



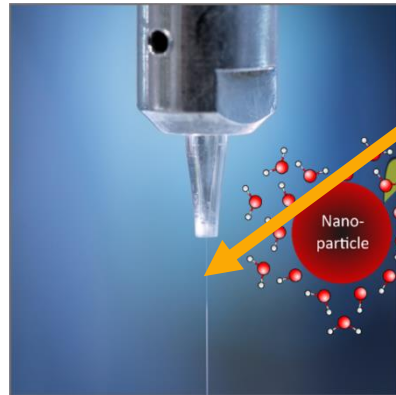
# Digital LEAPS – STARS proposal

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LEAPS Plenary Meeting, 21 October 2021

# STARS - Surveying Technology for Advancing Remote Services

## A bit of background:

### Sample



Flowing liquid microjet in vacuum to investigate nanoparticle solutions.  
Credit: HZB/R. Seidel



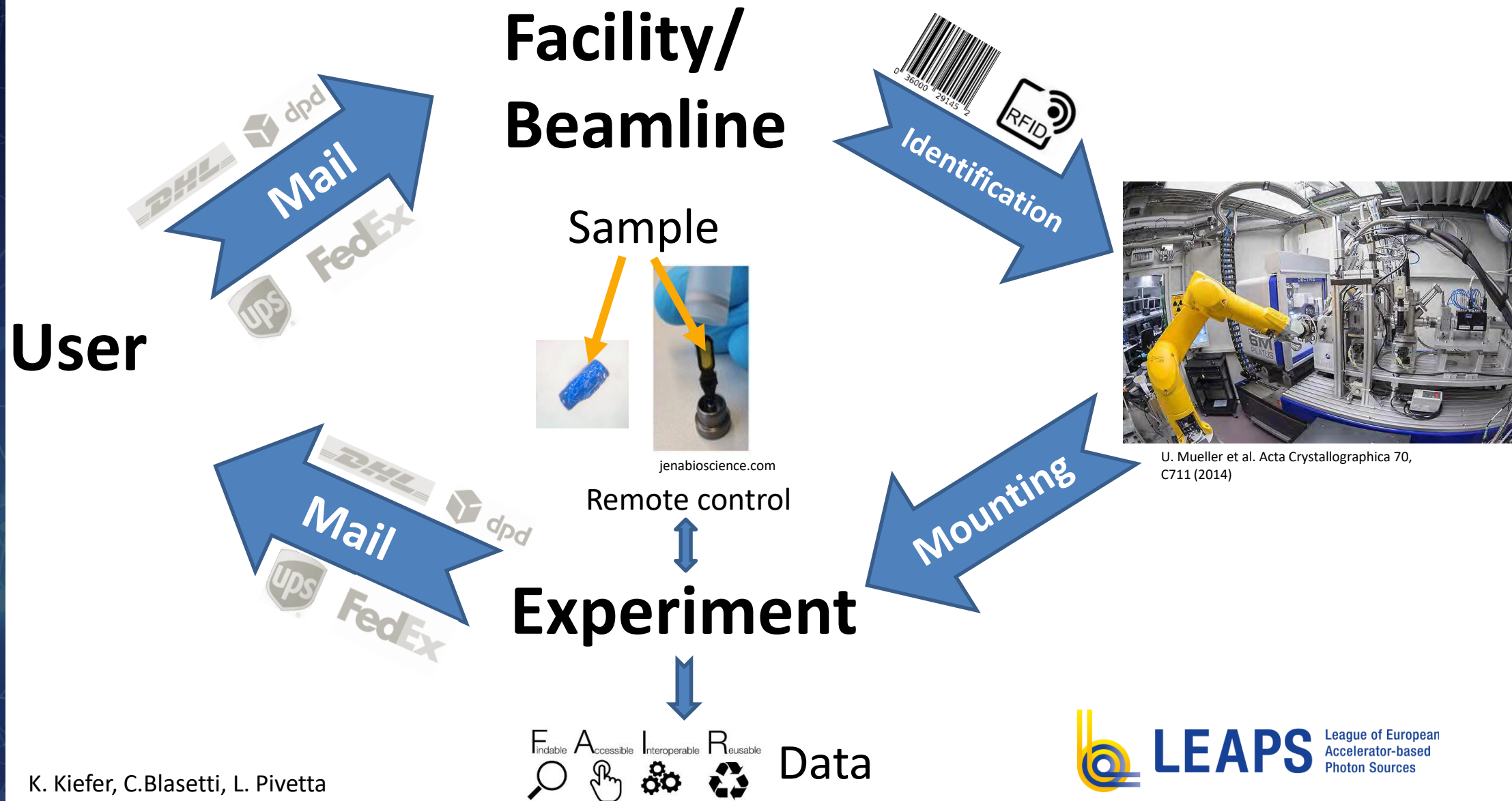
Sample holder for protein  
X-ray crystallography  
jenabioscience.com



