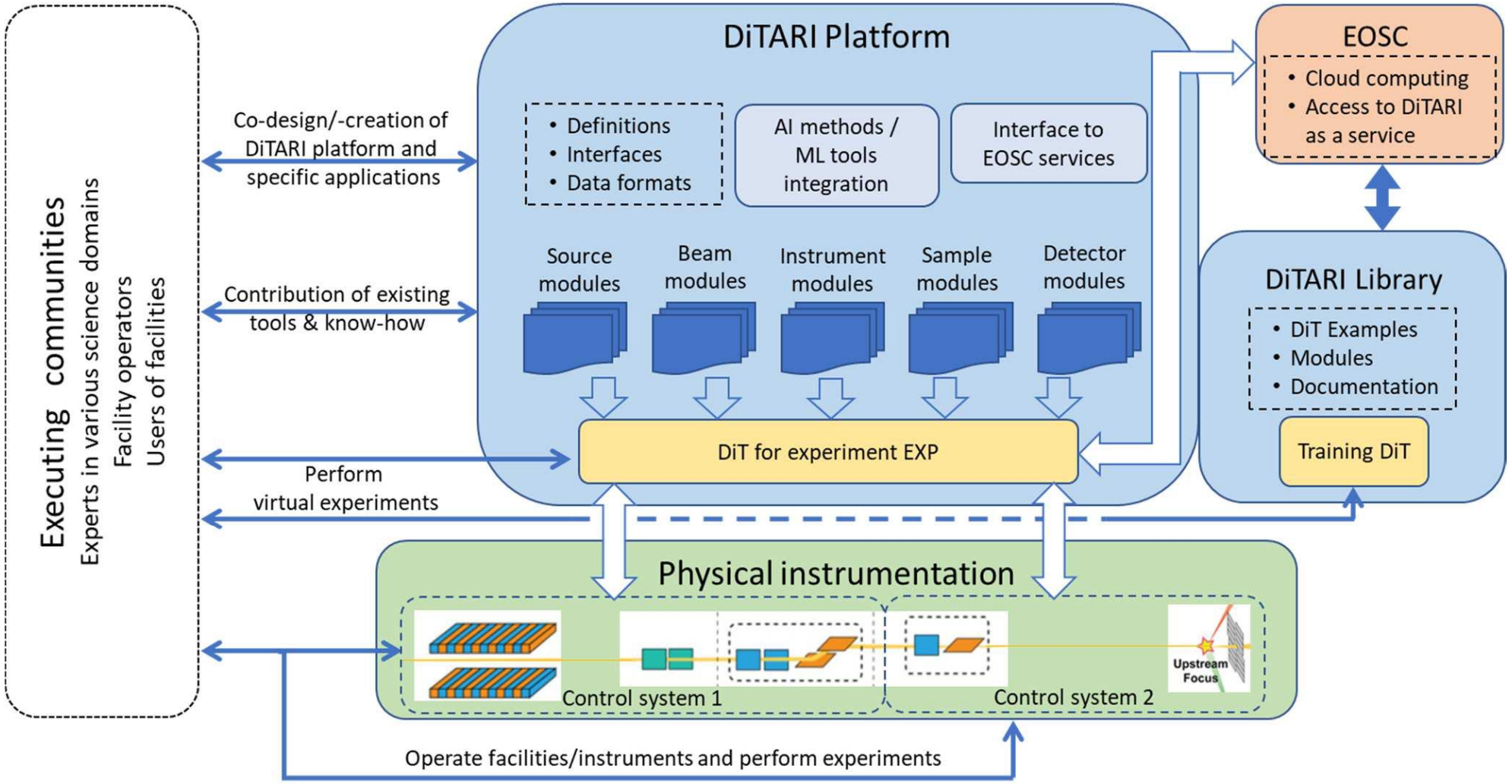
On the use of Digital Models

during life cycle of an experiment

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 offers to address all 3 different types of digital models
- Issue of real-time data exchange is addressed, but limitations will apply

The DiTARI eco-system



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

Four science problems addressed by DiTARI

- Understanding the mechanisms that control the **assembly of nature's nanoscale components** into hierarchical functional material with the aim to develop new fabrication processes and to elucidate the properties and use of such materials (SAXS, KTH)
- Studying the structure-function relationship of **next generation for solar cells** for efficient energy harvesting (SANS, TUM)
- Predictive modelling of **damage initiation in structural materials** (XRD microscopy, INSA/ARMINES)
- **Virtual diagnostics** measuring hidden beam properties (e-beam diagnostics + ML, PSI et al.)

