

# Deliverables

<b>Deliverable Number</b>	<b>D24.1</b>
<b>Deliverable Title</b>	<b>Report on Kick-off Workshop for the CALIPSOplus partners to present their needs for a remote data analysis</b>
<b>Lead Beneficiary</b>	<b>PSI</b>
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## Deliverable report

### WP24

## Demonstrator of a Photon Science Analysis Service (DaaS)

#### WORK PACKAGE

WP24

#### WORK PACKAGE LEADER

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Co-lead Andy Götz (ESRF)

#### ESTIMATED INDICATIVE PERSONMONTHS FOR THE DELIVERABLE

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#### DELIVERABLE DESCRIPTION

Kick-off workshop for the CALIPSOplus partners to present their needs for remote data analysis

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11

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## Premise

The present deliverable describes the first kick-off workshop of JRA2, i.e. WP24 Demonstrator of a Photon Science Analysis Service (DaaS). Participants were the partners of the CALIPSOplus collaboration (see participant list at the end of the document).

Light sources are generators of big volumes of complex scientific data and their users need assistance in analysing the scientific data. The aim of this JRA is to build up demonstrators for remote data analysis for a small number of archetypal experiments. The demonstrators will build on the HPC platforms of each participating institute. The demonstrators will be cloud based in those institutes where cloud technology is deployed. In the other institutes the demonstrator will run on standard HPC hardware. A web portal will ensure users to have a common user experience.

## Description of Work

### WP24: Demonstrator of a Photon Science Analysis Service (DaaS)

#### 1. Introduction

The kickoff meeting for the JRA2 work package of the CALIPSOplus project, organised by ESRF, took place from 26-28 June on the EPN campus in Grenoble in the IBS seminar room. The goal of JRA2 (i.e. WP24) is to build a Remote Data Analysis Demonstrator for photon science.

#### 2. Outline of the workshop

The kickoff meeting was 3 days long and addressed the different tasks of the work package. The second day was entirely focused on WP24 and each partner presented their plans for the task(s) they are responsible for (see <https://indico.esrf.fr/indico/event/8/timetable/#20170626.detailed>). The first part of the meeting (day 1) was dedicated to the UmbrellaID federated identity system and its connection to the JRA. The third part of the workshop (day 3) was on invitation only and was reserved for discussing the LEAPS IT work package and its connection to Umbrella ID and JRA2. For more info on the LEAPS initiative refer to <https://www.leaps-initiative.eu/about/>.

#### 3. Beneficiaries JRA2, i.e. WP24

Beneficiaries	Description	TOT Costs <u>incl</u> travel
PSI (leader)	30 PM	322 k€
ESRF (co-leader)	28 PM	248 k€
DESY	15 PM	120 k€
DLS	6 PM	50 k€
CELLS	12 PM	53 k€
<u>Elettra</u>	12 PM	64 k€
Soleil	6 PM	40 k€
EUXFEL	observer	2 k€
TOT (incl. 25% indirect costs)		899 k€

Table 1: Beneficiaries participating in WP24

## 4. Workshop program

Workshop program 3 days 26-28.06.2017

(see: <https://indico.esrf.fr/indico/event/8/timetable/#20170626.detailed> )

Day 1: 26.06.2017

Umbrella, Calipsoplus JRA2 Kickoff +LEAPS-IT / Programme

Monday 26 June 2017

### Umbrella, Calipsoplus JRA2 Kickoff +LEAPS-IT

## Monday 26 June 2017

### UmbrellaID - IBS Seminar Room (14:00-18:30)

#### *Developments around UmbrellaID*

time	[id]	title	presenter
14:00	[15]	Welcome	DIMPER, Rudolf
14:10	[16]	Status Umbrella	VAN DAALEN, Mirjam
14:30	[18]	CALIPSOplus & Umbrella	VAN DAALEN, Mirjam
15:00	[19]	EduTeams	ABT, Björn Erik
15:20		Coffee	
15:50	[20]	Moonshot @ Diamond	PAETOW, Stefan
16:10	[21]	OPEN IRIS & Umbrella	ABT, Björn Erik
16:30	[22]	Umbrella IdP	PERRIN, Jean-François
16:50	[37]	ESRF Umbrella status	PORTE, Dominique
17:05	[23]	EduGAIN & Key Cloak	ROUX, Antoine
17:25	[17]	Umbrella sustainability	VAN DAALEN, Mirjam
18:00	[24]	Roadmap & Discussion	