Picture of the skull of a juvenile *Mussaurus patagonicus*, of roughly 2 years of age. Size of the skull: 10cm long.  
Credit: @ESRF/C.Argoud

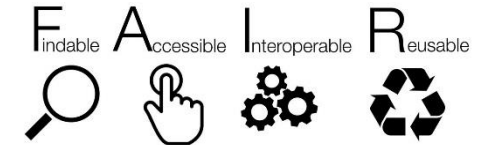


# STARS – Sample Life Cycle

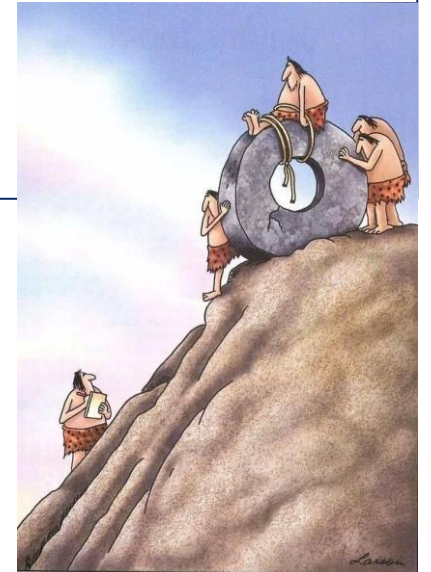


## STARS - Goals

- Make **sample information F.A.I.R. compliant**
- Bring **EOSC standards** into sample handling
- Help users and user offices to **manage samples**
- Foster **automation** and **remote operation** at beamlines



**EUROPEAN OPEN  
SCIENCE CLOUD**




Early experiments in transportation

*Joint work of User Offices, IT, Facility scientists*

# Example: sample identification and tracking at MX beamlines

## ISPyB (Information System for Protein CrystallographY Beamlines)

[About Us](#) [For Users](#) [Industry](#) [Public](#) [Science](#) [Instruments](#) [Careers](#) [More ▾](#)  [Search](#)

Macromolecular Crystallography

In This Section

MX Responsive Beamtime Guide Manual

Preparing for Beamtime ISPyB/SynchWeb

Select a Proposal

Add Lab Contact

Create a shipment

Registering a protein

Registering Samples

Prepare Experiment

Data Management

Data Management

Mobile Access

Sample Holders

Shipping Samples

Sample Changer

Remote Access

Data Collection Software

Mini Kappa

Data Analysis

Data Backup

Webcams

Acknowledging MX beamlines

Introduction to Eiger2 X

Detectors for MX at Diamond

Redhat 7 user environment

Science Highlights

Beamtime shift Patterns

Useful Calculators

### Registering Samples

#### Registering Samples in Container

To register samples, it is first necessary to create a new shipment, and detail information on all proteins.

1. [Ensure sample registered on UAS](#)
2. [Create Shipment](#)
3. [Create Protein](#)
4. [Register Samples](#)

Once a Shipment has been created click the "Add Container" button on a dewar in the shipment

#### Shipment Contents

Select a dewar by clicking on the row in the table below. Dewar details are then shown below. Click the + icon to add a container to the selected dewar

Name	Barcode	Facility Code	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers
DLS-01-0001	cm4950-0003872	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	opened		0 <a href="#">+</a>
Dewar1	cm4950-1-03-0003870	<a href="#">Click to edit</a>	cm4950-1	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	opened		<a href="#">Click to add a container</a> <a href="#">+</a>
rt	cm4950-0003871	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	opened		0 <a href="#">+</a>
DLS-01-0001	cm4950-0003873	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	opened		0 <a href="#">+</a>
DLS-01-0001	cm4950-0003874	DLS-01-0001	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	<a href="#">Click to edit</a>	opened		0 <a href="#">+</a>

This will take you to the register container page. Here you can register samples for this puck.

