CALIPSOPlus JRA2 Meeting

MAY 13th – 15th 2019 at Paul Scherrer Institut

Villigen – CH







MONDAY, MAY 13th

Time	Торіс	Speaker
13:30	Start of the Meeting	Gerd
	Welcome to PSI	Mann
	General Presentation of PSI	
	Work Break Down Structure for SLS 2.) PSI Goals	
13.45	Update on LEAPS developments, plans and future activities	Mirjam
	Mirjam van Daalen (PSI) introduces an update on the LEAPS project.	van
		Daalen
	16 Members: all SR and FELs operating in EU agree to work coherently to:	
	Shape future science & technology at accelerator-based light sources	
	 Collective landscape document and strategy across European facilities 	
	 Periodical update of roadmaps and action plans for key technologies 	
	 Develop future policies with stakeholders (e.g. European Commission) 	
	 Engage more effectively with industry and boost innovation 	
	Improve and broaden user access and enhance European integration	
	 Promote Open Science, education, training and exchange of staff, 	
	common indicators, communication and outreach	
	6 LEAPS Working Groups - 13 pilot projects > 100 experts from all member	
	countries working together	
	• devising technology roadmaps for advanced and disruptive technologies	
	new era of European cooperation	
	 more efficient and more cost-effective technology development 	
	smart specialization of European expertise	
	benefit for European industry	
	Current projects: first glimpse of what will be possible in the coming years. More	
	PR for the FEL and SLS community is needed and LEAPS is striving to do that.	
	SESAME welcomed as 1 st LEAPS Associate - 13 pilots projects presented	
	WG1 – Beamline technology - Five Pilot Projects presented:	
	1. High Throughput X-ray Spectroscopy Detector System	
	2. Detector Toolbox	
	 Superflat -industrial production of flat X-ray mirror and grating substrates 	
	4. NeXtgrating – Next generation diffraction gratings	
	5. Positioning and scanning systems for speed and accuracy	
	WG2 – Photon sources -1 Pilot Project:	
	1. LEAPS R&D Topic Insertion Devices (LIDs):	
	R&D on novel undulator technology pushing the parameters for	
	 high field / short period 	
	advanced schemes for EPU (elliptically polarizing undulator)	
	optimize production cost	

WG 3 – Informa	ation Technology - 2 Pilot projects:	
1. Data re	eduction and compression	
2. IT strat	egic blueprint	
WG 4 – Industr	was provider and user - 2 Pilot Projects	
1 Industr	ial Innovation through Light Sources (III S)	
2. SME In	novation through Light Sources Services	
WG 5 – User se	ervice and impact - 2 Pilot Projects	
1. Wayfor	light as a new e-infrastructure serving the user community	
2. Impact	assessment and standardized metrics for LEAPS	
MC 6 Educati	on training 9 outwood 1 Dilat Drainst	
1 Sciontif	fis focal points for new countries, new communities, new users	
I. Scientin	nd inductor	
SIVIES d	nd maastry	
GA4 and NFA R	oundtable Brussels 3-4 April 2019	
For this LEAPS \	will first participate in the INFRAINNOV-04-2010 call of H2020	
In HZ Europe Fu	unds for LEAPS will come out of pillar 1 "Excellent Science" of HZ	
Europe program	nme:	
Short to	erm vision: prepare for a co-fund action under HZ Europe (Funding	
rate (A	rt 30 FP): at least 30% of the total eligible costs and in identified	
and du	ly justified cases up to 70%).	
 Long-te 	erm vision: possibility to go for a European Partnership (e.g.	
EuroFu	sion) in the second part of HZ Europe programme.	
Need to have n	olitical support for the funding route for H7 Europe by the many	
countries that (do NOT host or have a direct interest in a synchrotron, either	
through their s	cientific community or (less directly) interest through notential	
commercial sur	anliers	
It is strongly su	ggested to meet the new responsible of the EU commission for RIs	
ASAP, as Phillip	e Froissard, Ales Fiala and JD. Malo will go to another division of	
the EU. Next m	eeting 21st of June	
NFA Round Tab	le: The interaction with the NFAs was very positive: national	
investments for	r RIs will be taken and coloured with the LEAPS colour. This money	
will then be ma	tched with at least 30% matching funds from the EU.	
It is clearly state	ed to NFA, that national and European funding will not be mixed.	
LEAPS has to as	sk for support by non-LEAPS facility countries (17): Belgium,	
Slovenia, Austri	ia, Czech Republic, Finland, Portugal, Croatia, Ireland, Estonia,	
Greece, Roman	ia, Hungary, Slovakia, Lithuania, Latvia, Bulgaria, Luxembourg,	
Malta, and Cyp	rus.	
	PORTANT DATES for LEAPS.	
2019		
Aug	LEAPS GA5	
Sept.	Meeting LEAPS CB	
Nov	2nd plenary meeting LEAPS at PSI 18-20.11.2019	
May-Dec.	Proposal writing for INFRAINNOV-04-2020 coordinated by DESY	
Dec	Deadline strategy of HE co-fund action ready	
2020	17th of March - INFRAINNOV-04	