### Dinner on-site - Chalet (18:30-21:00)

Day 2: 27.06.2017

Umbrella, Calipsoplus JRA2 Kickoff +LEAPS-IT / Programme

Tuesday 27 June 2017

## Tuesday 27 June 2017

### **JRA2 Kickoff - IBS Seminar Room (09:00-12:15)**

#### ***Presentation of work packages***

time	[id] title	presenter
09:00	[0] Introduction	VAN DAALEN, Mirjam
09:20	[1] Task 1 - Design of DAAS platform	GOETZ, Andrew
09:50	[2] Task 2 - Select use cases + software	EGLI, Stephan
10:10	[10] Industrial Use Cases	MITCHELL, Edward
10:20	Coffee	
10:40	[4] Task 4 - Portal	SALVAT, Daniel
11:00	[6] Task 6 - Authentication + Identity	ABT, Björn Erik
11:20	[7] Task 7 - Test use cases	KOUROUSIAS, Georgios
11:40	[3] Task 3 - Deployment	GOETZ, Andrew

### **Lunch - Guest Room Site Restaurant (12:00-14:00)**

### **JRA2 Planning - IBS Seminar Room (14:00-18:00)**

#### ***Plan the next steps and overall work plan for JRA2***

time	[id] title	presenter
14:00	[14] DAAS prototype @ ILL	HALL, Jamie
14:30	[8] Planning + Deliverables	VAN DAALEN, Mirjam GOETZ, Andrew
14:50	[9] Working together	VAN DAALEN, Mirjam GOETZ, Andrew
15:10	[11] Discussion	
15:30	Coffee	
15:45	[12] Breakout	
16:30	[13] Next steps	

### **Dinner Bar Le Zinc downtown - IBS Seminar Room (18:30-21:00)**

Day 3: 28.06.2017

Umbrella, Calipsoplus JRA2 Kickoff +LEAPS-IT / Programme

Wednesday 28 June 2017

## Wednesday 28 June 2017

### **LEAPS IT - IBS Seminar Room (08:00-17:00)**

#### ***Preparation meeting for the LEAPS IT pilot project***

time	[id] title	presenter
09:00	[26] Coffee	
09:15	[25] Welcome	DIMPER, Rudolf
09:30	[27] Introduction to LEAPS	VAN DAALEN, Mirjam
10:00	[28] LEAPS IT	HERON, Mark
10:30	Group Photo + Coffee	
11:00	[30] EOSC	REICHERT, Harald
11:30	[31] PaNdata + PaNDaaS wrt LEAPS	GOETZ, Andrew
12:00	[32] Lunch	
13:00	[33] Input from LEAPS facilities	
15:00	[34] Summary of LEAPS input	HERON, Mark
15:30	Coffee	
15:45	[35] LEAPS Pilot projects	GOETZ, Andrew
16:30	[36] Next steps	HERON, Mark

## 5. Distribution of tasks within WP24

**Day 2** of the workshop was specifically dedicated to planning of the work within the joint research activity (WP24). The main task was to distribute the work within JRA2 is to build a Remote Data Analysis Demonstrator for photon science. The different tasks of the work package were addressed and presented by the task leaders from the different facilities (see workshop program above). The tasks (see list below) were discussed at the meeting and each partner could declare interest to participate in the different tasks.

### Task list WP24:

#### Task 24.1 Task lead ESRF Andrew Goetz

**Description:** Design a platform which satisfies the requirements for Remote Data Analysis as a Service. The design will take into account the current situation at the partner institutes. Study approaches which increase re-usability of solutions like component based software engineering and development of scientific/algorithmic libraries. Evaluate different container concepts as deployment strategies, like classical installation procedures, shipping of virtual machines and/or Docker containers.

