
ESRF
The European Synchrotron

STREAMLINE

INTRODUCTION & OVERVIEW

Michael Krisch

On behalf of the Streamline Executive Team

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Outline of the presentation

- Acknowledgments
- Streamline in the context of the ESRF Upgrade Programme
- Project organization and structure
- Project overview and highlights
- Introduction of the next speakers

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

ACKNOWLEDGEMENTS

Former STREAMLINE coordinators: **Jean Susini and Harald Reichert**

Members of the Executive Team & Project Support Team: **Gary Admans, Patrick Bruno, Ennio Capria, Marine Cotte, Delphine Chenevier, Chiara Facoetti, Andy Götz, Gema Martinez Criado, Joanne McCarthy, Ed Mitchell, Stephanie Monaco, Annalisa Pastore, Eleonore Ryan, Anne Talucci**

All STREAMLINE participants

ESRF Senior Management

Project Advisor, European Research Executive Agency: **Christos Chatzimichail, Angela Lahuarta-Marin**

Project Reviewers: **Lars Osten Christer Frojd, Axel Steuwer**

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STREAMLINE IN A NUTSHELL

STREAMLINE

SusTainable REseArch at Micro and nano X-ray beamLINEs

- **EU Programme Call: H2020 INFRADEV-2018-2019 (RIA)**
- **Topic: Infradev-03: Sustainability of RIs**
- **Funding: 4997.5 M€**
- **Single beneficiary: ESRF**
- **Duration: 15th Nov. 2019 – 14th May 2024**

streamline.esrf.eu

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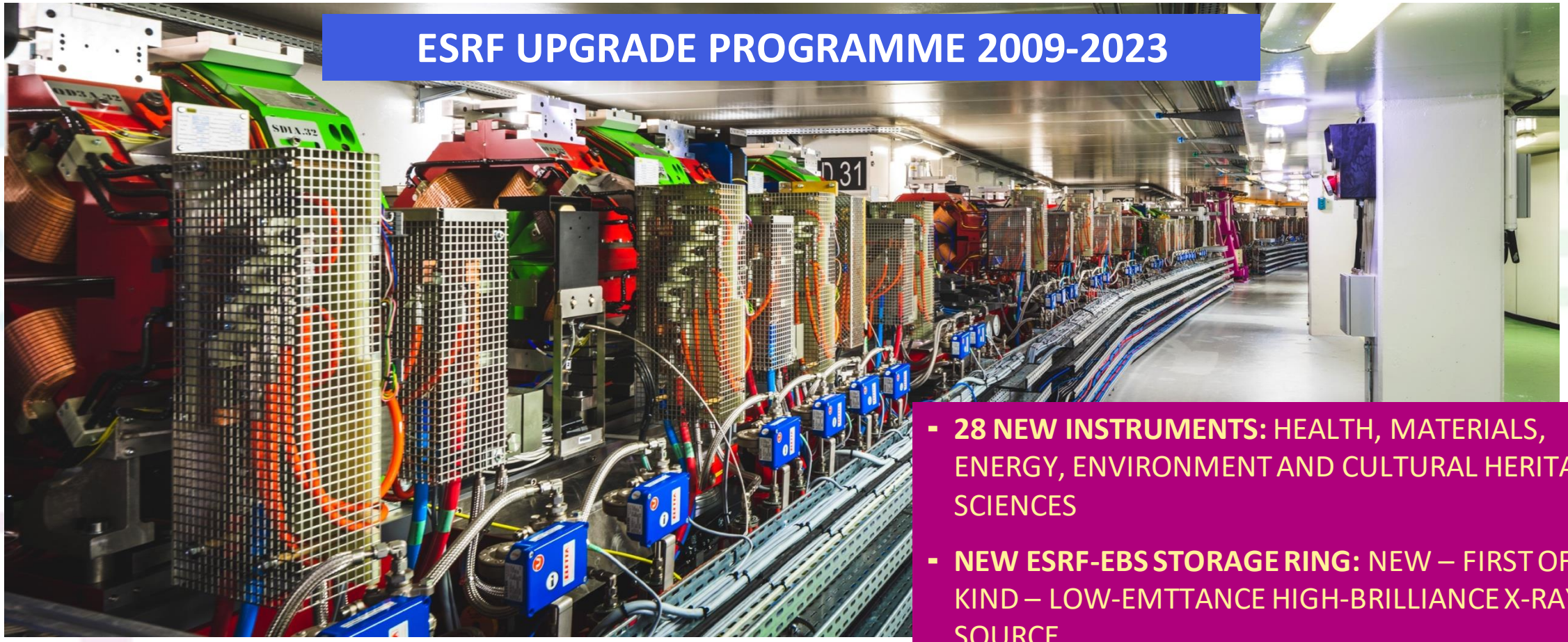
STREAMLINE AS ESSENTIAL PART OF ESRF-EBS SCIENTIFIC SUSTAINABILITY



ESRF UPGRADE PROGRAMME 2009-2023

- **28 NEW INSTRUMENTS:** HEALTH, MATERIALS, ENERGY, ENVIRONMENT AND CULTURAL HERITAGE SCIENCES
- **NEW ESRF-EBS STORAGE RING:** NEW – FIRST OF A KIND – LOW-EMTTANCE HIGH-BRILLIANCE X-RAY SOURCE
- **PIONEERING NEW BIG&OPEN DATA IT INFRASTRUCTURE**
- **25% OF ENERGY SAVINGS (16.6 GWH/year)**

ESRF UPGRADE: ON THE ESFRI ROADMAP SINCE ITS INCEPTION

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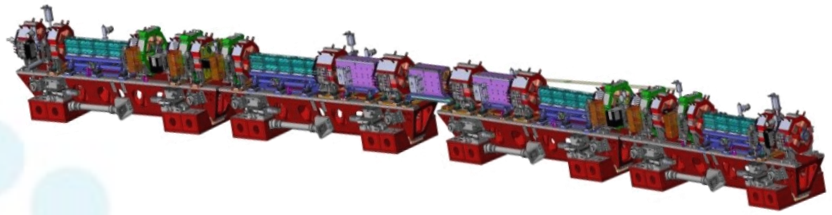
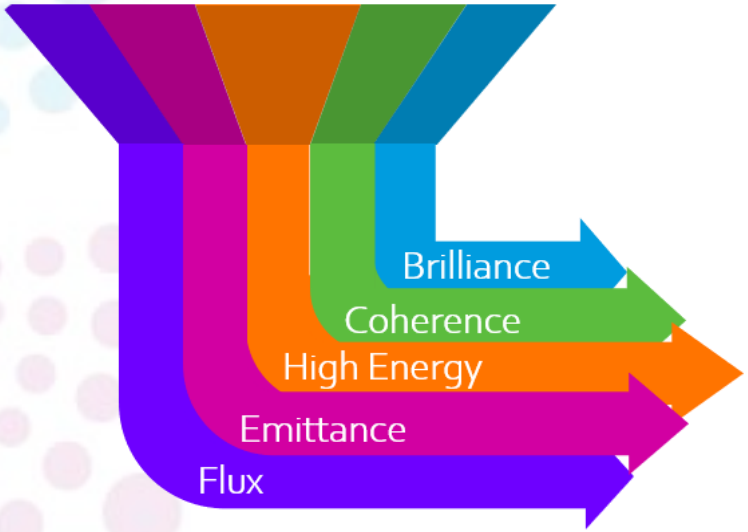
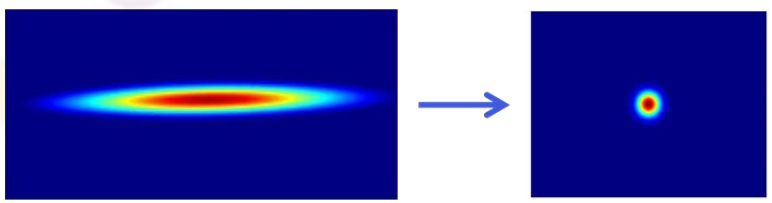
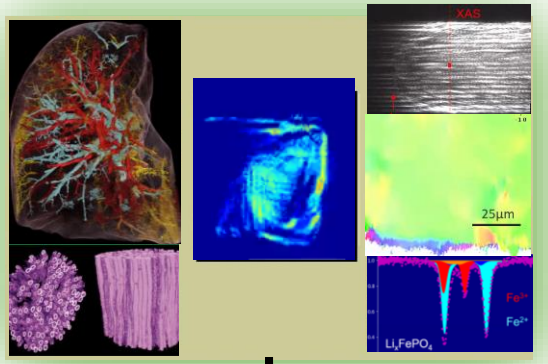
ESRF-EBS IMPACT ON THE EXPERIMENTAL PROGRAMME



HMBA lattice







× 30 Trans. Coherence | **× 100 Brilliance** | **÷ 100 Hor. Emittance**

- ✓ Multiscale (mm → µm → nm)
- ✓ Pump probe experiments
- ✓ Time resolution
- ✓ Conditions: extreme (T,P), *in-situ*, *operando*
- ✓ Better capabilities: energy resolution, sensitivity, throughput, selectivity..
- ✓ Machine learning algorithms…

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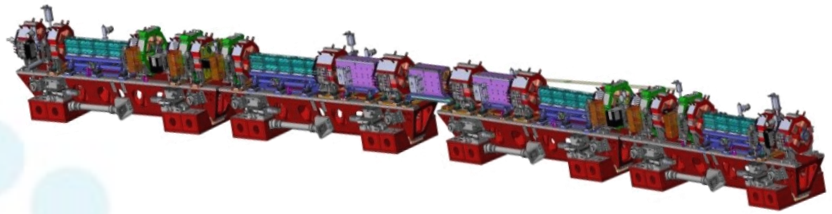
ESRF-EBS IMPACT ON THE EXPERIMENTAL PROGRAMME



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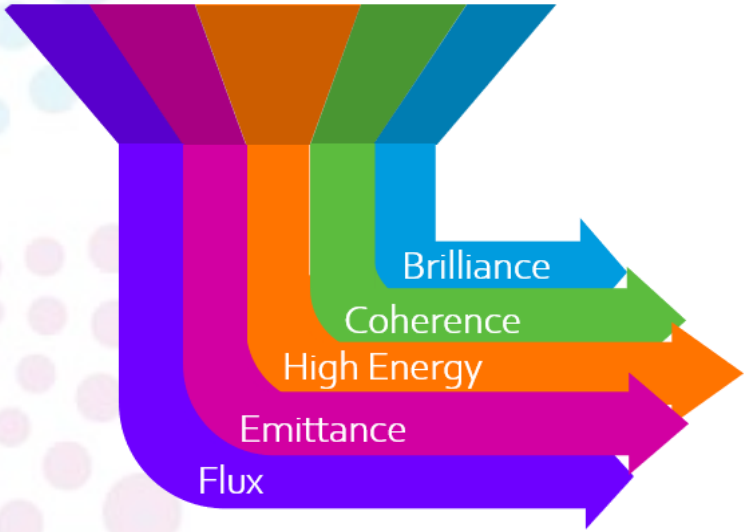

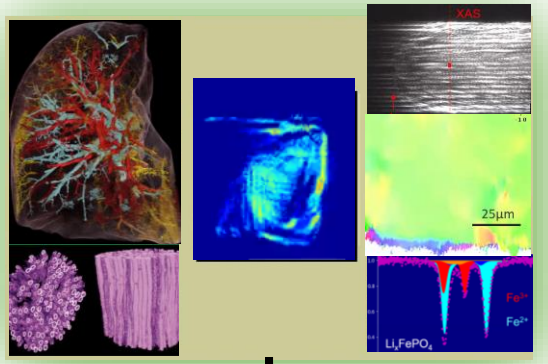

× 30 Trans. Coherence

× 100 Brilliance

÷ 100 Hor. Emittance

- ✓ New source
- ✓ New, long beamlines
- ✓ New instrumentation
- ✓ New data analysis & management tools

Improved experimental conditions by factors of 100 to 10 000

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STREAMLINE - Sustainable research at micro and nano X-ray beamlines

ESRF-EBS
Extremely Brilliant Source

NEW

Source
Beamlines
Infrastructure
+
Brighter X-ray beams

STREAMLINE

Access &
Data services
+
Enhanced capacity
Modernisation of tools
Community outreach

NEW

NEW SCIENCE → **+** / **−** **Socio-economic impact** **Environmental footprint** ← **INCREASED EFFICIENCY & USABILITY**

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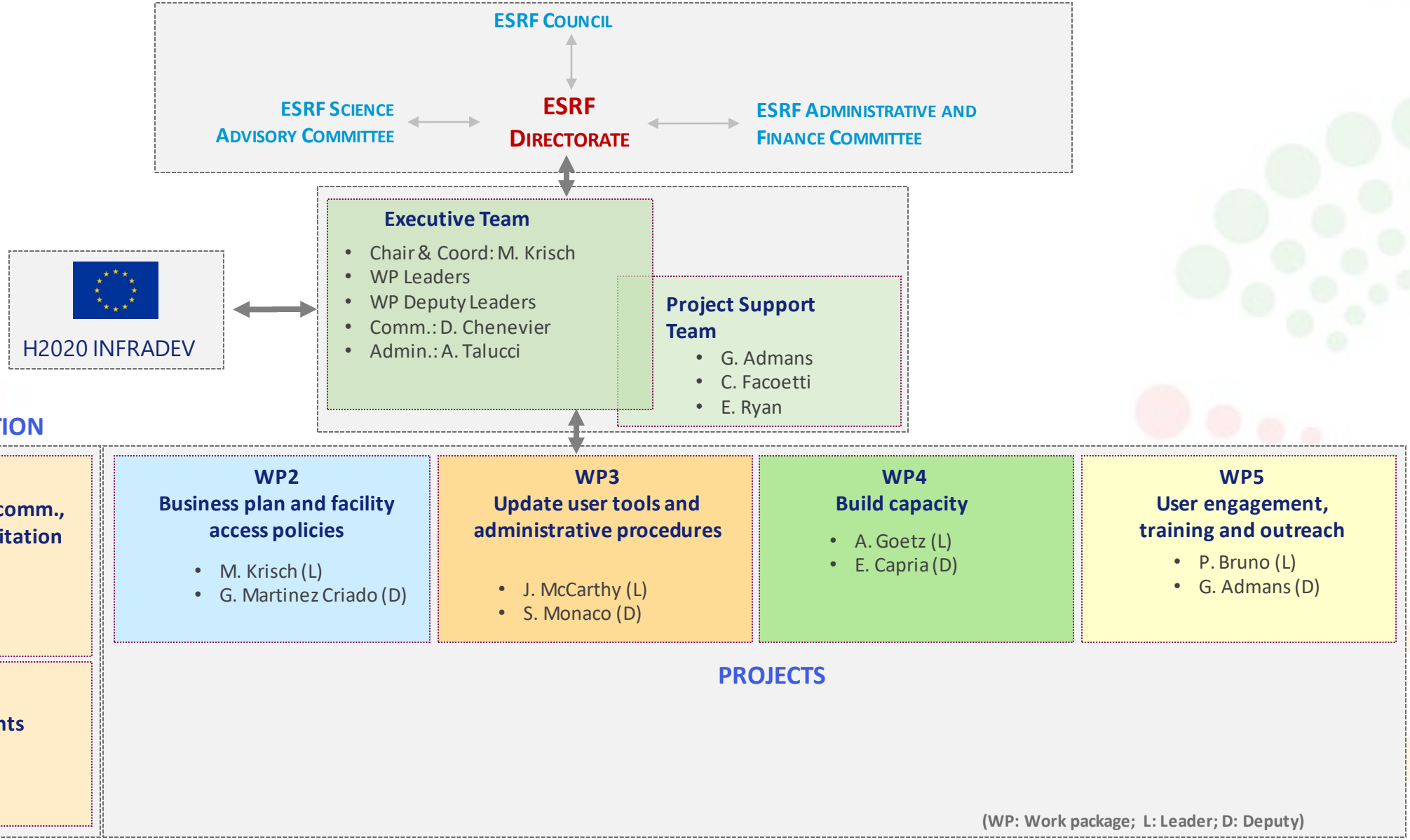
STREAMLINE PROJECT MANAGEMENT AND ORGANISATION



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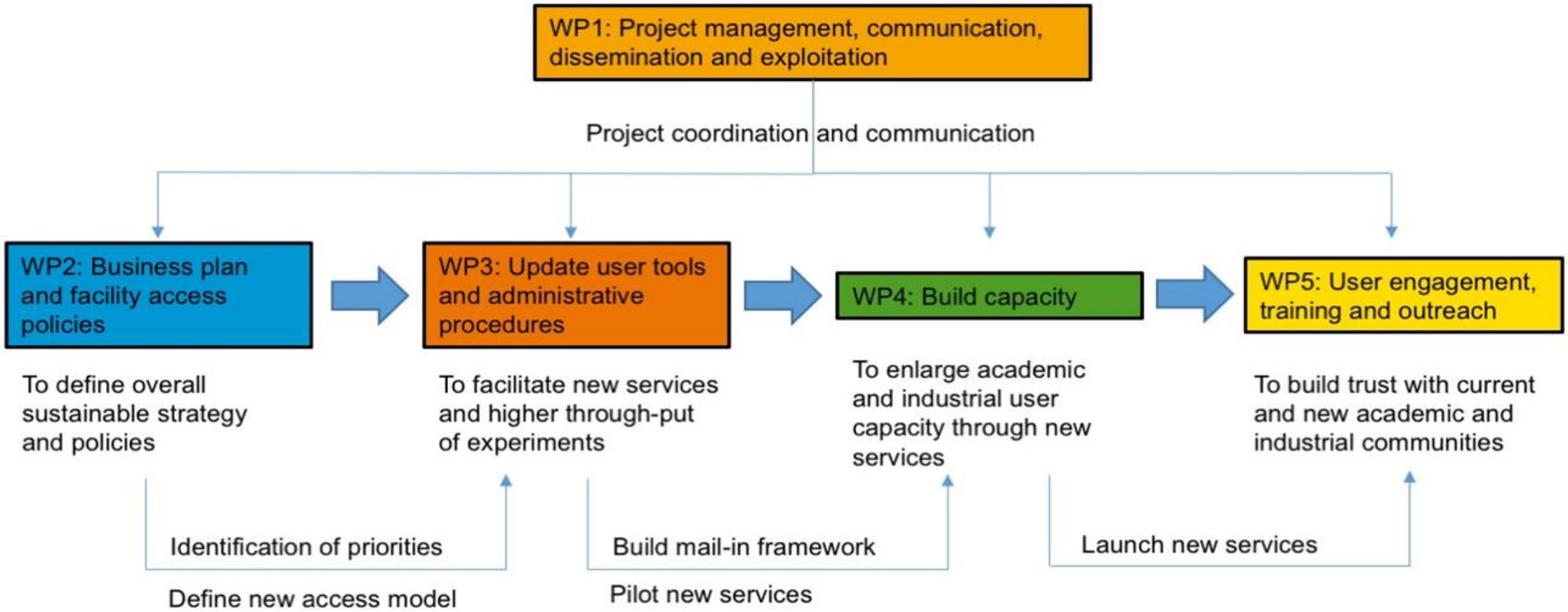
EXECUTION SEQUENCE: from definition to implementation



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Publications

Adapting the European Synchrotron to industry

Ennio Capria[1], Andrea Ciuffini[1], Jakub Drnec[1], Wou
Frey[1], Bernd Hinrichsen[2], Veijo Honkimäki, Ma
Mitchell[1], Manuel Munoz[3], Athanasios Papazoglou[1]

[1] European Synchrotron Radiation Facility, 71 avenu
[2] Momentum Transfer - A Venture of Chemova
Germany
[3] Geosciences Montpellier, Université de Montpellie

1. Introduction

In the 1990s the European Synchrotron Radiation Fa
synchrotron in the world, boasting new tec
instrumentation. The ESRF welcomed its first comm
brilliance beamline "BL4" at the time and now ID02
industry use of third-generation synchrotrons has g
worldwide, demonstrating their relevance to sup
ecosystem from commercial use supported sometir
9]. As this use has grown, most synchrotrons have
with industry contact officers who are often PhD qu
techniques and able to bridge synchrotron-to-indus
is complemented strongly by external bridges via r
with their industry-heavy networks and collaborate
companies providing an entry point to research infr

In 2019, the ESRF started its long closure for the
upgrade [10,11], and reopened in summer 2020
synchrotron with beam properties typically betwee
on the X-ray technique. A game-changer for
unprecedented opportunity for industry, opening up
X-rays for commercial research and innovation. The
adapt the synchrotron world to what industry need
new, but with the increasing pressure from stakeh
investments in large-scale research infrastructures,
constructively with industry now has a much differe

to be published in Sync
special on industry

X-ray science using the ESRF-E
Source

Patrick Bruno[1*], Jean-Claude Biasci
Rudolf Dimper[1], Michael Krisch[1], Ge
Mohamed Mezouar[1], Christian Ne
Pantaleo Raimondi[1,2], Harald Reichert
Jean Susini[1,4], Paul Tafforeau[1],

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Abstract

The Extremely Brilliant Source (EBS), the first
radiation source, constructed at ESRF and based
Hybrid Multi Bend Achromat (HMBA), has start
25th, 2020. We report here on selected recent sci
greatly improved performances of this novel X-ray

March 28, 2024

Keywords: X-ray science, synchrotron radiation source

Synchrotron Radiation News

ISSN: (Print) (Online) Journal homepage: https://www.tand

ESRF Prepares New User Acce

J. McCarthy & H. Reichert

To cite this article: J. McCarthy & H. Reichert (2022): ES
Synchrotron Radiation News, DOI: 10.1080/08940886.20

To link to this article: https://doi.org/10.1080/089408

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Marine Cotte, Kathleen Dollman, Vinc
Frederik Vanmeert, Letizia Monico, Ca
Loïc Huder, Stuart Fisher, Wout de Nol
Murielle Salomé, Marta Ghirardello, D
Tafforeau

To cite this article: Marine Cotte, Kathleen Dollm
Frederik Vanmeert, Letizia Monico, Catherine Dej
Fisher, Wout de Nolf, Ida Fazlic, Hiram Castillo-M
Daniela Comelli, Olivier Mathon & Paul Tafforeau
ESRF to the Cultural and Natural Heritage Comm
10.1080/08940886.2022.2135958

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Article

The "Historical Materials BAG": A New Facilitated Access to Synchrotron X-ray Diffraction Analyses for Cultural Heritage Materials at the European Synchrotron Radiation Facility

Marine Cotte [1,2,*], Victor Gonzalez [3,*], Frederik Vanmeert [4,5,*], Letizia Monico [4,6,7,*], Catherine Dejoie [1], Manfred Burghammer [1], Loïc Huder [1], Wout de Nolf [1], Stuart Fisher [1], Ida Fazlic [1,8], Christelle Chauffeton [9,10,11], Gilles Wallez [9,11,12], Núria Jiménez [13], Francesc Albert-Tortosa [13], Nati Salvadó [13], Elena Possenti [14], Chiara Colombo [14], Marta Ghirardello [15], Daniela Comelli [15], Ermanno Avranovich Clerici [4,16], Riccardo Vivani [17], Aldo Romani [6,7], Claudio Costantino [6,7], Koen Janssens [4,5], Yoko Taniguchi [18], Joanne McCarthy [1], Harald Reichert [1] and Jean Susini [1,†]

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check for updates

Citation: Cotte, M.; Gonzalez, V.; Vanmeert, F.; Monico, L.; Dejoie, C.; Burghammer, M.; Huder, L.; de Nolf, W.; Fisher, S.; Fazlic, I.; et al. The "Historical Materials BAG": A New Facilitated Access to Synchrotron X-ray Diffraction Analyses for Cultural Heritage Materials at the European Synchrotron Radiation Facility. *Molecules* **2022**, *27*, 1997. https://doi.org/10.3390/molecules27061997

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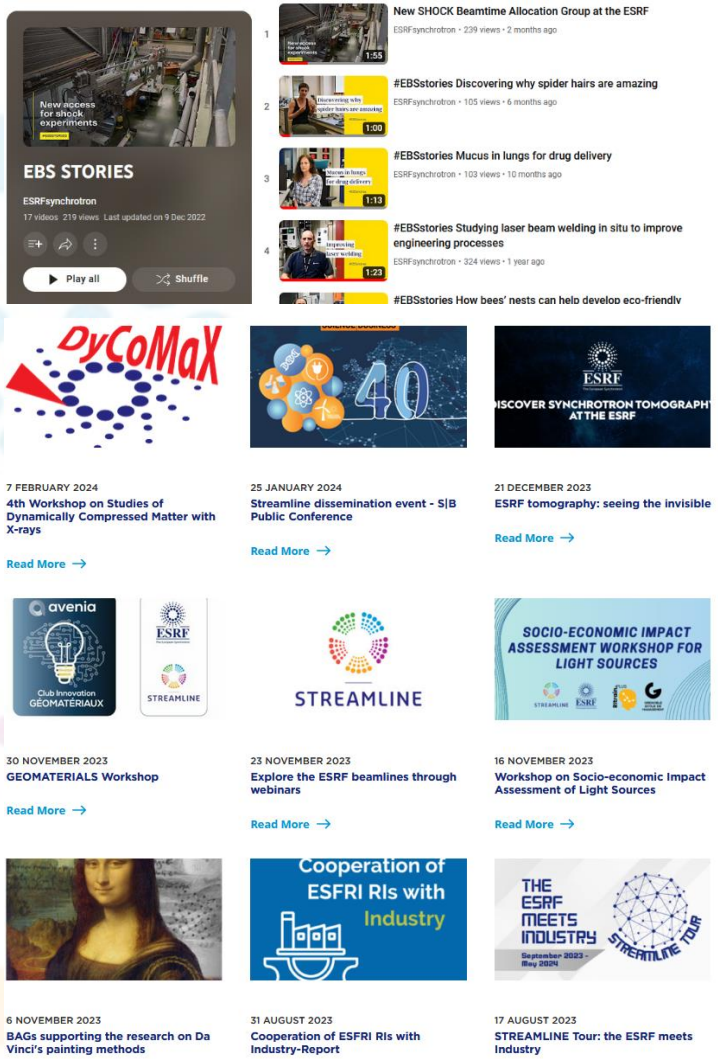
Abstract: The European Synchrotron Radiation Facility (ESRF) has recently commissioned the new Extremely Brilliant Source (EBS). The gain in brightness as well as the continuous development of beamline instruments boosts the beamline performances, in particular in terms of accelerated data acquisition. This has motivated the development of new access modes as an alternative to standard proposals for access to beamtime, in particular via the "block allocation group" (BAG)

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Project web and live presence



COMMS ACTIONS & STATS

75 Web items
(News & Events)

333 total posts
226 followers

85 Videos on YouTube
+25.000,00 views

+100 Events, webinars & workshops

Dissemination via others websites/Newsletters

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Scientific roadshow & Outreach to industry

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STREAMLINE TOUR –ESRF meets Industry

EVENT NAME	LOCATION	EVENT NAME	LOCATION
FEMS Euromat 2023	Germany	Battery Innovation Days 2023	France
ICBR 2023 – International Congress for Battery Recycling	Spain	CARAC 2023	France
Nano Innovation 2023	Italy	ICT – International Conference on Industrial Computed Tomography	Austria
Les Rendez-Vous Carnot 2023	France	Beyond Additive – NDT Technologies for new Hybrid AM PROCESSES	Italy
G-RADNEXT	Switzerland	GEOMATERIALS Workshop	ESRF
31st PSDI – Protein Structure Determination in Industry	UK	New High-throughput services at the ESRF: HT – XRD day **(with MT)**	ESRF

12 EVENTS

7 COUNTRIES

CLOSING EVENT ORGANISED AT THE ESRF IN PARTNERSHIP WITH MOMENTUM TRANSFER (Monday 15 April 2024)

Goal: To enhance the ESRF marketing and business development programme

How? Targeting actions that will include a broad range of disciplines, to promote the ESR-EBS new opportunities.

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Streamline dissemination event – Science Business Public Conference 13 Feb 2024

Next gen' infrastructures as enablers to solve tomorrow's industrial and societal challenges

Breakout session – 2 speeches + panel discussion

270 attendees (150 on site & 120 online)

SCIENCE|BUSINESS®

Extremely brilliant: Will synchrotrons help to unlock the secrets of the universe?

DG Plenary Speech + Q&A session

300 attendees (200 on site & 100 online)

Article and recordings available on the Streamline website, ESRF YouTube and Science Business channels.

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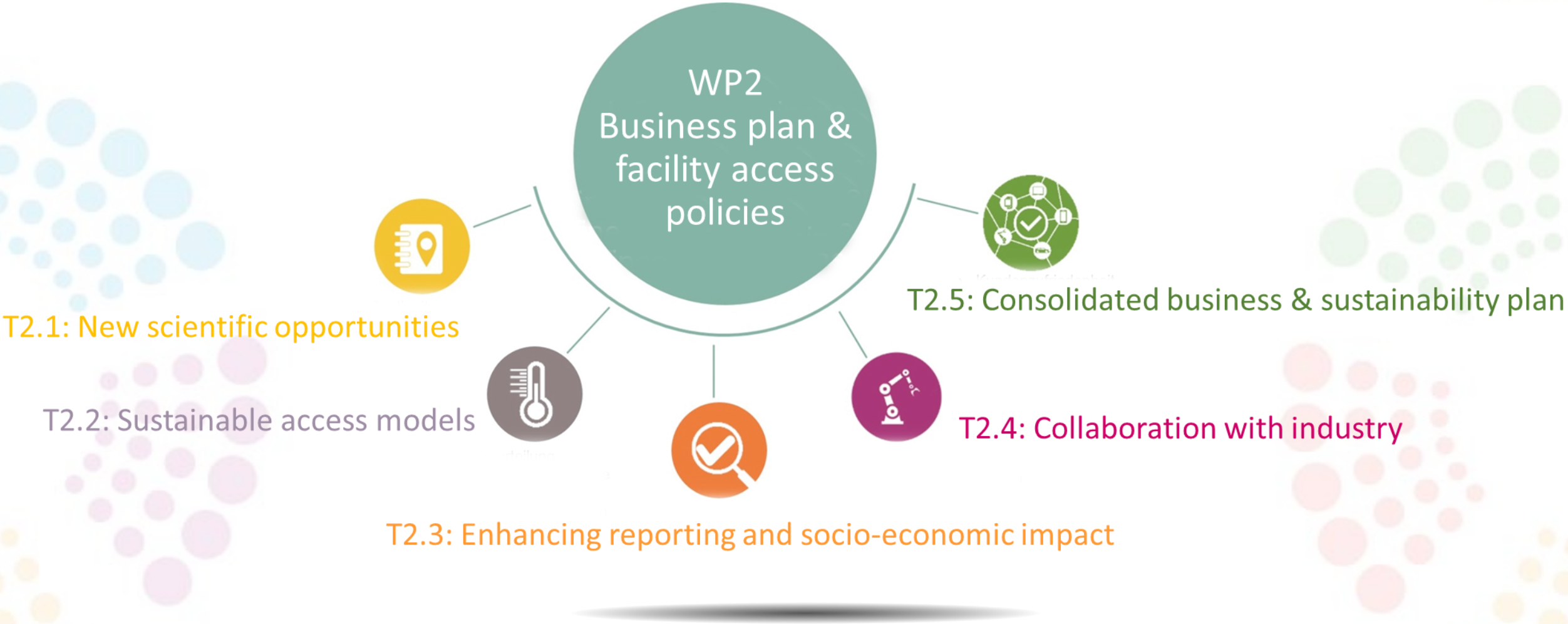
Business plan and facility access policies



Foundation for the medium- and long-term sustainable operation of the ESRF-EBS

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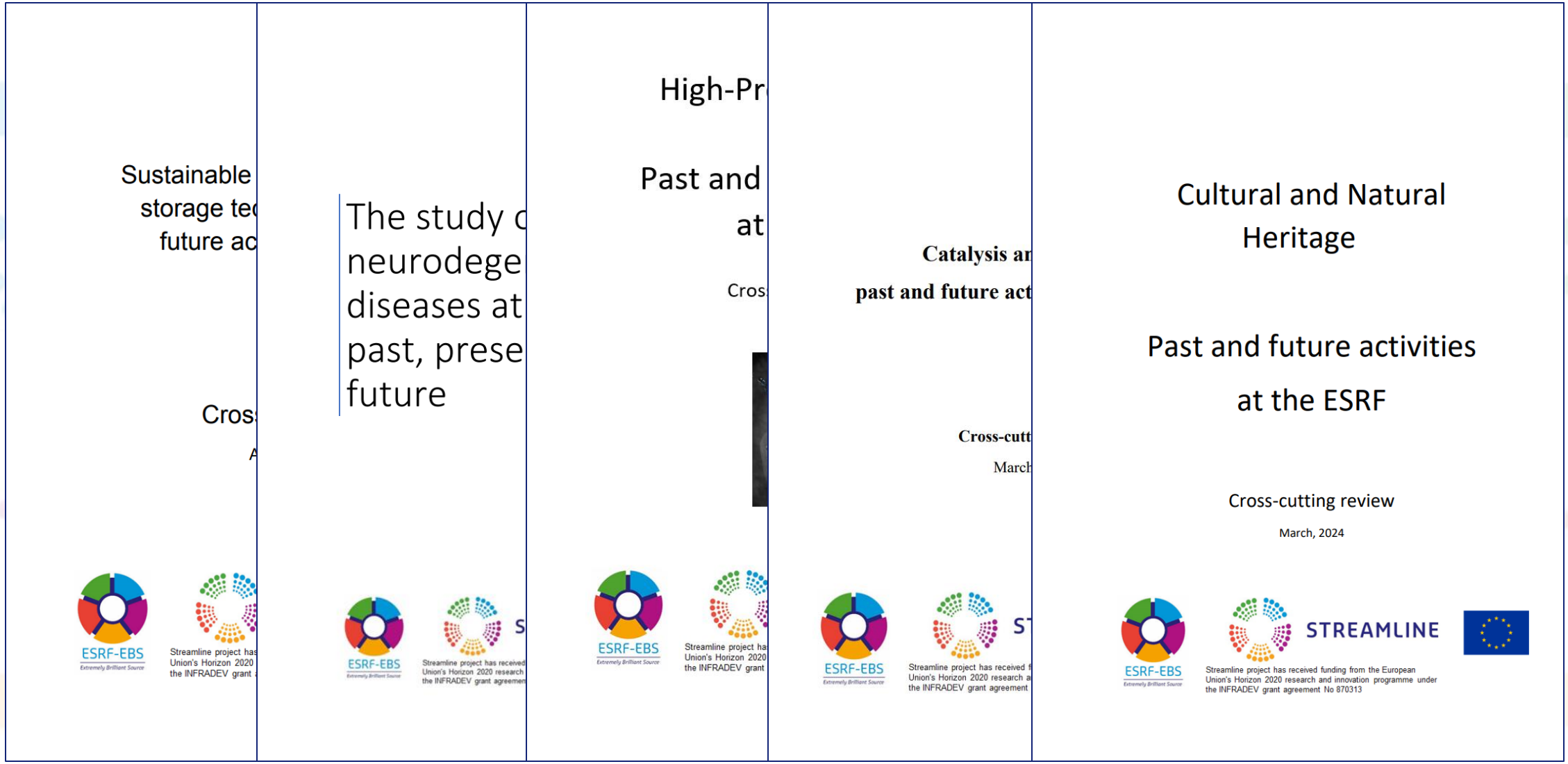
New scientific opportunities – cross cutting reviews



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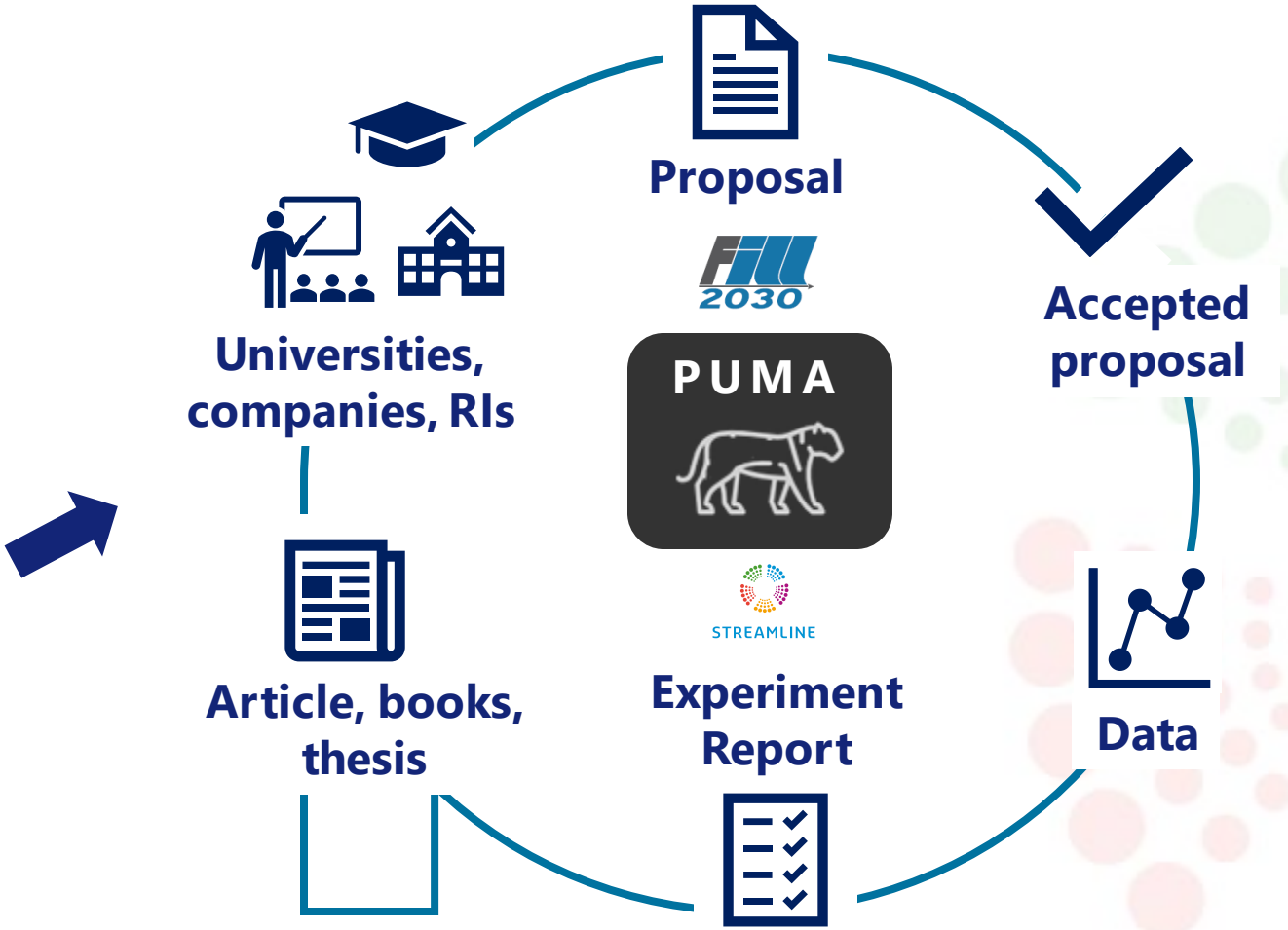
GETTING TO GRIPS with IMPACT and OUTPUT



PUblication **MA**tching using Business Intelligence
Real time reporting for scientists and facility strategy.