14:30	LEAPS IT Pilot Phase Projects Update and Evolution	Mark Heron
	Mark Heron (DLS) gives a quick overview while updating on the LEAPS IT pilot phase.	
	In 2018 the Coordination board requested we consider three funding options for projects under LEAPS: 1. LEAPS technology projects funded by H2020 Innovation Call	
	 Not funded via the EC call 2019/2020 funded by other EU projects INFRAEOSC-4/5, 	
	 Not funded via the EC call 2019/2020 funded by other already running H2020 projects 	
	2 & 3 are about showing where we are working together And are covered by ExPaNDS, PaNOSC and CalipsoPlus	
	Work Groups were asked to revisit pilot projects and consider which of the Pilot Projects will be included in the INFRAINNOV-04-2020: Innovation Pilots Call.	
	 From Work Group 3 IT: IT Strategic Blueprint and Data Reduction and Compression 	
	From Work Group 1 Detectors: Detector ToolBox This meeting should meet the following shipstives:	
	This meeting should meet the following objectives:	
	 Agreement on content of pilot project proposals for LEAPS II Agreement on pilot project proposal(s) to go back to CB Agreement on participating of facilities 	
	 Agreement on Pilot Project leads 	
	IT Strategic Blueprint	Daniel Salvat
	Daniel Salvat (ALBA) gives an overview of the LEAPS WP3 IT Strategic Blueprint. Scientific capability and capacity of LEAPS facilities are determined the quality of their data management and software ie IT infrastructure.	
	To exploit the full scientific potential of LEAPS facilities require substantial and ongoing developments in IT.	
	A strategic blueprint has to be developed to define future IT needs. Propose to establish a European wide coordinated effort to investigate and understand the challenges faced by LEAPS facilities in IT. Define	
	Functional requirement from end users across the various science domains of LEAPS facilities.	
	Translate the science drivers into technical requirements/ specification for IT systems.	
	Assess IT solutions and technology to best address.	
	Tasks 1 to 5 of pilot project	