The task leader proposed that in view of the different infrastructures on each sites it is better to adopt a functional architecture approach. The approach would consist on agreeing on the different functional requirements and then adapting these to the local infrastructure solutions. The NIST Big Data functional architecture has been proposed as starting point (see fig below). The next step will be to involve the architects from the different sites to agree on the functional components.

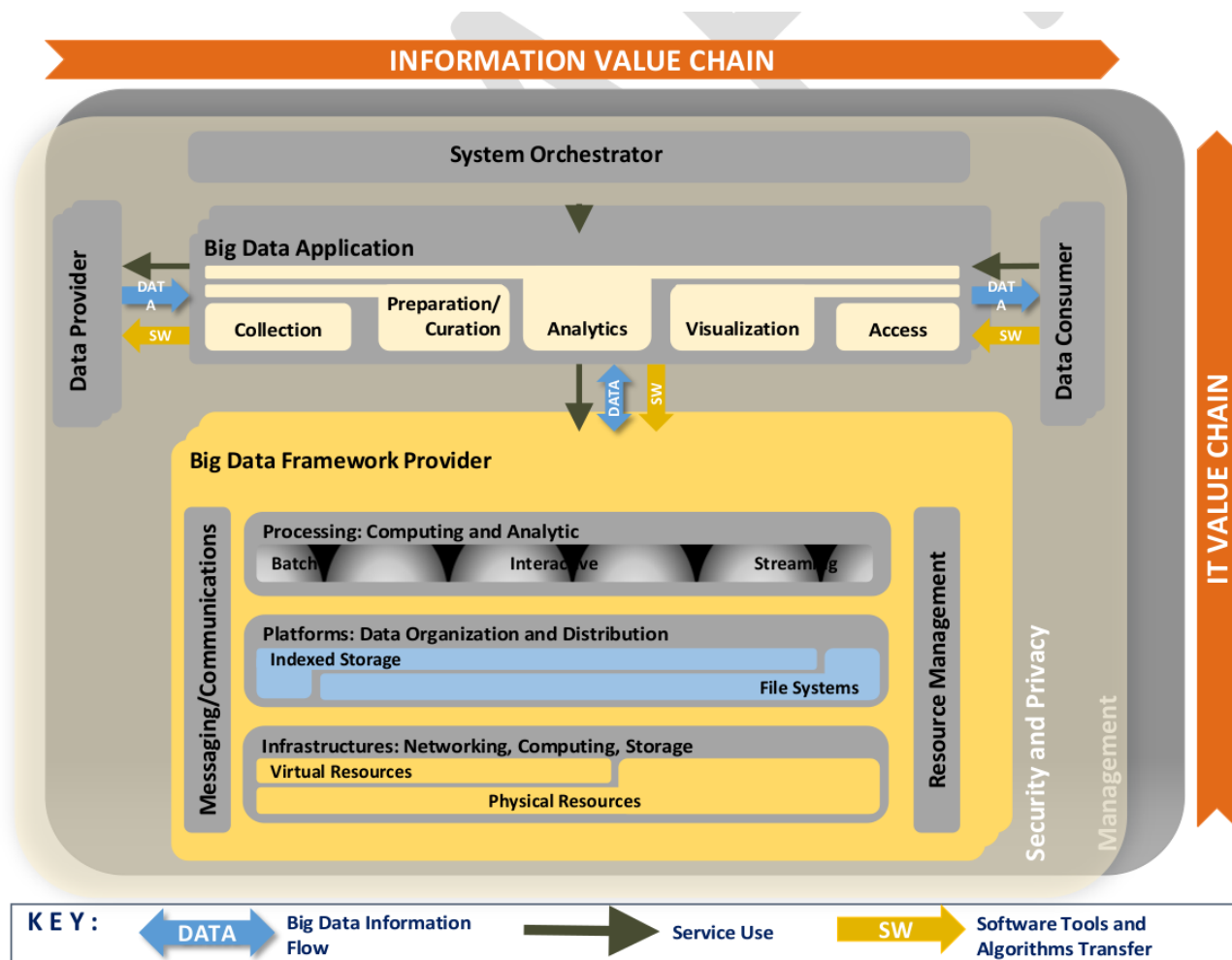


Figure 2: NIST Big Data Reference Architecture (NBDRA)