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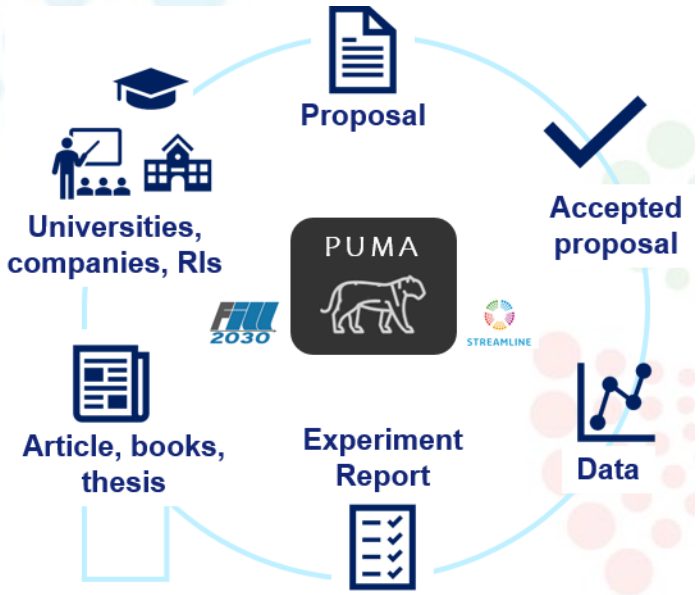
Common Beamline Indicators Database as a Science & Innovation strategy tool

Powerful tool to adapt and steer the science programme



Common Beamline Indicators to assess overall impact, science reach & optimal use of resources.

Part A	Executive Summary (past, present and future of the beamline)	1
Part B	Facts and Figures 2015 – 2022 Bibliometric, user access & relevant metrics	2
Part C	Current *scientific* status and medium-term plans 2023 - 2027	3
Part D	Current *technical* status and medium-term plans 2023 - 2027	4

- Uniqueness of the science programme
- Size of the user communities
- Competitiveness and relevance
- Required investments to stay at the forefront

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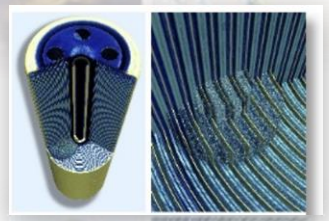
Community Access Pilots

Launched in 2021

Historical Materials BAG

Battery HUB



Launched in 2022

Shock BAG

Launched in 2023

ReMade@ARI
A hub for materials research

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ESRF-EBS Beamline Portfolio Strategy Meetings

- Autrans Meeting 1: 17 – 18 October 2022
- Autrans Meeting 2: 4 & % July 2023
- Autrans Meeting 3: 29 & 30 April 2024
- IT Strategy Meeting: 19 December 2023
- Science & Students Days Val Cenis: 16 – 18 October 2023
- EoI for the future biomedical science programme
- Sandpit: Nano-imaging beamline for life and biological sciences

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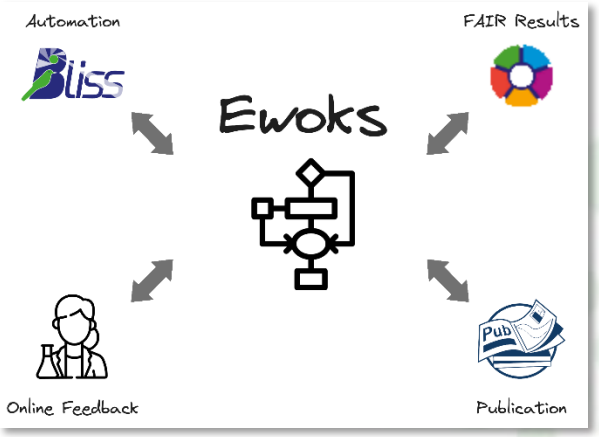
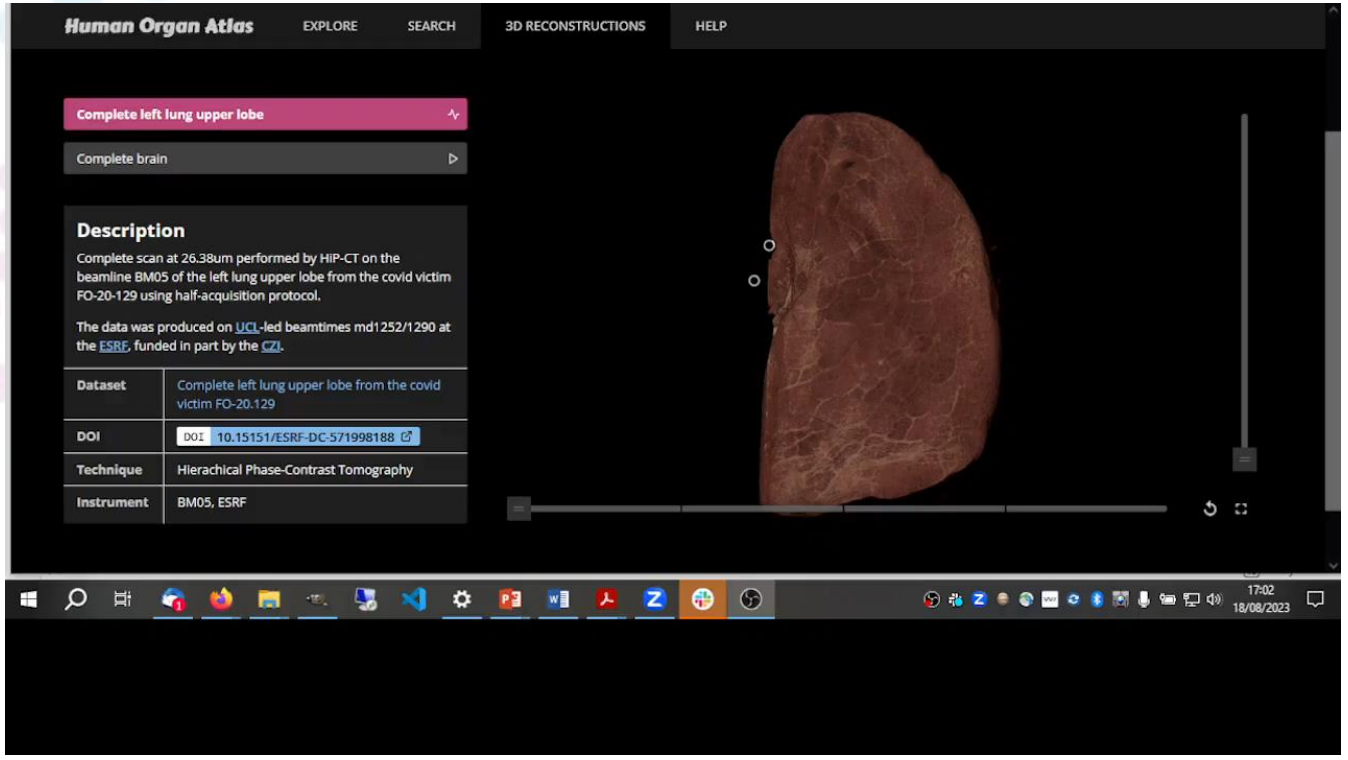
STRETCHING SERVICES: STREAMLINE is revolutionising efficiency and innovation by EWOKS

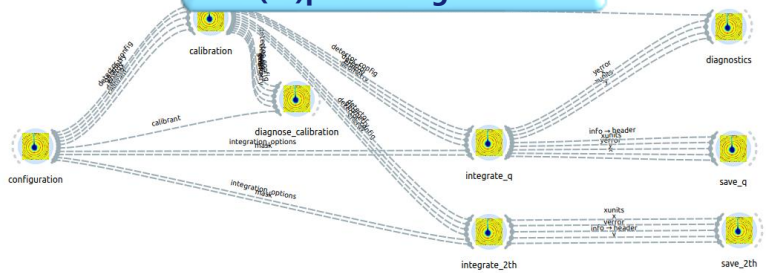
- ✓ **A meta-workflow controller**, for local or cluster-based workflows
- ✓ **Online monitoring** and **visualisation**
- ✓ **Linked to data portal** for easy and, eventually, open access data
- ✓ **Unified sample tracking** and LIMS for all techniques
- ✓ **Code is open source available to the community**
- ✓ **Used on 25 beamlines** to accelerate data (re)processing and evaluation



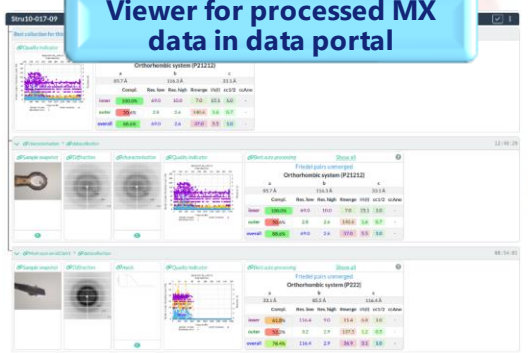
The Human Organ Atlas – an example of FAIR data



Workflows for (re)processing HTPD



Viewer for processed MX data in data portal



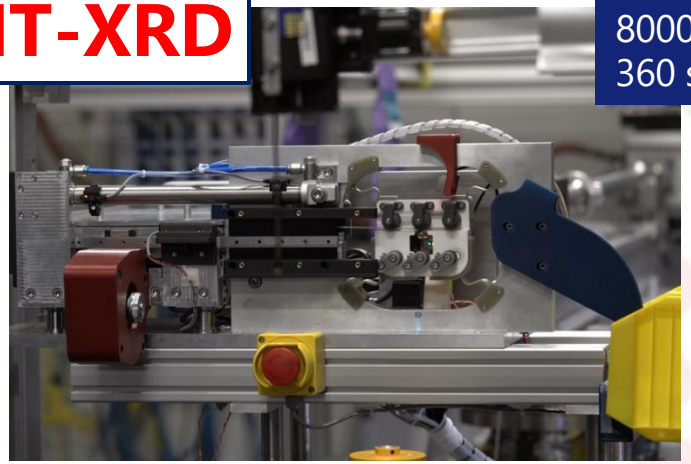
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

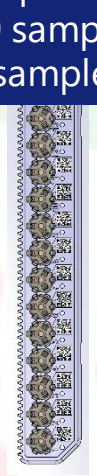
Novel high throughput characterisation services for industry and academia

Acceleration of **new material discovery** with EBS X-rays and innovative instrumentation, coupled with **automation of data acquisition** and **streamlined data reduction**

50.000 samples in 2 years
160 samples/hour

HT-XRF & HT-XRD





Creation of a new start-up
6 unique clients in 1.5 years
8000 samples in 2years
360 samples/hour

- **Designed**, **Developed** and **Launched: 2 new customised services** tailored to meet the challenging need of academic researchers and industrial clients
- Established **Standard Operating Procedures** to ensure **consistency** and **reproducibility** in experimental workflows, enhancing the **quality** and **reliability** of experiment results + **EWOKS**
- Services **co-designed and co-developed** with relevant representatives of the user community: **Uni Montpellier and BASF**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

User engagement, training and outreach

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Nurturing new communities: ESRF hosted workshops

Title	Date	Type	Hosting	Participants
Cultural and Natural Heritage at ESRF-EBS	22-24 January 2020	Workshop	In person	151
Dark Field X-ray Microscopy (DFXM)	5-7 May 2021	Sandpit	Virtual	105
3rd DyCoMaX workshop: Studies of Dynamically Compressed Matter with X-rays	14-15 January 2021	Workshop	Virtual	161
New Frontiers in the Study of Molecular Crowding	29 June - 1 July 2022	Workshop	In person	52
Quantum Materials	5-7 October 2022	Sandpit	In person	50
Advanced Methods for Ambient Crystallography at ESRF-EBS	21-23 Nov 2023	Sandpit	In person	29
X-ray Spectroscopy of Magnetic Materials	11-13 Dec 2023	Workshop	In person	103
New Opportunities in Diffraction Microscopy	8-11 Jan 2024	Workshop	In person	101
4th Workshop on Studies of Dynamically Compressed Matter with X-rays	12-14 March 2024	Workshop	In person	71
Fluid Dynamics meets Synchrotron X-ray High-speed Imaging	21-22 March 2024	Sandpit	In person	67

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Nurturing new communities: ESRF hosted workshops

Workshops hosted in 2024

New Opportunities in Diffraction Microscopy, 8-11 Jan 2024

Fluid Dynamics meets Synchrotron X-ray High-speed Imaging, 21-22 March 2024

Studies of Dynamically Compressed Matter with X-rays, 12-14 March 2024

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Insight programme – Observation of an experiment

Aim: To provide opportunities for potential future users to gain insight into the practicalities of running an experiment at a beamline

Achieved via individual visits and training for small groups associated with workshops:

- Advanced Methods for Ambient Crystallography at ESRF-EBS
- 4th Workshop on Studies of Dynamically Compressed Matter with X-rays
- Hercules 2024
- Industry day 2024

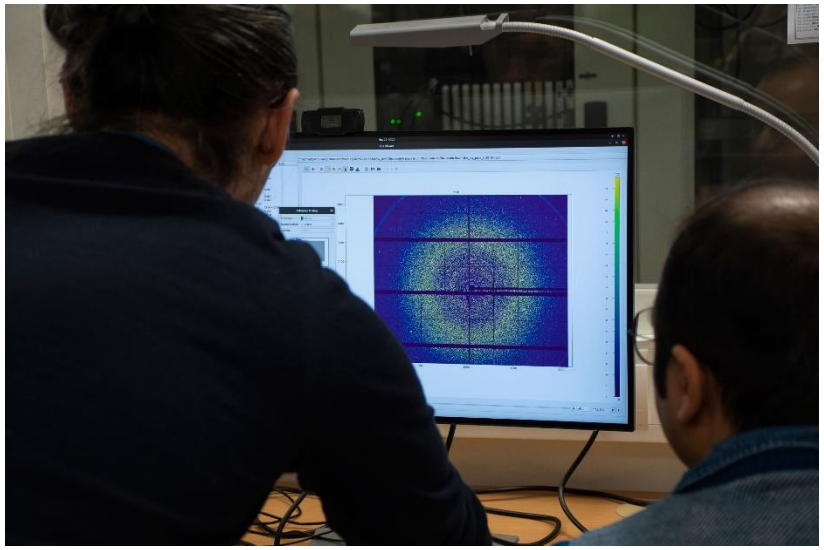
Streamline has given about 40 young researchers their first hands-on experience at a beamline

Professor Graciela Diaz de Delgado and Analio Dugarte from Universidad de Los Andes, Venezuela joined Andy Fitch and Catherine Dejoie for hands-on training at powder diffraction beamline ID22 in November 2022.

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Insight programme – Observation of an experiment

Insight training associated with workshop: Advanced Methods for Ambient Crystallography at ESRF-EBS, 21-23 Nov 2023



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Ambassador programme: Focus by country, example of Greece

2022 Outreach to Greek scientists

ESRF Information Day - The Use of Synchrotron Radiation in Science, 6 May 2022, University of Patras, Greece

100 participants + webcast to 5 sites

Followed up by ESRF participation in summer school on synchrotron radiation at **Aristotle University of Thessaloniki**, 5-8/09/2022.

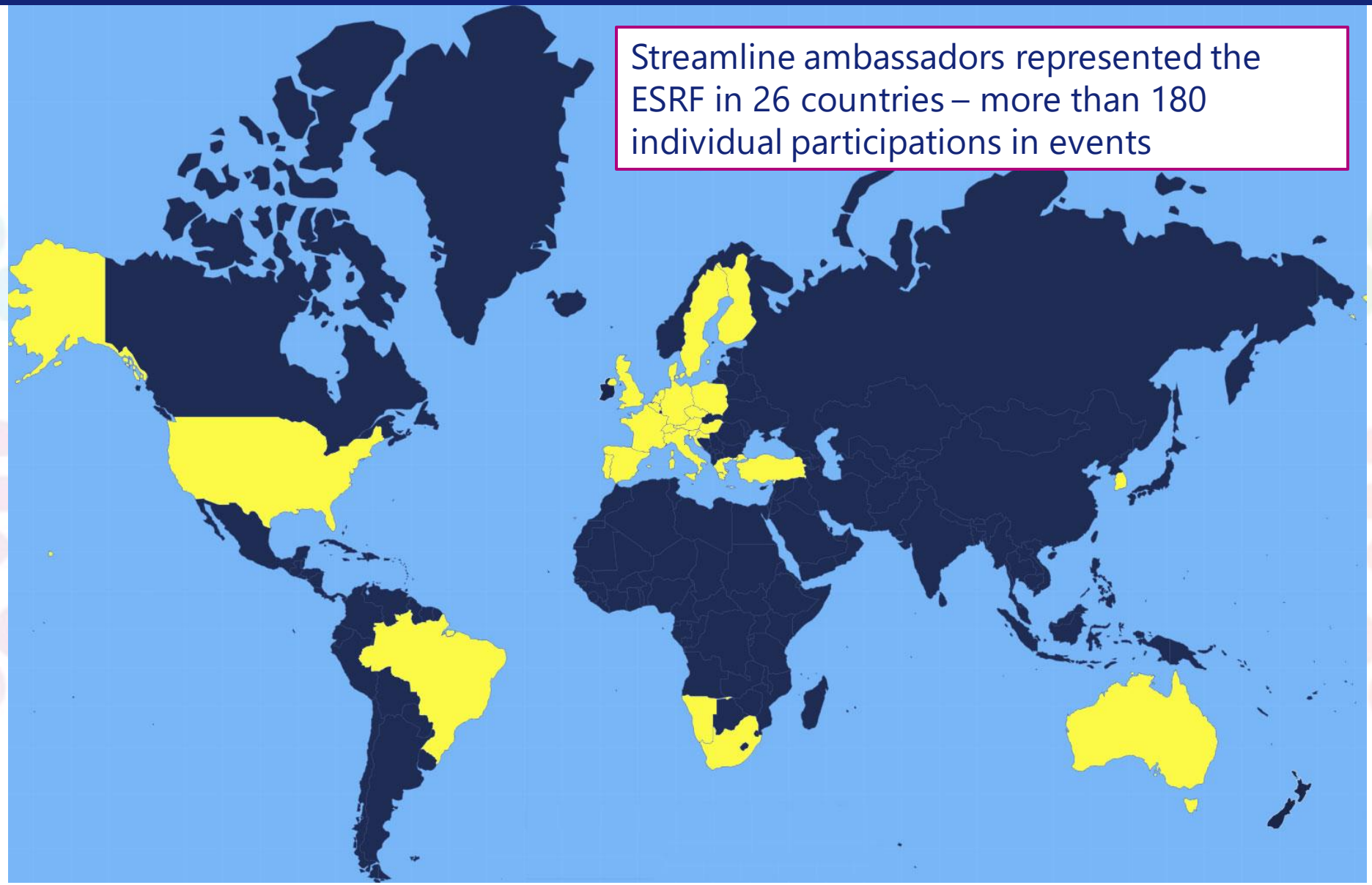
2024 A workshop to promote benefits of ESRF Membership

ESRF membership: Catalyzing Greek Scientific Excellence, 13-14 March 2024, Acropolis Museum, Athens, Greece

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant a

Scientific roadshow; Ambassador programme

Streamline ambassadors represented the ESRF in 26 countries – more than 180 individual participations in events



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

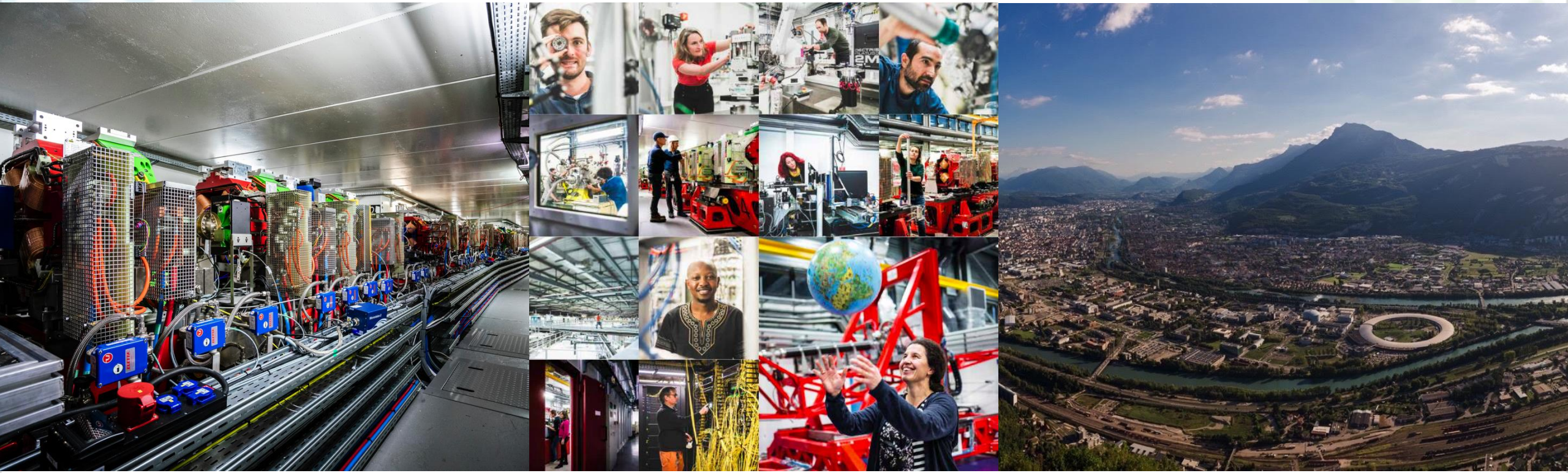
What's next: the programme of this afternoon

TIMINGS	SPEECH/ACTIVITY	PERSON IN CHARGE
14:00 – 14:30	Streamline project introduction/overview	Michael Krisch
14:30 – 15:00	PUMA/ Facility metrics	Stephanie Monaco/ Renaud Duyme
15:00 – 15:30	EWOKS+ICAT/ Workflows + Processed data	Andy Götz
15:30 – 16:00	Coffee break in the Auditorium	/
16:00 – 16:30	New industry services	Ennio Capria/Thanos
16:30 – 17:00	Novel Access framework (BAGs, HUBs..)	Joanne Mc Carthy
17:00 – 17:15	Wrap up & ESRF future perspectives	

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

THANK YOU FOR YOUR ATTENTION

CREATING TOGETHER VALUE FOR ALL
SCIENCE FOR SOCIETY



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

PUMA
Publication and **U**ser experiment **M**etadata **A**nalyser

STREAMLINE - 2024/04/11

S. Malbet-Monaco & R. Duyme

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

ESRF scientific activity in details: Need for a tool

Proposal
>94,000

ESRF
User Portal

Universities,
companies, RI
~110,000

Accepted
proposal
>62,000

PUMA

Instrument
experiment
48

Data

Publication,
book, thesis

~48,000
ESRF Library
database

>21,000

Experiment report

?

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

PUMA: Publication and User experiment Metadata Analyser

V2

STREAMLINE

ESRF development
EU H2020 funded
project Streamline

- Based on **ESRF library validation** ("acknowledgement section")
- **Enhancement of dashboards & Search tool**

V3

STREAMLINE

Common ILL/ESRF project
EU H2020 funded project
Streamline
Aim for a **dissemination** package

V1

FILL 2030

ILL development
EU H2020 funded
project FILL 2030

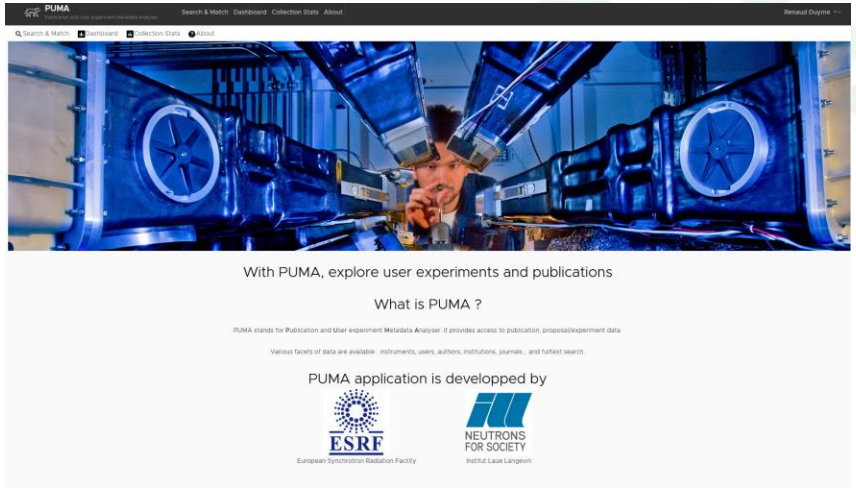
- Based on **mapping** between publications and proposals & **validation** by facility staff
- **Instrument dashboard & bibliometrics**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

PUMA V2 & V3

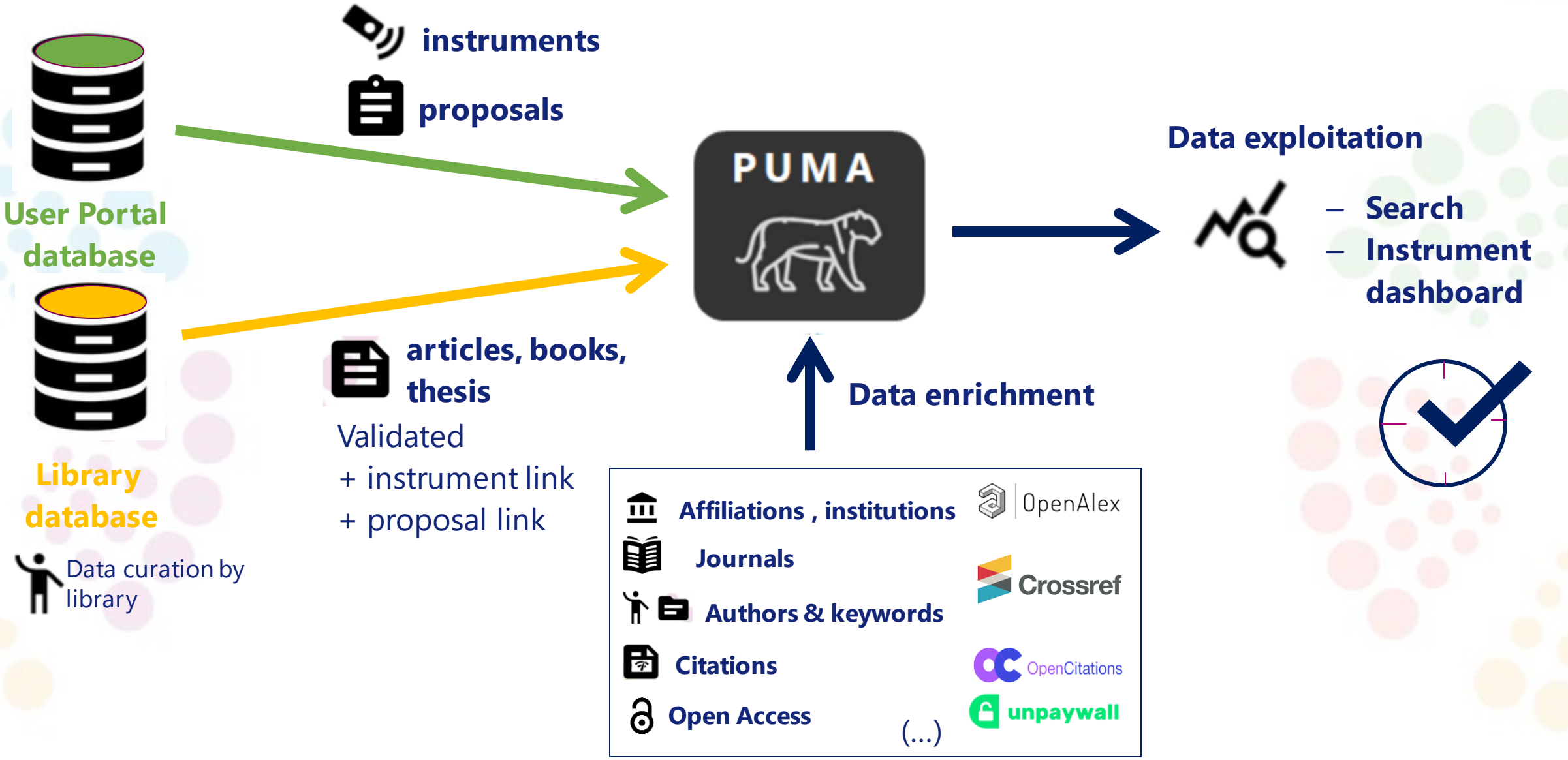
Rely only on the 'acknowledgment' section for the mapping between publications and proposals

- **Dashboards enhancement with new graphs** (open access, common instrument bibliometrics indicators, collaboration…)
- **History of instruments**: instrument move on synchrotron during upgrades (i.e. HRPD instrument from ID31 to ID22).
- Addition of an **institution repository**
- Addition of **facets** (filters) in the **search tool**: instruments, institution, keywords, search keywords highlighted, aggregation graphs
- Usage of **open data services** for publications (citations, authors affiliations, open access status)