#### Add New Container

This page shows the contents of the selected container. Samples can be added and edited by clicking the pencil icon, and removed by clicking the x

Shipment

Dewar

Container Type

Container Name

Registered Container

Priority Processing

Automated Collection

Owner

Comments

Dewar1

Puck

High2DIALS

☐

Elser Nielsen (You)

1

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### ISPyB project

The ISPyB (Information System for Protein CrystallographY Beamlines) is a LIMS dedicated to protein crystallography experiments on synchrotron beamlines, it has been extended in 2013 to BioSaxs beamlines and in 2018 to CryoEM.

The ISPyB project was a joint development between ESRF/spine and BM14/MRC/eHTPX, based on the PXWeb ESRF project.

It is now deployed also at SOLEIL, EMBL Hamburg, Max IV, ALBA, HZB, and also at APS and NSLS for tests. A MOU was signed on January 2017 with other European institutes to define the frame of a collaboration.

For more information on ISPyB at ESRF you may contact [ispyb@esrf.fr](mailto:ispyb@esrf.fr).





## **STARS** - Structure

### **3 Work packages:**

**WP1:** Overview of procedures for mail-in sample handling

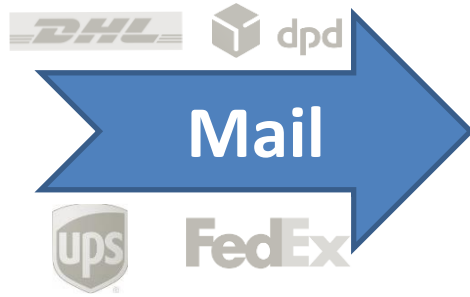
**WP2:** Overview of IT tools for remote access

**WP3:** Digital Sample Handling

Proposed starting date: **December 1st, 2021**

Month 6 milestone → May 2022

# **STARS – WP1:** Overview of procedures for mail-in sample handling



**Only first year (M1-12):**

**Task 1.1:** Overview of mail-in sample handling procedures at LEAPS and LENS facilities

## **STARS – WP2:** Overview of IT tools for remote access

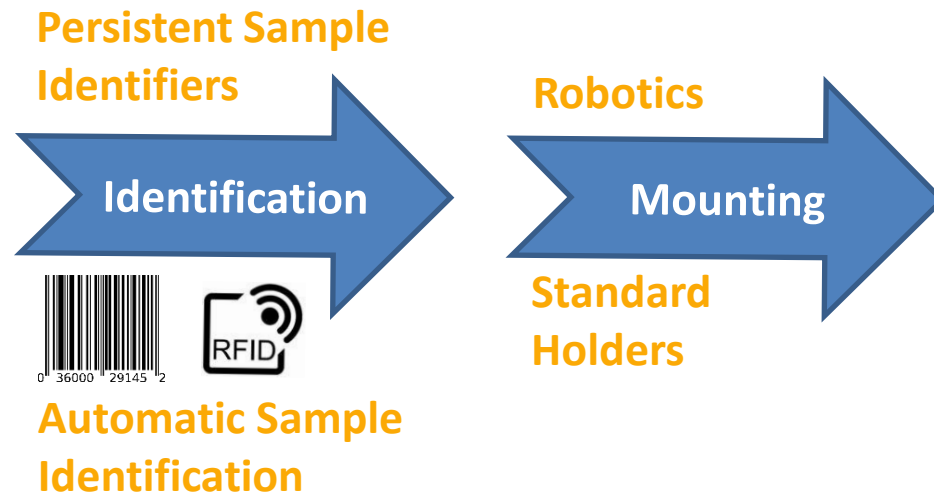


**Only first year (M1-12):**

**Task 2.1:** Overview of existing tools in use at LEAPS and LENS facilities



## STARS – WP3: Digital Sample Handling



MX beamline Bessy II, U. Mueller et al. Acta Crystallographica 70, C711 (2014)

