LEAPS League of European Accelerator-based Photon Sources

“LEAPS perspective on projects outcome and sustainability”

Caterina Biscari

LEAPS Chair
Director of ALBA synchrotron

2nd European PaN EOSC Symposium

October, 26th 2021

LEAPS

League of European Accelerator-based Photon Sources

+35000 users from all EU & beyond

+300 operating End Stations

+25000 publications In last 5 years

offering +800000 h/year

LEAPS-members primary goal is to actively and constructively ensure and promote the quality and impact of the fundamental, applied and industrial research carried out at their respective facility to the greater benefit of European science and society.

19 facilities in 16 institutions

LEAPS League of European Accelerator-based Photon Sources

Vision

A world where European science is a **catalyst for solving global challenges**, a key driver for competitiveness and a compelling force for **closer integration and peace** through scientific collaboration.

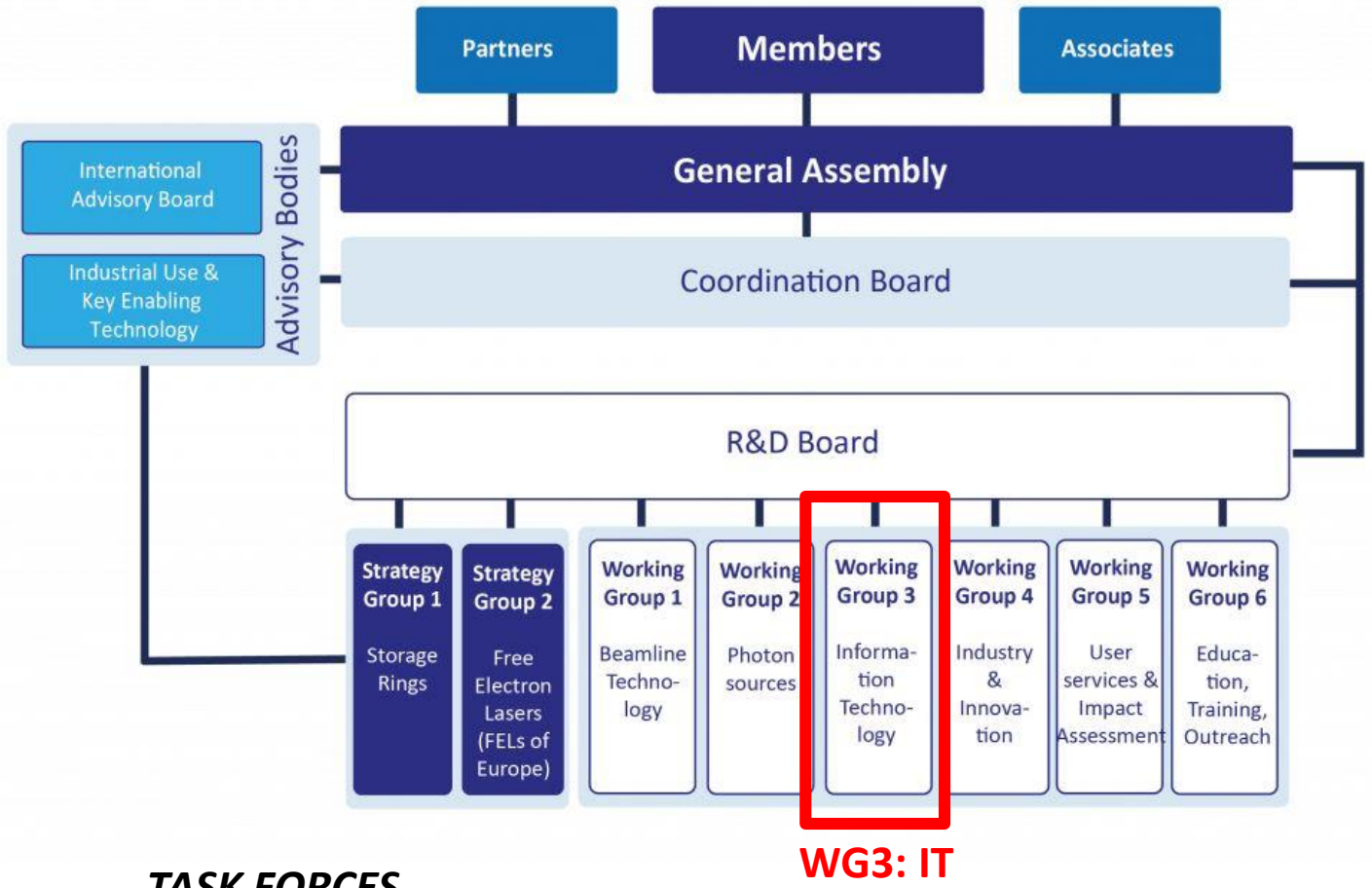
Mission

LEAPS use **the power of its combined voice** to ensure that member light source facilities continue to be world - leading, to act as a powerful tool for the development and integration of skills with a view to address 21st century global challenges, and to consolidate Europe's leadership in the field.

European LEAPS Strategy for new ERA

- LEAPS is the joint force of great national and international facilities
- LEAPS provides a forum for growing together in a concerted commitment serving the European Research Area
- LEAPS Landscape is in fast evolution thanks to technical advancements, digitalization, **open data and open science**
- European industry needs LEAPS for its competitiveness to develop
- All Member States researchers benefit from LEAPS instruments
- 2022: European LEAPS Strategy for new ERA

LEAPS organization



WG3: IT

LEAPS chairs

(Present/past/incoming)

General Assembly
Caterina Biscari (ALBA)
Helmut Dosch (DESY)
Lenny Rivkin (PSI)

Coordination Board
Gastón García (CMAM-UAM)
Rafael Abela (PSI)
Ute Krell (DESY)

TASK FORCES
- *ESUO*
- *IDEA- Inclusion, Diversity, Equity and Anti-discrimination*
- *Internal project funding*
- *LEAPS positioning on the ERA*
- *Strategic Access*