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

PUMA data flow

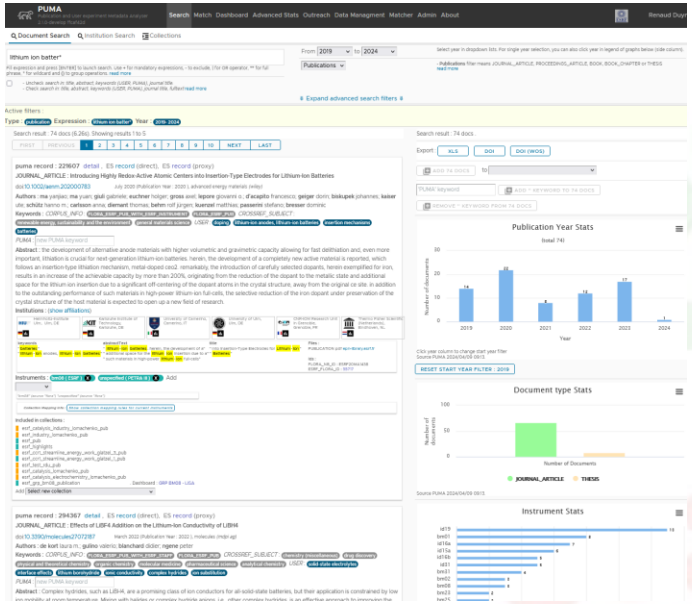


STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

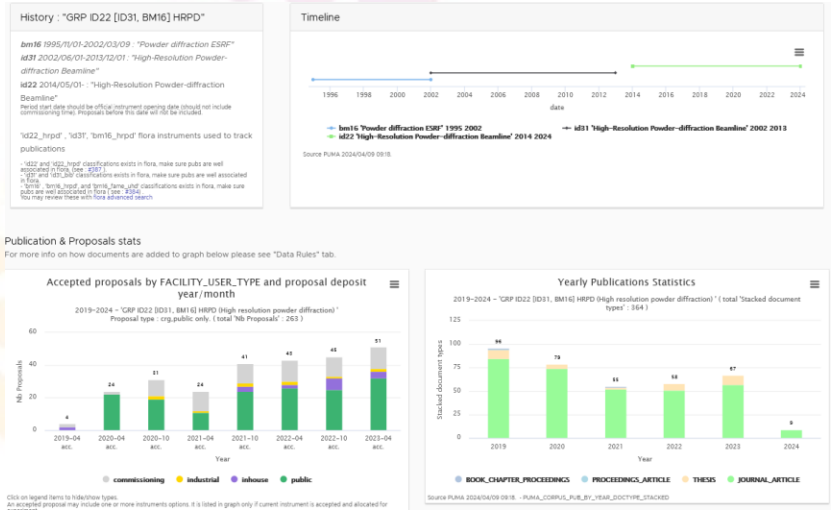
Examples of PUMA features

Facility Dashboard

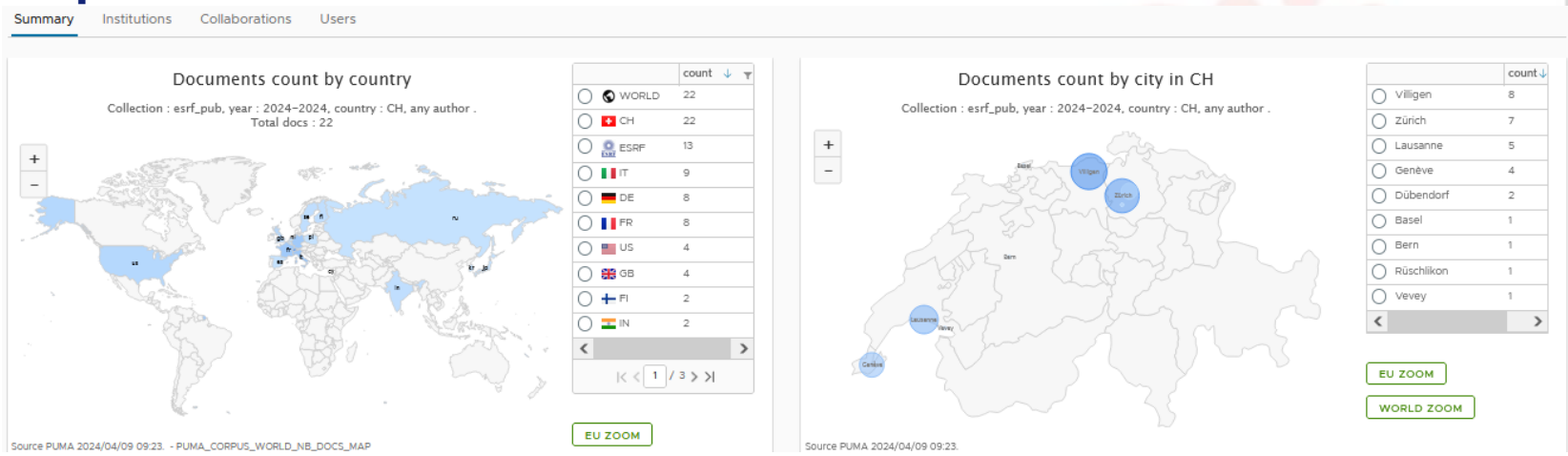
Advanced Search



Instrument Dashboard

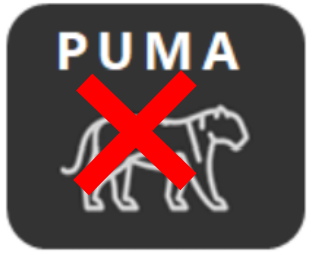


Maps



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

In summary



PUMA is not:

- a substitute to librarians and existing Library databases (corpus validation essential)
- a tool to replace User Portal to manage proposals and to schedule experiments

PUMA:

- **Centralizes** data related to science stored in **proposals and publications**
- Tool for **viewing up-to-date real-time data**
- Allows **reporting** for countries, institutions, instruments,…
- Allows the **in-depth study** of a scientific topic
- **Free from paid-access** platforms (except for the IF)
- Allows the study of **metadata aggregations** that were not envisageable before (i.e collaborations)

PUMA provides a **quantifiable view of the data**, not only enabling **conclusions about the science currently** being carried out at the ESRF, but also helping to **identity trends**.

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

STREAMLINE

ESRF
The European Synchrotron

PUMA advanced Search

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Open Data entities

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

PUMA - lithium ion battery

Document Search | Institution Search | Collections

lithium ion batter*

From 2019 to 2024

Publications

Fill expression and press [ENTER] to launch search. Use + for mandatory expressions, - to exclude, | for OR operator, "" for full phrase, * for wildcard and () to group operations. read more

Search result : 74 docs (0.21s). Showing results 1 to 5

FIRST | PREVIOUS | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | NEXT | LAST

puma record : 221607 detail , ES record (direct), ES record (proxy)

JOURNAL_ARTICLE : Introducing Highly Redox-Active Atomic Centers into Insertion-Type Electrodes for Lithium-Ion Batteries

doi:10.1002/aenm.202000783 July 2020 (Publication Year : 2020) advanced energy materials *(wiley)*

Authors : ma yanjiao; **ma** yuan; **giuli** gabriele; **euchner** holger; **gross** axel; **lepore** giovanni o.; **d'acapito** francesco; **geiger** dorin; **biskupek** johannes; **kaiser** ute; **schütz** hanno m.; **carlsson** anna; **diemant** thomas; **behm** rolf jürgen; **kuenzel** matthias; **passerini** stefano; **bresser** dominic

Keywords : *CORPUS_INFO :* FLORA_ESRF_PUB_WITH_ESRF_INSTRUMENT FLORA_ESRF_PUB *CROSSREF_SUBJECT :* renewable energy, sustainability and the environment general materials science *USER :* doping lithium-ion anodes, lithium-ion batteries insertion mechanisms batteries *PUMA :* new PUMA keyword

Abstract : the development of alternative anode materials with higher volumetric and gravimetric capacity allowing for fast delithiation and, even more important, lithiation is crucial for next-generation lithium-ion batteries. herein, the development of a completely new active material is reported, which follows an insertion-type lithiation mechanism, metal-doped ceo2. remarkably, the introduction of carefully selected dopants, herein exemplified for iron, results in an increase of the achievable capacity by more than 200%, originating from the reduction of the dopant to the metallic state and additional space for the lithium ion insertion due to a significant off-centering of the dopant atoms in the crystal structure, away from the original ce site. in addition to the outstanding performance of such materials in high-power lithium-ion full-cells, the selective reduction of the iron dopant under preservation of the crystal structure of the host material is expected to open up a new field of research.

Institutions : (show affiliations)

Helmholtz-Institute Ulm, Ulm, DE | Karlsruhe Institute of Technology, Karlsruhe, DE | University of Camerino, Camerino, IT | University of Ulm, Ulm, DE | CNR-IOM Research Unit in Grenoble, Grenoble, FR | Thermo Fisher Scientific (Netherlands), Eindhoven, NL

keywords: "batteries" "lithium-ion anodes, lithium-ion batteries"

abstractText: "lithium-ion batteries. herein, the development of a" "additional space for the lithium ion insertion due to a" "such materials in high-power lithium-ion full-cells"

title: "into Insertion-Type Electrodes for Lithium-Ion" "Batteries"

Files : PUBLICATION pdf epn-library.esrf.fr

Ids : FLORA_NB_ID : ESRF20MA1438 ESRF_FLORA_ID : 55717

Instruments : bm08 (ESRF) unspecified (PETRA III) Add

"bm08" (source "flora") "unspecified" (source "flora")

Journal

Authors

Keywords

Institutions

Instruments

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Focus - Institution profile

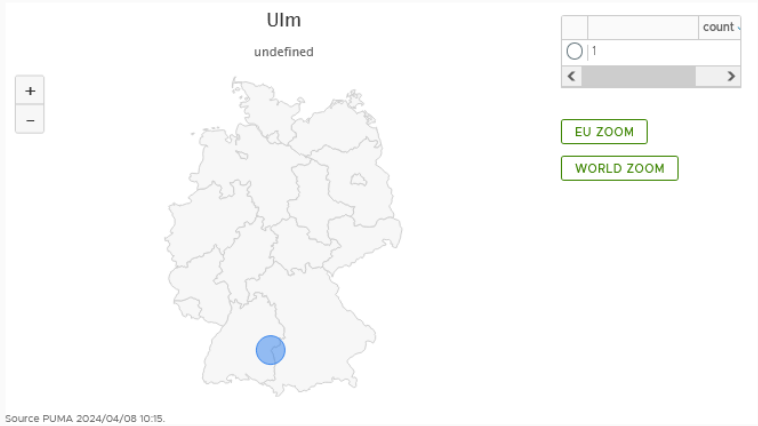
"Helmholtz-Institute Ulm, Ulm, DE" (puma-grid.461900.a)

Institution basic profile page. For more info see also: Institution dashboard

Summary | Persons | Documents | Affiliations

puma-grid.461900.a : "Helmholtz-Institute Ulm"	
Puma Id	puma-grid.461900.a*
Puma code	puma-grid.461900.a
city	Ulm
state	DE-BW
country	DE
www	http://www.hiu-batteries.de/en/
labels	• Helmholtz-Institut Ulm
acronyms	• HIU
Grid types	• Government
Puma types	• research

* Puma institutions reference is based on Grid, Grid mainly is a subset of wikidata (prefix 'puma-grid'). Additional entries are taken from Wikidata (prefix 'puma-Q'), Hal (prefix 'puma-H') and custom Puma entries (prefix 'puma-P')

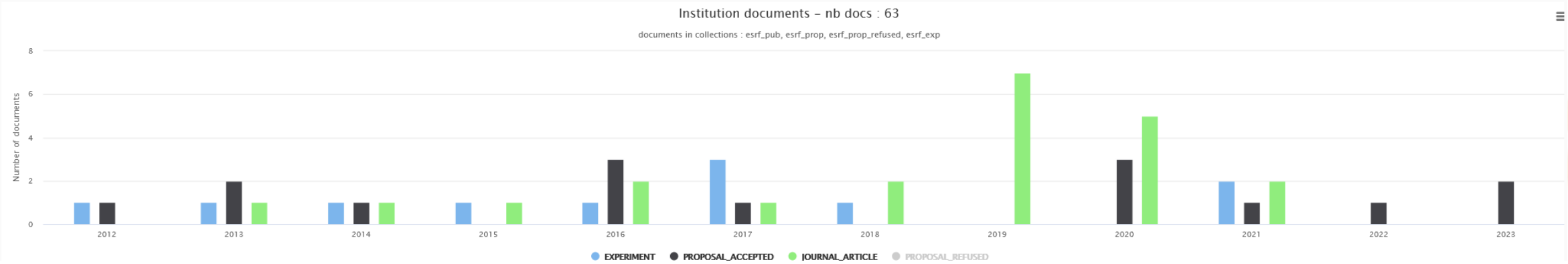


Related institutions

Helmholtz Association of German Research Centres Berlin - DE PARENT

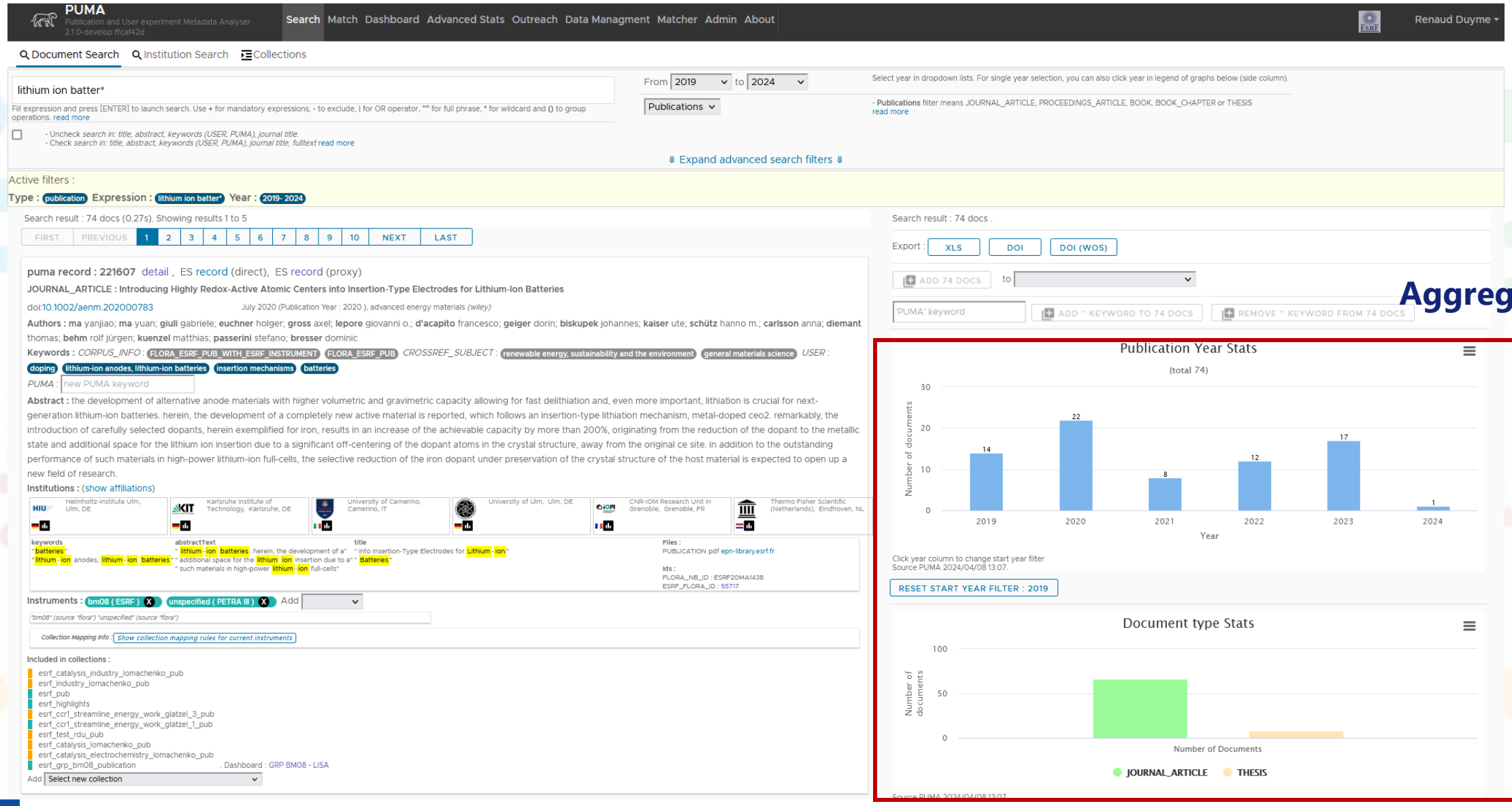
Karlsruhe Institute of Technology Karlsruhe - DE PARENT

2/2 institutions displayed



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

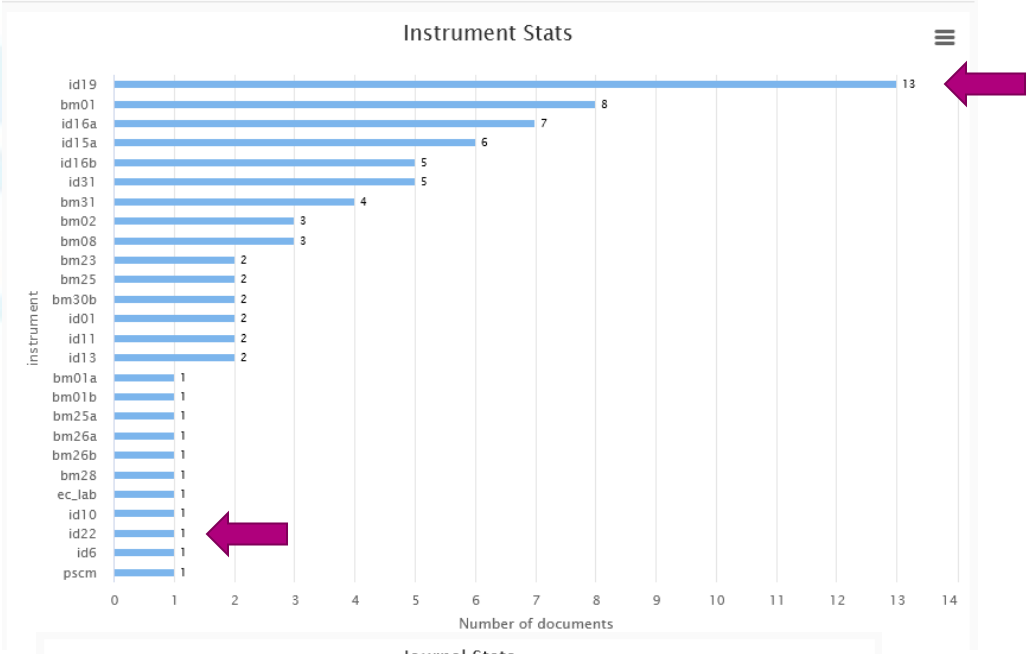
Search aggregations

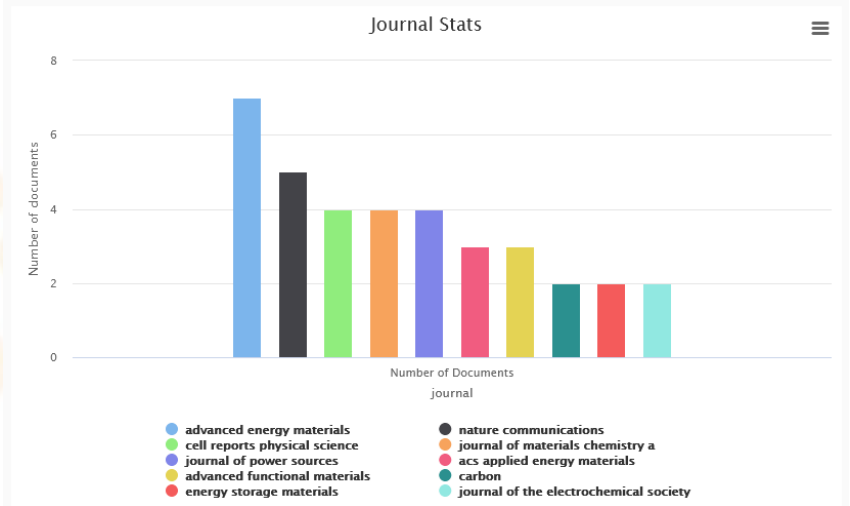


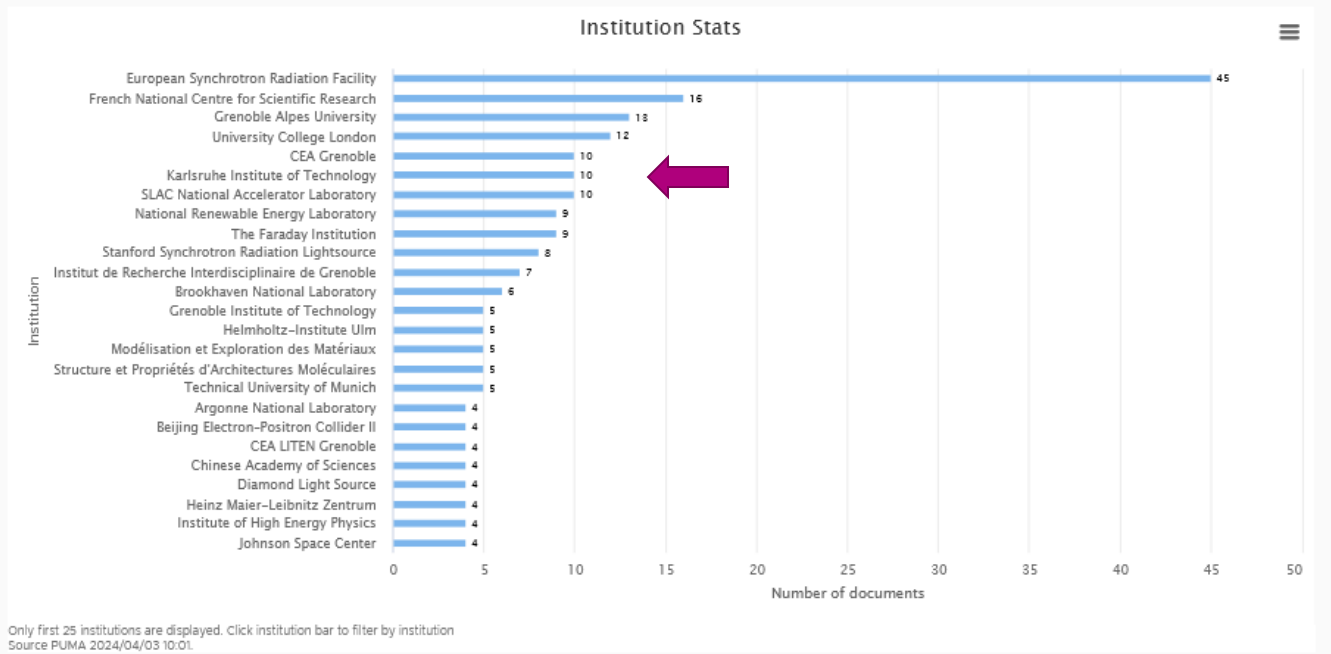
Aggregations

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

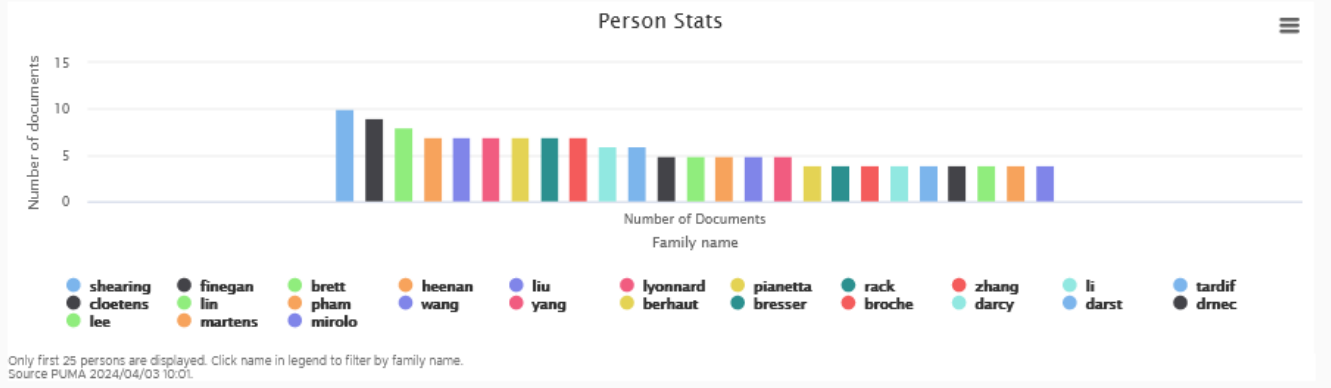
Search aggregation - facets







For detailed institution country/city map please select a collection



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Focus Instrument - ID22

lithium ion batter*

Fill expression and press [ENTER] to launch search. Use + for mandatory expressions, - to exclude, | for OR operator, "" for full phrase, * for wildcard and () to group operations. read more

- Uncheck *search in: title, abstract, keywords (USER, PUMA), journal title.*
- Check *search in: title, abstract, keywords (USER, PUMA), journal title, fulltext* read more

From 2019 to 2024 Select year in

Publications - Publications read more

Collection Any (all database)

⇓ Expand advanced search filters ⇓

Instruments id22

puma record : 215412 detail , ES record (direct), ES record (proxy)

JOURNAL_ARTICLE : Understanding the structural changes in lithiated graphite through high-resolution operando powder X-ray diffraction

doi:10.1016/j.carbon.2019.06.103 November 2019 (Publication Year : 2019), carbon *(Elsevier BV)*

Authors : mathiesen jette k.; **johnsen** rune e.; **blennow** ane s.; **norby** poul

Keywords : *CORPUS_INFO :* FLORA_ESRF_PUB FLORA_ESRF_PUB_WITH_ESRF_INSTRUMENT *CROSSREF_SUBJECT :* General Materials Science General Chemistry

PUMA : high resolution powder diffraction X lithium-ion battery X in-situ study X new PUMA keyword

Abstract : to develop more efficient and safer batteries, a deeper understanding of lithium ion intercalation and de-intercalation dynamics upon operation in lithium-ion batteries is of great importance. we have performed operando high-resolution powder x-ray diffraction (pxrd) studies of the intercalation and de-intercalation process in a graphite electrode material using custom-made capillary-based lithium-ion battery cells. using high-resolution pxrd, it was possible to resolve the diffraction peaks from a number of lithiated graphite phases occurring during intercalation/de-intercalation of lithium and obtain information about the transformation processes, both related to the staging process and the in-plane transformation. in the staging related to the intercalation of lithium, two-phase and solid-solution behavior is identified. similar phase behavior is observed when examining the in-plane parameters. the mechanism of intercalation is proposed to involve charge transfer between the lithium ion and the π orbitals of the graphene layer. broadening of the hk0 peaks may be related to non-uniform reduction of the graphene layers depending on the staging number and the graphene layer neighboring environment.

Institutions : (show affiliations)

Technical University of Denmark, Kongens Lyngby, DK

University of Copenhagen, Copenhagen, DK

Siemens (Denmark), Ballerup, DK

instruments.code	abstractText	keywordsPumaType
"id22"	" lithium-ion batteries is of great importance. we" " lithium-ion battery cells. using high-resolution pxrd" " deeper understanding of lithium ion intercalation" " lithium ion and the π orbitals of the graphene layer" "to develop more efficient and safer batteries. a" " during intercalation/de-intercalation of lithium " " to the intercalation of lithium, two-phase and"	"lithium-ion battery"

Files :
PUBLICATION pdf epn-library.esrf.fr

Ids :
FLORA_NB_ID : ESRF19MA1567
ESRF_FLORA_ID : 52910
OPENALEX_ID : W2955665841

Instruments : id22 (ESRF) X Add **Instruments category :** hrpd

"id22" (source "flora")

"hrpd" (source "flora")

"high resolution powder diffraction" (source "") "lithium-ion battery" (source "") "in-situ study" (source "")

Collection Mapping Info : Show collection mapping rules for current instruments

Included in collections :

esrf_pub
esrf_ccr1_streamline_energy_work_glatzel_3_pub
esrf_ccr1_streamline_energy_work_glatzel_1_pub
esrf_grp_id_hrpd_publication . Dashboard : GRP ID22 [ID31, BM16] HRPD

STREAMLINE has received funding fror

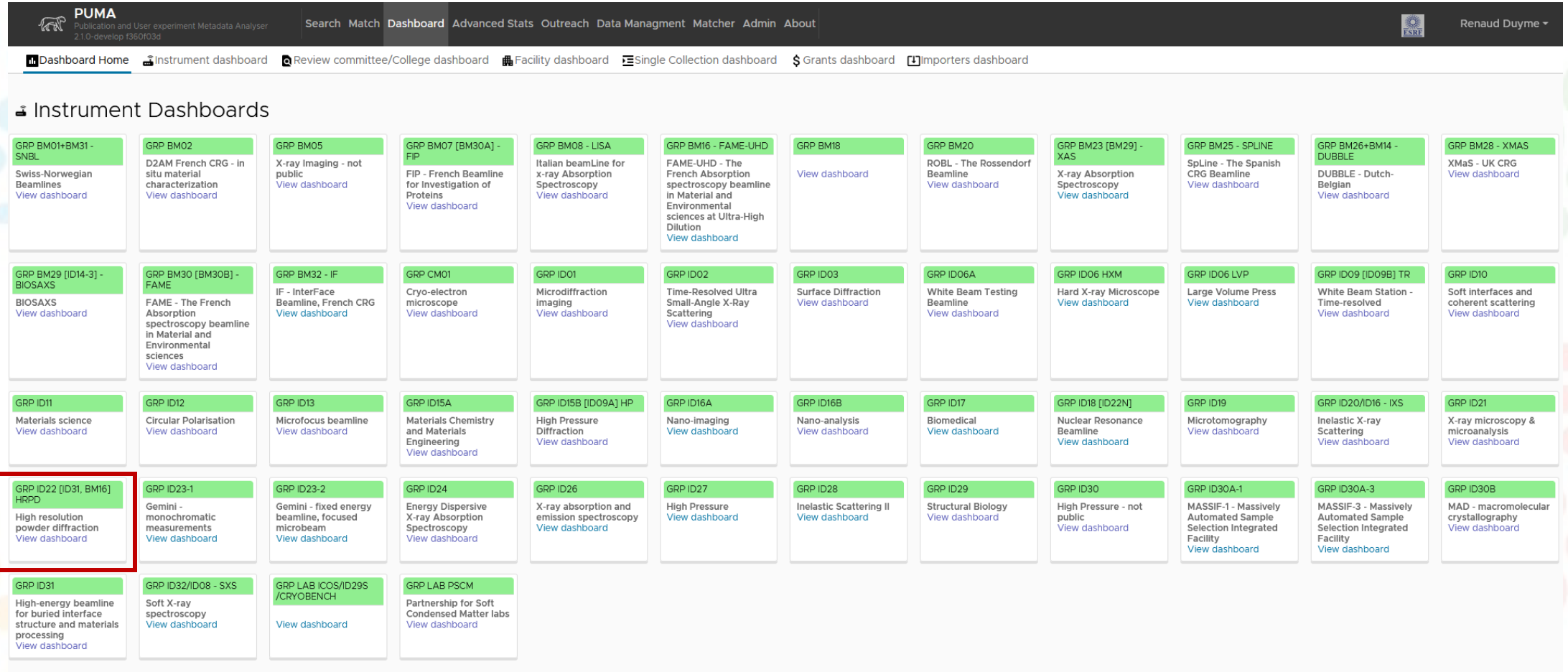
STREAMLINE

ESRF
The European Synchrotron

PUMA Instrument Dashboard

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Instrument Dashboard - ESRF Instruments



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Instrument Dashboard - ID22

summary | bibliometrics | documents | keywords | pub instruments | prop instruments | journals | open access | users | institutions | exp to pub delay | data rules

History : "GRP ID22 [ID31, BM16] HRPD"

bm16 *1995/11/01-2002/03/09 : "Powder diffraction ESRF"*

id31 *2002/06/01-2013/12/01 : "High-Resolution Powder-diffraction Beamline"*

id22 2014/05/01- : "High-Resolution Powder-diffraction Beamline"

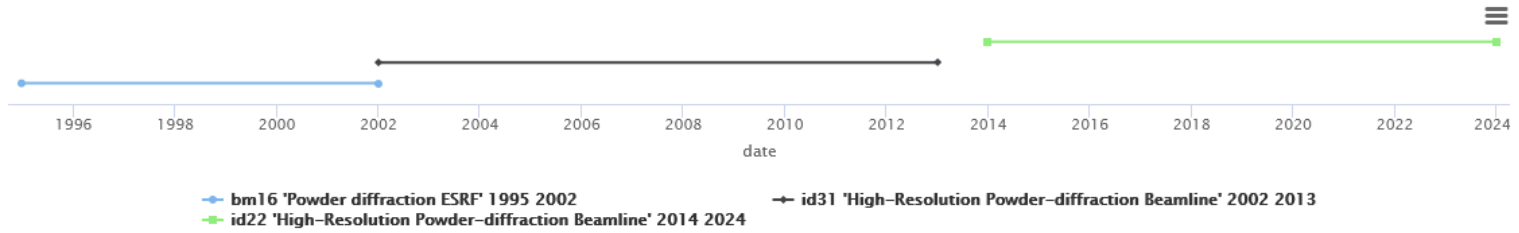
Period start date should be official instrument opening date (should not include commissioning time).
Proposals before this date will not be included.

'id22_hrpd' , 'id31', 'bm16_hrpd' flora instruments used to track publications

- 'id22' and 'id22_hrpd' classifications exists in flora, make sure pubs are well associated in flora. (see : #387).
- 'id31' and 'id31_bib' classifications exists in flora, make sure pubs are well associated in flora.
- 'bm16' , 'bm16_hrpd', and 'bm16_fame_uhd' classifications exists in flora, make sure pubs are well associated in flora (see : #384) .

You may review these with flora advanced search

Timeline



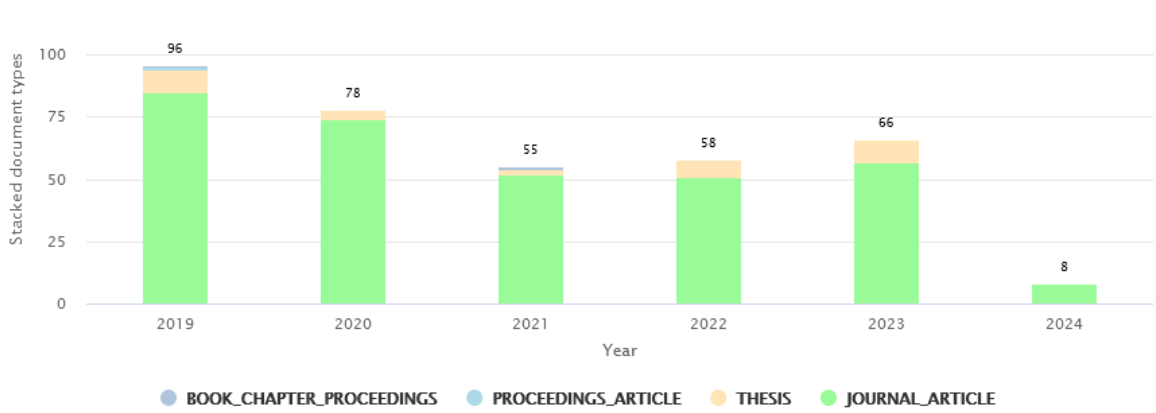
Source PUMA 2024/04/03 11:09.