### First year (M1-12):

**Task 3.1:** Survey on Digital Sample Handling

**STONE month 6:** Decision on program and budget for years 2-4

**Task 3.2:** Persistent Unique Identifiers for Samples

**Task 3.3:** Automatic Sample Identification

**Task 3.4:** Automatic/remote Sample Handling

# STARS - Resources

Participant short name	WP1 (M1-12)		
	Own contribution*	Request ed LEAPS resources	3rd party funding
ALBA*	0.25 PM UO		
DESY*	0.25 PM UO		
DIAMOND*	1 PM UO		
ELETTRA*	1 PM co-leader + 0.5 PM UO		
ESRF*	2.5 PM UO (Coordination + UO)		
EuXFEL*	0.25 PM UO		
FELIX*	0.25 PM UO		
HZB*	1 PM UO		
HZDR*	0.25 PM UO		
INFN*	0.5 PM UO		
ISA*	0.25 PM UO		
MAXIV*	0.25 PM UO		
PSI*	0.25 PM UO		
PTB			
SESAME*			
SOLARIS*	1 PM UO + 1 PM Coord		
SOLEIL*	1 PM UO		

\*confirmed by facility

## Resource tables not finalized

Participant short name	WP2 (M1-12)		
	Own contribution	Request ed LEAPS resources	3rd party funding
ALBA ?	0.5 PM IT		
DESY	0.5 PM IT		
DIAMOND	0.5 PM IT		
ELETTRA	1 PM Coord + 0.5 PM IT		
ESRF	0.5 PM IT		
EuXFEL	0.5 PM IT		
FELIX	0.5 PM IT		
HZB	0.5 PM IT		
HZDR?	0.5 PM IT		
INFN*	0.5 PM (IT/BL)		
ISA*	0.25 PM (IT/BL)		
MAXIV	0.5 PM IT		
PSI	0.5 PM IT		
PTB			
SESAME			
SOLARIS	0.5 PM IT		
SOLEIL	0.5 PM IT + 0.5 PM BL		

\*stated by facility

Participant short name	Task 3.1 (M1-12)		
	Own contribution	Requested LEAPS resources	3rd party funding
ALBA	0.5 PM IT + 0.5 PM SE		
DESY	0.5 PM IT + 0.5 PM SE		
DIAMOND	0.5 PM IT + 0.5 PM SE		
ELETTRA*	0.5 PM IT + 0.5 PM SE		
ESRF ?	0.5 PM IT + 0.5 PM SE		
EuXFEL	0.5 PM IT + 0.5 PM SE		
FELIX	0.5 PM IT + 0.5 PM SE		
HZB (leader)*	0.5 PM IT + 0.5 PM SE + 0.5 BL + 2 PM Coord		
HZDR*	0.25 PM IT + 0.25 PM SE (realistic, but further Coord needed)		
INFN*	0.5 PM (IT/SE)		
ISA*	0.25 PM (IT/SE)		
MAXIV *	0.5 PM IT + 0.5 PM SE		
PSI	0.5 PM IT + 0.25 PM SE		
PTB	0.5 PM IT + 0.5 PM SE		
SESAME			
SOLARIS	0.5 PM IT + 0.5 PM SE		
SOLEIL (co-leader 3.1)*	0.5 PM IT + 0.5 PM SE + 0.5 BL + 1 PM Coord		

\*stated by facility

# **STARS** – levels of standardization for digital sample handling

*European and  
worldwide  
data initiatives*



**Global standards  
Central resources**



*Consortia of  
facilities and  
users*



**Requirements  
Use cases**



**Adaptation  
of standards**



*Experiments at  
the facilities*



**Implementations**



## **STARS** - Summary

Key messages:

**STARS** addresses **problems** that **every facility will have to face ANYWAY** in the next years.

**If we work together, we will:**

- Solve the problem
- Save resources
- Offer a better service to our users

Cooperation between IT, SE, UO, BL

# Commitment needed