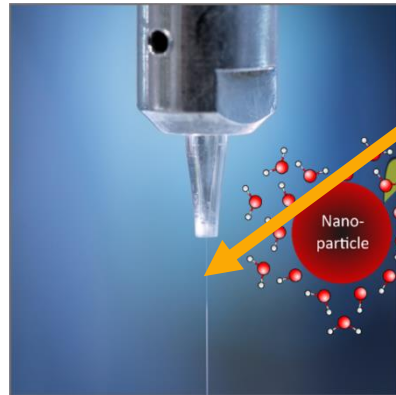# Digital LEAPS – STARS proposal

Klaus Kiefer , Cecilia Blasetti, Lorenzo Pivetta,

LEAPS Plenary Meeting, 21 October 2021

A bit of background:

Sample

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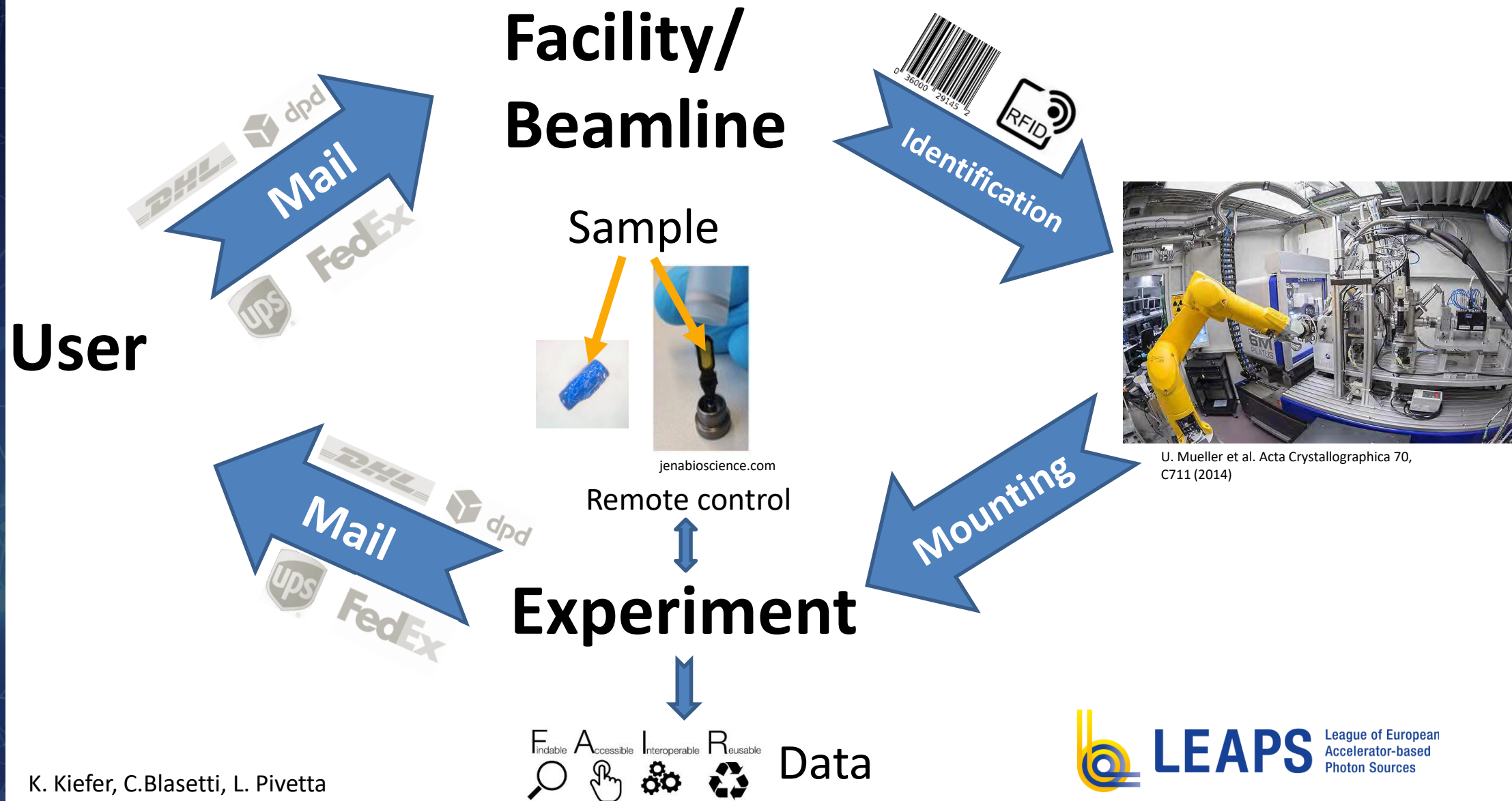Credit: HZB/R. Seidel