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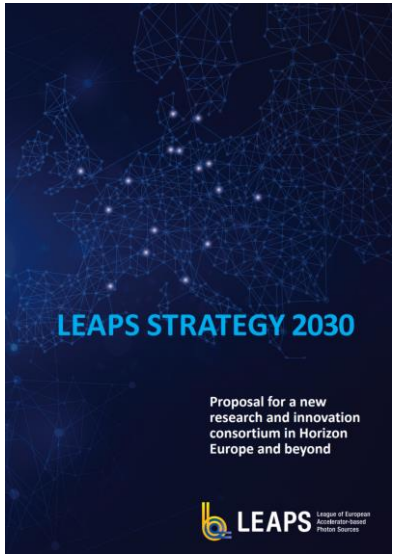
LEAPS activities

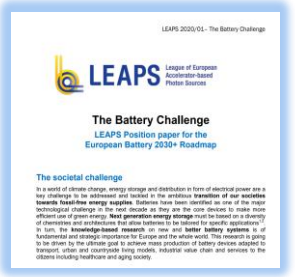


LEAPS description and vision

2017: LEAPS Brochure
2018: LEAPS Strategy 2030
2019: LEAPS Landscape

LEAPS position papers 2020 - 2021

HE Missions
LEAPS facilities fighting COVID-19
LEAPS Strategy 2030
Battery Roadmap 2030
DIGITAL LEAPS



Aligned with EU Commission priorities

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2021: LEAPS IDEA - Inclusion, Diversity, Equity and Antidiscrimination

LEAPS IDEA

LEAPS Statement on Inclusion, Diversity, Equity, and Anti-discrimination (IDEA)

The League of European Accelerator-based Photon Sources (LEAPS) brings together Synchrotron Radiation and Free Electron Laser user facilities in Europe in a strategic consortium that aims to actively and constructively ensure and promote the quality and impact of fundamental, applied and industrial research for the benefit of European science and society.

As international large-scale research infrastructures where interdisciplinary

individuals informed by their own experience, circumstances, unconscious biases and greater society.

In order to achieve the goals of inclusion, diversity, equity and anti-discrimination, it is our commitment to provide a range of specific tools, tailored to each of the LEAPS facilities, making them the ideal location for large international, interdisciplinary and intermixed teams to thrive and achieve their highest potential.

LEAPS

LEAPS_IDEA #1

May is European Diversity Month

LEAPS

We are committed to **strengthening diversity** as we are aware of owing our success to the talents, ideas

As a European consortium focusing on scientific excellence, LEAPS is committed to strengthening diversity and is acutely aware of owing its success to the talents, ideas, cooperation, and collective and complementary collaboration of its scientists. The ingredients to this success are respect and fairness, appreciation and openness. Ensuring equity and achieving an inclusive environment, free from discrimination at all levels, is LEAPS's responsibility.

Seminar at the 4th LEAPS Plenary Meeting (21st Oct 2021)

12:40 - 13:30	**Seminar promoted by the LEAPS-IDEA TF**	*Chair: H. Dosch (DESY, LEAPS vice chair)*
12:40	The Science of Inclusion	*S. Estradé (IN2UB and iiEDG, U. Barcelona)*

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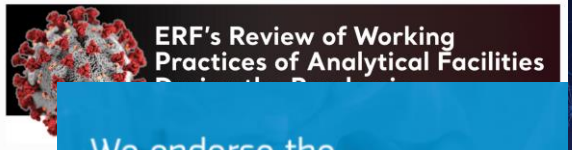
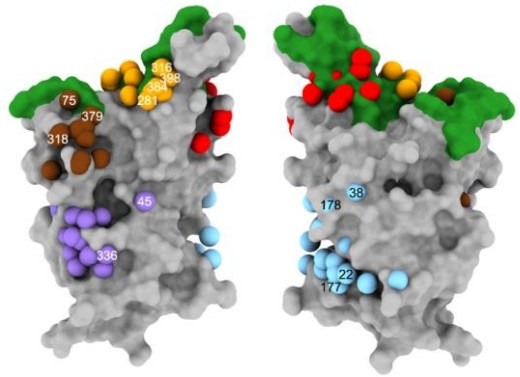
LEAPS, providing solutions for the pandemic

*Dedicated **fast track access mode** on almost all LEAPS facilities, addressed to Academy and Industry from the very first moment, compatibly with each country pandemic conditions*

See Tim Salditt and Dave Stuart talks, in Plenary Meeting, Session 2

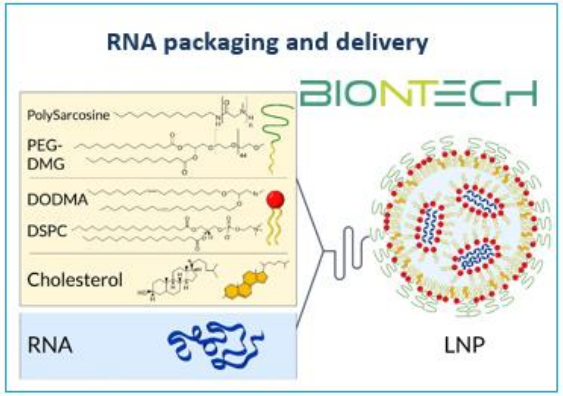
ERF's Review of Working Practices of Analytical Facilities During the Pandemic





https://doi.org/10.1016/j.cell.2021.02.032

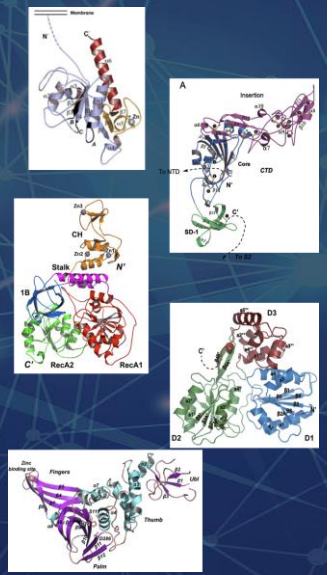
Academy



Industry

Developing the new generation of mRNA vaccines with enhanced transfection efficiency and overall effectiveness of the vaccine.