### Task 24.2 Task lead PSI, Stephan Egli

**Description:** Collect and compare offline (post experiment) data analysis requirements and existing software solutions from users of at least three different sites. Analyse which of these use cases and/or solutions are suitable candidates for providing harmonised solutions which can be transferred from one site to another site. This is done for the use case domains selected i.e. SAXS, tomography, diffraction (including MX).

The task leader proposed to define 3 sites, each with a use case. Each site has the role of "leading house" for their selected application e.g. PSI selects cSAXS Ptychography Software, and makes it available for other sites. The JRA2 will then make it deployable on new platform. Contact persons would need to be defined for each site. Start from existing software catalog <https://software.pan-data.eu/> (entries so far from ALBA, ESRF, ILL)? Concentrate on applications for offline analysis which are at the end of an analysis chain (and therefore hopefully quite generic)? A questionnaire will be sent around for selecting application candidates and corresponding institutes and contact persons.

### Task 24.3 Task lead ESRF Andrew Goetz

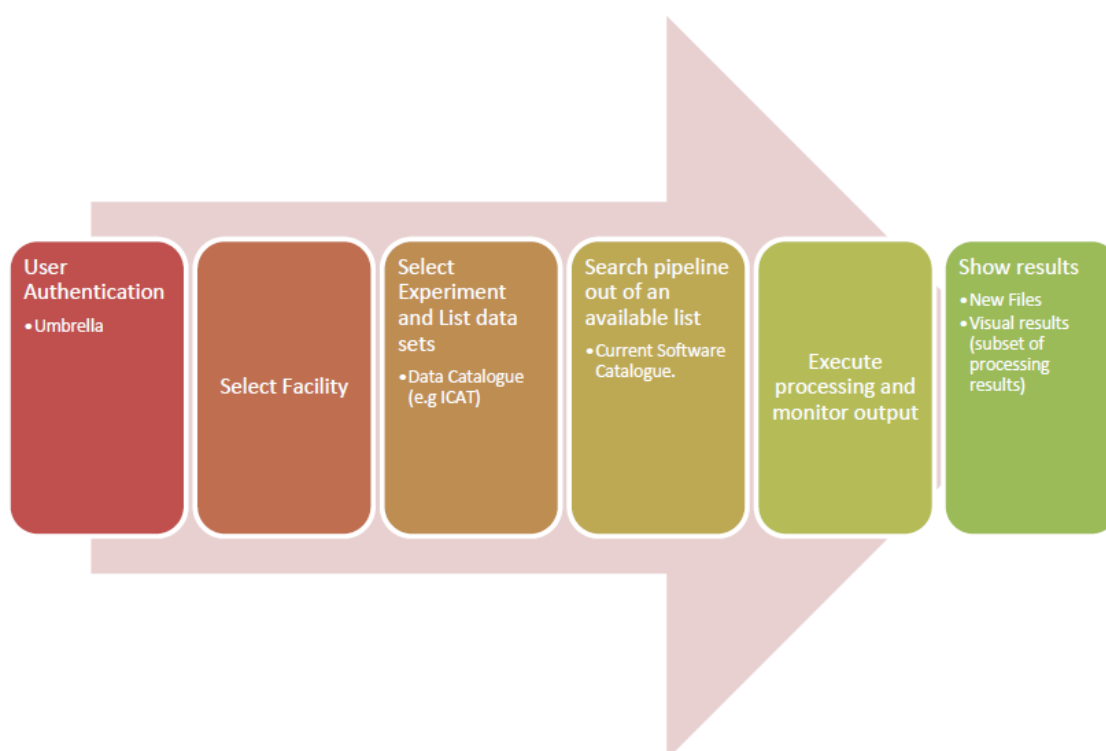
**Description:** Implement DaaS on the local platform at each site with remote access to compute and storage resources using dedicated hardware resources supplied by each site.