Publication & Proposals stats

For more info on how documents are added to graph below please see "Data Rules" tab.

Accepted proposals by FACILITY_USER_TYPE and proposal deposit year/month

Yearly Publications Statistics



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Instrument Dashboard - Citations

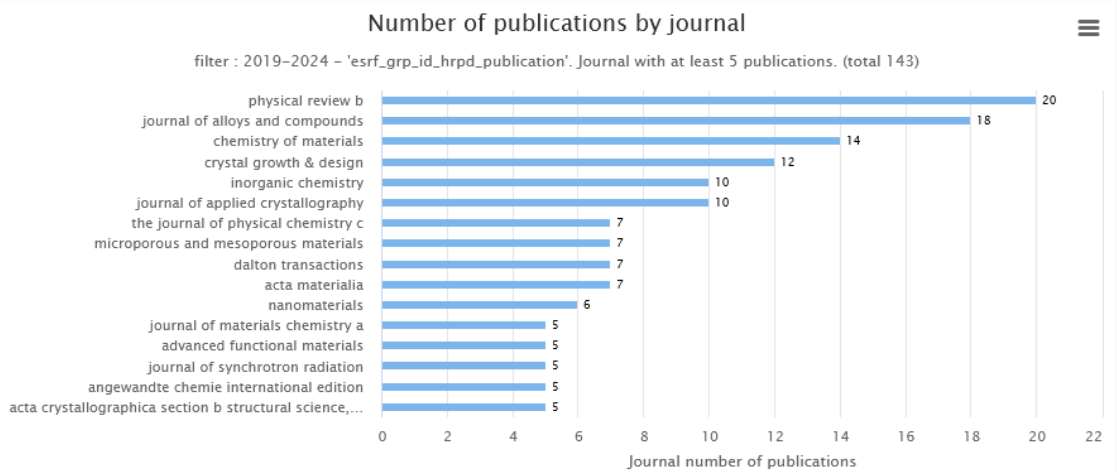
20 best cited publications

2019-2024 - 'GRP ID22 [ID31, BM16] HRPD (High resolution powder diffraction) '

Year	Publication	Nb Citations.	Impact Factor	Puma Id
2019	**a hydrated crystalline calcium carbonate phase: calcium carbonate hemihydrate** *zou z.; habraken w.; matveeva g.; jensen a.; bertinetti l.; hood m.; sun c.; gilbert p.; polishchuk i.; pokroy b.; mahamid j.; politi y.; weiner s.; w* 10.1126/science.aav0210 - science	141	41.845	search 215028
2019	**Gapless spin-liquid state in the structurally disorder-free triangular antiferromagnet NaYbO2** *ding l.; manuel p.; bachus s.; grußler f.; gegenwart p.; singleton j.; johnson r.; walker h.; adroja d.; hillier a.; tsirlin a.* 10.1103/PhysRevB.100.144432 - physical review b	91	3.575	search 214316
2019	**on the heterogeneous nature of deformation in a strain-transformable beta metastable ti-v-cr-al alloy** *lilensten l.; danard y.; brozek c.; mantri s.; castany p.; gloriant t.; vermaut p.; sun f.; banerjee r.; prima f.* 10.1016/j.actamat.2018.10.003 - acta materialia	79	7.656	search 214169
2019	**structural insight into strong pt–ceo2 interaction: from single pt atoms to ptox clusters** *derevyannikova e.; kardash t.; stadnichenko a.; stonkus o.; slavinskaya e.; svetlichnyi v.; boronin a.* 10.1021/acs.jpcc.8b11009 - the journal of physical chemistry c	65	4.189	search 215287
2019	**In-depth study of the mechanism of heavy metal trapping on the surface of hydroxyapatite** *ferri m.; campisi s.; scavini m.; evangelisti c.; carniti p.; gervasini a.* 10.1016/j.apsusc.2018.12.264 - applied surface science	65	6.182	search 215531
2019	**Development of a high strength Al–Zn–Si–Mg–Cu alloy for selective laser melting** *casati r.; coduri m.; riccio m.; rizzi a.; vedani m.* 10.1016/j.jallcom.2019.06.123 - journal of alloys and compounds	64	4.65	search 214039
2020	**Endogenous Nanoparticles Strain Perovskite Host Lattice Providing Oxygen Capacity and Driving Oxygen Exchange and CH 4 Conversion to Syngas** *kousi k.; neagu d.; bekris l.; papaioannou e.; metcalfe i.* 10.1002/anie.201915140 - angewandte chemie international edition	64	15.336	search 222499

Publications stats all journals

To be displayed below a journal must have at least number of publications : 5



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PUMA Country Dashboard

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Country dashboards

Facility : European Synchrotron Radiation Facility

European Synchrotron Radiation Facility

European Synchrotron Radiation Facility (puma-grid.5398.7)
Facility ESRF View dashboard
ESRF proposals and publications

Recent dashboards links :
Home : 'European Synchrotron Radiation Facility'
Instrument : 'GRP ID22 [ID31, BM16] HRPD'
Facility - Country/Institution : 'Facility ESRF - CH'
Collection : 'esrf_grp_id10_cs_publication'

Facility ESRF - dashboards by country

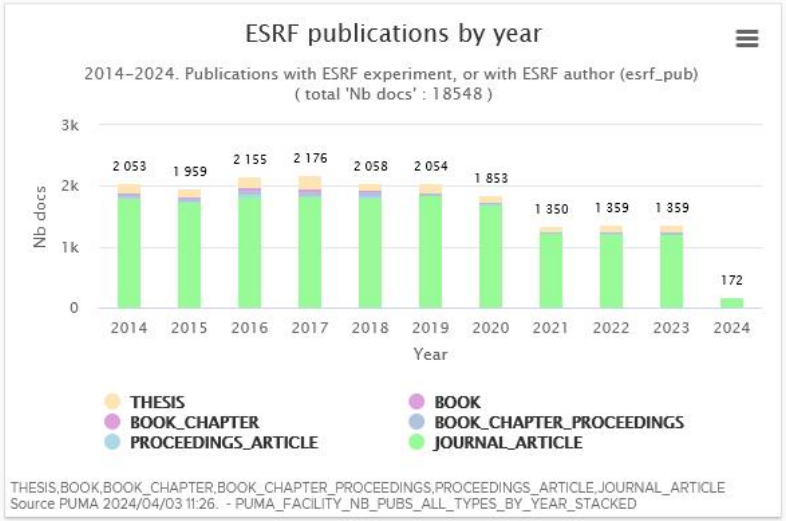
Members & associates :

Additional :

Other

National Institutions :

Universities :



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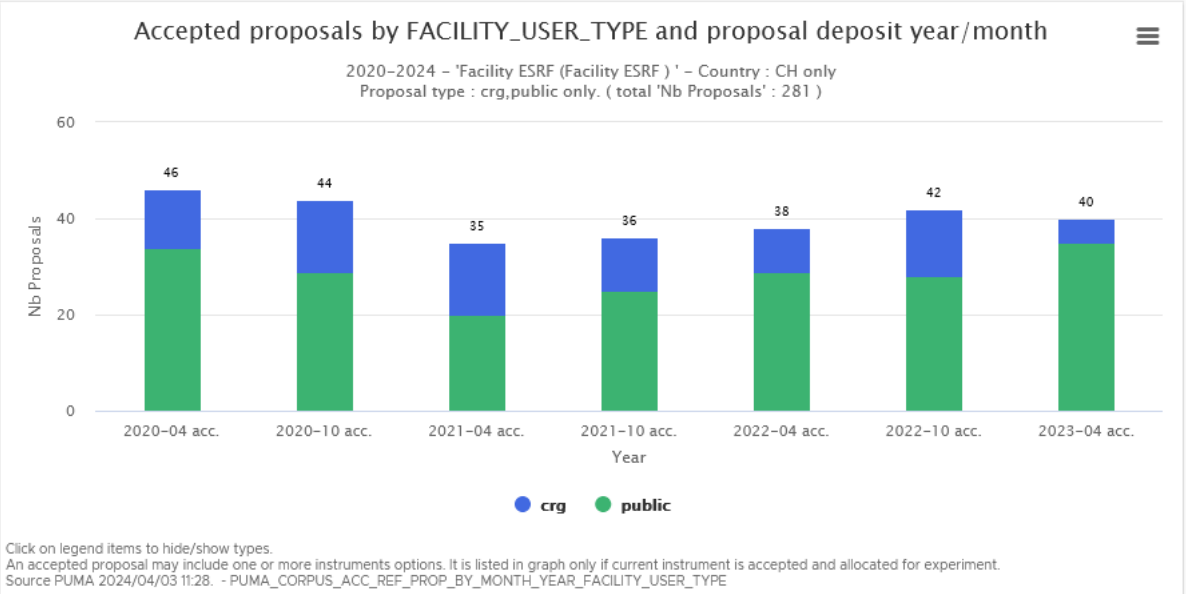
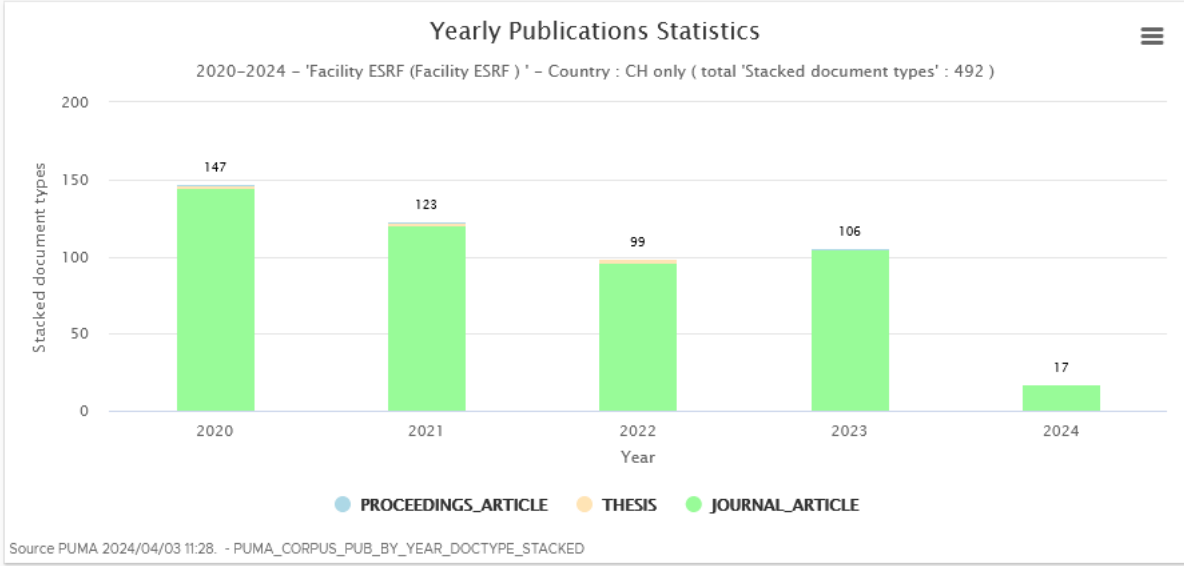
Focus - Switzerland

Dashboard : Facility ESRF CH

summary | bibliometrics | documents | keywords | pub instruments | prop instruments | journals | open access | users | institutions | data rules

Publication & Proposals stats





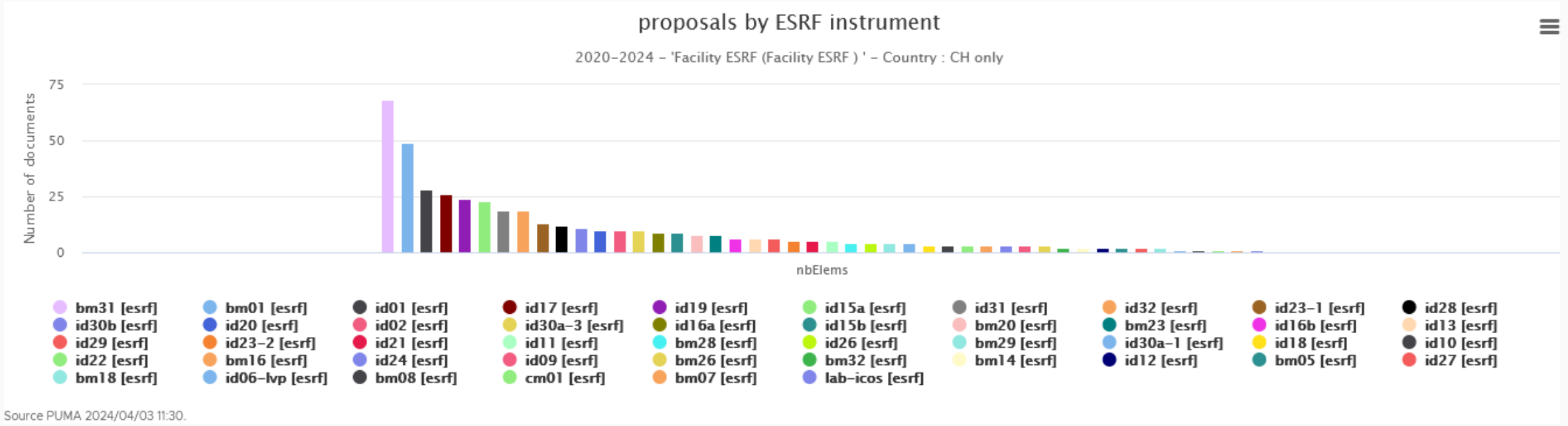
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Switzerland - Instruments

Dashboard : Facility ESRF CH

summary | bibliometrics | documents | keywords | pub instruments | prop instruments | journals | open access | users | institutions | data rules

Multiple instruments may be involved in proposals documents. The current page shows statistic from proposals related to *2020-2024 - 'Facility ESRF (Facility ESRF) ' - Country : CH only.*



Source PUMA 2024/04/03 11:30.

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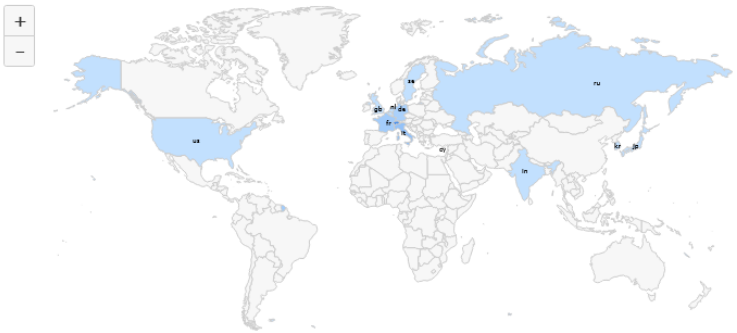
Switzerland - Country collaboration - publications

Summary | Institutions | Collaborations | Users

Documents count by country

Collection : esrf_pub, year : 2024–2024, country : CH, any author .
Total docs : 17



	count
CH	17
WORLD	17
ESRF	8
IT	7
FR	5
DE	4
SE	1
RU	1
US	1
KR	1

1 / 2

EU ZOOM

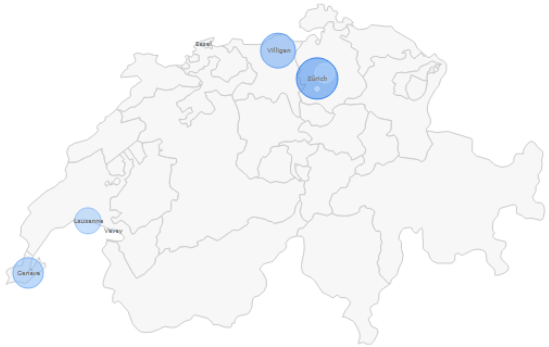
Source PUMA 2024/04/02 14:59. - PUMA_CORPUS_WORLD_NB_DOCS_MAP

All authors of documents are counted. A document is linked to a country if at least one author affiliation is located in the country. In the graph below, a document can then be counted in multiple countries.
NO_AFF : Number of documents with main user without affiliation available
NO_AFF_TO_ANALYSE : Number of documents where author affiliations are not yet loaded by PUMA
NO_INST : Number of documents with main user affiliation not associated to any PUMA institution.
NO_COUNTRY : Number of documents with main user not associated to any country.
Affiliation debug. See : Affiliation to institution match stats

PIE CHART MODE

Documents count by city in CH

Collection : esrf_pub, year : 2024–2024, country : CH, any author .



	count
Zürich	7
Villigen	5
Genève	4
Lausanne	3
Dübendorf	2
Basel	1
Rüschlikon	1
Vevey	1

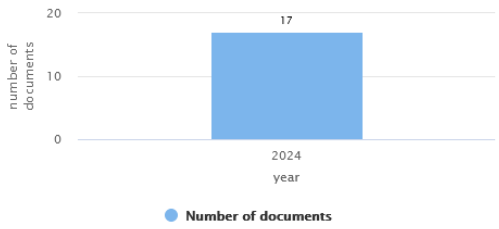
EU ZOOM | WORLD ZOOM

Source PUMA 2024/04/02 14:59.

Select a city to display related institutions stats

Evolution of documents involving country : CH

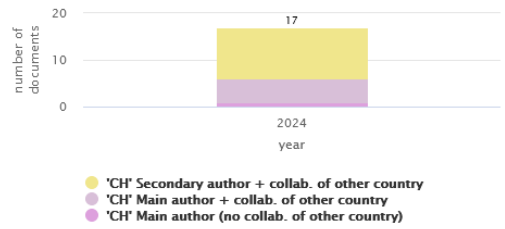
Collection : esrf_pub, year : 2024–2024, country : CH, any author . (total 'number of documents' : 17)



Source PUMA 2024/04/02 14:59.

Evolution of collaboration with CH

Collection : esrf_pub, year : 2024–2024, country : CH (total 'number of documents' : 17)



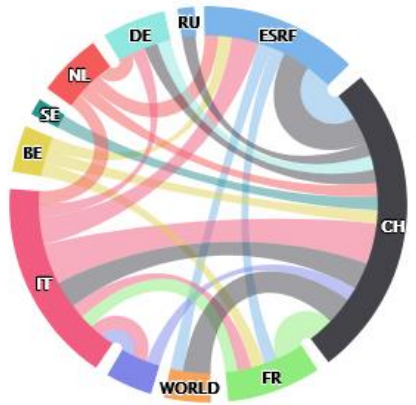
Source PUMA 2024/04/02 14:59.

Main institutions in CH.

ETH Zurich () Zürich - CH 7 docs	Paul Scherrer Institute () Villigen - CH 5 docs	University of Geneva () Genève - CH 3 docs
École Polytechnique Fédérale de Lausanne () Lausanne - CH 3 docs	Swiss Federal Laboratories for Materials Science and Te... () Dübendorf - CH 2 docs	Swiss Light Source () Villigen - CH 2 docs

Country collaboration stats

Collaborations from main author to secondary authors only.
Collection : esrf_pub, year : 2024–2024, country : CH



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Next Steps

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Current PUMA instance. ESRF, ILL.

Facility : European Synchrotron Radiation Facility

European Synchrotron Radiation Facility

European Synchrotron Radiation Facility (puma-grid.5398.7)
Facility ESRF View dashboard

ESRF proposals and publications

Recent dashboards links :
Home : 'European Synchrotron Radiation Facility'
Instrument : 'GRP ID22 [ID31, BM16] HRPD'
Facility - Country/Institution : 'Facility ESRF - CH'
Collection : 'esrf_grp_id10_cs_publication'

Facility ESRF - dashboards by country

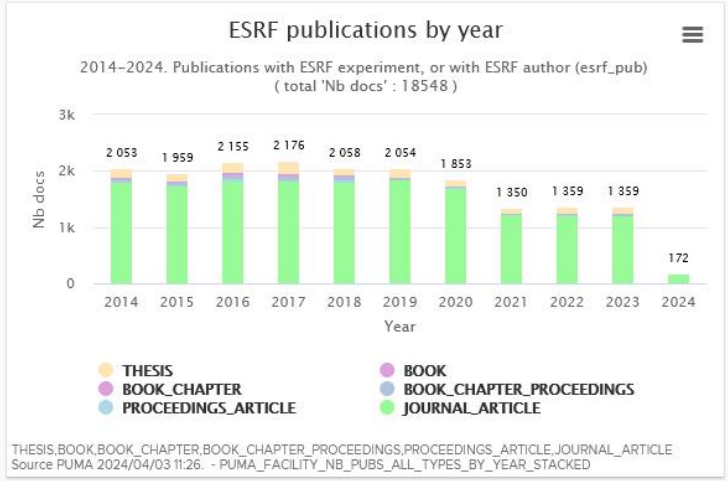
Members & associates :

Additional :

Other

National Institutions :

Universities :



Facility : ILL Facility

ILL Facility

ILL Facility (puma-grid.156520.5)
Facility ILL View dashboard

Recent dashboards links :
Home : 'ILL Facility'
Instrument : 'DSH_PSCM_ILL'
Facility - Country/Institution :
Collection : 'ill_prop'

Facility ILL - dashboards by country

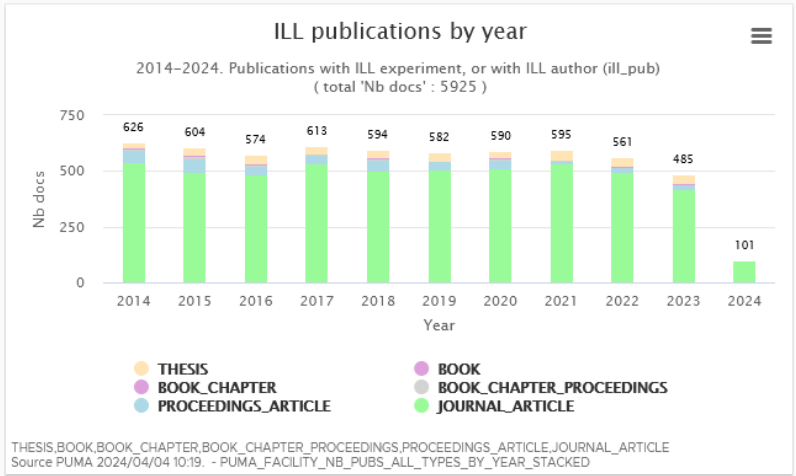
Members & associates :

Additional :

Other

National Institutions :

Universities :



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

How to set up new PUMA instance in a facility ?

User Portal database

Library database

Data curation by library

instruments

proposals

articles, books, thesis

Validated
+ instrument link
+ proposal link

PUMA

Data enrichment

Data exploitation

- Search
- Instrument dashboard

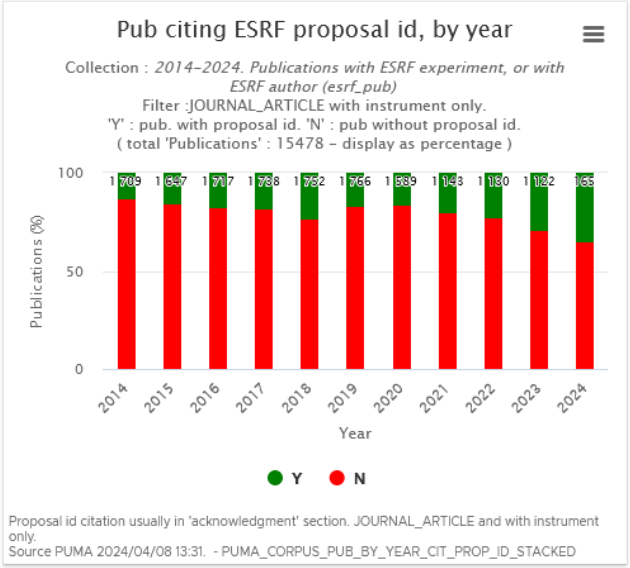
Requirements for new graphs in instrument dashboards

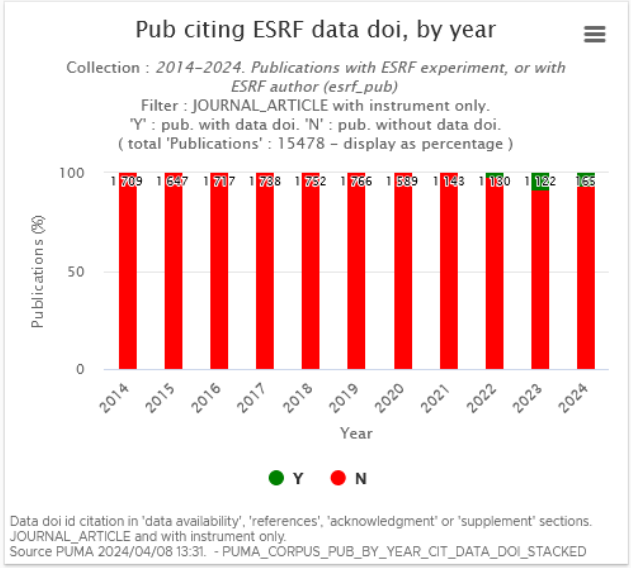
- **Data imports technical analysis for integration. Connection to User Portal and Library repositories**
- **Facility specific needs: experiment duration shifts/cycle, proposal types, proposal rounds…**

Work In Progress

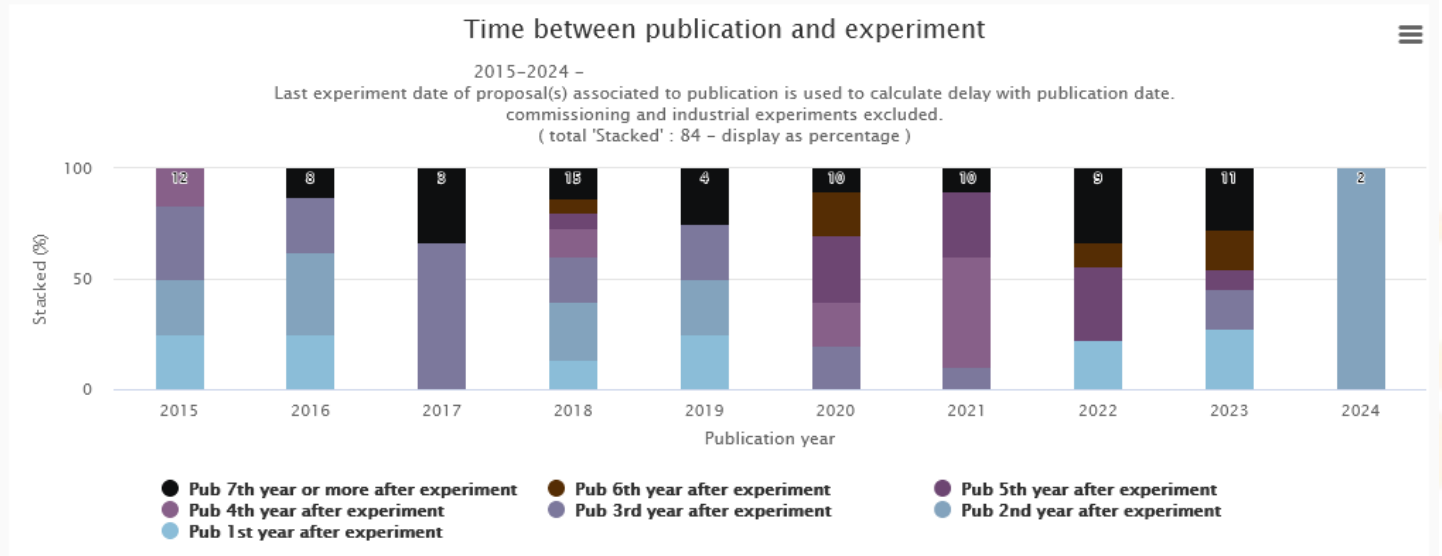
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Next Steps - Time between experiment and publication





Work In Progress



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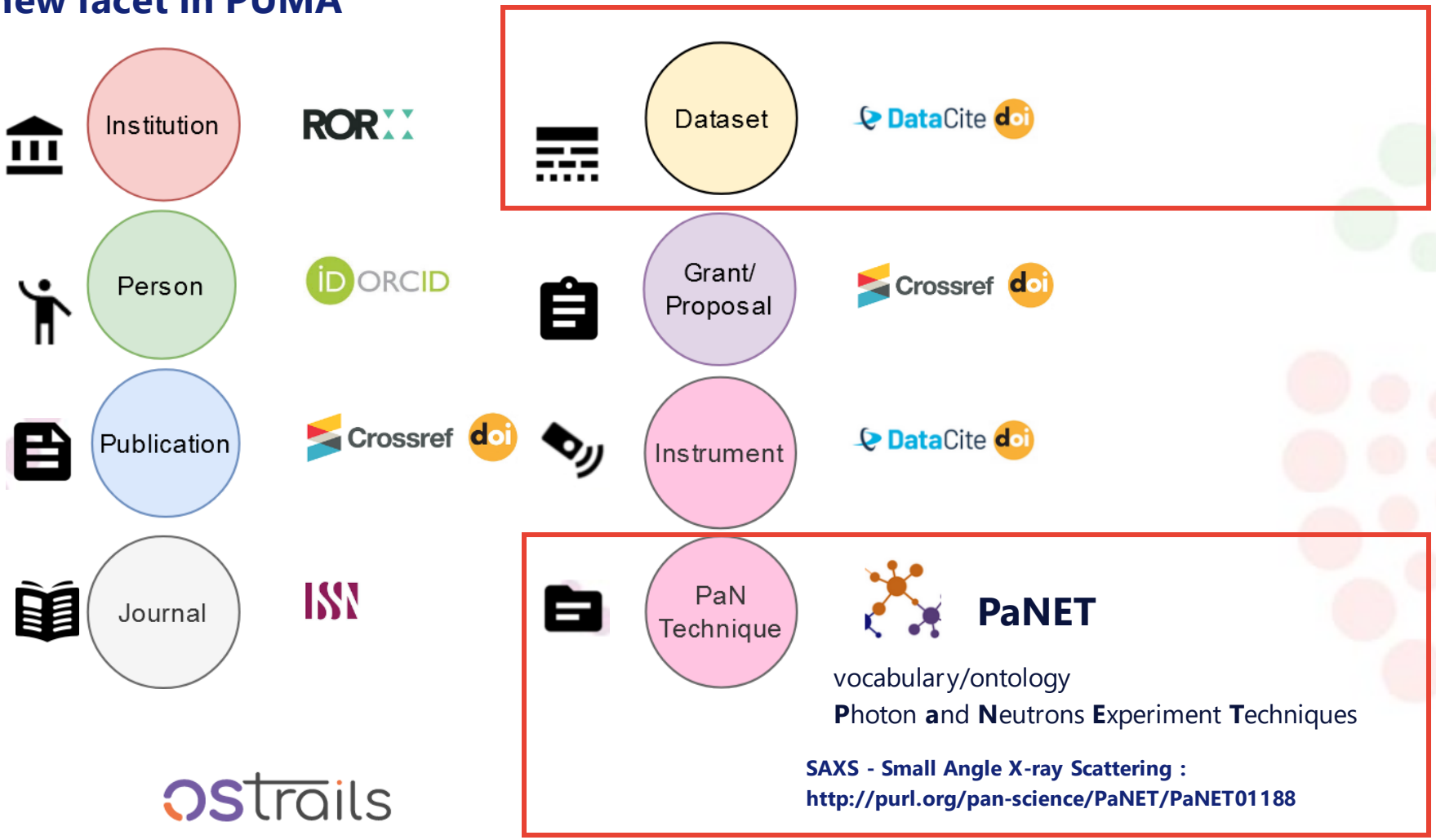
Next Steps - Experiment technique as a new facet

- **Enhance ESRF datasets with experiment technique**
- **Technique as a new facet in PUMA**



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Acknowledgments

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Solange Delageniere
Jean François Perrin

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Marine Cotte, Vincent Fernandez
Kirill Lomachenko
Mohamed Mezouar
Pieter Glatzel
Montse Soler Lopez, Gordon Leonard, Christoph Mueller-Dieckmann
Andy Fitch

Jacques Jestin, Mark Johnson

Erwan Le Gall

Ludovic Leroux, Cédric Ortiz, Fabien Pinet, Stuart Caunt

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Virginie Teissier

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Jean Susini

Brigitte Gagey
Majid Ounsy

Idrissou Chado

Frédérique Fraissard

Jean-Marc Lucacchioni

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WP4 : Data Processing & Processed Data

Andy Götz on behalf of

Mael Goanach, Alex de Maria, Marjolaine Bodin, Olof Svensson, **Ioannis Koumoutsos**, Wout de Nolf, Loic Huder, Axel Bocciarelli, Henri Payno, Thomas Vincent, **Quentin Bruel**, Vincent Favre-Nicolin, and ALL Beamlines who helped test the software!

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Revolutionising Data Processing with **EWOKS** and **ICAT**

ESRF
The European Synchrotron

STREAMLINE has r ent No. 870313.

Why a Revolution ?!

A Revolution is judged by the Impact it has in the long term

WP4 - Vision

· **WP4 will enlarge capacity at the ESRF to serve academic and industrial communities with enhanced experiment services beyond data acquisition,** and with a specific focus on the creation and launching of a new package of access services.