Sample holder for protein X-ray crystollography
jenabioscience.com

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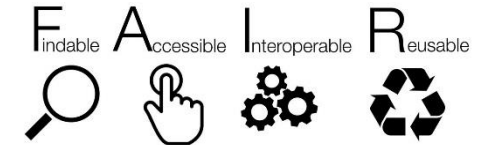Credit: @ESRF/C.Argoud

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STARS – *Sample Life Cycle*

Facility/Beamline

Mail

User

Sample

jenabioscience.com

Remote control

Identification

Mounting

U. Mueller et al. Acta Crystallographica 70, C711 (2014)

Mail

Experiment

Findable Accessible Interoperable Reusable Data

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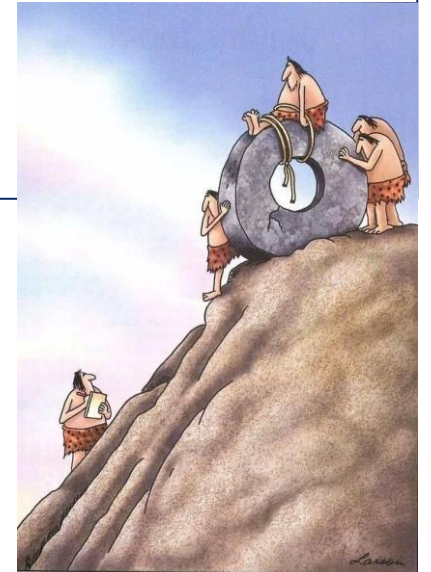League of European Accelerator-based Photon Sources

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**

Joint work of User Offices, IT, Facility scientists

F.indable A.ccessible I.nteroperable R.eusable

EUROPEAN OPEN SCIENCE CLOUD

Early experiments in transportation

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Example: sample identification and tracking at MX beamlines

ISPyB (Information System for Protein CrystallographY Beamlines)

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.**

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

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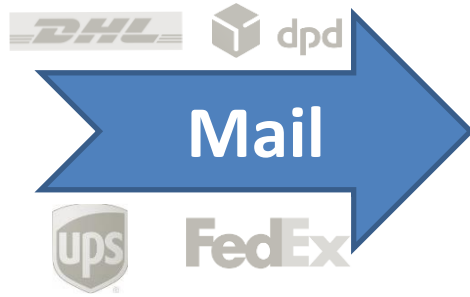
Mail

Only first year (M1-12):

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

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STARS – WP2: Overview of IT tools for remote access

Digital User Office

Only first year (M1-12):

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

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STARS – WP3: Digital Sample Handling

Persistent Sample Identifiers

Identification →

Robotics

Mounting →

Standard Holders

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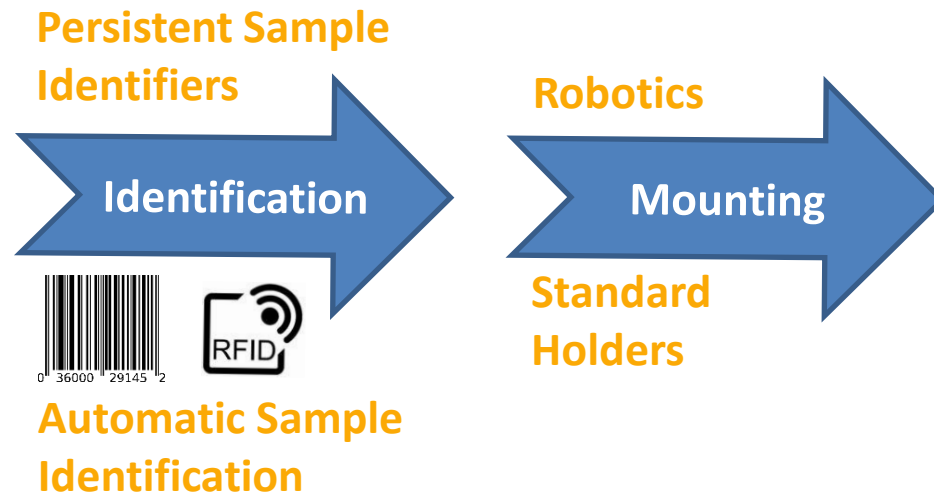
MX beamline Bessy II, U. Mueller et al. Acta Crystallographica 70, C711 (2014)

First year (M1-12):

Task 3.1: Survey on Digital Sample Handling

MILESTONE 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

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STARS - Resources

Resource tables
not finalized

Participant short name	WP1 (M1-12)		
	Own contribution*	Requested 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

Participant short name	WP2 (M1-12)		
	Own contribution	Requested 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

*stated by facility

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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

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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

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