This task depends on the choices made in Task 24.1 and was not discussed in detail. Each site will have to do their own deployment to fit with their local infra-structure.

### Task 24.4 Task lead ALBA, Daniel Salvat

**Description:** Design and implement Remote Data Analysis as a Service portal demonstrator.

The aim of this task is to provide a fully web-oriented user experience to remote users, integrate current established services among the different facilities, take advantage of current maturity of web frameworks and technologies. The UmbrellaID will be the the main (only?) login. The process for implementing this task is depicted below:





**Task 24.5 Task lead DESY, Frank Schlutzen**

**Description:** *Package and deploy data analysis packages for at least two use cases / site.*

This task was not discussed due to the absence of someone from DESY at the meeting. The main direction proposed is to use containers (Docker or others) for packaging.

**Task 24.6 Task lead PSI, Björn Abt**

**Description:** *Extend and deploy the Umbrella authentication system as the standard authentication mechanism to fully support different non-web-based authentication mechanisms to be able to service a broader range of facilities (eduGain + JISC Assent) with differing needs and capabilities.*

The task leader explained that the two main authentication mechanisms to be added to UmbrellaID are MoonShot and OpenID. The former is needed for authentication non-web applications and the latter will simplify use of UmbrellaID in web applications. A demonstrator for MoonShot in UmbrellaID exists but needs to be made production level ready.

**Task 24.7 Task lead Elettra, Georgios Kourousias**

**Description:** *Test data analysis software for Use Cases with test data and users.*

The task leader explained how Elettra what DAAS services they have implemented and their experience. Their experience will be very relevant for carrying out the tests.

## 6. Synergies with Other WP's of CALIPSOplus

**Synergies with WP4 European Light Sources for Industrial Innovation plus (ELSIplus)**

Synergies with WP4 were discussed, during and after the presentation of WP4 leader Ed Mitchell from ESRF (see workshop program). As CALIPSOplus wants to improve the industrial client experience, synergies have to be used here between both work packages. The first task is to get WP24 in contact with the industrial advisory board IAB of WP4 and discuss the needs of industry in data analysis for the different use cases of WP24.

**Synergies with WP2 User tools for access and data management**

Synergies of WP24 with WP2 were discussed during the kick off meeting of CALIPSOplus project in Dresden 18-19.05.2017. Synergies between the two WP's will be mainly focussing on the developments for the Umbrella ID.

## 7. Workshop participants



Figure 1 LEAPS and CALIPSOplus JRA2 Kickoff workshop participants 26-28.06.2017 ESRF Grenoble (for names see list at end of document)

## Conclusion

Three workshops related to JRA2 (WP24) were held from 26-28 June 2017 at the ESRF in Grenoble. The first workshop on UmbrellaID highlighted the wide deployment of Umbrella as a secondary authentication system. A number of presentations described the ongoing developments to add support for different authentication protocols e.g. openID, KeyCloak, MoonShot.

The CALIPSOplus JRA2 kickoff meeting included presentations by each of the task leaders who explained the state of the art in their institute and presented their plans for implementing their tasks. First work within WP24 was started and distributed between the different participating facilities. The task leaders will start their work and report in monthly telephone conferences to the WP lead. Mailing lists will be made available by WP1 and 2 face to face meetings a year will be strived for.

The third and final workshop linked to CALIPSOplus JRA2 was dedicated to the LEAPS-IT working group. LEAPS is an initiative of the accelerator-based photon sources in Europe to seek EC funding for research and development over the next 9 years. The IT working group meeting at the ESRF brought all partners on board by explaining the current status of this initiative and gathering input from all the partners on what their main needs in IT are. During the meeting it was clear that the current and future challenges are huge and we will have to deal with detectors producing gigabits to terabits per second, experiments producing hundreds of terabytes up to petabytes per week and archives which will approach the hundreds of petabytes if not exabytes over the next 10 years.

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