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

WP4 - Objectives

1. *To create effective **experiment work flows** and **database tools** supporting the mail-in services from **sample tracking**, **data collection** and **meta data modelling** and **delivery of data** and **useable results**;*

2. *To **provide online data analysis** by building upon the generic services developed in the PaNOSC H2020 project, providing a platform for data analysis as a service, **targeting the implementation of this across all ESRF beamlines**; These services will be designed for direct exploitation within the European Open Science Cloud. The services will encourage and enable **Open Science**;*

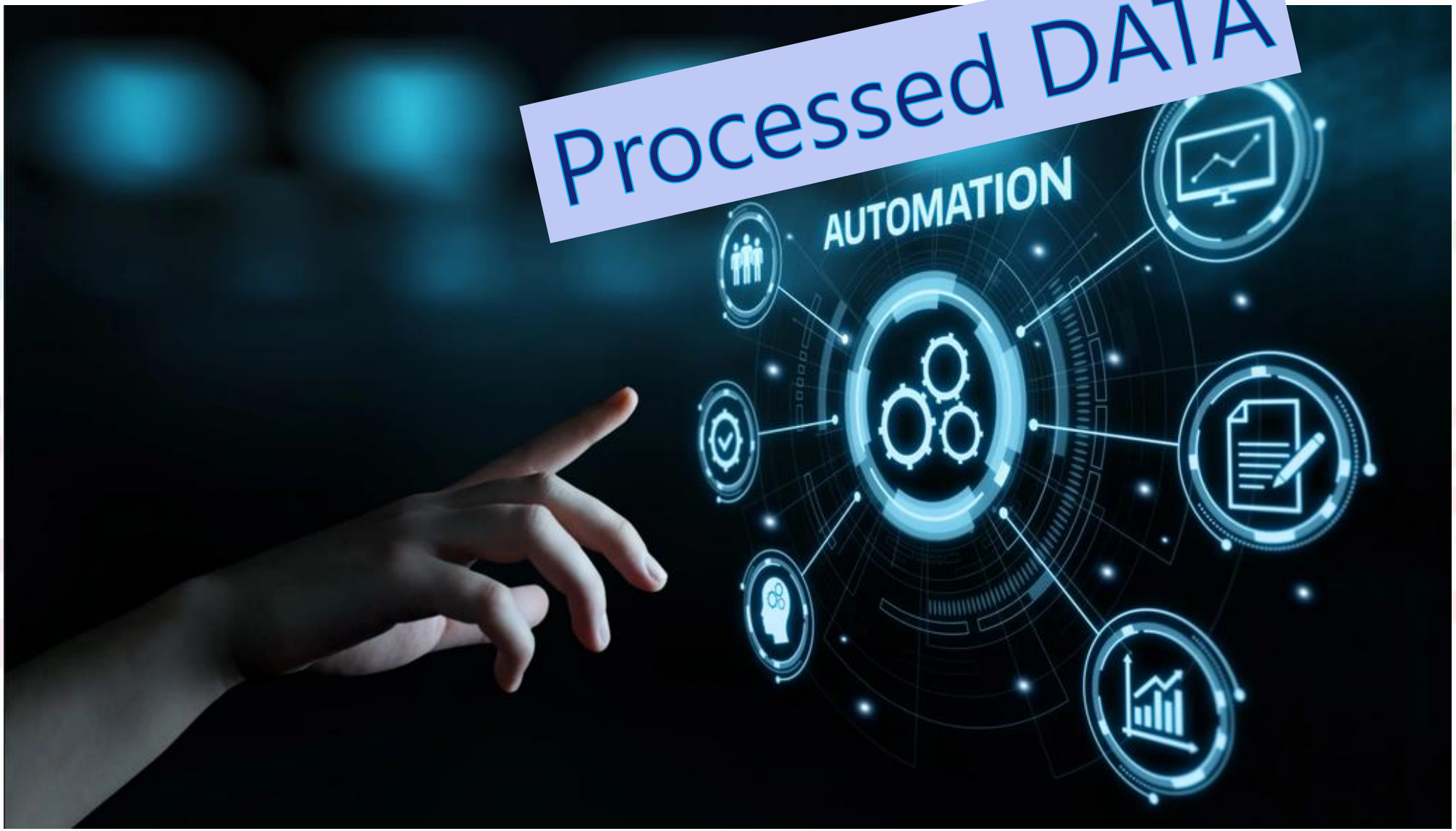
3. *To **enhance data collection** and **data analysis** through the exploitation of **artificial intelligence**, notably the deployment of **machine learning** algorithms to accelerate beamline processes, **reduce data volumes** and automate certain aspects of data analysis, for example reducing operator input for routine and time-consuming tasks;*

4. *To define **standard operating procedures** (SOP) and to test the new procedures and services;*

5. *To launch a new mail-in service package.*

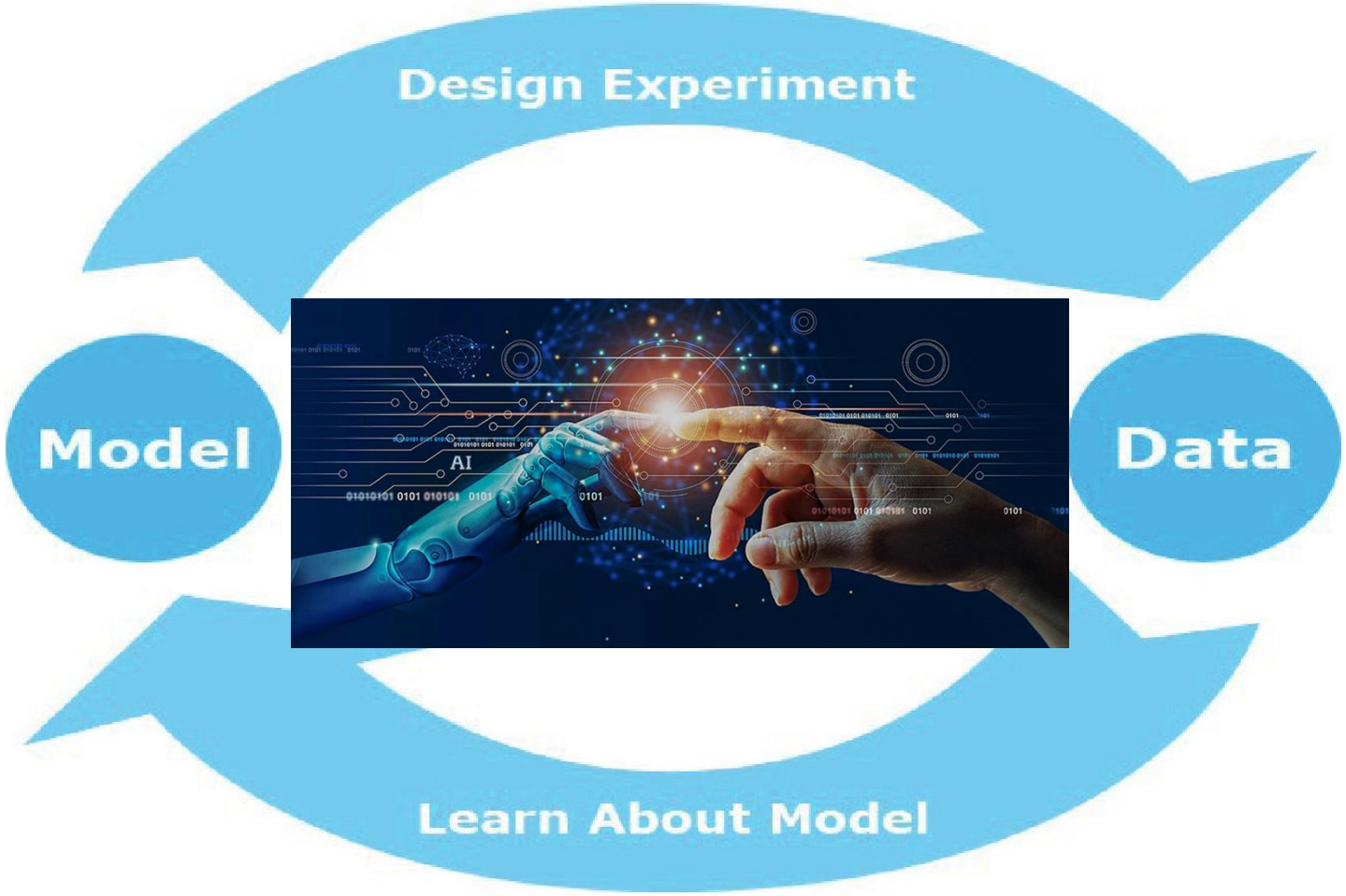
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Our Revolution is the Automation of Processed Data



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

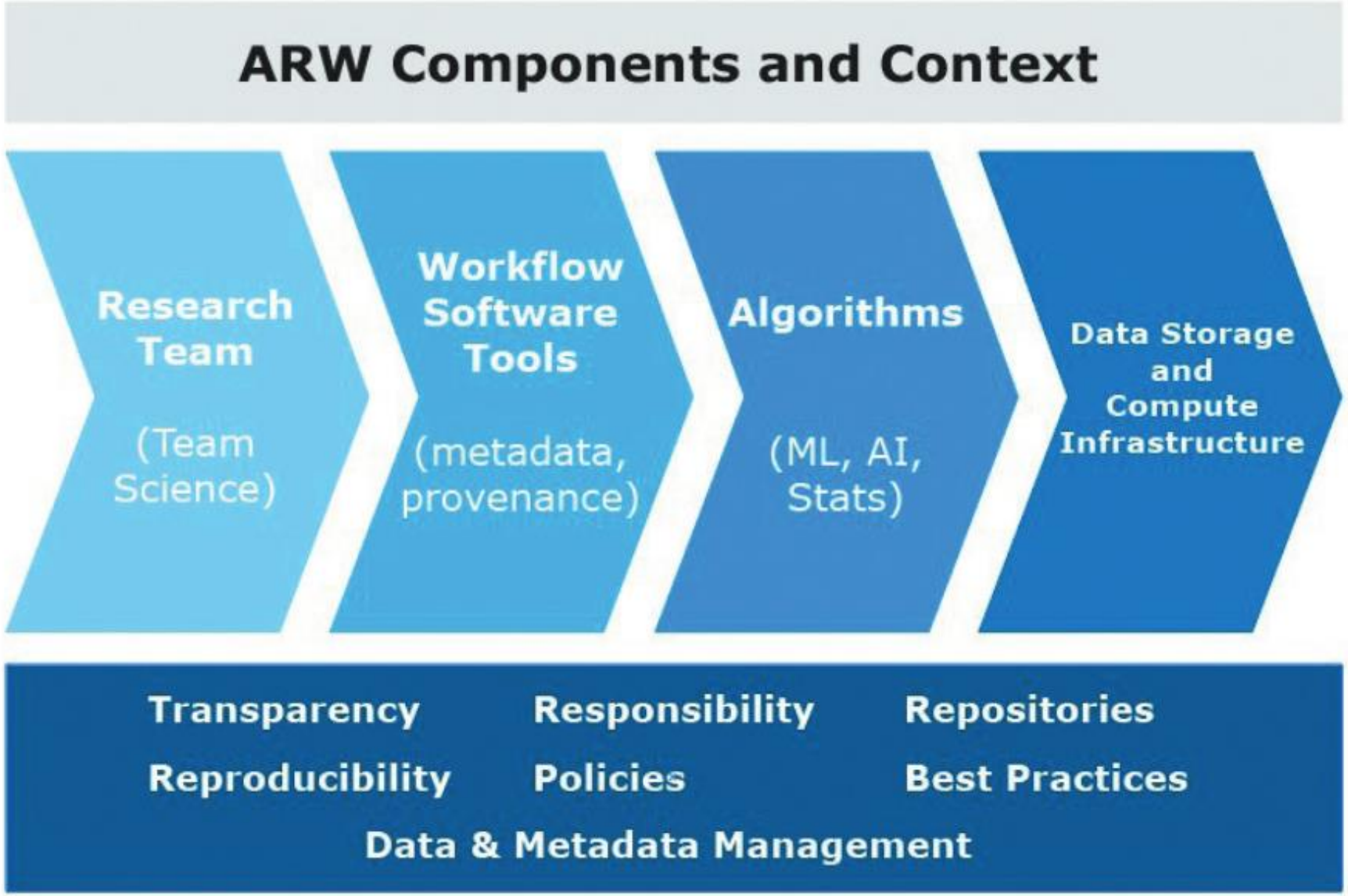
Automating data processing to accelerate discovery



https://doi.org/10.17226/26532

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

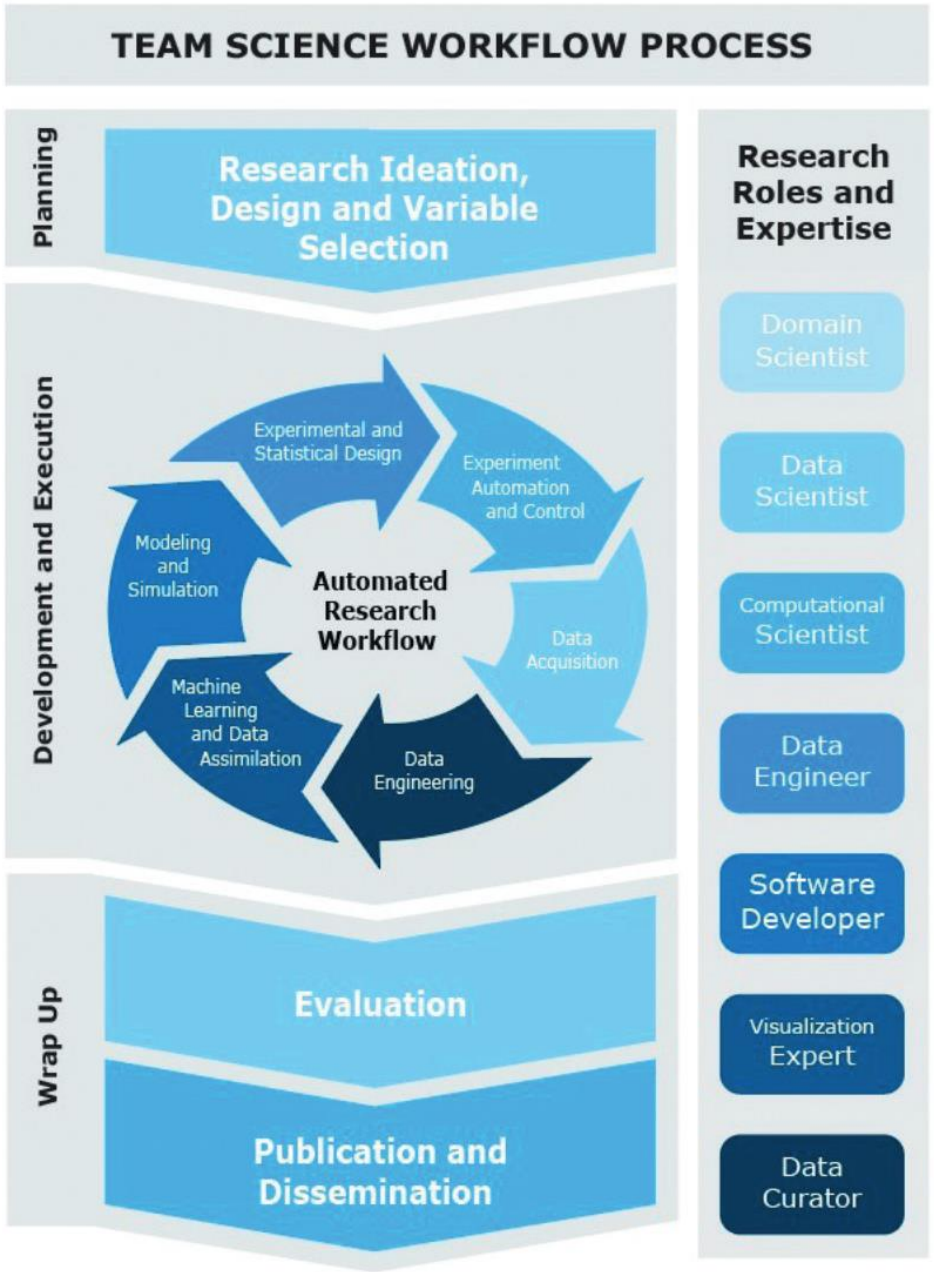
Automating data processing requires multiple components



https://doi.org/10.17226/26532

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Automating data processing requires a team of highly skilled experts



Users

Beamline scientists

Data scientists (ADA)

Software engineers (BCU)

Data automation + viz engineers (DAU)

Data managers (DAU)

IT engineers (TID)

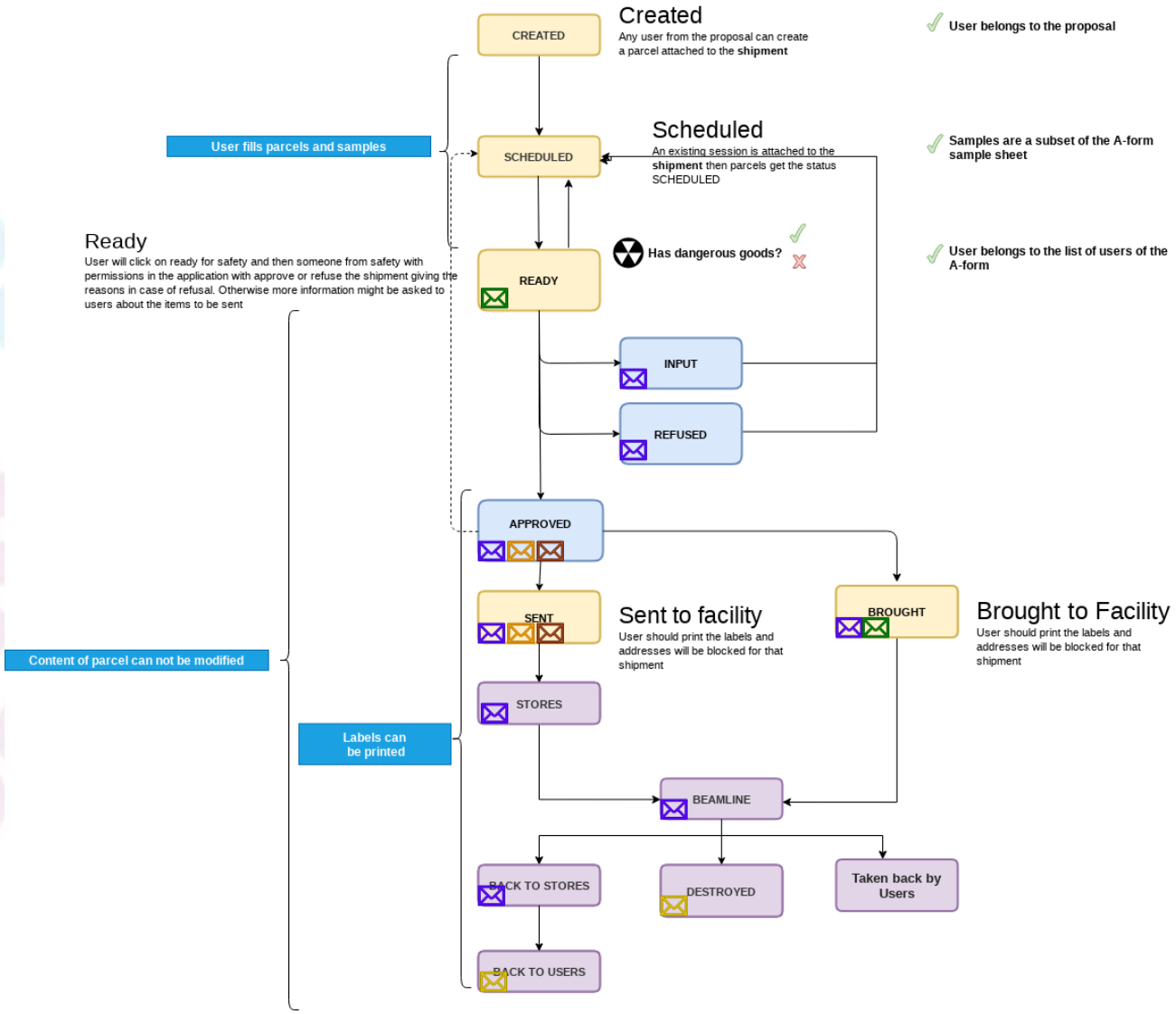
https://doi.org/10.17226/26532

Task 4.3: LIMS for new mail-in services *(Software Group)*

1. Objective was to create a **Mail-in** service for **all Beamlines**
2. **COVID-19** lockdown pushed the **priority** to **VERY HIGH**
3. A development was started based on **ICAT** in **April 2020** and ready by **August 2020**!
4. Next step was to **unify** the Mail-In based on **ICAT** with Mail-In based on **ISPyB** (for MX)
5. This was implemented as part of the **new data portal** in 2024

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Task 4.3 : MAIL-IN SAMPLE TRACKING - WORKFLOW



LEGEND

- Notification to expsaf@esrf.fr if contains dangerous goods
- Notification to safety group (expsaf@esrf.fr)
- Notification to users
- Notification to users, local contact and BDO (industry@esrf.eu) in case of IM/IN
- Notification to esrftransport@esrf.fr
- Notification to users and BDO (industry@esrf.eu)in case of IM/IN

Action done by users

Action done by safety

Action done by staff (stores or local concatcts)

Credits: **Alex de Maria**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Sample Tracking statistics for all non-MX beamlines from 2020 to 2024

1929 parcels shipped!

Summary

Test parcels are filtered! A parcel is considered as test if the beamline associated is **ID00**

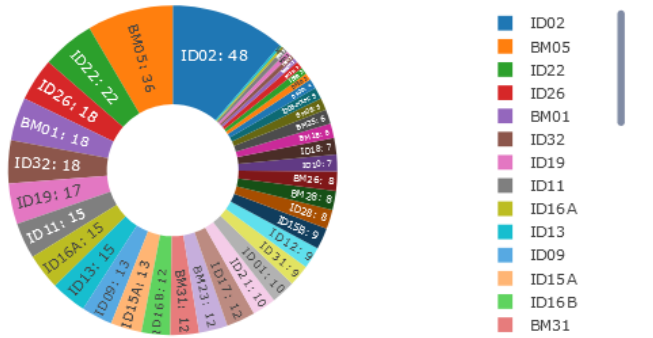
Parcels	1929
Beamlines	45

Items

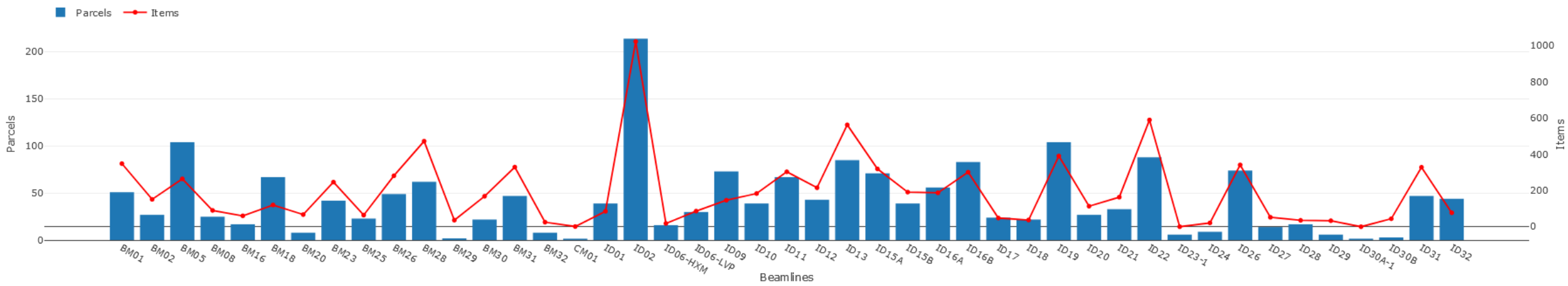
Samples	6567
Tools	775
Others	1269
Total items	8611

CREATED	0
SCHEDULED	150
READY	0
APPROVED	504
REFUSED	0
INPUT	1
SENT	180
STORES	111
BEAMLINE	426
BACK_STORES	37
BACK_USER	476
DESTROYED	44

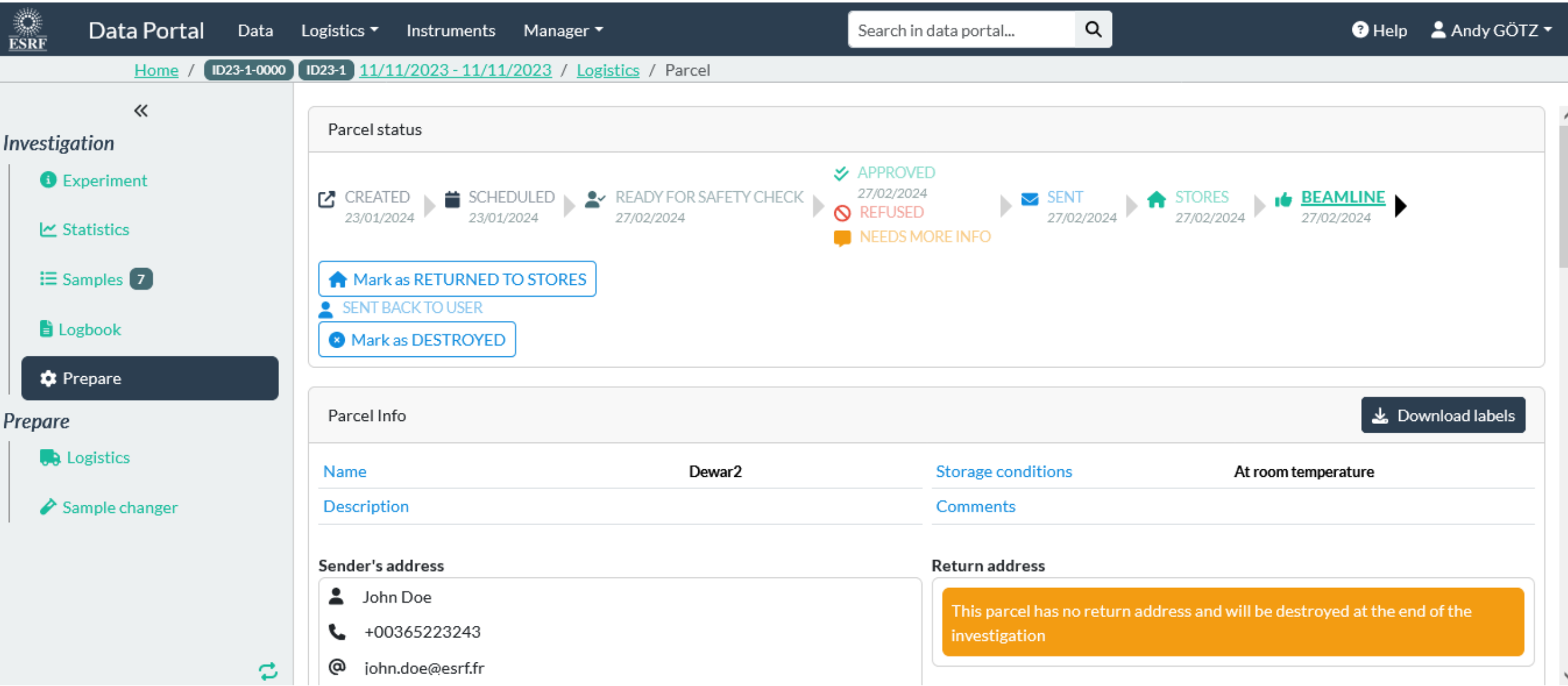
Parcels currently on beamlines



Parcel and items/Beamlines



Unified interface for Sample Tracking



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Unified interface for Sample Tracking – sending many samples

Data Portal | Data | Logistics | Instruments | Manager | Search in data portal... | Help | Andy GÖTZ

Home / ID23-1-0000 ID23-1 11/11/2023 - 11/11/2023 / Logistics / Parcel

Investigation

- Experiment
- Statistics
- Samples 7
- Logbook
- Prepare

Prepare

- Logistics
- Sample changer

Content

Table | Containers

Import file | Export data | Download template

Supported formats: CSV, XLS, XLSX

Columns should match the table below. You can download the template file to fill in the data.
Import will overwrite the current table data.

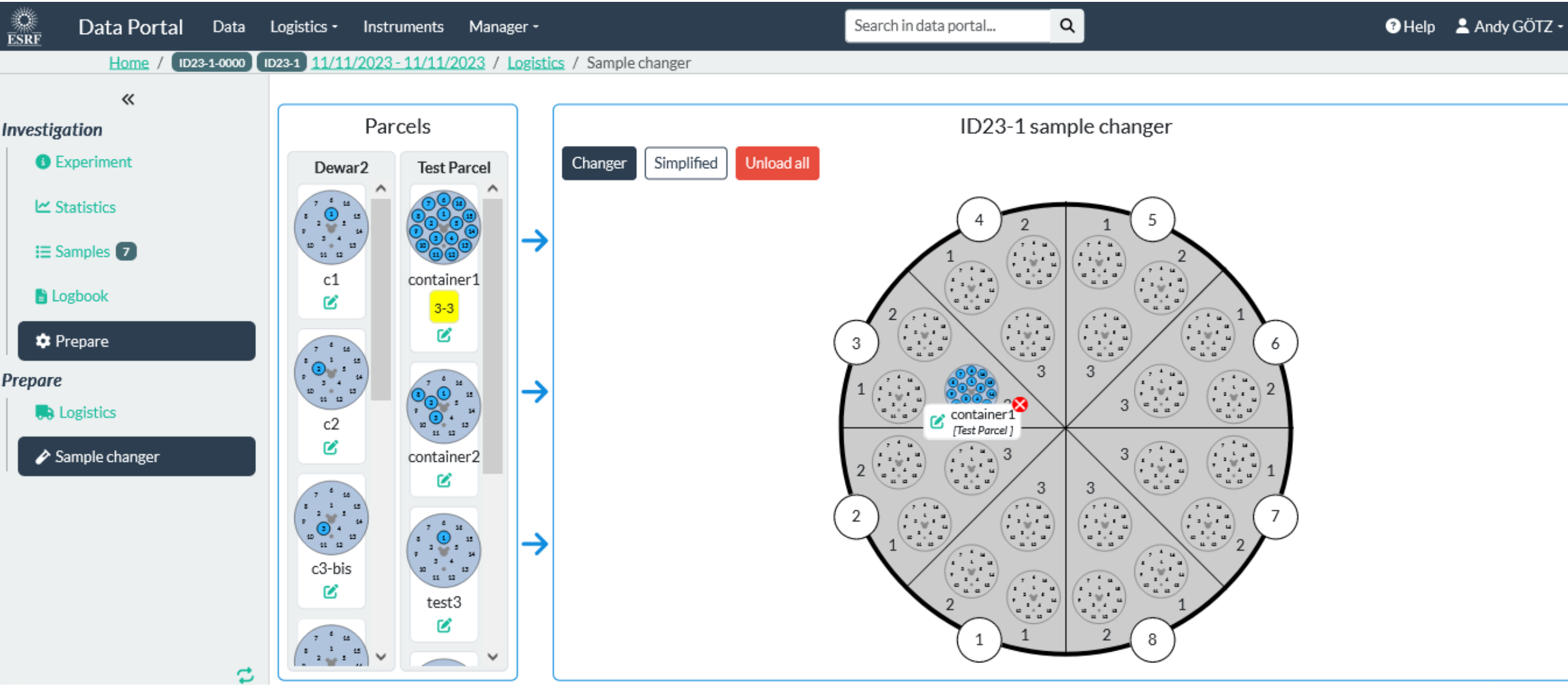
Save | Discard changes | Fullscreen | No changes to save.

Same values have same color.