EMBL DESY.



https://leaps-initiative.eu/leaps-and-covid-19-one-year-later/

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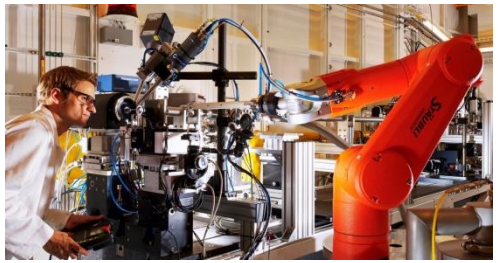
Digital LEAPS

From 2020 idea to 2021 pillar proposals

Users
Training
Green operation



Stretegic elements for a transition to a green DIGITAL LEAPS

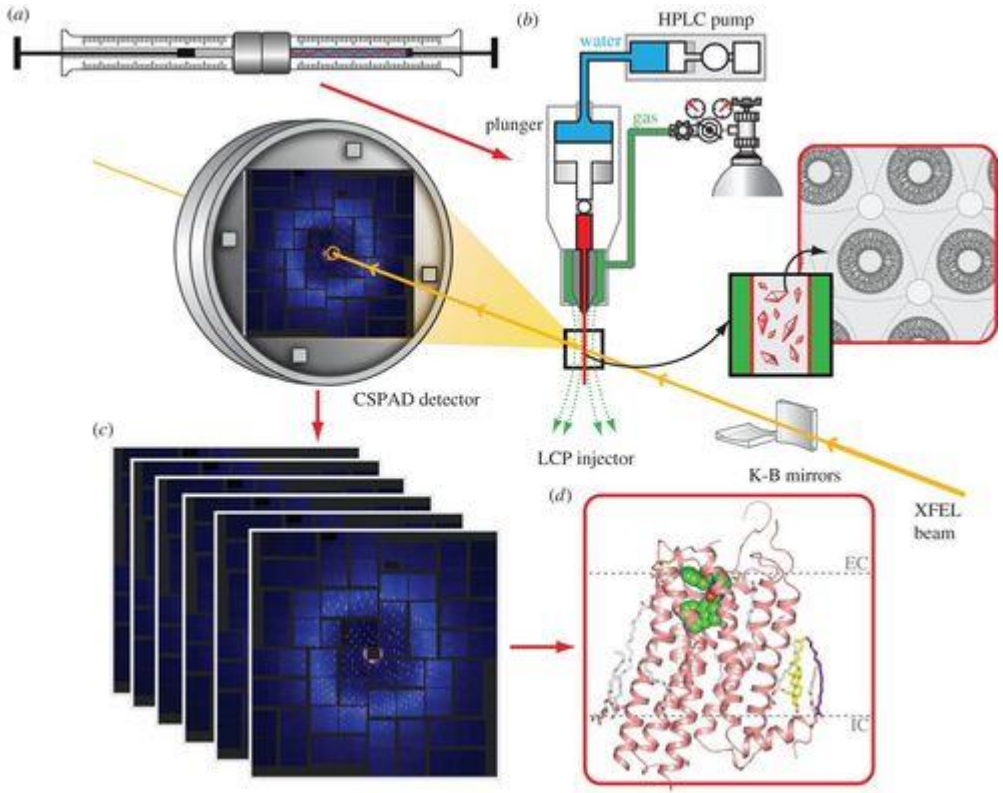
- Remote User Operation
- Digital Communication
- Digital Training
- Resilient & energy saving operation
- AI-assisted molecular infection fight
- Advanced materials for digital transformation & circular economy

DIGITAL LEAPS pillars

STARS | HR⁴ | LIP

Impact to ERA and societal challenges

LEAPS facilities become more resilient and more green & serve better the scope of European Green Deal and resilience to future pandamics & serve Missions of Horizon Europe



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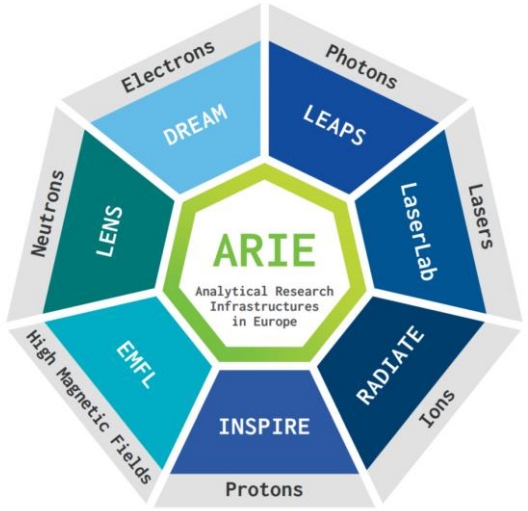
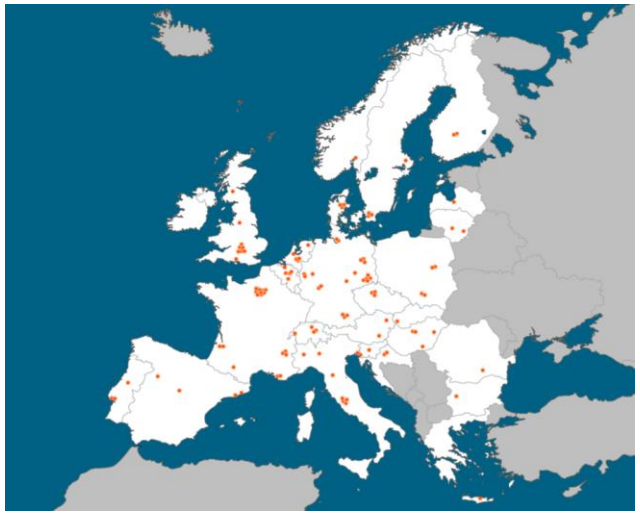
Cooperation with other European Analytical RIs:
a powerful tool for solving societal challenges