	Funding requested was 1.6 Mio, general assembly got 200k Euros / therefore	
	need to re-scope the project, opting for other options:	
	Common workshops *2x / year), meetings	
	Results of the poll	
	Data Paduction	Mark
		Heron
	Objectives> data reduction and compression	
	5 basic tasks	
	Update on Detector Toolbox	Bernd
		Schmitt
	Bernd Schmitt (PSI) updates on the WG 1 pilot project - Description of work	
	He highlights that is essential to make the data backend system a part of LEAPS IT	
	as there is a need for a common approach towards detectors and their	
	integration.	
	Colleboration Loons Detectors and IT	
	COAL from Detector side:	
	Development of a tealbax from Sensor to file on disk	
	• Development of a coolbox from sensor to file of disk	
	Euture Detectors will get close to 178/te/s	
	Patertors and data backend not independent	
	Common approach/Toolbox required	
	hetween LEAPS Detectors and LEAPS IT	
	hetween Facilities in general	
	Discussion on Inkind Contributions of the different facilities	Chair:
		Mark
	Gerd Mann suggests creating a closer link with the Detector project, in order to	Heron
	push a little more towards data reductions	
	Work package leaders:	
	Sandor Brockhausen from European XFEL volunteers to lead the WP on data	
	compression.	
16:00	Introduction to ExPaNDS	Knut
		Sander
	Kurt Sander (DESY) gives a broad overview of the ExPaNDS project, its objectives	
16.15	and its current activities.	
16:15	Update from ExPaNDS	Mark
	Mark undeter on the latest about Γ_{V} DONDS, its six (6) M/DS and relatives tasks	Heron
	Mark also mentioned planned and prospect collaborators	
	The PaNOSC and ExPaNDS projects tend to overlap concerning the technical	
	objectives. To keep in mind:	
	• ExPaNDS cannot duplicate what PaNOSC is funded to do	
	ExPaNDS must build on PaNOSC	

	There are some critical dependencies on PaNOSC :	
	PaNOSC Catalogue Service Deliverable	
	PaNOSC Analysis Deliverable	
47.45		
17:15	PaNOSC overview and Status	Andy
	Andy Götz (ESPE) presents an overview of the PaNOSC project and its status	GOTZ
	The project will run for four years and has six (6) partner infrastructures. The	
	mission of the project is to reduce on-site data and link all scientific data and	
	output together.	
	9 WPs with relative tasks.	
	PaNOSC, ExPANDS and EOSC are about making science RELIABLE and	
	REPRODUCIBLE.	
	PaNOSC's objectives:	
	1. Participate in the construction of the EOSC by linking with the e-infrastructures	
	and other ESFRI clusters.	
	2. Make scientific data produced at Europe's major Prioton and Neutron sources	
	3 Generalise the adoption of open data policies standard metadata and data	
	stewardship from 15 photon and neutron RIs and physics institutes across	
	Europe.	
	4. Provide innovative data services to the users of these facilities locally and the	
	scientific community at large via the EOSC. (Jupyter is the first common data	
	service to be provided).	
	5. Increase the impact of RIs by ensuring data from user experiments can be used	
	beyond the initial scope. (ILL developed a metric tool called PUMA, which will	
	help in this objective).	
	6. Share the outcomes with the national Ris who are observers in the proposal	
	data stewardship and the EOSC	
	There is a need to find common ground to link PaNOSC and ExPaNDs together	
	through concrete actions. This should be regulated by an official agreement,	
	allowing collaboration and sharing of outcomes.	
	Andy suggests that all ExPaNDs' WP leaders will be observers in PaNOSC.	

TUESDAY, MAY 14th

08:30	Introduction to technical topics and objectives	Mark Heron
	 We are meeting twice per year to develop the IT input into the LEAPS roadmap. The objectives of the project are long-term and include: Pilot project 2020+? Co-fund activities 2023+? 	