	Container			Item								
	Type	Name	Sample position	Type	Short name	Name	Description	Comments	a	b	c	Alp
1	UNIPUCK	container1	1	SAMPLESHEET	Lysoz	l1	test	test	1	2	3	4
2	UNIPUCK	container1	2	SAMPLESHEET	Lysoz	l2			1	2	3	4
3	UNIPUCK	container1	3	SAMPLESHEET	Lysoz	l3			1	2	3	4
4	UNIPUCK	container1	4	SAMPLESHEET	Lysoz	l4			1	2	3	4
5	UNIPUCK	container1	5	SAMPLESHEET	Lysoz	l5			1	2	3	4
6	UNIPUCK	container1	6	SAMPLESHEET	Lysoz	l6			1	2	3	4

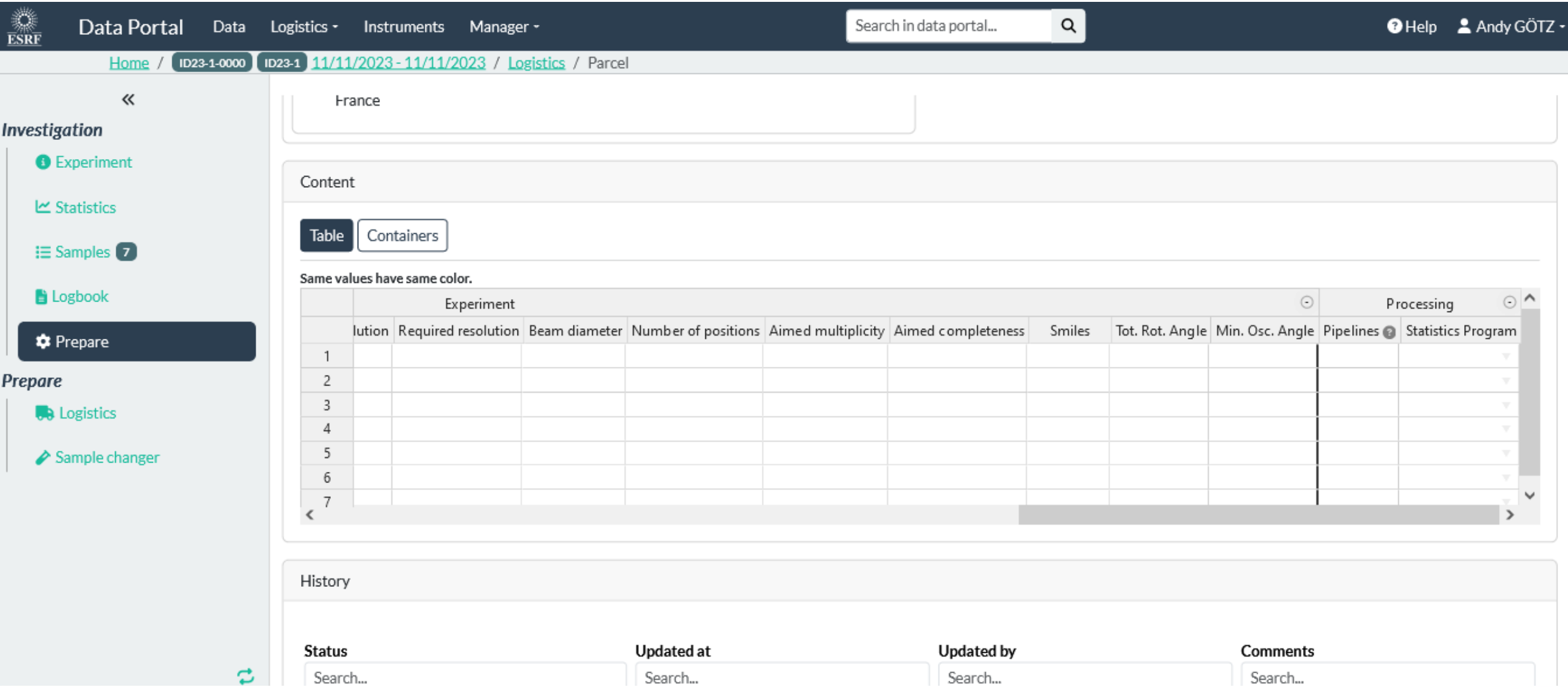
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Unified interface for Sample Tracking – preparing MX sample changer



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

MX Experiment + Processing Plan in ICAT LIMS



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Task 4.3 : LIMS for ALL techniques based on ICAT

1. ISPyB is a Laboratory Information Management System (LIMS) originally developed at ESRF for MX experiments.

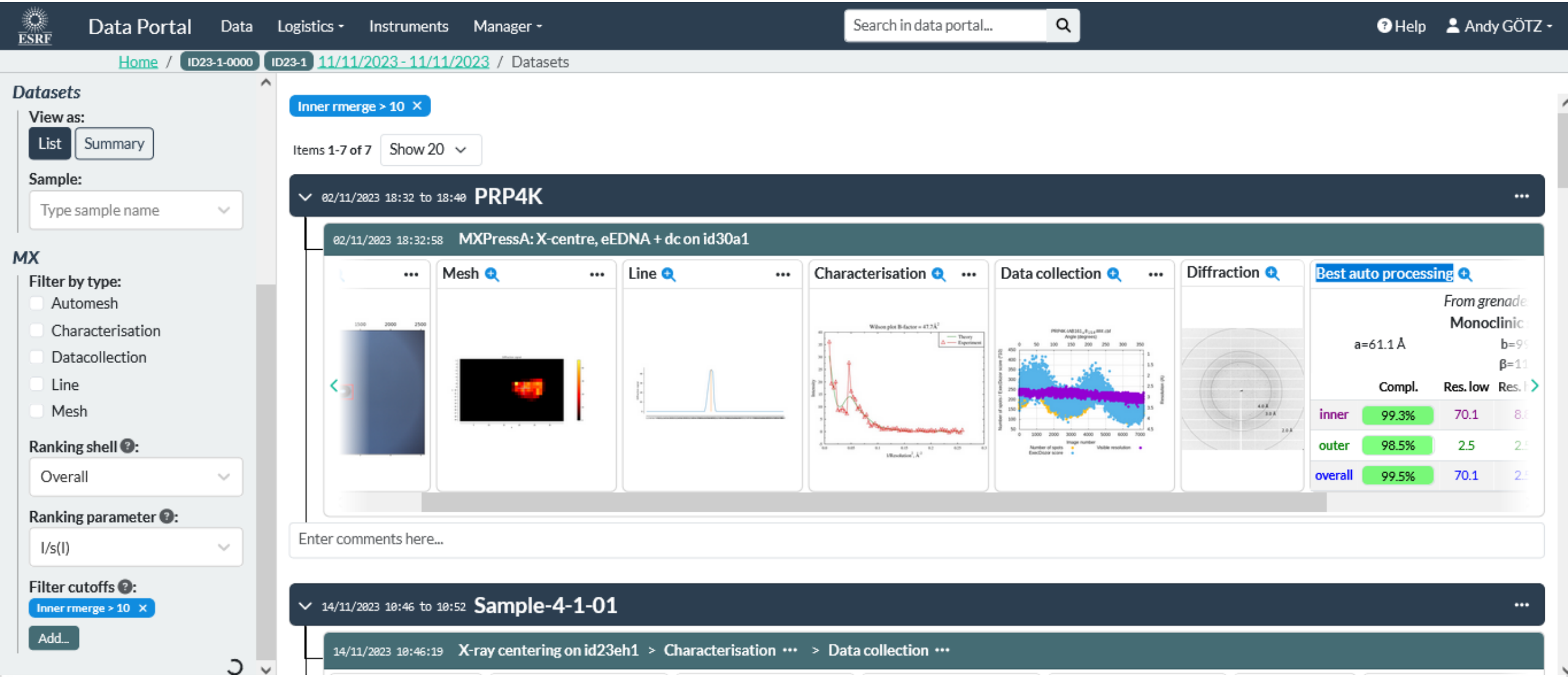
2. In STREAMLINE we unified the LIMS system at ESRF by replacing ISPyB with ICAT

3. Sample tracking for MX has been unified with the other beamlines

4. All techniques are now deployed on the new LIMS with the same powerful features as MX+SSX

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

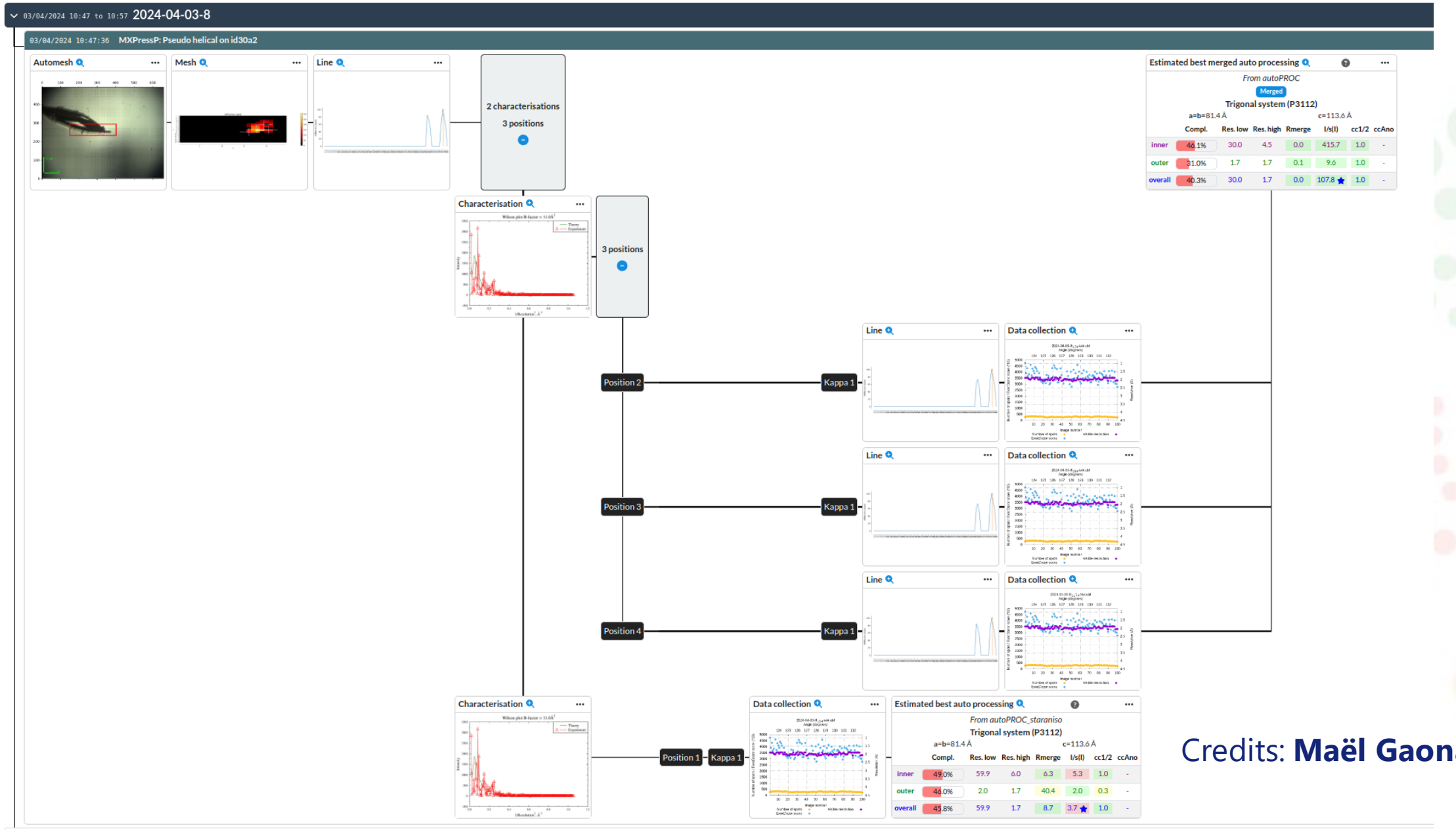
ICAT LIMS allows displaying all processed results e.g. MX experiment on ID23-1



https://data2.esrf.fr/investigation/1405067863/datasets

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

ICAT LIMS provides new possibilities to display processed data e.g. MX merged results



Credits: **Maël Gaonach**

Serial Crystallography (SSX) @ ID29 – work in progress

Credits: **Maël Gaonach**

What are the data processing challenges of the ESRF-EBS?

1992-2018

ESRF

2020-present

ESRF-EBS
Extremely Brilliant Source

Produce Data

Policy until 2015: data were deleted after 6 months!

Produce Results

Policy since 2021: raw and processed data are kept for 10 years

OPEN SCIENCE

Findable Accessible Interoperable Reusable

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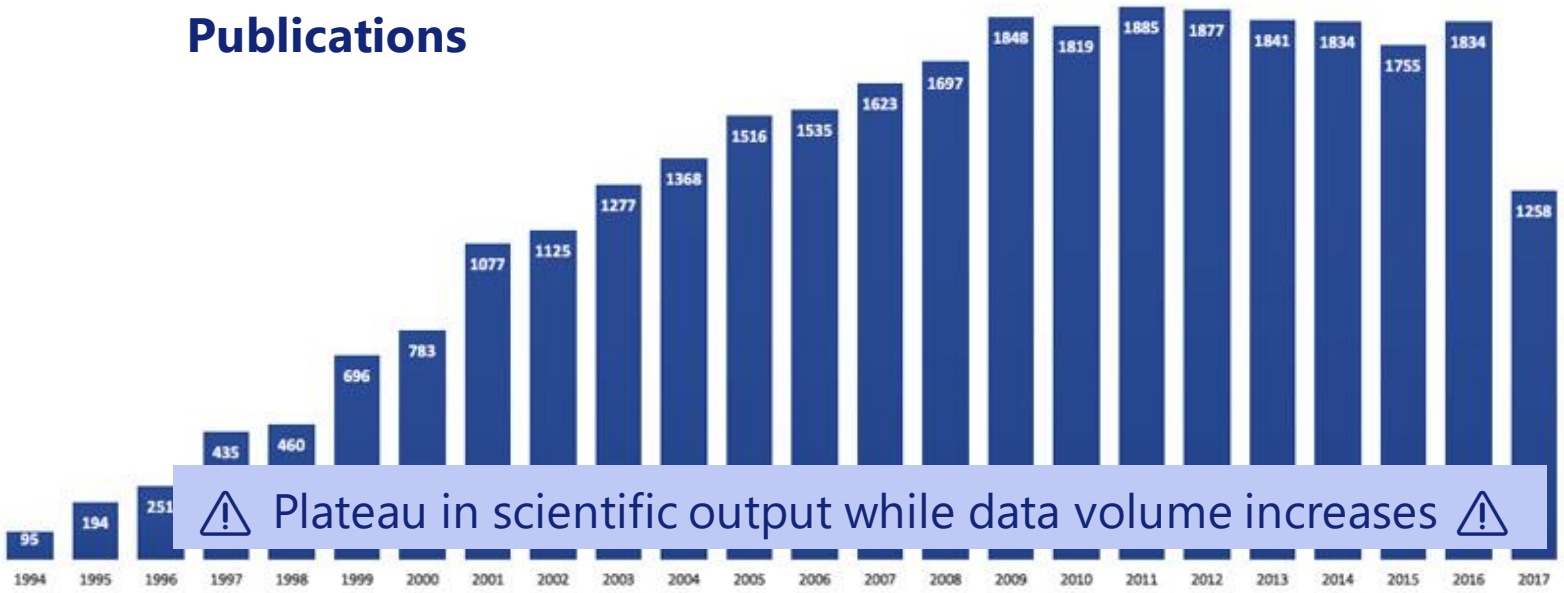
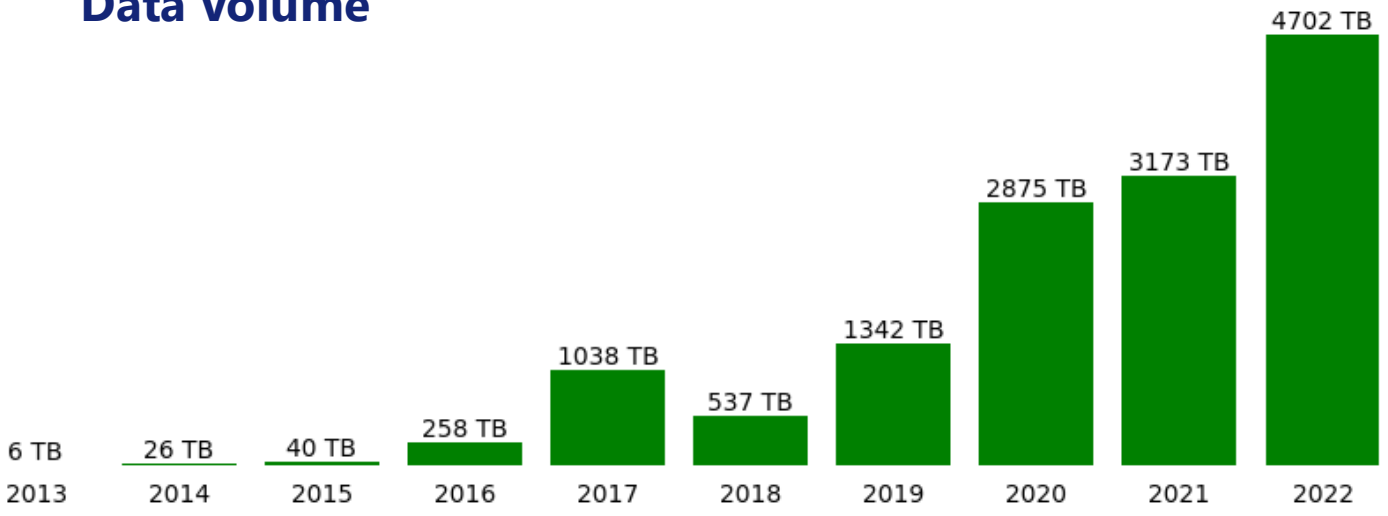
Data are increasing but not publications

Publications



⚠ Plateau in scientific output while data volume increases ⚠

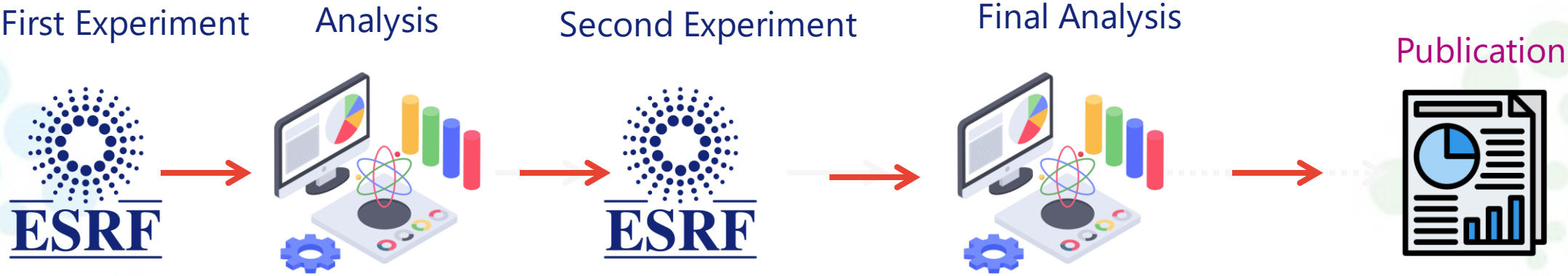
Data Volume



Credits: **Wout de Nolf**

STREAMLINE has receivec agreement No. 870313.

Time to publish can be long



Timescale of months at best, often one year or more

Steep learning curve for **new users** from a **wide range of scientific domains**
Growing the **synchrotron community has reached its limits**

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

The goal of data automation is to reduce the time to publish significantly

- **Visualize the experiment** for humans, not the way X-ray detectors see it
- Produce **domain specific results** when possible, X-ray results when necessary

➥ **Integrate scientific software in the experiment** (acquisition control system and data portal)

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Before STREAMLINE and ESRF-EBS there was no common solution

- **Visualize the experiment** for humans
- Produce **domain specific results** when possible

➥ Integrate scientific software in the experiment

Attempts at the ESRF to do this are domain or beamline specific.

For example the *Structural Biology Services* at the ESRF (e.g. macromolecular crytallography) allow for completely automated experiments.

- custom designed workflow system that orchestrates the experiment and data analysis
- ISPyB based Laboratory Information Management System (LIMS) combining sample tracking and experiment reporting

Other attempts are all beamline specific with custom software.
➥ reinvent the wheel for every beamline
➥ no shared tools or technologies
➥ very labor intensive
➥ relies on a single expert per project (knowledge leaves when they leave)
➥ no professional devops (users cannot run the software at home)

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

STREAMLINE WP4 needed to address these needs

Visualize the experiment for humans

Produce **domain specific results** when possible

➥ Integrate scientific software in the experiment

We needed a domain and beamline agnostic solution with the following properties:

1. **easy to install** (runs everywhere from laptops to clusters)
2. **reproducible** data processing (*executable data provenance document* saved with the results)
3. **modular** (share common data processing steps, e.g. SAXS - WAXS, XRF mapping - XRF tomography, needs to evolve with the state-of-the-art)
4. **interactive** vs. non-interactive
5. different types of **interfaces** for humans and machines (GUI with plots and buttons, job scheduling on a cluster, web service)
6. scientific software (often in python) needs to be **integrated**, not re-written
7. can be provided as **service** of the facility maintained by a group, not reliant on individual experts

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

After STREAMLINE we have EWOKS workflows for ESRF-EBS

Visualize the experiment for humans

Produce **domain specific results** when possible

➥ Integrate scientific software in the experiment

A **workflow-based solution** was chosen for the ESRF because

1. A workflow is an **executable data provenance document**.
2. It encapsulated the decisions taken by an **expert** so the learning curve for non-experts is less steep: “how do I use this workflow” not “how do I process this diffraction data”.
3. A workflow can be **reused** to process other data (the “R” in FAIR).
4. Workflows can be developed by experts and **maintained and deployed** by the facility.

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 870313.

WORKFLOWS – USED @ ESRF before ESRF-EBS

	Purpose	WMS
MX workflows	Automate data collection and processing	**BES (Passarelle/pypushflow) ID23-1, ID23-2, ID30A-1, ID30A-3, ID30B**
Tomwer	Data processing	**Orange3 (ID19, BM05, ID11, ID16b)**
Est	Data processing	**Orange3 (BM23)**
Darfix	Data processing	**Orange3 (ID06, ID11)**
Oasys	Simulation	**Orange3**
CryoEM	Data processing	**Scipion (CM01)**
Image stitching	Data processing	**Orange3 (Opticslab)**
Data policy	Data mining	**Apache Camel**
Lima2	Online data processing	**oneTBB**

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Many workflow engines exist – which is the best one for ESRF-EBS ?

TABLE 2-1 Examples of Workflow Engines and Related Tools

Airflow	https://airflow.apache.org
Bigtable	https://cloud.google.com/bigtable
Chimera	https://github.com/hysds/chimera
Cromwell	http://cromwell.readthedocs.io/
Cyverse Discovery Environment	https://cyverse.org/discovery-environment
Fireworks	https://materialsproject.github.io/fireworks
Hadoop	https://hadoop.apache.org
Galaxy	https://galaxyproject.org
iRODS	https://irods.org
Jupyter	https://jupyter.org
Kepler	https://kepler-project.org
Nextflow	https://www.nextflow.io
Open Science Framework	https://osf.io
Luigi	https://luigi.readthedocs.io/en/stable/workflows.html
Parsl	http://parsl-project.org
Pegasus	https://pegasus.isi.edu
Snakemake	https://snakemake.readthedocs.io/en/stable
Spark	https://spark.apache.org
Starfish Storage	https://starfishstorage.com
Wolfram	https://www.wolframcloud.com

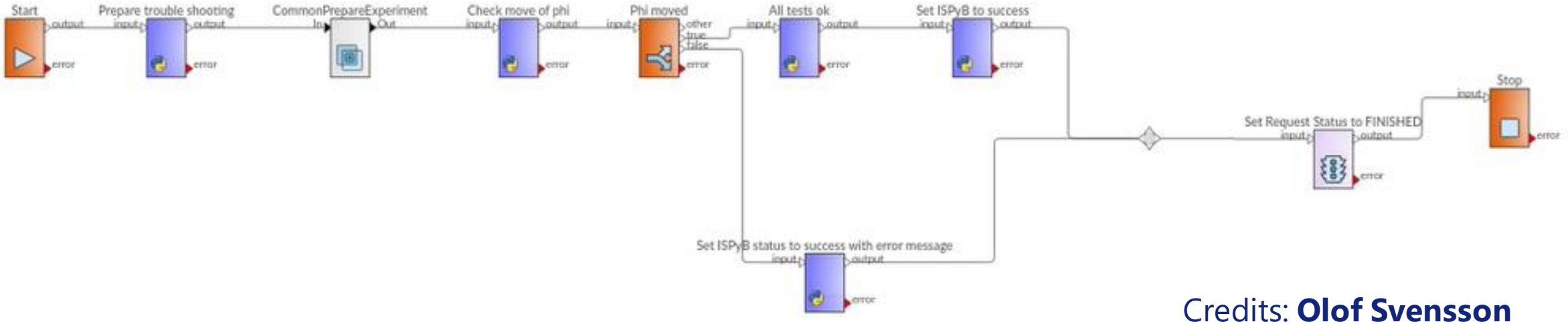
NOTE: Many of these tools are tracked by workflow community initiatives such as WorkflowHub (https://workflowhub.eu) and WorkflowsRI (https://workflowsri.org).

https://doi.org/10.17226/26532

ogramme under grant agreement No. 870313.

Beamline automation for MX - before STREAMLINE

1. **Kappa reorientation**
2. **Visual reorientation**
3. **Line scan**
4. **Mesh scan**
5. **X-ray centring**
6. **Enhanced EDNA characterisation**
7. **Dehydration workflow**
8. **Burn strategy**
9. **Pseudo-helical data collection**
10. **Automated data collections**
11. **Trouble shooting workflow**



Credits: **Olof Svensson**

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EWOKS workflows – the concept

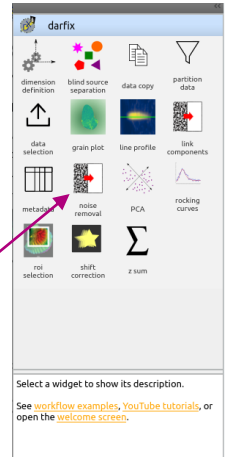
Ewoks representation (JSON)

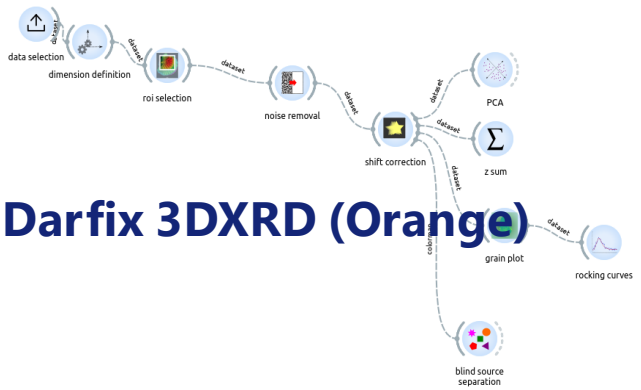
Ewoks
Ewoks
Ewoks automated execution

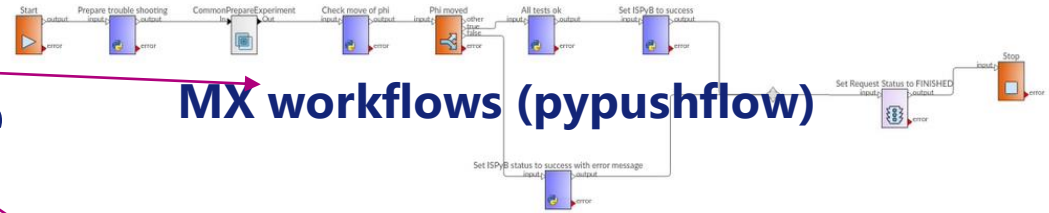
Ewoks Monitoring database (MongoDB)

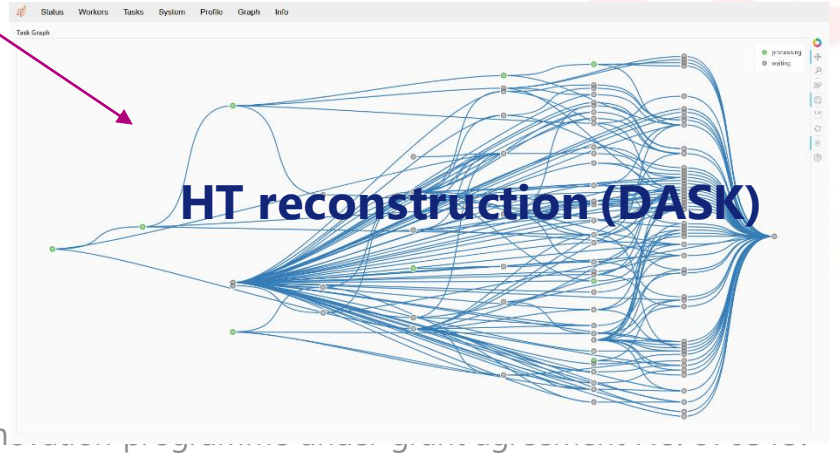
Ewoks provenance (HDF5)

Workflow Management System(s)







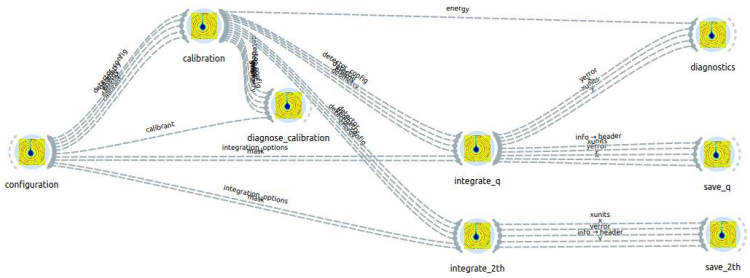


STREAMLINE has received funding from the European Union's Horizon 2020 research and inn

Typical setup for online data processing at the ESRF

Acquisition control system
(Bliss, Daiquiri, MxCube)

Execute EWOKS workflow on
- local machines (immediate feed)
- compute cluster



Visualization

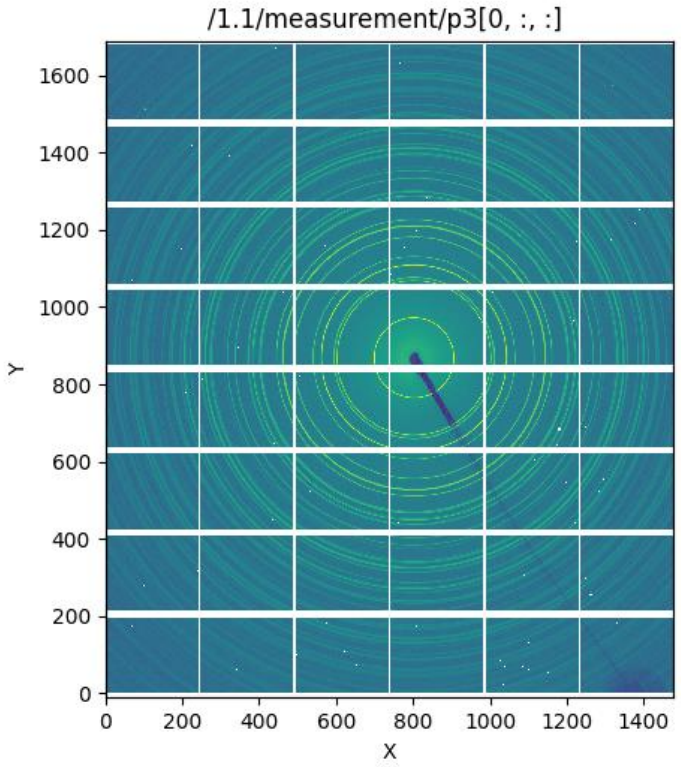
Persist result for further analysis + reuse

Data portal
(FAIR results including the workflows with DOI for publication)

Credits: **Wout de Nolf**

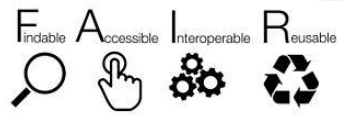
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

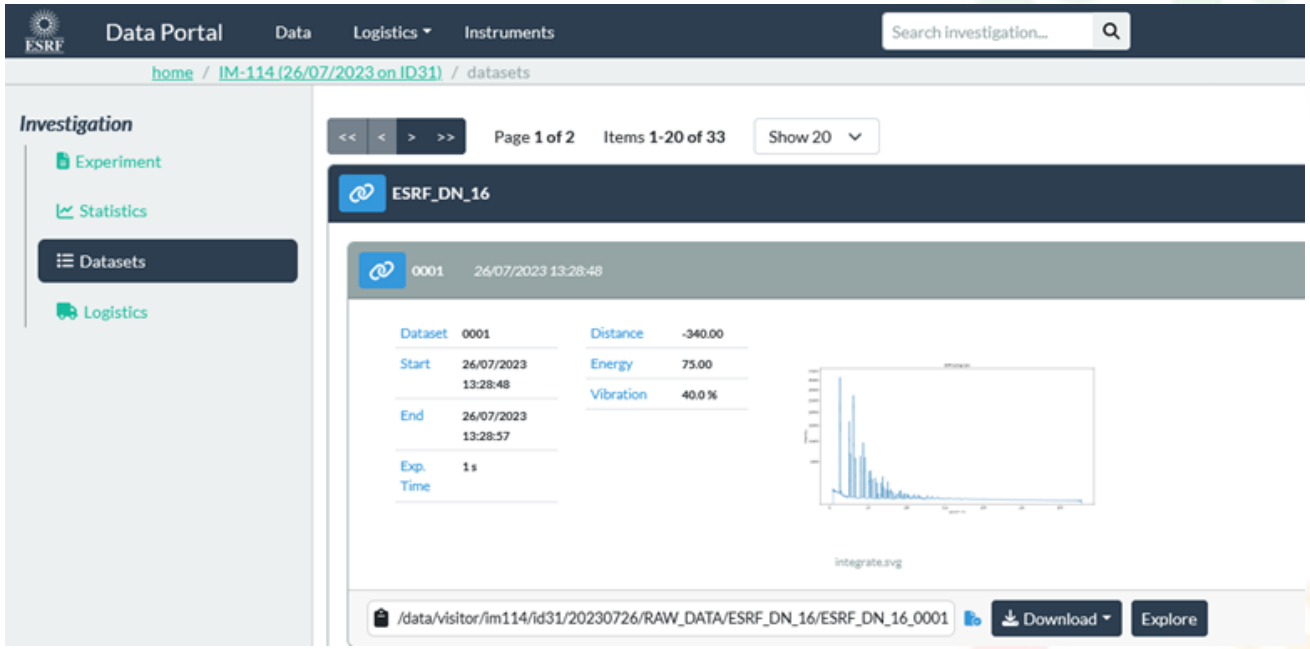
Diffraction (SAXS/WAXS): convert synchrotron data to traditional powder diffractograms



- **images + metadata** (flux, energy, geometry)
- **calibration** (pyFAI)
- **integration** (pyFAI)
- **save** (HDF5)

EWOKS





Further analysis to be brought online in the future

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

EWOKS supports different modes of execution

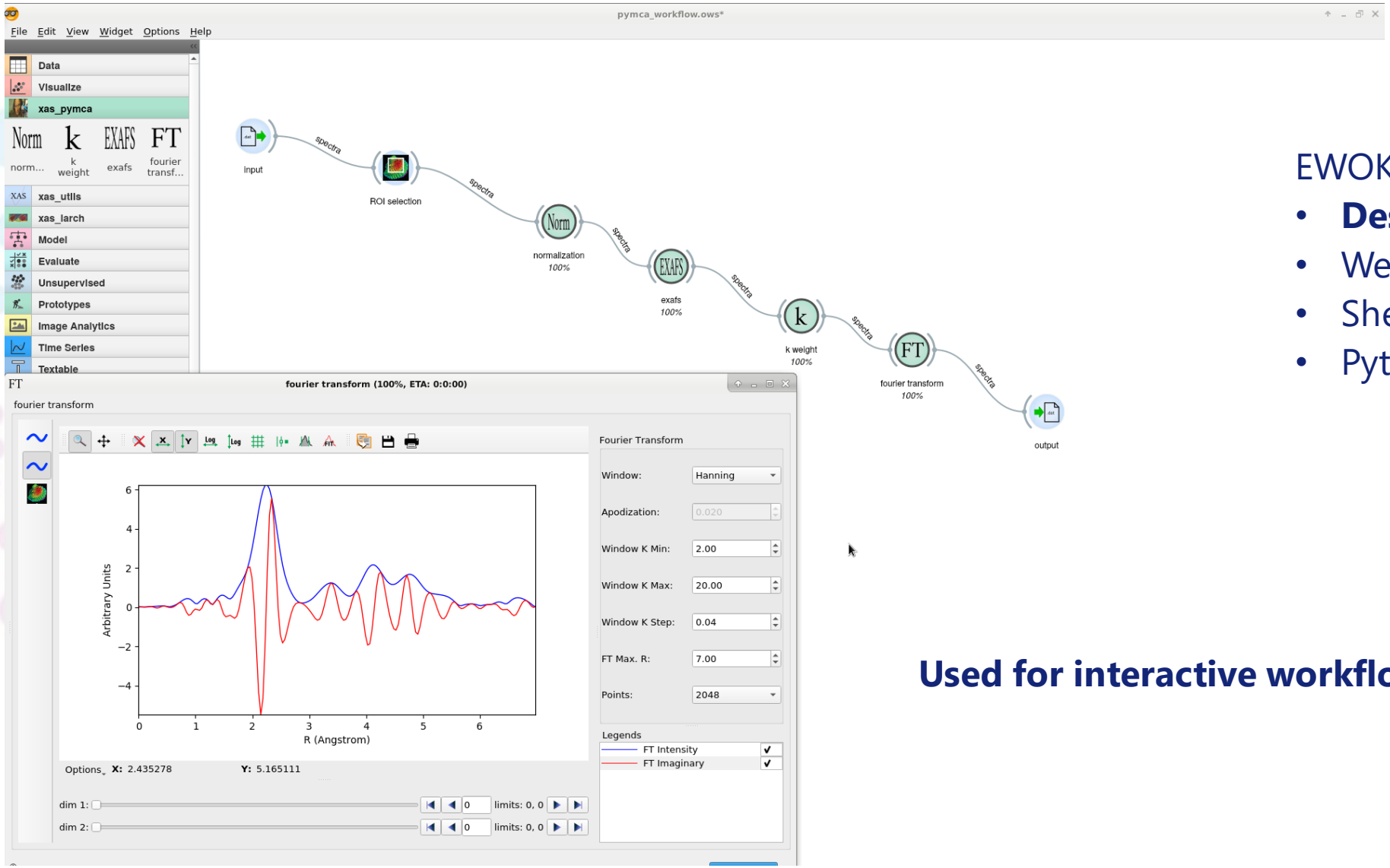
EWOKS is **unique** in that it supports

- **Desktop** (interactive workflows)
- **Web** (workflows as a service)
- **Shell** (headless execution)
- **Python** (integration for developers)