More than 120 European RIs

*The **ARIEs**, accessed by tens of thousands of researchers every year, also serve as interdisciplinary training platforms for students, future scientists, engineers and technicians, and are paradigms for European collaboration in large, high-tech projects.*

Complementary
Multi-scale
Multi-modal

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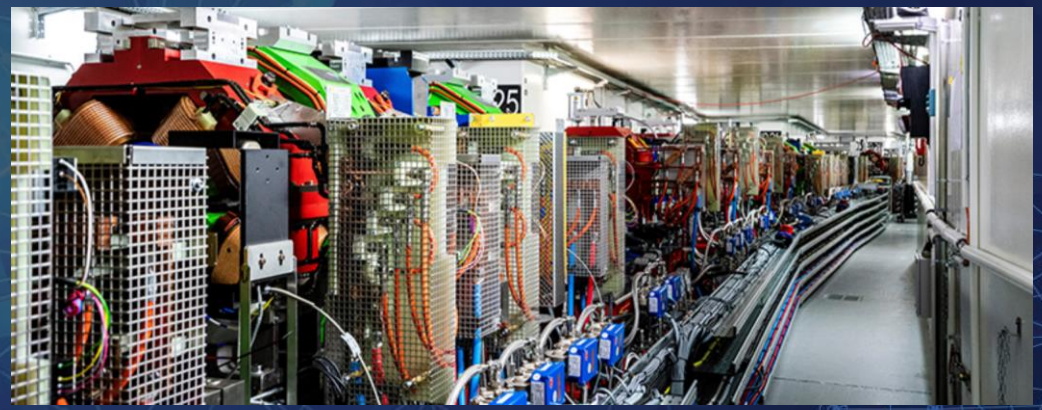
World leadership in technologies

At the front end of synchrotrons and FELs technologies

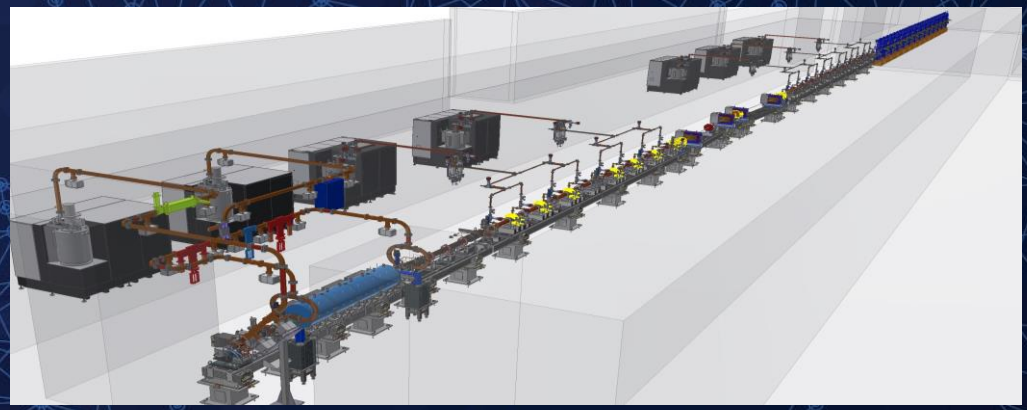
MaX IV, the first 4th gen Synchrotron

EuXFEL the highest energy FEL

ESRF-EBS, the first upgraded from 3rd to 4th



EuPRAXIA - in construction, LNF

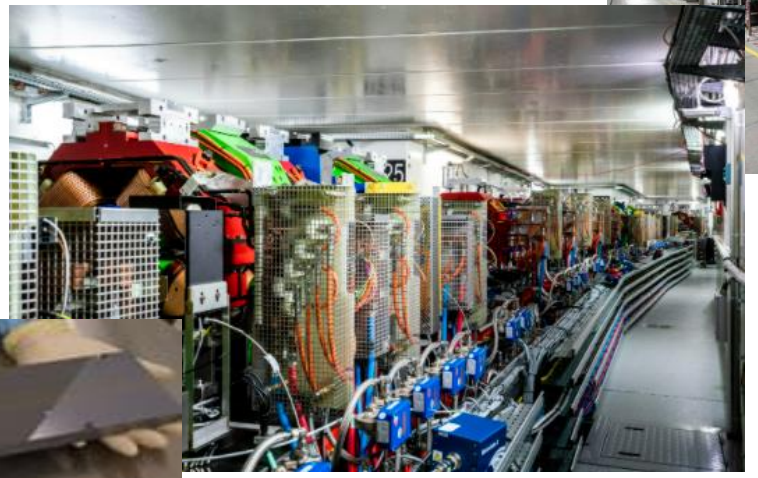


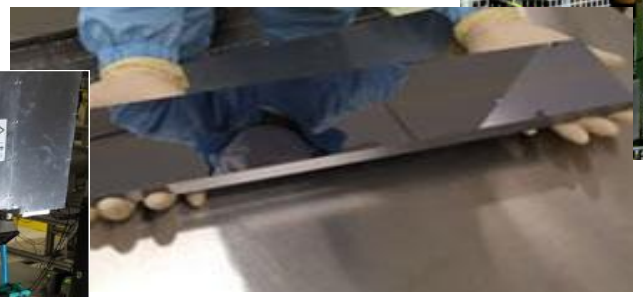
Its example followed all over the world. @ LEAPS: Alba, BESSY II, Diamond, Elettra, Petra III, Soleil, SLS