Conclusions

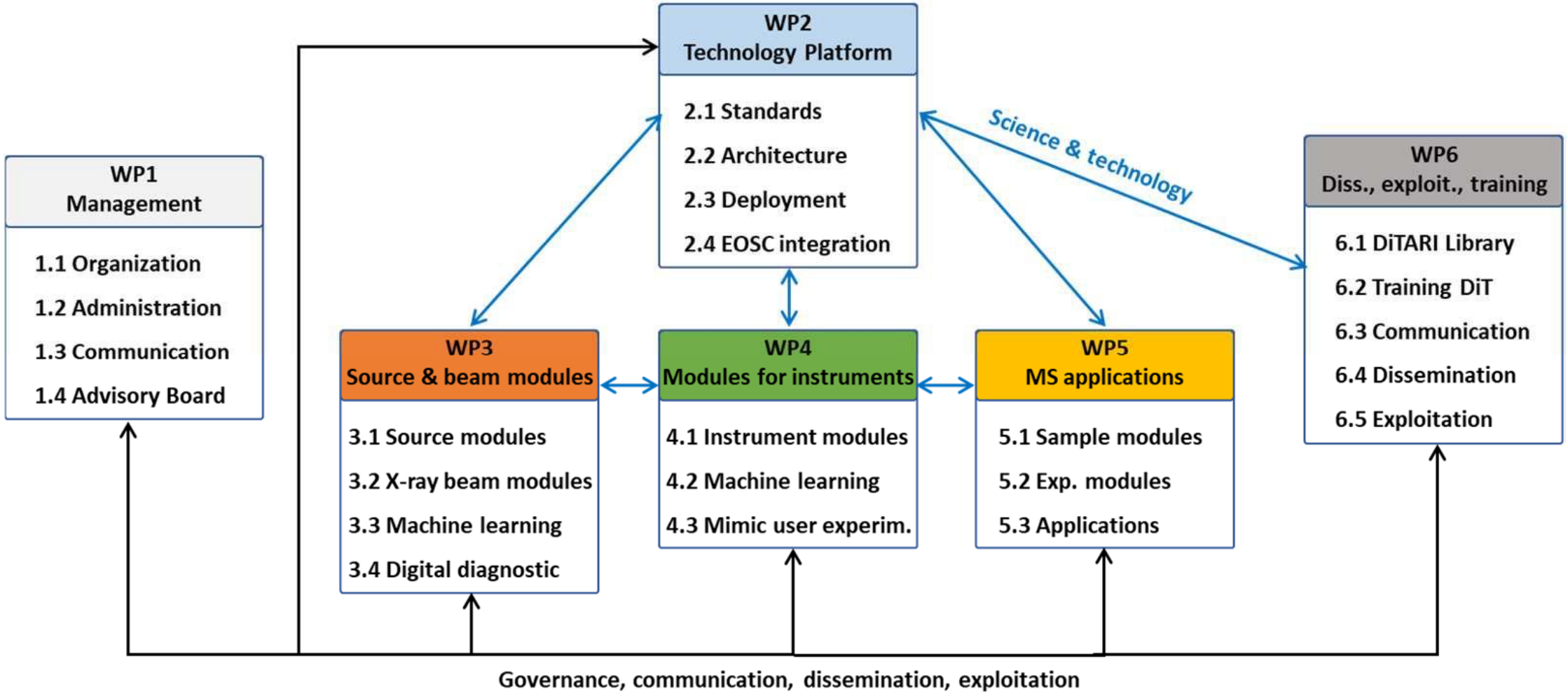
- Machine Learning will be the key for the success of DiTARI
- If positively received by the EC and adequately financed, DiTARI can foster the development and integration of ML methods for light sources and beyond
- You are all welcome to contact me if you want to have more info
- We are looking forward to reach out a larger community

Spare slides

DiTARI objectives and more

- **Objectives**
  - Support complex experiments using Analytical Research Infrastructures
  - Enable new science applications
  - Enable access by new communities, both expert and learning
  - Improve operation and performance of Analytical Research Infrastructures
- **Methodology**
  - Enable building of DiTs to describe ARI experiments
  - Build a joint technology platform allowing to connect specific modules for the virtual description
  - Integrate and develop modules performing the virtual description
  - Co-design platform and modules through expertise by application and facility experts
- **Deliverables**
  - Platform, few functional DiTs (TRL6+), Library

Workpackages



DiTARI Overview

- **Name**
  - the **Di**gital **T**win Platform for **A**nalytical **R**esearch **I**nfrastructure Experiments – **DiTARI**
  - ditari [latin] = enrich (engl.), bereichern (dts.),
- **Main purpose**
  - Provide a platform for digital twinning of complex experiments at ARI facilities
  - Enable new science; make complex experiments and operation more efficient; address new communities
- **Deliverables**
  - DiTARI platform enabling to assemble digital twin applications (DiT), DiTARI Library, 4 operational DiTs
- **Long-term aim**
  - Become the common tool for digital twinning of ARI facilities, user communities
- **Resources**
  - 11.5 M€ over 4 years

DiTARI terms

- **Technology platform** – the framework to be created by DiTARI to build specific Digital Twin applications
- **DiT** – short for Digital Twin application. In this project used as an application allowing to simulate physical processes or a combination of many physical processes. The DiTs will be specific for an application, addressing the entity of relevant physical processes contributing to an accelerator, beam transport, instrument experiment.
- **Modules** – software tools or sophisticated packages that already exist or will be developed to make the Digital Twins functions
- **Library** – a special repository to place documentation, sample DiTs, and Training material
- **Experiment** – Use this term to describe the physical process to be simulated. No matter whether it takes place in the accelerator or instrument.
- **Source, beams, instruments** – the three major sections of an ARI addressed by the project