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

EWOKS on the desktop



EWOKS interfaces

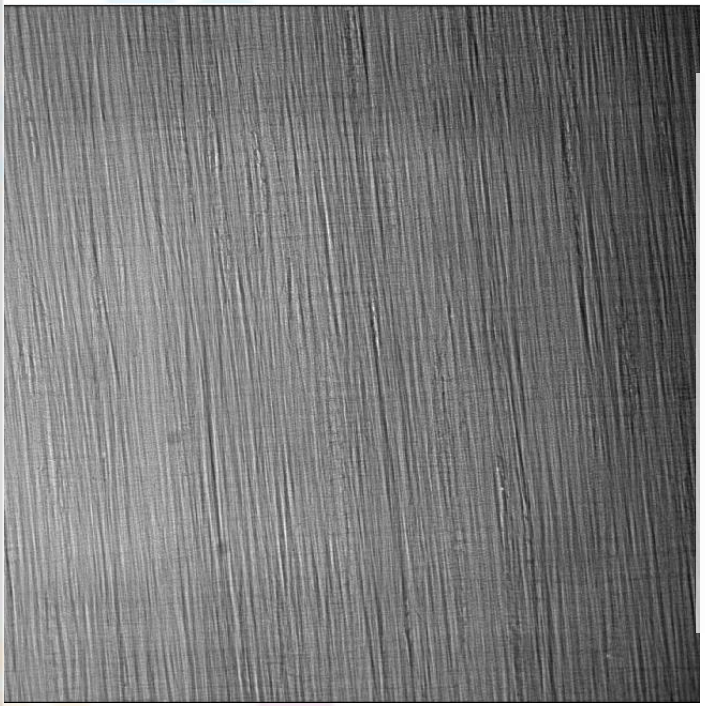
- **Desktop**
- Web
- Shell
- Python

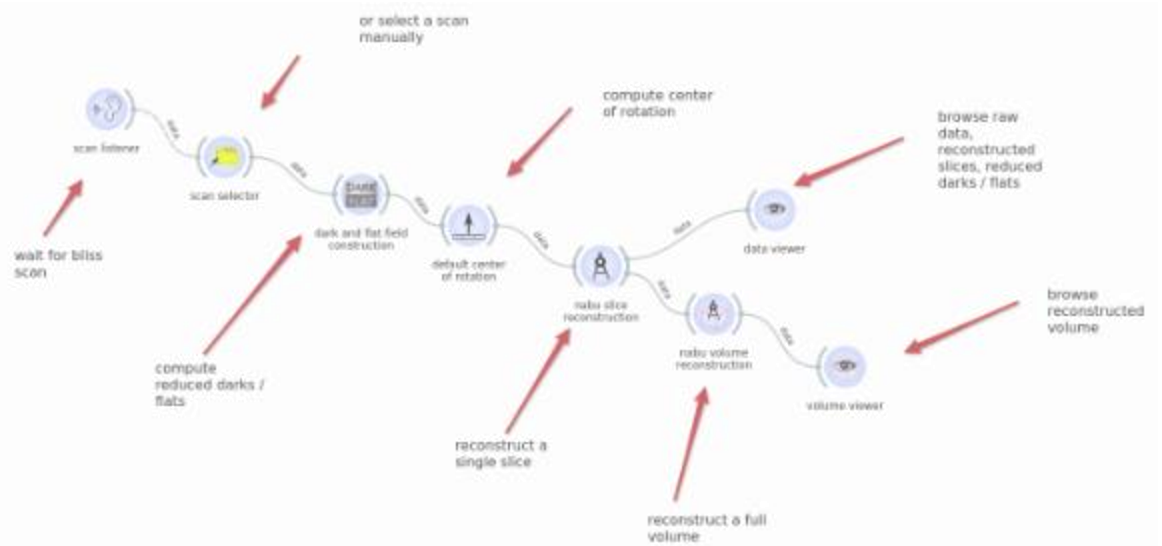
Used for interactive workflows

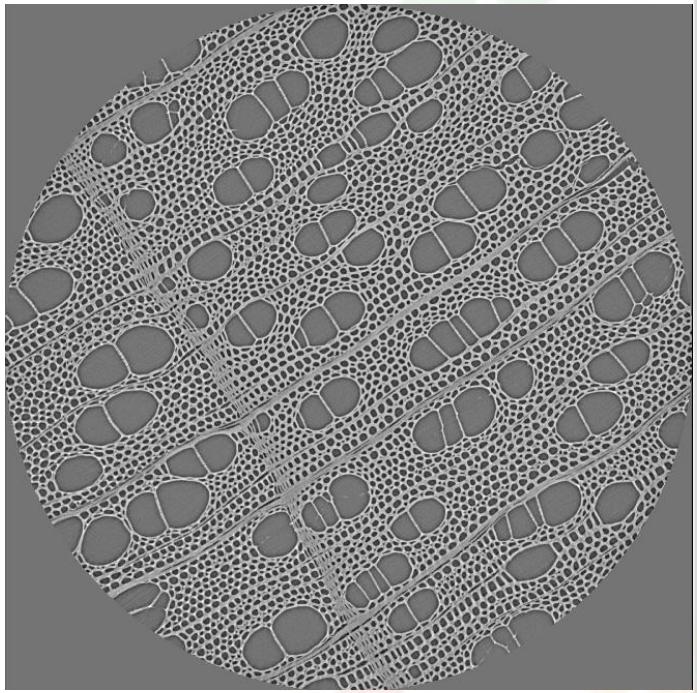
Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Diffraction (SAXS/WAXS): convert synchrotron data to traditional power diffractograms







Inputs
Images of the sample in transmission + dark field images + flat field images + metadata

EWOKS

Outputs
Reconstructed volumes

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

EWOKS on the web

EWOKS interfaces

- Desktop
- **Web**
- Shell
- Python

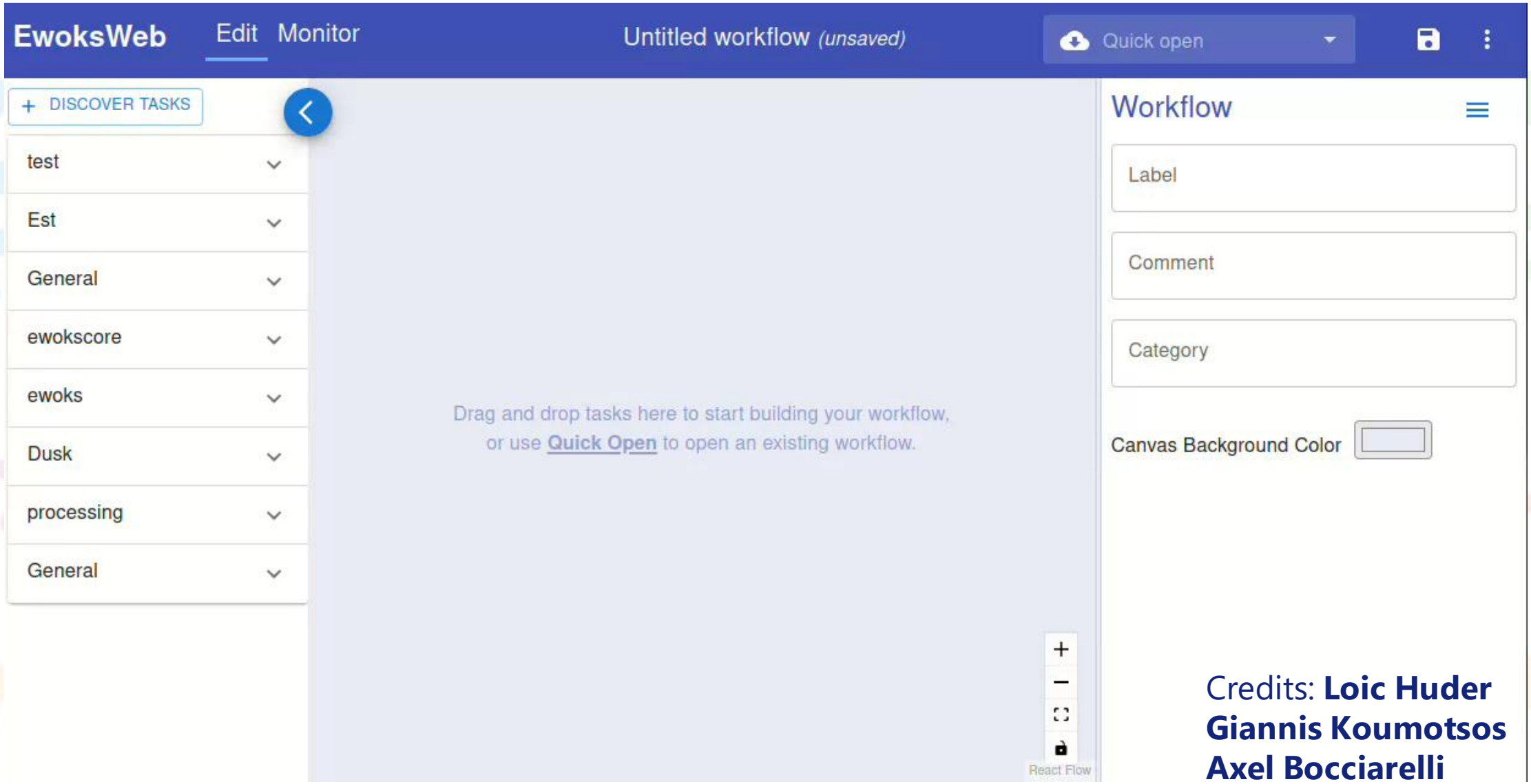
Used to edit and visualize workflows that don't have graphical components

Standalone + **frontend** (similar to Jupyter notebooks)

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

EWOKS on the web



Credits: **Loic Huder**
Giannis Koumotsos
Axel Bocciarelli

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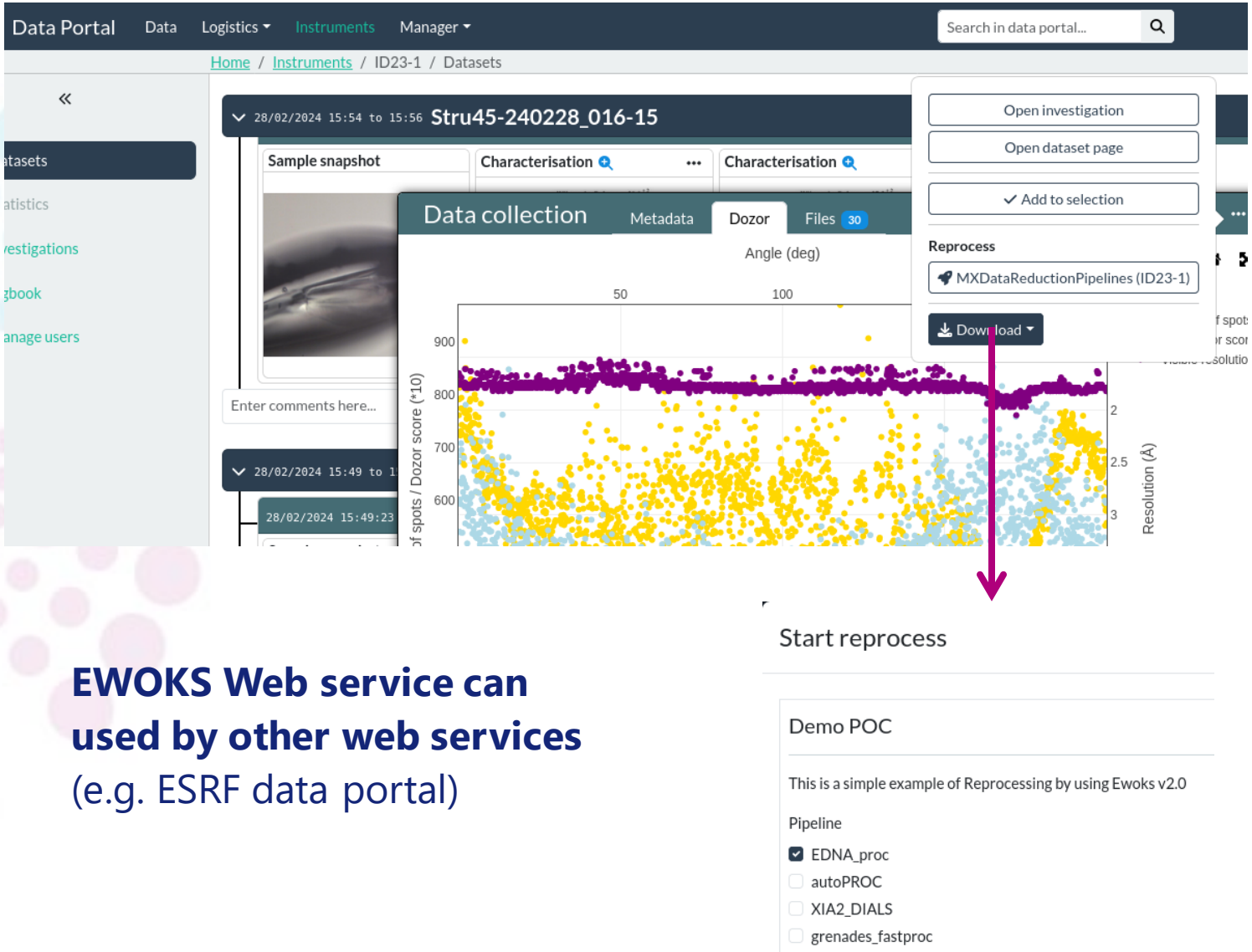
EWOKS reprocessing results for MX from data portal



EWOKS Web service can used by other web services
(e.g. ESRF data portal)

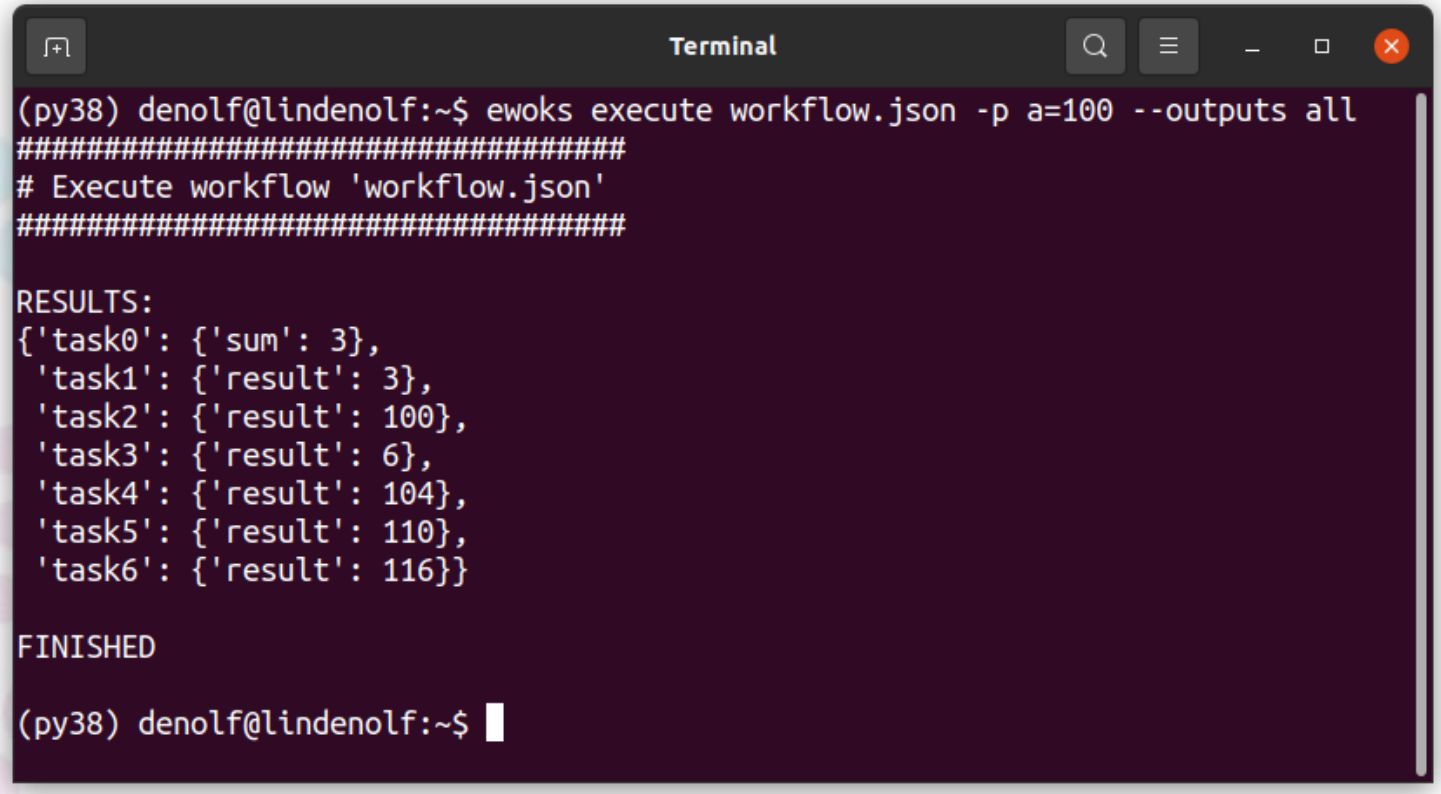
EWOKS interfaces

- Desktop
- **Web**
- Shell
- Python

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

EWOKS running from the command line



EWOKS interfaces

- Desktop
- Web
- **Shell**
- Python

Used for headless execution

Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

EWOKS being called from Python

```python
from ewokscore import Task
from ewokscore import execute_graph

# Implement a workflow task
class SumTask(
    Task, input_names=["a"], optional_input_names=["b"], output_names=["result"]
):
    def run(self):
        result = self.inputs.a
        if self.inputs.b:
            result += self.inputs.b
        self.outputs.result = result


# Define a workflow with default inputs
nodes = [
    {
        "id": "task1",
        "task_type": "class",
        "task_identifier": "__main__.SumTask",
        "default_inputs": [{"name": "a", "value": 1}],
    },
    {
        "id": "task2",
        "task_type": "class",
        "task_identifier": "__main__.SumTask",
        "default_inputs": [{"name": "b", "value": 1}],
    },
    {
        "id": "task3",
        "task_type": "class",
        "task_identifier": "__main__.SumTask",
        "default_inputs": [{"name": "b", "value": 1}],
    },
]
links = [
    {
        "source": "task1",
        "target": "task2",
        "data_mapping": [{"source_output": "result", "target_input": "a"}],
    },
    {
        "source": "task2",
        "target": "task3",
        "data_mapping": [{"source_output": "result", "target_input": "a"}],
    },
]
workflow = {"graph": {"id": "testworkflow"}, "nodes": nodes, "links": links}

# Define task inputs
inputs = [{"id": "task1", "name": "a", "value": 10}]

# Execute a workflow (use a proper Ewoks task scheduler in production)
varinfo = {"root_uri": "/tmp/myresults"}  # optionally save all task outputs
result = execute_graph(workflow, varinfo=varinfo, inputs=inputs)
print(result)
```

EWOKS interfaces

- Desktop
- Web
- Shell
- **Python**

Developer usage like triggering workflows from the acquisition control system.

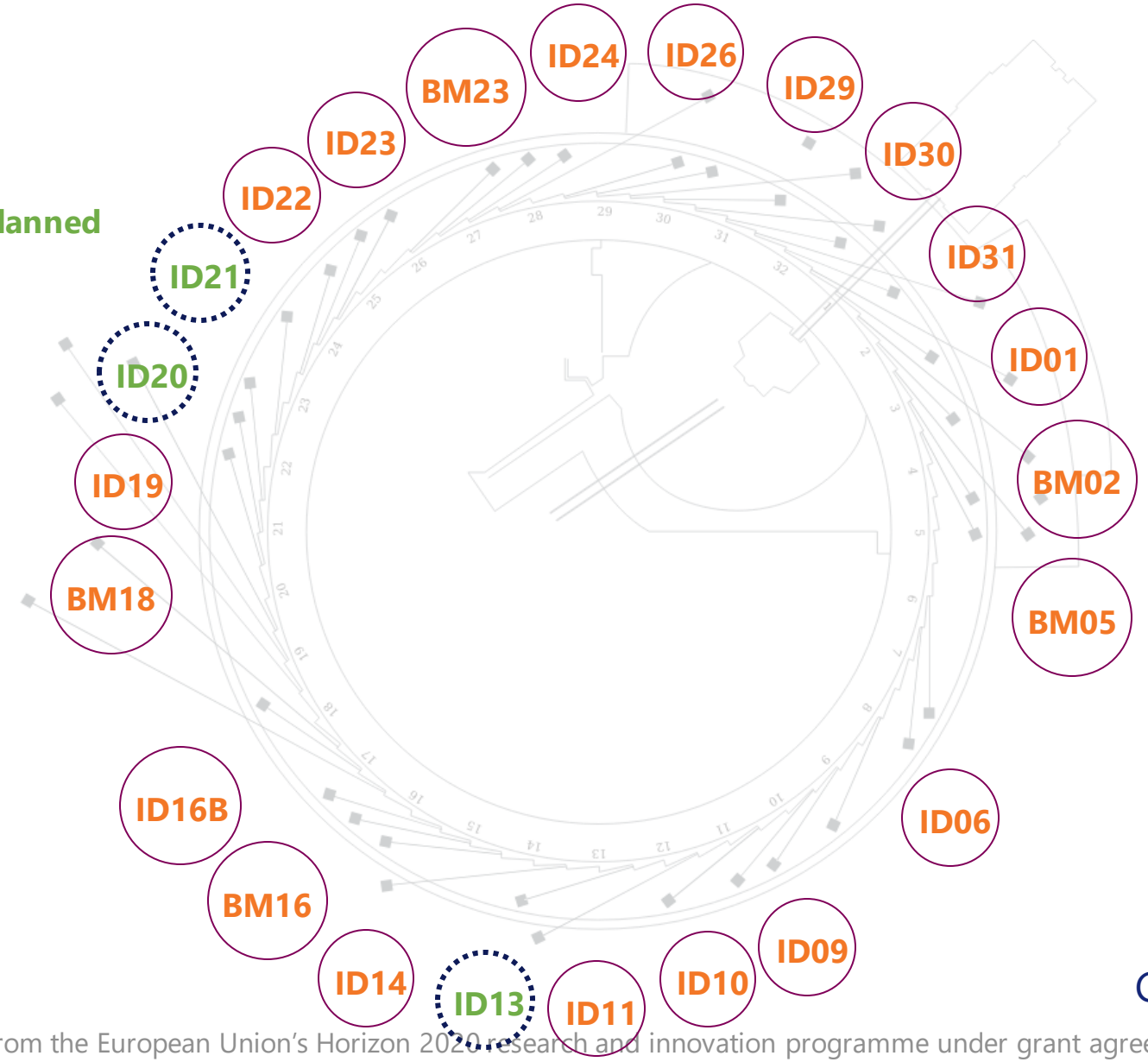
Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

EWOKS workflows in production / development on 23 beamlines i.e. 50% of ESRF beamlines

BM/ID In production

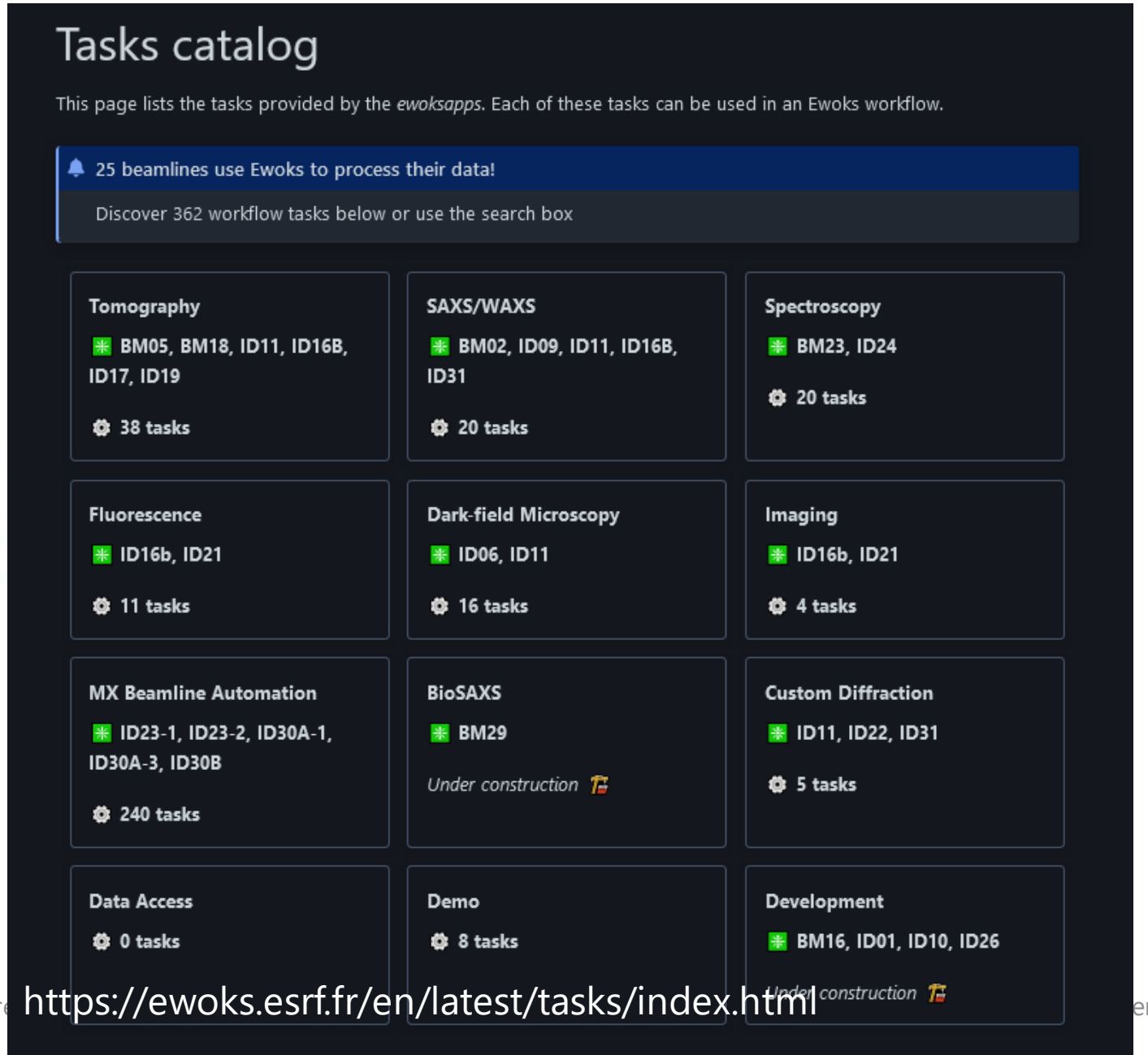
BM/ID In development/planned



Credits: **Wout de Nolf**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

EWOKS tasks catalog has over 360 workflow tasks today



https://ewoks.esrf.fr/en/latest/tasks/index.html

STREAMLINE has re er grant agreement No. 870313.

EWOKS is a MAJOR contribution of STREAMLINE which is revolutionizing data processing!

Increase the scientific output of the ESRF

- **Visualize the experiment** for humans
- Produce **domain specific results** when possible, X-ray specific otherwise

➥ Integrate scientific software in the experiment

➥ Workflow based solution (**executable data provenance**)

➥ **Meta approach**: decouple workflows and implementation from systems

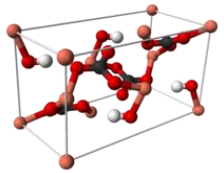
https://ewoks.esrf.fr

Credits: **Wout de Nolf**

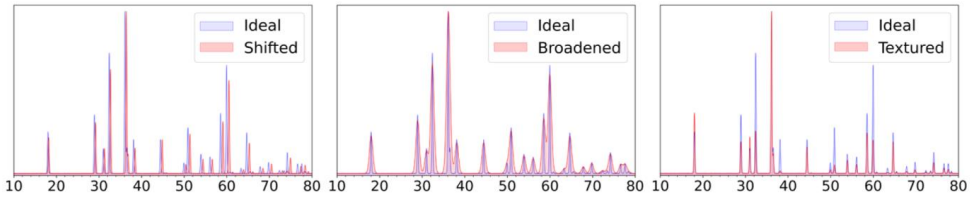
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Probabilistic phase detection using AI/ML

- **Powder Xray Diffraction (PXRD) patterns are simulated and used for training a neural network to identify phases in a sample**
  - ***Provides a probability of presence for each phase of a specified set in a PXRD pattern (handles mixtures)***



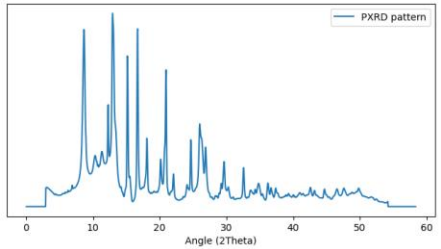
PXRD augmented simulation →



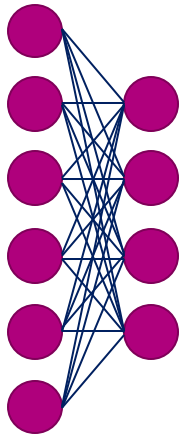
https://pymatgen.org/

Trains ↓

PXRD raw data



→



Neural network

→

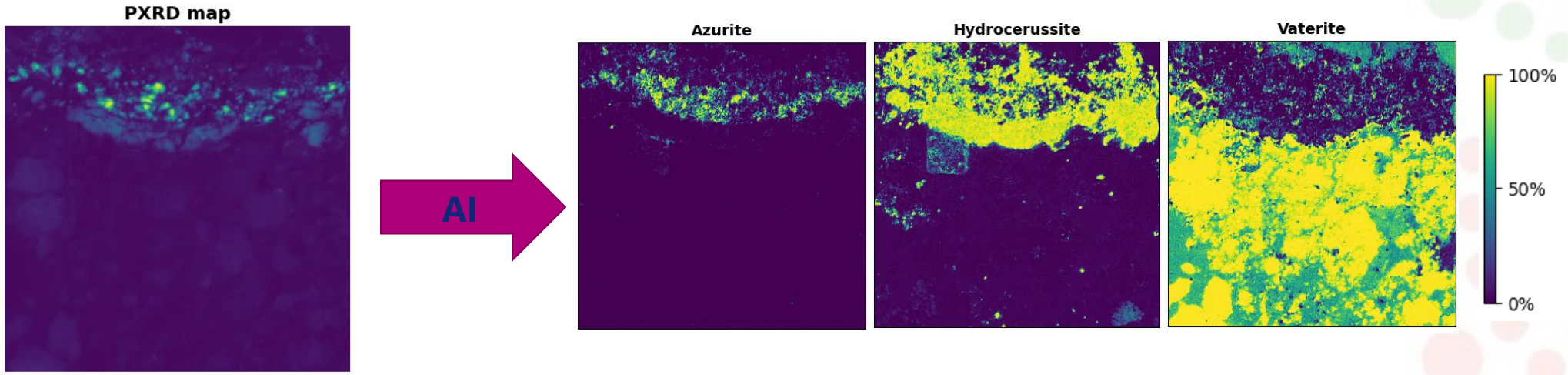
Azurite	**57%**
Hydrocerussite	**80%**
Vaterite	**7%**

Credits: **Quentin Bruel**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Probabilistic phase mapping of a full dataset

- **The neural network can be used of a full 2D dataset**
  - ***Allows to locate the phases on the sample even though they have a low relative contribution to the signal***
  - ***Fast online analysis can allow to select the next area to scan during acquisition***



µXRD map in cartesian coordinates of a historical sample from the famous *Cena* fresco.Voxels represent the integrated intensities of the PXRD patterns.