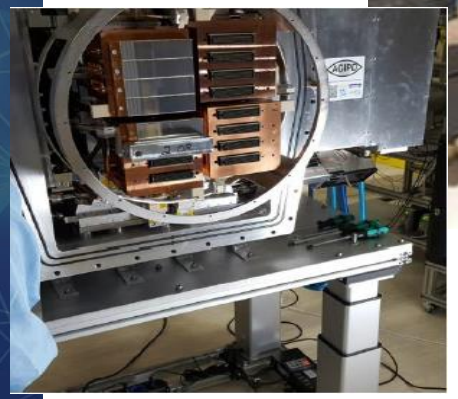
the 1st plasma acceleration based FEL facility, based on H2020 EU design study

LEAPS technology step change

- Synchrotrons Leaping from 3rd to 4th generation
- Brilliance increase
- Faster detectors
- Faster FEL experiments







Technology step change has a huge impact on data dimension

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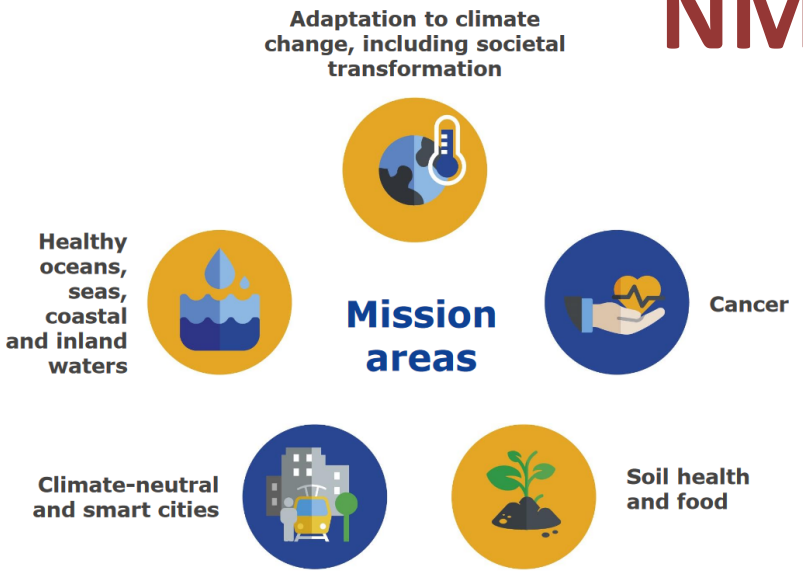
LEAPS technology step change and the other ARIE networks

Lasers

NMR



EM

Neutrons

Complementary

	Strength	Weakness
LEAPS	• Very high brightness (photons/mm²/s/mrad², 0.1% bandwidth) reaching 10^{23} at the 4G SRs and 10^{33} at XFEL and very broad wavelength range • Up to ~ 100% coherence • Tunability, full polarization options • Variable penetration depth • Time resolution over a wide range approaching few fs range • Multipurpose multi-user specialized beamlines offering many state-of-the art techniques, very reliable • Sensitive to chemical environment	• Radiation damage limits • Time resolution still limited to fs range
Lasers	• Broad wavelenght range from THz-IR to X-ray reaching MeV energies with Compton Source • Fully coherent pulses down to attosecond range • Multipurpose facilities offering different capabilities	• ≈2 orders of magnitude lower peak brightness and lower repetition rate compared to MH X-ray FELs • Limited tunability at shorter wavelengths, limited polarizatio
Neutrons (LENS)	• High penetration power • Isotopic contrast • Good for very light elements, e.g. excellent probes for hydrogen, major constituent of organic-life matter • Sample environments for ultra-low temperature, high magnetic field, etc. • Very well suited for large samples • μeV energy resolution for inelastic scattering • Multipurpose multi-user facilities offering different capabilities, very reliable	• Low brightness source • Limited spatial resolution • Limited time resolution • Sample activation for some isotopes
EM	• Very high spatial resolution in crystals, excellent phase measurements • CryoEM to look at non-crystallizing macro-molecules • Requires limited infrastructure	• Penetration depth limited to microns • 3D imaging is destructive for sample • MX only at cryo temperatures, long acquisition time
NMR	• Biological molecule structures without crystallization • Non-invasive, hazardless • Widely used in clinical medicine	• Limited to atoms with net spin • Needs large samples • Not applicable to very large biomolecules