	We should use LEAPS IT WG meetings to share the current activities in each	
	facility. Therefore, we are going to have a series of technical talks today in	
	order to share knowledge and experience between facilities.	
	A doodle pool with a number of suggested topics: HDF5 and Nexus standards	
	was the subject that encountered most interest.	
08:45	Status, experience and plans for using NEXUS at your facility	
_		
12:30		
	Tech Talk PSI 20'	Mark
		Koennecke
	Nexus at SINO, SLS, SwissEEL	
	Nexus is a container that can possibly contain everything	
	SINO has been writing Nexus files since 1996 / more than 2 Min files which	
	have been written, analysed and scientific results obtained from	
		A
	Tech Talk ESRF 20	Armando
		Sole
	I ECH TAIK MAX IV 20	Darren
		Spruce
	DMP doing it through the university library – because it is linked to the	
	funding.	
	Tech Talk SOLEIL 20'	Majid
	Tech Talk ELETTRA 20'	Lorenzo
		Pivetta
	Tech Talk DLS 20'	Alun Ashton
	Summary of Technical Talks	Mark Heron
	Mixed up take of Nexus across photon facilities	
	Facilities have similar objectives	
	• Similar reasons for limited take up	
	• Facilities need a "Nexus Champion" to promote.	
	Nexus is caught between the pragmatism of getting experiments going and	
	delivering results versus delivering perfectly-described data	
	It is essential to promote the added value of Nexus to science and user	
	communities Therefore, it is important to work with communities to get	
	applications definitions agreed upon	
	applications definitions agreed upon.	
	this is appreciable	
	To dev	
	Address misconceptions in terms of overhead in writing Nexus	
	 Engagement with communities on FAIR and Open data 	
	Facilities could possibly use Data Policy to influence take up of Nexus as the	
	data standard. Data Management Plan and long-term curation may help.	

Working Group for NEXUS: LEAPS IT representatives should nominate a person to be part of the group.	
It would be valuable to have 1 example of Nexus file for each facility	
We will have a working group meeting during the LEAPS Plenary in November 2019 – half a day for the update and half a day for a chosen topic of interest.	

13:30	Status Update JRA2	Mirjam van
	Mirjam van Daalen (PSI) gives an overview on JRA2 objectives, its benefits for the users and WP24 Demonstrator of a Photon Science Analysis Service (DaaS).	Daalen
	Review Brussels	
	Update on Deliverables – submitted on time	
14:00	Design and Features of Portal (ALBA)	Daniel Salvat
	Daniel Salvat (ALBA) presents the project from its initial ideas to its current status and features, which include the following:	
	 Landing Page: List of available facilities. Authentication: Local Authentication allowed using REST API. UmbrellaID is also available. OpenID implemented (ESRF use case). Dataset retrieval From the DB. From an external endpoint (e.g. ICAT) Authorized access to resources is configurable. Access to Docker containers with no attached experiments. Extra features: Command line for adding/updating/deleting: Users Experiments Session Single record or CSV files are allowed. 	
14:30	Design of Data Analysis Service Infrastructure (ESRF)	Aidan
15:00	Results of Portal Tests by Site (ELETTRA)	Chair / Andy Götz
	What does the portal need in order to get into operation?	
	 Moving data from one side to another 	
	- Combine data	

	- Use case	
	Issues with UmbrellaID– authentication is only web-based There are currently some limitations (for ex. The need to insert credentials multiple times.)	
16:15	Intro Umbrella ID	Mirjam van Daalen
16:30	Feedback from the WG "Future of Umbrella ID Infrastructure"	Björn Abt
	Björn Abt (PSI) introduces project reminding that the umbrellaID collaboration connects the photon and neutron communities, consisting of more than 35000 users and gives this community a strong image amongst other research communities. It is highly important to preserve this visibility and keep ownership and governance within the community.	
	A crucial technical aspect of the collaboration is the attribute EAAHash, which is a unique and persistent identifier of a user.	
	The community workflow contains a large part of non-web-based interactions where there is still a need for user-friendly solutions.	
	The PaN community is user-centric and international, whereas most of the existing AAA federations in the research communities have an institute-based vision.	
	The rapidly growing security constraints and legal requirements drive us to explore further collaborations in order to increase our capacity to respond to users' needs in a stable, secure and trusted environment.	
	Furthermore, with the growing number of facilities entering the European Open Science Cloud (EOSC) project, there is a need to ensure global and comprehensive interoperability with services outside of the Photon and Neutron domain. Strong collaboration with other EOSC partners is becoming essential.	
	 The platform offered by GÉANT can: Fulfil the current status quo offered by umbrellaID Meet the upcoming needs towards EOSC Integrate new technical developments to the federation Provide a good user support Provide an outstanding uptime and performance 	
	Stefan Paetow (JISC) gives an overview of Moonshot, what it is and how it works, its pros and cons. Moonshot supports web and non-web Moonshot is a technology and doesn't depend on UmbrellaID	Stefan Paetow
17.00	Presentation EDU Teams in the context of Umbrella ID Presentation of the Service eduGAIN. eduTFAM	Christos Kanellopoulos
L		