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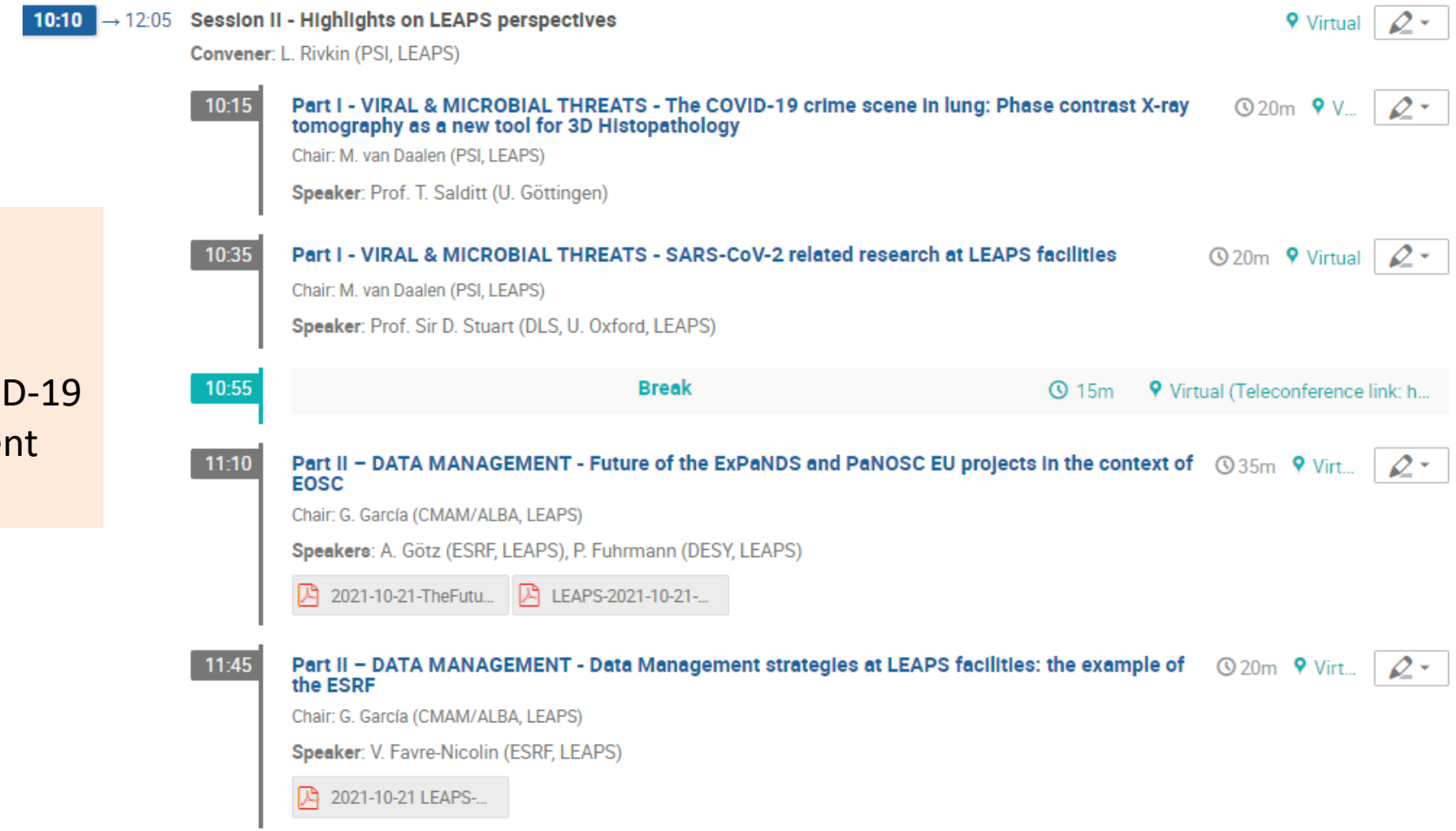
LEAPS and its DATA
Example: Plenary meeting last week

Two key highlights

- Research in COVID-19
- DATA Management



Inspiring talks by Andy, Patrick and Vincent

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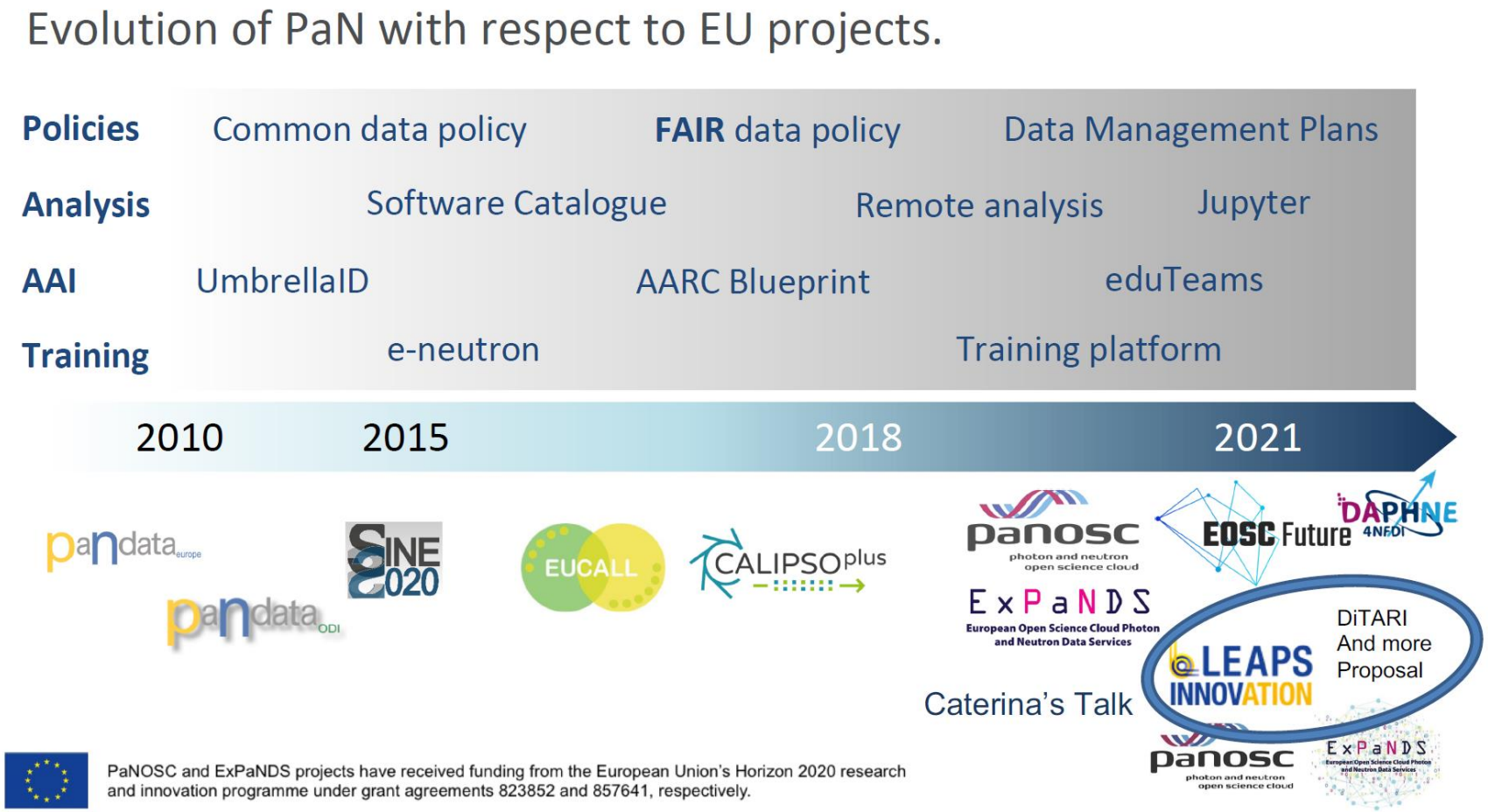
Cooperation with LENS on Data established years ago



PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

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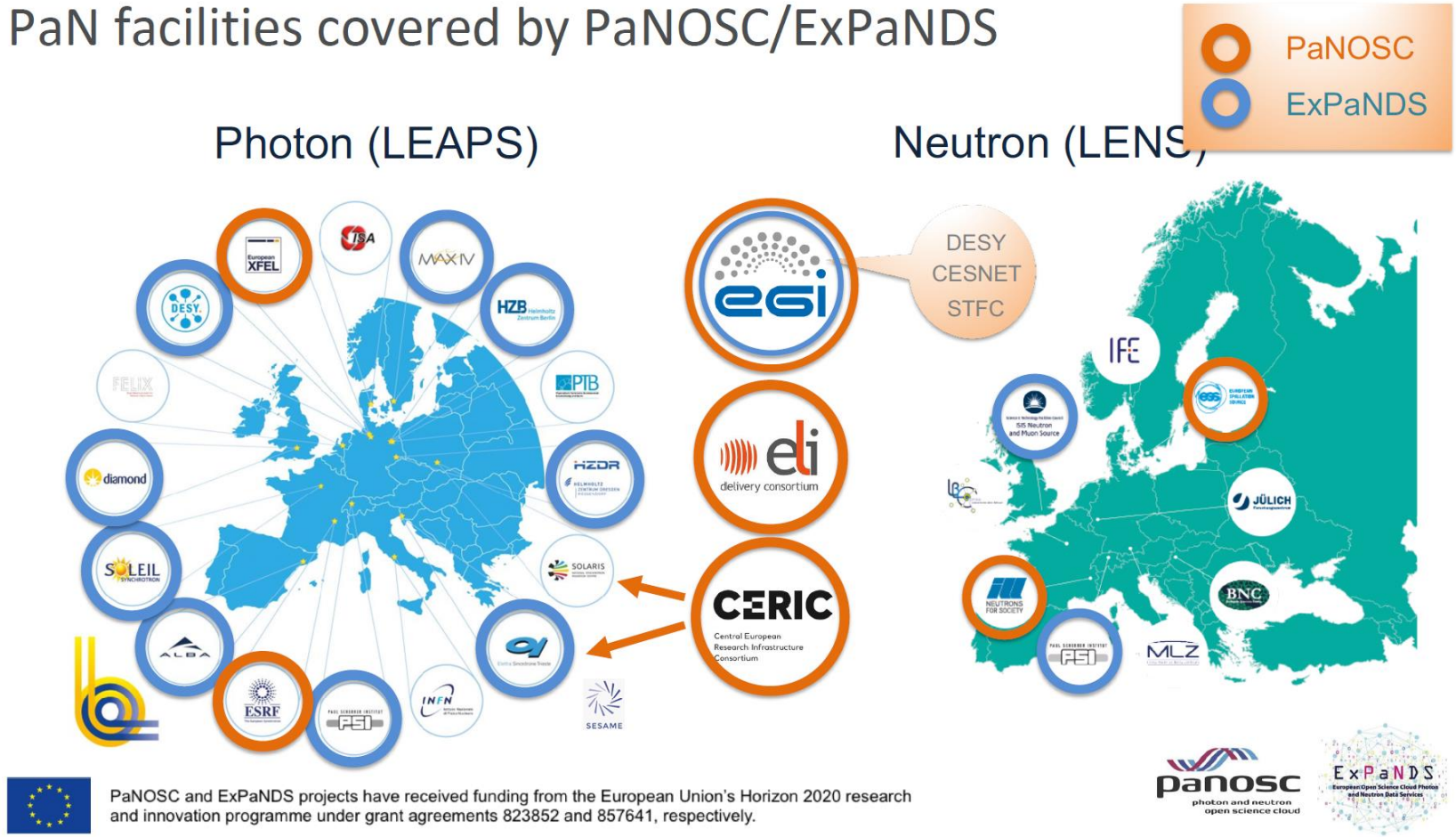
Cooperation with LENS on Data established years ago



Answer to PaNOSC + ExPaNDS survey – see Andy's talk

Q1: LEAPS facilities uptake of PaNOSC+EXPaNDS outcomes

Yes, already adopted (Y)
Not Planning to be adopted (N)
In progress of being adopted (WIP)
Planned to be adopted (P)
Under evaluation (U)

FACILITY	FAIR data policy	DMPs	DOIs	Nexus HDF5	Search API	Open Data Portal	AAI	JupyterLab	VISA	SIMEX	Pan-learning/ training
ALBA	P	P	WIP	WIP	P	P	U	P	U	U	U
DESY	WIP	P	P	Y	WIP	P	WIP	Y	U	N	WIP
DIAMOND											
ELETTRA	Y	WIP	Y	Y	WIP	WIP	Y	Y	WIP	Y	WIP
ESRF	Y	WIP	Y	Y	WIP	WIP	Y	Y	WIP	Y	WIP
EuXFEL	WIP	WIP	Y	WIP	WIP	WIP	WIP	Y	WIP	Y	WIP
FELIX	Y	P	WIP	U	U	WIP	U	U	N	N	U
HZB	Y, N, P [1]	P	WIP [2]	Y	P	Y	P	U	U	U	U
HZDR	WIP	WIP	Y	N	N	WIP	WIP	WIP	P	N	Y
INFN	U	U	U	U	U	U	U	U	U	U	U
ISA*	U	U	U	U	U	U	U	U	U	U	
MAX IV											
PSI	WIP	WIP	Y	WIP	Y	Y	WIP	WIP	N	N	N
PTB	Y	WIP	Y	WIP	N	Y	N	N	N	N	N
SOLARIS #											
SOLEIL	U	P	WIP	Y	P	P	WIP	U	WIP	U	Y

PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

Data Strategy: QUESTIONNAIRE to LEAPS facilities - GENERAL CONSIDERATIONS

Adoption of the PaNOSC and ExPaNDS outcomes

Q1: LEAPS GA members answers with WIP and P items converted to Y (assumes they are completed in the near future)

FACILITY	FAIR data policy	DMPs	DOIs	Nexus HDF5	Search API	Open Data Portal	AAI	JupyterLab	VISA	SIMEX	Pan-learning/ training
ALBA	Y	Y	Y	Y	Y	Y	U	Y	U	U	U
ELETTRA	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
ESRF	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
EuXFEL	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
FELIX	Y	Y	Y	U	U	Y	U	U	N	N	U
HZB	Y	Y	Y	Y	Y	Y	Y	U	U	U	U
HZDR	Y	Y	Y	N	N	Y	Y	Y	Y	N	Y
PSI	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N
PTB	Y	Y	Y	Y	N	Y	N	N	N	N	N
SOLEIL	U	Y	Y	Y	Y	Y	Y	U	Y	U	Y
DESY											
DIAMOND	* Will fill-in after Oct 25										
INFN	U	U	U	U	U	U	U	U	U	U	U
ISA*	U	U	U	U	U	U	U	U	U	U	
MAX IV											
SOLARIS #											

Yes, already adopted (Y)
Not Planning to be adopted (N)
In progress of being adopted (WIP)
Planned to be adopted (P)
Under evaluation (U)

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From LEAPS Plenary meeting last week

What do we need from the LEAPS (and LENS) partners

Data Steward

"I ensure data usage complies with our policies."

Data Steward. Falling between the cracks of library and domain science

- To make sure the ontologies, as bases of our NeXus rendering and catalogue entries are followed up upon and regularly updated;
- The Data Policies, FAIR rules and DMP are up to date;
- Data Handling at the facility is following the Data Policies and DMPs;
- Provides regular beamline and dataset FAIR assessment.
- Involved in international groups on definitions and standards, like RDA, NFAC and national initiatives.
- Role: "Ensures data usage complies with our policies"

LEAPS members are considering the suggestion

PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement [illegible]52 and 857641, respectively.

From LEAPS Plenary meeting last week

What do we need from the LEAPS and LENS partners

- Teaching and Learning Platform
  - Sustained installment of the two platforms;
  - Teaching and training material from the facilities to be harvested or added to those platforms.
- AAI
  - Connect the facility services to the PaN-oxy system(s);
  - Fees might apply for GEANT or EGI to support our AAI.
- Data Management
  - Further evaluation of DM solutions for data transfer;
  - Stay in touch with professional DM projects like ESCAPE ,DOMA etc.;
  - Possible fees e.g. for GlobusOnline, EGI DataHub or others.

LEAPS members are considering the suggestion

PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively

Apply for EOSC Association membership ....

either through your facilities, national science associations or your country!

From LEAPS Plenary meeting last week

LEAPS Data should be getting more attention

- Why it's important
  - attribution of published data to our facilities: impact, visibility
  - globalisation of research
- What PaNOSC+ExPaNDS do
  - **FAIR data policy** framework for PaN
  - support for implementation: metadata catalogues, active **DMPs**, **PID** infrastructures...
  - open data harvested and searchable in **EOSC**
- What we need from LEAPS
  - commitment to FAIR data management
  - means + resources to implement data policies
  - → **recommend updating of policies and hiring data managers**

LEAPS members are considering the suggestion

☞ cf. demo at ExPaNDS mid-term review

Q2: Does LEAPS GA members share the vision of a common open data portal for open data from LEAPS facilities?

Mixed answers:

- Few totally endorsing the idea
- Most in favor of combined common/individual portal
- Some worried by legal issues

Q3: Do you want a common LEAPS strategy paper on Open Science and Data and would you contribute to it?

- In general all positive comments
- Some totally in favor and ready to provide support
- Need of clarifying the strategy and the implementation schedule
- Need of defining the resources for the common paper

LEAPS support to PaNOSC and ExPaNDS

✓ **Most of the LEAPS facilities have interest in adopting the outcomes of PaNOSC and ExPaNDS:**

- Half of the facilities have already adopted some of the tools or are in the process to adopting it;
- The tools considered more useful or urgent to implement are:

FAIR data policy, DMPs, Nexus HDF5, DOIs and Open data portal

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LEAPS vision in relation to PaN Open Data Commons

✓ **Most of the LEAPS facilities share the vision of a common open data portal.**

- In few cases the possibilities to implement it could be limited by the facilities legal status.
- How it would be implemented is under debate but could:
  - Imply that all LEAPS facilities implement an open data portal locally, including the federated search API

OR

  - Some LEAPS facilities would implement an open data portal locally while others would rely on the common portal to upload and store data centrally.

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Some thoughts about what comes next

- ✓ EXPANDS/PANOSC are guiding us towards what facilities have to do anyhow
- ✓ **We should aim at an ambitious HE project (2023-…) to support the joint effort to implement EXPANDS/PANOSC in LEAPS (and LENS) facilities**
- ✓ In parallel the conditions may be favorable to plan for an internal LEAPS project to bridge over from the end of 2022 to the start of a new project, and to complement once it starts
- ✓ Joint data developments may lead to a long-term ´´federated´´ approach for some services, if more efficient together
- ✓ 26 November – General Assembly – DATA Strategy in the agenda
- ✓ LEAPS is looking forward to a intensive interplay with you during the coming year in order to clarify the strategic directions to be taken

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https://leaps-initiative.eu

"The strength of LEAPS lies in its staff and users, hailing from all European countries, beyond those which host the facilities."

Tak
Tack
Thanks
Bedankt
Danke
Dziękuję
Merci
Grazie
Gracias

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LEAPS Initiative

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