Pilot demo	
Costs: the GÉANT project will cover all the costs for the initial years. Support within normal working hours is also provided.	
Integration with EOSC and other communities	J F Perrin
Typical use case from PaNOSC	

WEDNESDAY, MAY 15th

8:30	Open questions and discussions	Björn Abt
	Attributes	or
	Authorization model	JF Perrin
	Migration steps	
	 Non-web Access (Moonshot, ssh,) 	
	IDPs (eduGain, UmbrellaID, ORCID,)	
9:15	Decision Process and Roadmap	Mirjam van
		Daalen and
		JF Perrin
10:45	Harmonization of Data Policies and Data Management Plans	Mirjam van
		Daalen
	On March 30^{tn} , we submitted D. 2.6 and D. 2.8 that were due within NA1. A	
	survey was sent among the CALIPSOPIus partners in order to gain information	
	on the status of each facilities data policy.	
	CAUDSOnlys facilities based on the DANDate framework. Out of 10 facilities	
	14 have adopted a policy based on the PANData data framework. This is an	
	increase with respect to the last survey done for D2.2. At that time 4 out of	
	the 14 policies mentioned before were still planned or in preparation. The	
	harmonisation process is still on its way and the 5 missing data policies are	
	planned to be implemented until the end of the CALIPOnlus project. However	
	it has to be mentioned that the facilities with missing data policies are	
	facilities with a minor amount of users compared to the other partners of the	
	collaboration. Thus, less data are produced, giving the facilities less urgency to	
	put policies in place.	
	In general, the implementation of data policies at the different facilities is an	
	ongoing long-term process involving installation of metadata catalogue	
	software (see D2.8), data analysis software and data storage. This process is	
	time-consuming (often multiple years) and involves roll out from beamline to	
	beamline.	
	New projects under H2020 such as European Photon and Neutron Data	
	Services (ExPaNDS) and Photon and Neutron Open Science Cloud (PaNOSC)	

will build on the results of CALIPSOplus and work on the extension of data policy harmonisation and making data FAIR. With regards to the Data Management Plan, the survey showed that ten (10) out of nineteen (19) facilities have a metadata catalogue in place now, which is a clear progress in comparison to the status 1.5 years ago during the last survey done amongst CALIPSOplus partners. Several different metadata catalogue software are used (iCAT, SciCAT, ISPyB). Implementation of the Data Policies is done step by step (i.e. roll out from beamline to beamline) at all facilities. This stepwise process implies that a DMP will only be complete once these processes at the different facilities have been finished. Only three (3) out of nineteen (19) partners have a DMP in place on the national level, here there was no increase with respect to the last survey done for D2.2. Overall, the survey shows that the partner facilities are moving towards a more advanced harmonised data management structure, by putting in place data policies, metadata catalogues, data analysis infrastructures and storage capacities. All accessible via the UmbrellaID.

May 15th - Parallel Session DaaS Portal

GOAL OF THE MEETING: RECEIVE FEEDBACK FROM ATTENDEES, SHARE PLANS FOR THE IMMEDIATE FUTURE AND AGREE ON THE CONTRIBUTIONS IN FUTURE DEVELOPMENTS OF THE PORTAL.

ESRF (Andy Goetz, Armando Solé, Aidan Campbell)

- 1. <u>Feedback</u>: A list of needs have been defined in order to make this portal suitable for the ESRF.
- 2. <u>Plans</u>: Having a production environment ready for November 2019 (6 months from now).
- 3. Contributions: Aidan Campbell will be working (almost) full time on the project. (1 FTE)
- 4. <u>Needs</u>:

a. Jupyterhub infrastructure to be linked (not integrated) to the Portal.

b. Installation procedure should be improved. The current one is too dense. Suggested the technical installation/setup (to be located at the README.md) from the description and additional information of the project (suggested /docs folder).

c. Include Admin section for statistics purposes (e.g. What are the most used images? What is the level of resources reserved?...)

- d. Improve User Experience (agreed on the fact that this is a continuous improvement process)
- e. Remove 1-user-1-container constraint on the non-experiment section.

f. Role management might be needed, and information on the roles might be retrieved from an external resource, out of the portal.

g. Improve guacamole installation.

5. <u>Comments</u>: Contributions to the project will be made visible, as they have been so far, on the Github repository: https://github.com/Calipsoplus

DESY (Johannes Reppin)

1. <u>Feedback</u>: Interested in testing real use cases. Portal up and running on Kubernetes – in the next year run experimental data. This doesn't imply changes to application.

- 2. <u>Plans</u>: No plans for production.
- 3. Contributions: Johannes Reppin will be working half of his time on this project. (0.5 FTE)
- 4. <u>Needs</u>: No specific needs.
- 5. Comments: Interested in running the portal on Kubernetes.

DSL (Alun Ashton)

- 1. Feedback: Interested in participating. Going to invest in GPU cluster for imaging
- 2. <u>Plans</u>: No plans for production yet.
- 3. <u>Contributions</u>: 3 people to be hired. (5 FTE) To be confirmed.
- 4. <u>Needs</u>: No specific needs.
- 5. <u>Comments</u>: GPU support.

FELIX (Martin van Breukelen)

- 1. Feedback: Acting as observers.
- 2. <u>Plans</u>: No plans for production.
- 3. Contributions: Might be willing to participate as testers. (To be confirmed)
- 4. <u>Needs</u>: No specific needs.
- 5. Comments: No comments.

European XFEL (Sandor Brockhauser)

- 1. <u>Feedback</u>: Acting as observers.
- 2. <u>Plans</u>: No plans for production.

- 3. Contributions: Infrastructure depends on DESY.
- 4. <u>Needs</u>: No specific needs.
- 5. <u>Comments</u>: No comments.

Soleil Synchrotron (Majid Ounsi and Grégory Viguier)

- 1. Feedback: Installation and setup is work in progress at Soleil.
- 2. <u>Plans</u>: Prototype for internal use by November 2019.
- 3. <u>Contributions</u>: As testers.
- 4. <u>Needs</u>: No specific needs.
- 5. Comments: No comments.

MAX IV (Darren Spruce)

1. <u>Feedback</u>: They are currently acting as observers of this project but will be starting hiring people to work on this in the next few years. Strategy online data processing through the university, which uses a different software

- 2. <u>Plans</u>: No plans for production.
- 3. Contributions: Might be willing to participate as testers. (To be confirmed)
- 4. <u>Needs</u>: No specific needs.
- 5. Comments: No comments.

PSI (Stefan Egli and Kai Kaminski)

- 1. <u>Feedback</u>: Acting as observers.
- 2. <u>Plans</u>: No plans for production.
- 3. Contributions: Might be willing to participate as testers. (To be confirmed)
- 4. <u>Needs</u>: Identified use case -> Students.
- 5. Comments: Is Guacamole removable? (Other options should be considered)

ALBA (Daniel Salvat)

- 1. Feedback: Active member of the development team.
- 2. <u>Plans</u>: No plans for production, yet. To be discussed internally.

3. <u>Contributions</u>: Alex Camps and Daniel Sanchez (and maybe others) might be able to participate (0.5 FTE) until September 2019, when the ExPaNDS project starts. To be confirmed.

4. <u>Needs</u>: No specific needs, for the moment.

5. <u>Comments</u>: UI to be improved

- a. Login page should be more user-friendly.
- b. Information shown on the Proposal page should be improved.