Oriols, N., Salvadó, N., Pradell, T., Jiménez, N., Cotte, M., Gonzalez, V., & Butí, S. (2022). Carbonation of fresco mural paintings with a dolomitic mortar. Cement and Concrete Research, 157, 106828

Credits: **Quentin Bruel**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

DEMO – try it !

https://data2.esrf.fr/investigation/1405067863/datasets

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Some tangible outcomes of WP4

1. ***Mail-In service for ALL*** *techniques and beamlines*

2. *ISPyB is being replaced by* ***ICAT LIMS*** *which means all techniques can profit from the pioneering work for automating data processing that is done for MX*

3. *A* ***new data portal*** *has been developed to support all the features for MX and other techniques, with new features for managing experiments, raw and processed data*

4. ***Workflows for automating data processing*** *have been unified under one meta-workflow system called* ***EWOKS*** *and been deployed on 50% of ESRF beamlines. EWOKS workflows will enable processed data to become the main result provided to users*

5. ***Processed data*** *has become a* ***FIRST CLASS citizen at the ESRF****, medium term goal for* ***ESRF-EBS*** *is that* ***all users can take home processed*** *data after their experiment in alignment with the* ***new ESRF scientific data policy***

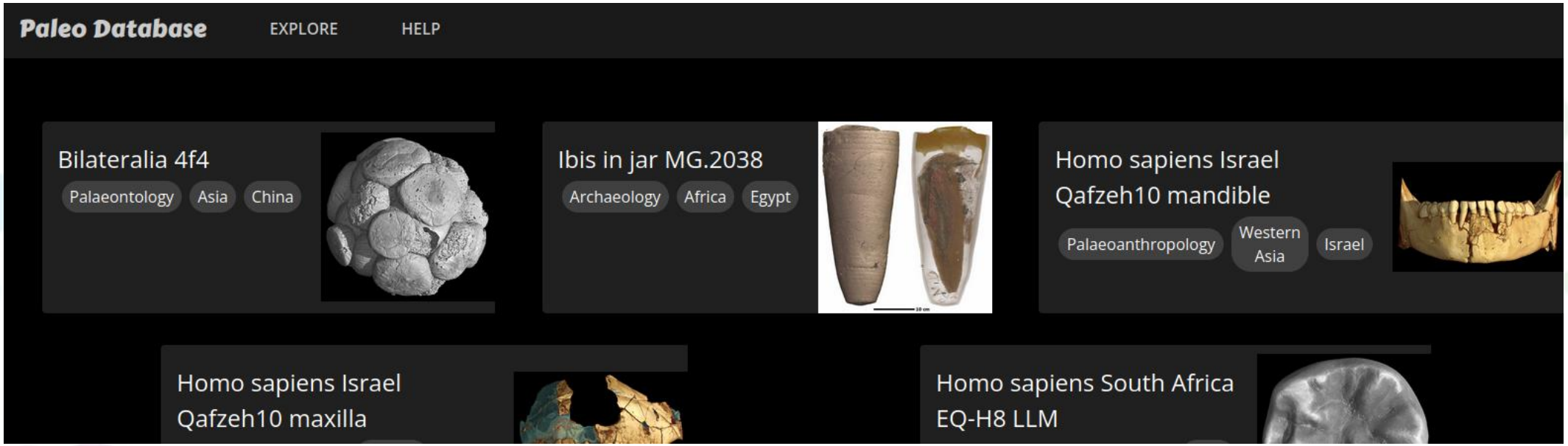
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant ag

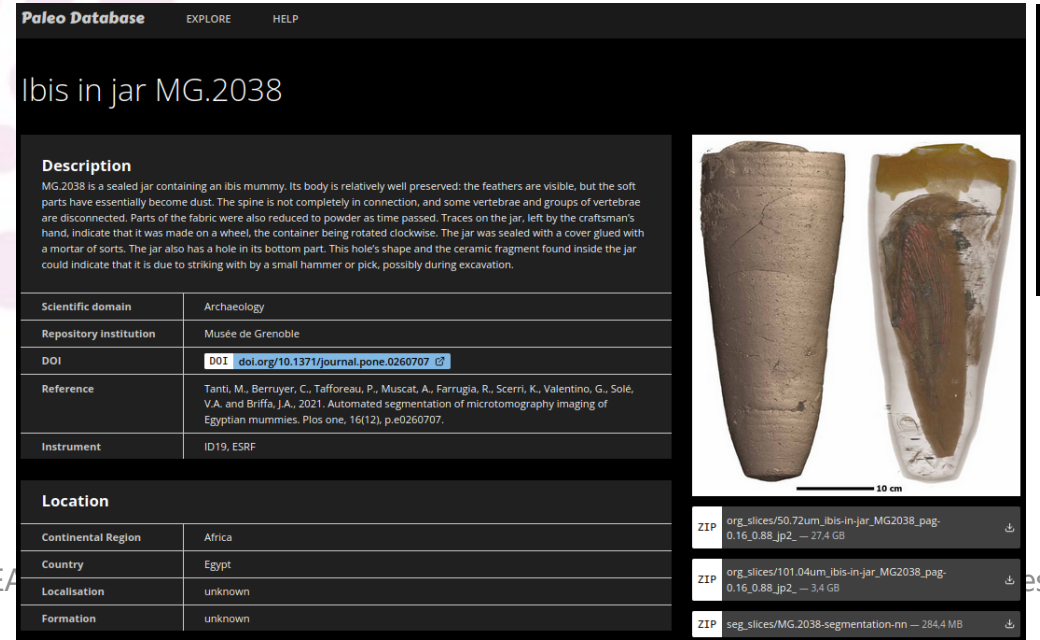
Next Steps - after the revolution comes evolution

1. Get **feedback from more beamlines** on the **new data portal**
2. Develop and deploy **basic EWOKS workflows** for **all beamlines**
3. Address **complex data processing workflows** to provide users with **results**
4. Improve the **display of processed data** for **non-MX** techniques
5. Improve the **metadata of raw + processed data** to make them **FAIRer**
6. Continue exploring **AI/ML for processing data** and **driving experiments**
7. **Share the outcomes** with the Photon and Neutron community

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Making data FAIRer – assign DOIs to paleontology data





Credits: **Guillaume Gaisné**
Marjolaine Bodin
Vincent Fernandez,
Paul Tafforeau

STREA esearch and innovation programme under grant agreement No. 870313.

Spectrocrunch - example of a complex workflow producing final results on ID21

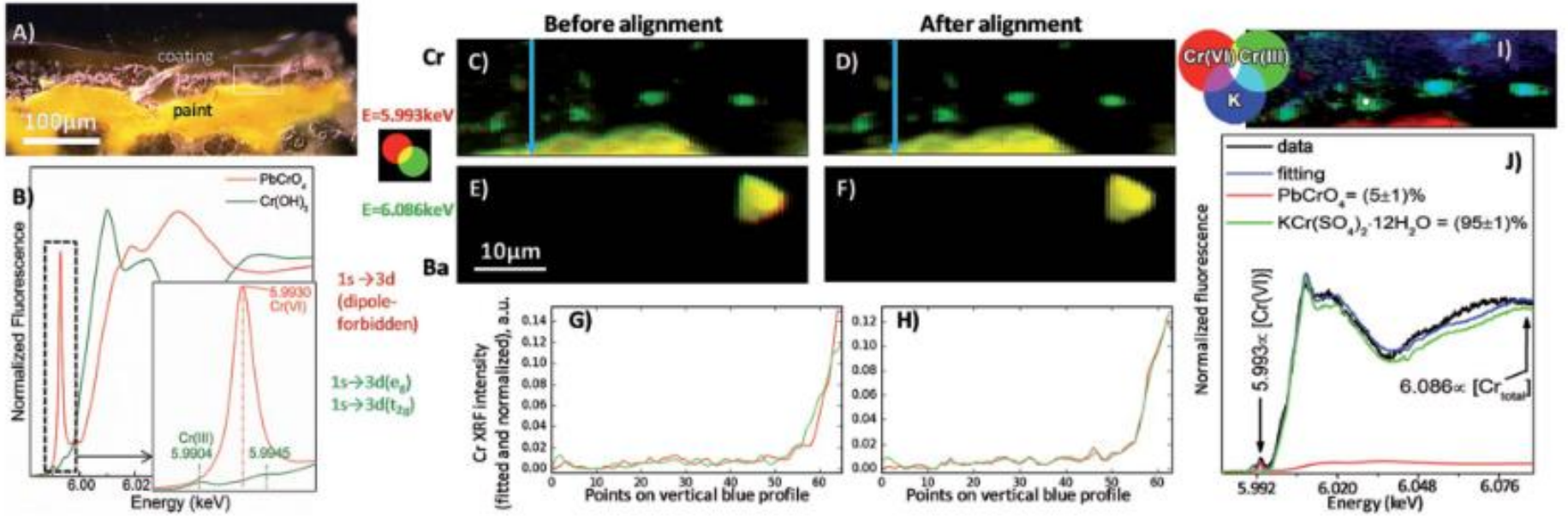


Fig. 3 Illustration of the "Spectrocrunch" package for hyperspectral map fitting, normalization and alignment on the analysis of chrome yellow alteration in Van Gogh paintings. (A) Visible light picture of a paint fragment from Falling Leaves (Les Alyscamps) (Arles, 1888; Kröller-Müller Museum, Otterlo, NL) embedded in resin and polished. The surface of the yellow paint layer is covered with a coating brown translucent layer. The white rectangle represents the area where the µXRF maps shown in (C–F) and (I) were collected. (B) Cr K-edge XANES spectra of $PbCrO_4$ (red) and $Cr(OH)_3$ (green) and inset on the pre-edge peak region. The dotted line highlights the position of the Cr(VI) pre-edge peak (5.993 keV). (C and D) Cr and (E and F) Ba µXRF maps recorded from the area shown in (A) at $E = 5.993$ keV (red) and $E = 6.086$ keV (green), (C–E) before and (D–F) after image realignment [map size (hor. × ver.): 49.7 × 16.25 µm^2; beam and step size (hor. × ver.): 0.7 × 0.25 µm^2]. Maps were normalized, dead-time corrected and fitted. (G and H) Cr XRF intensity obtained over the vertical profile shown by a blue arrow in (C) and (D). (I) Composite RGB distribution maps of Cr(VI) (red), Cr(III) (green) and K (blue). (J) Result of the linear combination fitting (blue) of $PbCrO_4$ (red) and $KCr(SO_4)_2 \cdot 12H_2O$ (green) to the µXANES spectrum (black) obtained from the particle indicated by a white circle in (I) (see[19,20] for further details).

https://doi.org/10.1039/C6JA00356G

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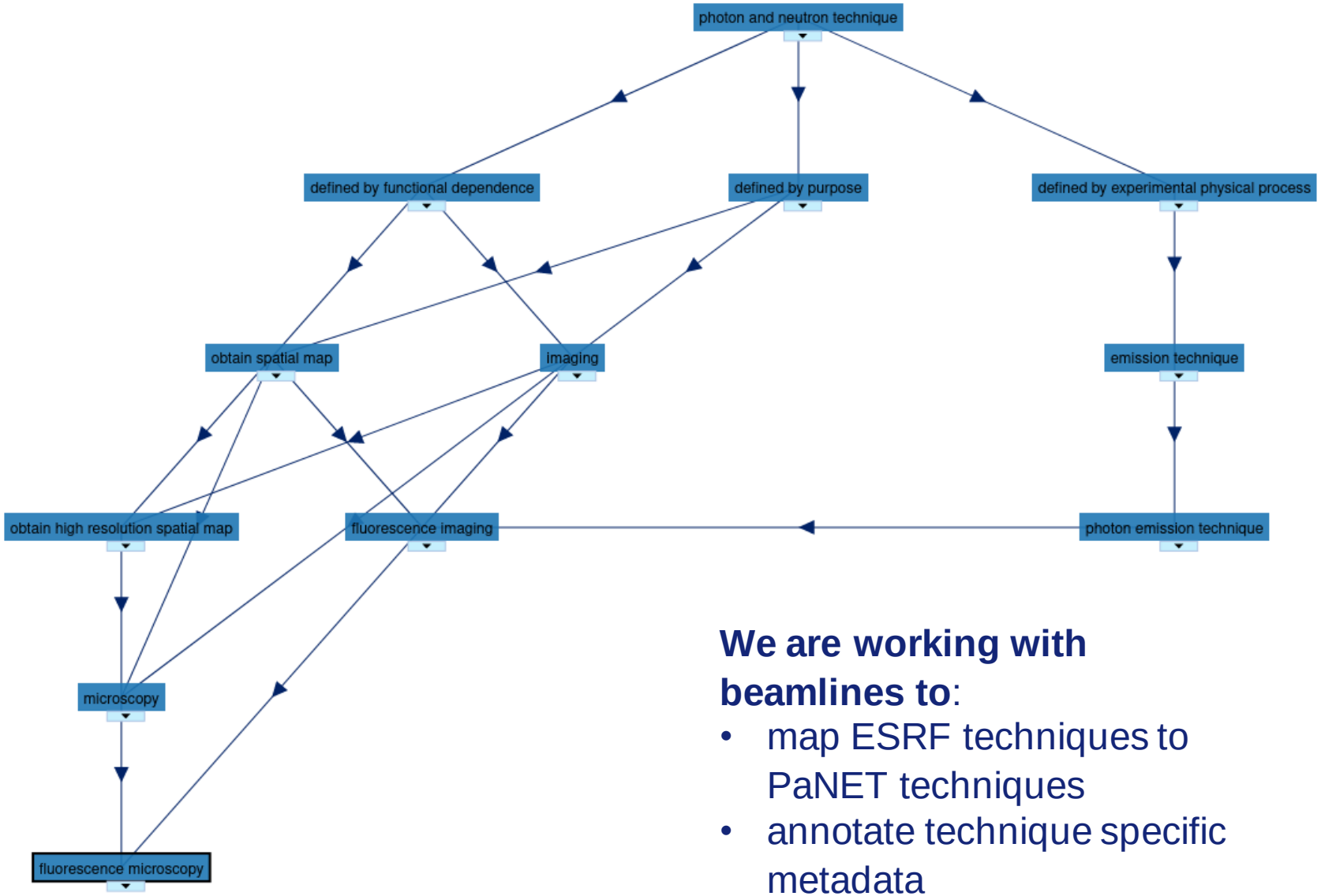
- Dataset
- Person
- photon and neutron technique
  - defined by experimental physical process
  - defined by experimental probe
  - defined by functional dependence
  - defined by purpose
    - characterize excitations
    - chiral determination
      - magnetochiral dichroism
      - natural circular dichroism
    - drug fragment binding
    - imaging
      - absorption contrast imaging
      - coherent diffraction imaging
      - cold neutron imaging
      - diffraction imaging
      - fluorescence imaging
        - **fluorescence microscopy**
      - high-resolution neutron imaging
      - holography
      - microscopy
      - neutron transmission radiography
      - obtain 3D spatial map
      - obtain high resolution spatial map
      - phase contrast imaging
      - scanning probe imaging
      - single-shot imaging
      - UV circular dichroism imaging
      - x-ray birefringence imaging
      - x-ray imaging
      - x-ray refraction imaging
    - manufacturing technique
    - medical application
    - obtain atomic structure
    - obtain dynamics
      - elastic neutron scattering spectroscopy
    - obtain electronic ground state properties
    - obtain internal field
    - obtain spatial map
    - testing
    - therapy



We are working with beamlines to:

- map ESRF techniques to PaNET techniques
- annotate technique specific metadata

https://bioportal.bioontology.org/ontologies/PANET

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Outcomes available for all facilities to re-use

1. **ALL software** is under an **Open Source licence @ https://gitlab.esrf.fr**

2. **Tutorials, documentation** and **training are available**

3. We are ready to help install and run the STREAMLINE software. **Some software** already running at **ALBA, HZB, SESAME, …**

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Acknowledgement to the WP4 Software contributors:

Software developers:

Mael Goanach, Alex de Maria, Marjolaine Bodin, Olof Svensson, **Ioannis Koumoutsos**, Wout de Nolf, Loic Huder, Axel Bocciarelli, Henri Payno, Thomas Vincent, **Quentin Bruel**, Vincent Favre-Nicolin, Jerome Kieffer, Pierre Paleo, Marcus Oscarsson, Antonia Beteva, and ALL Beamline Control Unit members

Beamlines – ALL beamlines, especially those who gave feedback on the software

Technical infrastructure division for IT infrastructure support

Experiment Division

Business and Development Office

User office

Thank you for your attention!

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STREAMLINE

ESRF
The European Synchrotron

Co-designed with industry: New high throughput routine services

Ennio Capria, Thanos Papazoglou

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

In which way the ESRF can contribute to industrial innovation?

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

In which way the ESRF can contribute to industrial innovation?

By contributing to the development of new products

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Contribution of ESRF to the development of new products

1. Develop the idea
2. Validate the idea
3. Build a prototype
4. Create the messaging
5. Build the product
6. Release the product
7. Improve the product

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Contribution of ESRF to the development of new products

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Contribution of ESRF to the development of new products

Academic access for publication

Long term collaborative approach; grant catalysed

Confidential access

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Contribution of ESRF to the development of new products

Process and product design and optimization

Materiomics Accelerated discovery platforms

Academic access For publication

Long term collaborative approach; grant catalysed

Confidential access

STREAMLINE has received funding from the European Union's Horizon 2020 resea

Contribution of ESRF to the development of new products

Process and product design and optimization

+

Benchmark

Materiomics
Accelerated discovery platforms

Academic access
For publication

Long term collaborative approach; grant catalysed

Confidential access

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Contribution of ESRF to the development of new products

Ad-hoc
In-situ
Operando
Low number of samples

Routine service
Ex-situ
Large number of samples

Academic access
For publication

Long term collaborative approach; grant catalysed

Confidential access

STREAMLINE has received funding from the European Union's Horizon 2020 resea

Contribution of ESRF to the development of new products

Ad-hoc
In-situ
Operando
Low number of samples

Routine service
Ex-situ
Large number of samples

Standard

Complexity

Academic access
For publication

Long term collaborative approach; grant catalysed

Confidential access

1 Develop the idea
2 Validate the idea
3 Build a prototype
4 Create the messaging
5 Build the product
6 Release the product
7 Improve the product

Pre-competitive phase

Confidential phase

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Genesis of a new service

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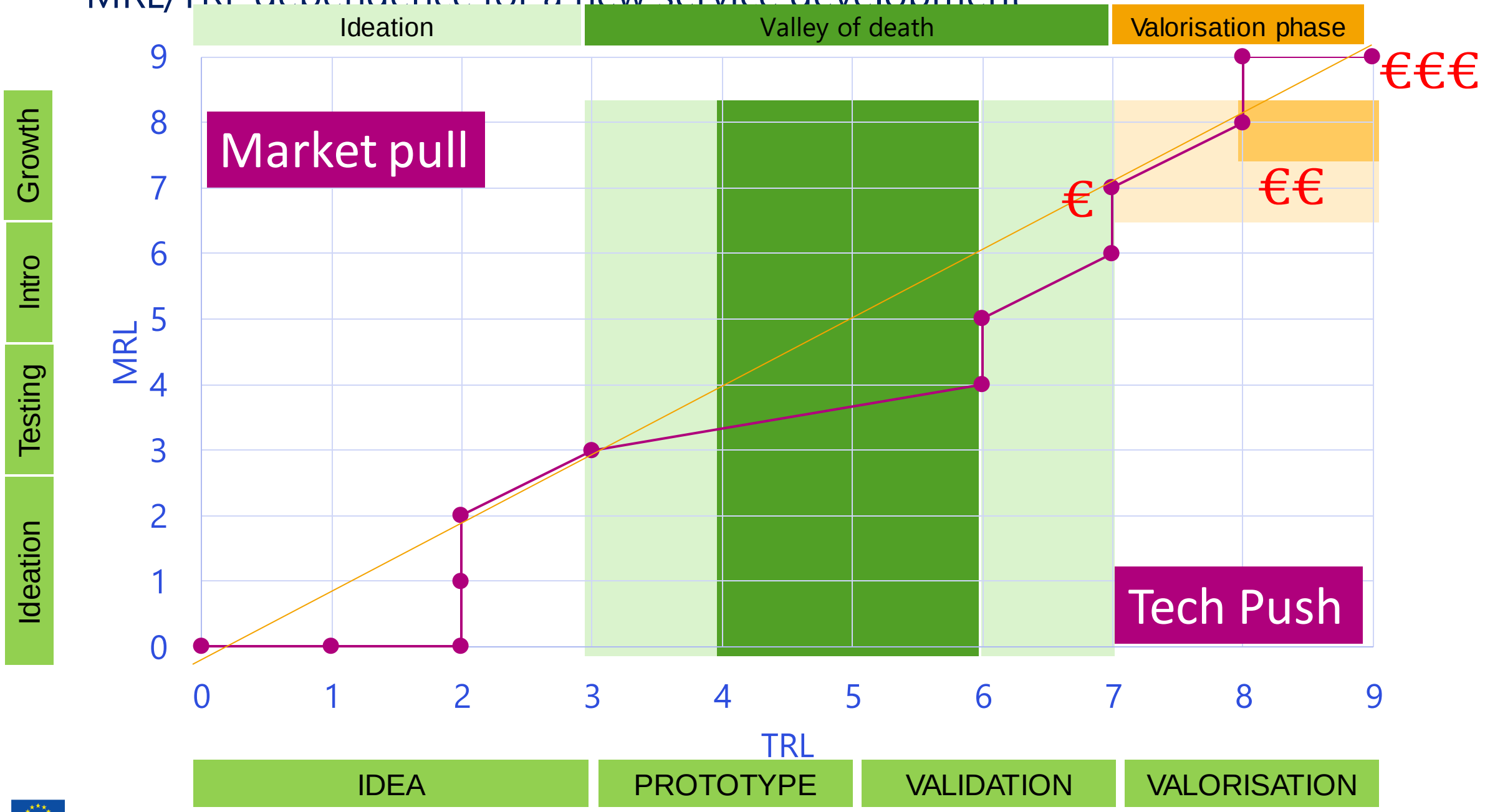
MRL/TRL dependence for a new service development



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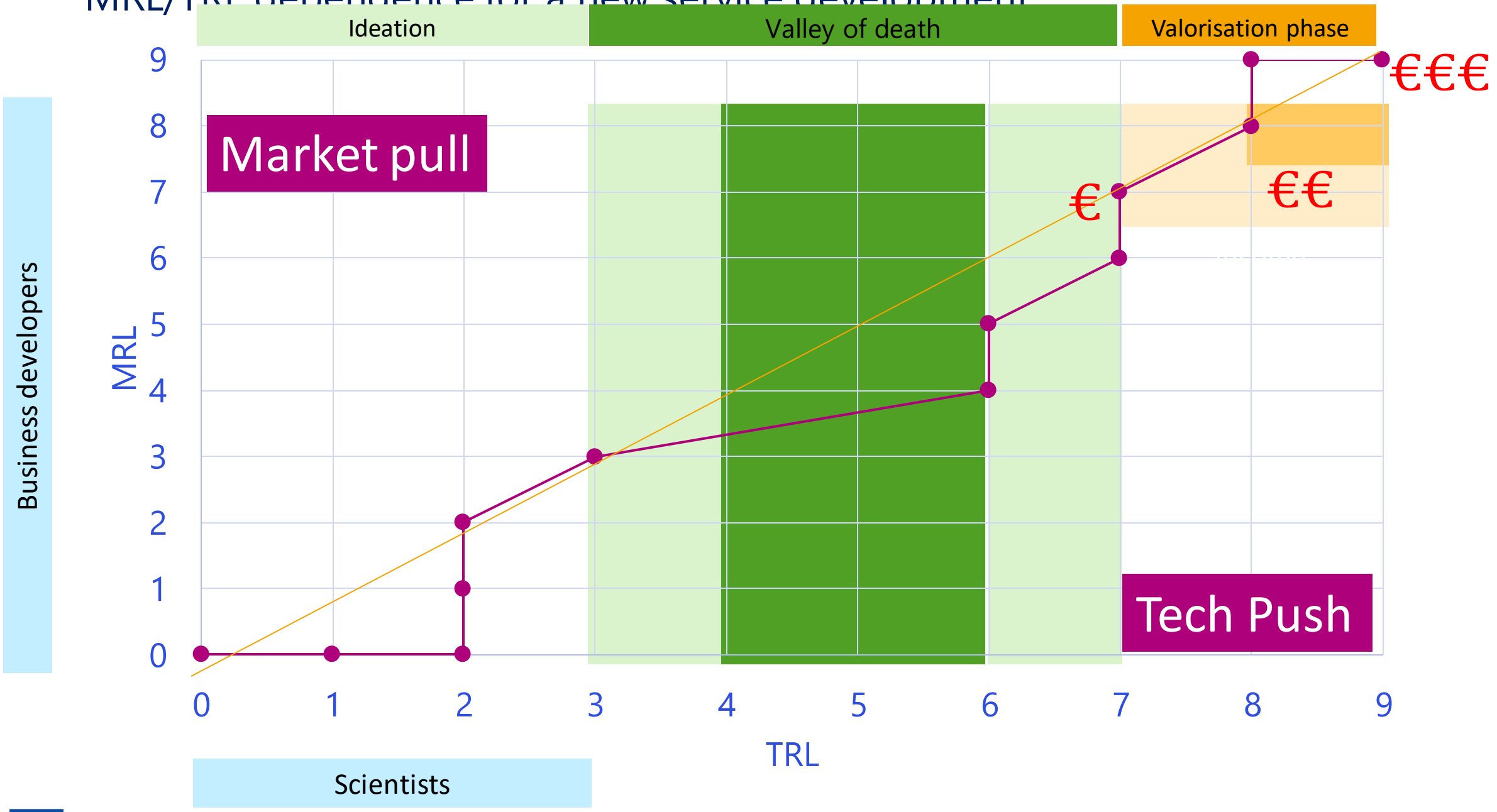
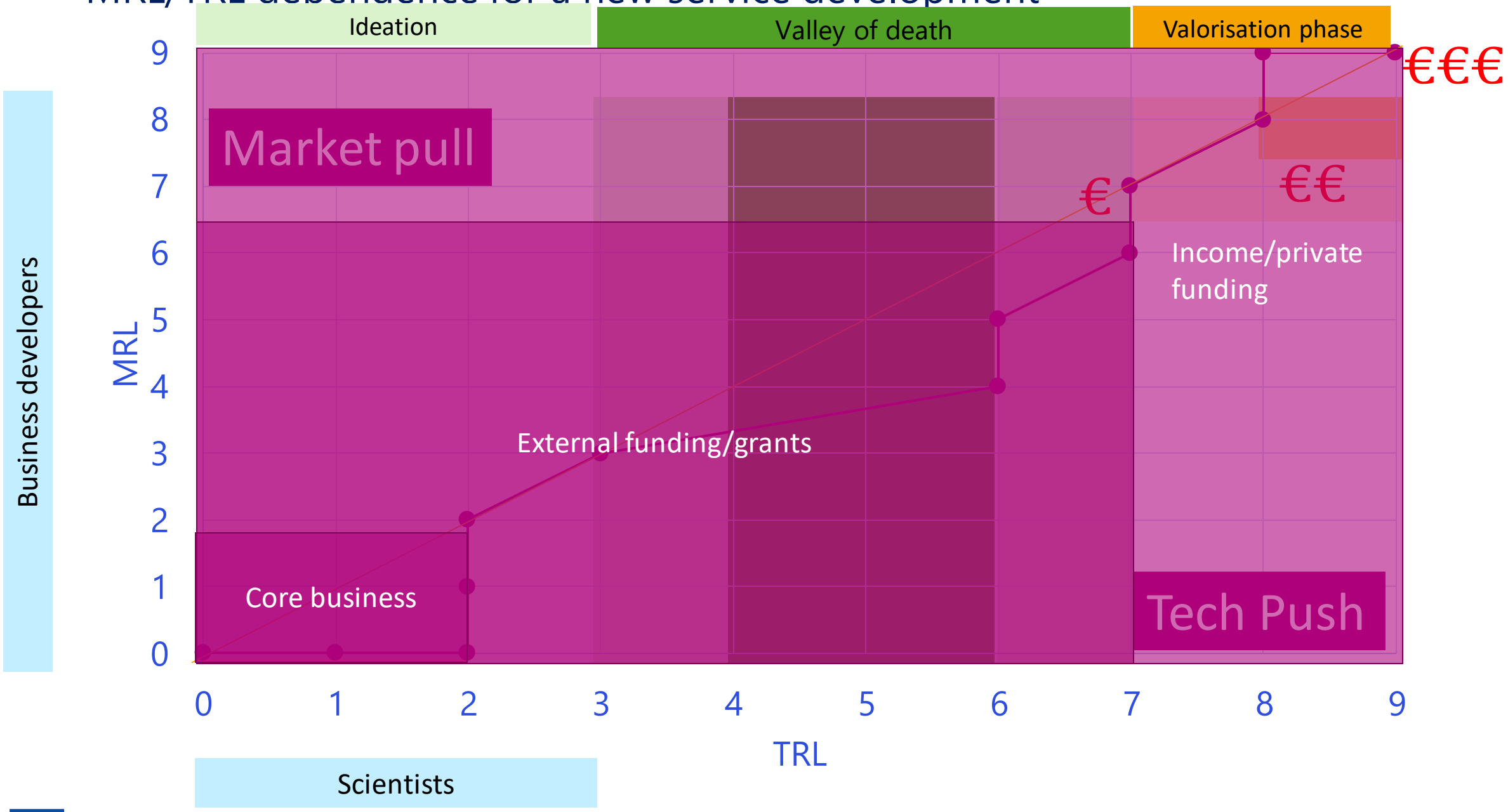
MRL/TRL dependence for a new service development



STREAMLINE has received funding from th 3.

MRL/TRL dependence for a new service development



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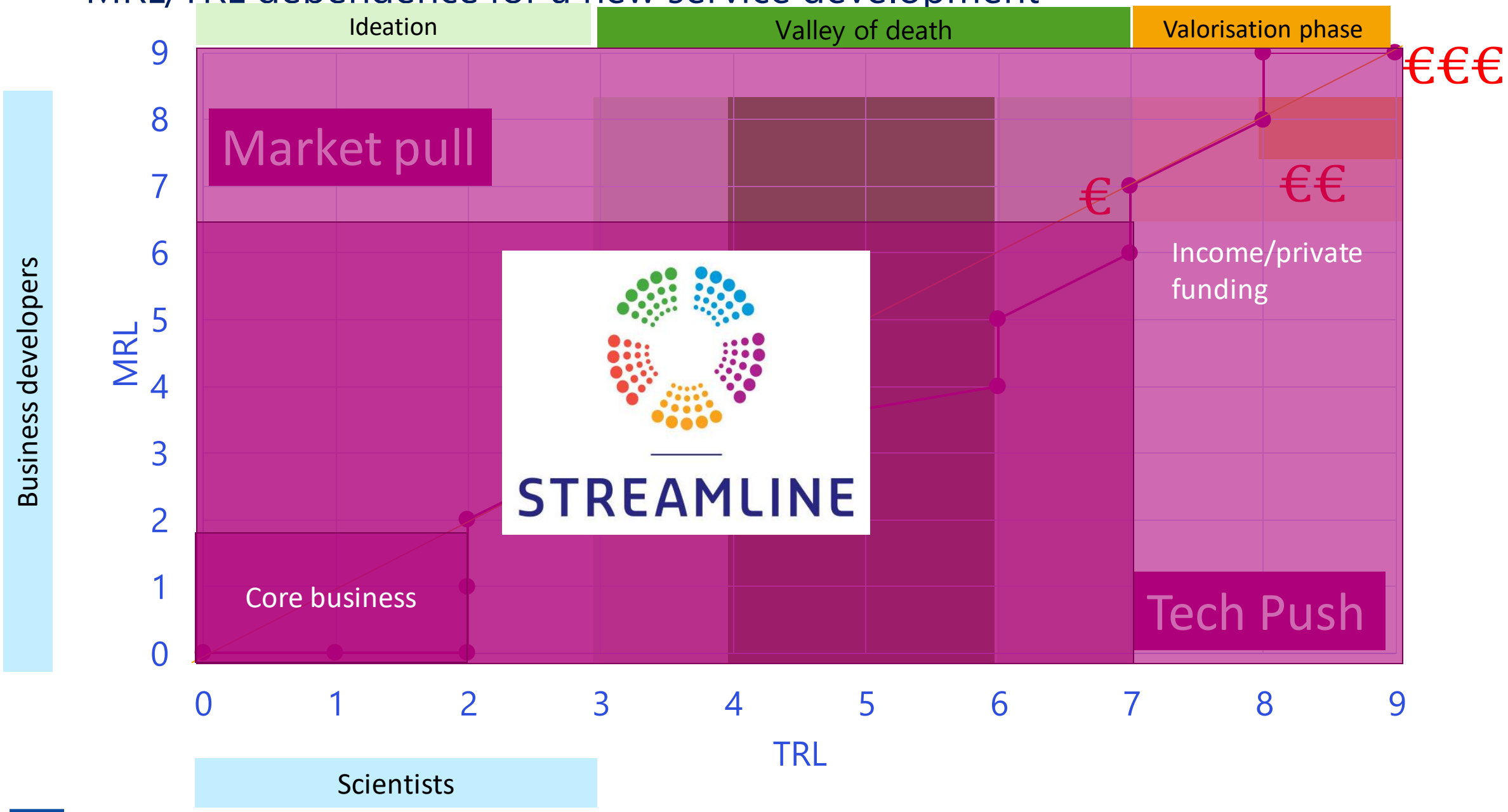
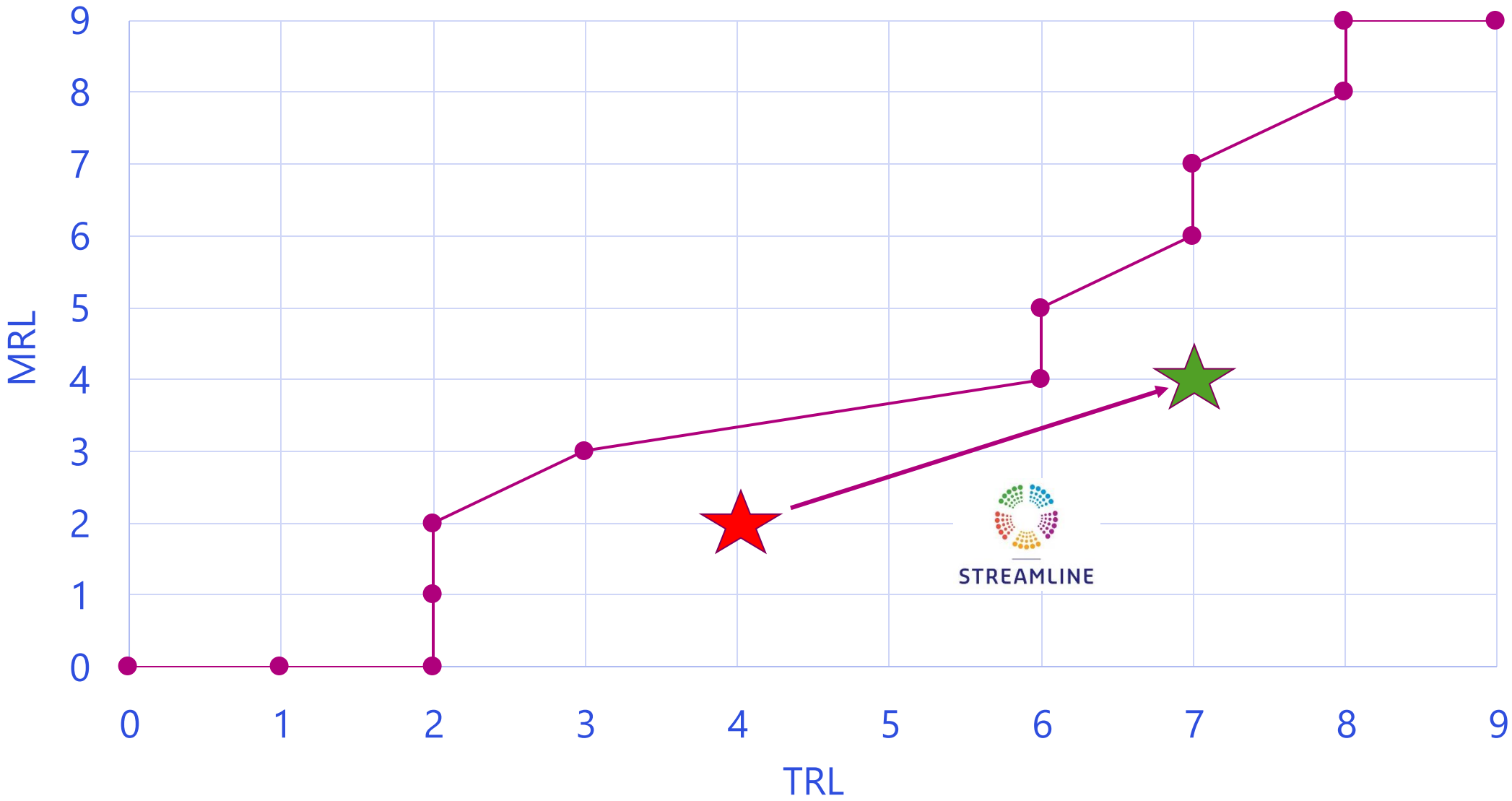
MRL/TRL dependence for a new service development



STREAMLINE has received funding from th 3.

HT services developed in STREAMLINE - XRPD & XRF



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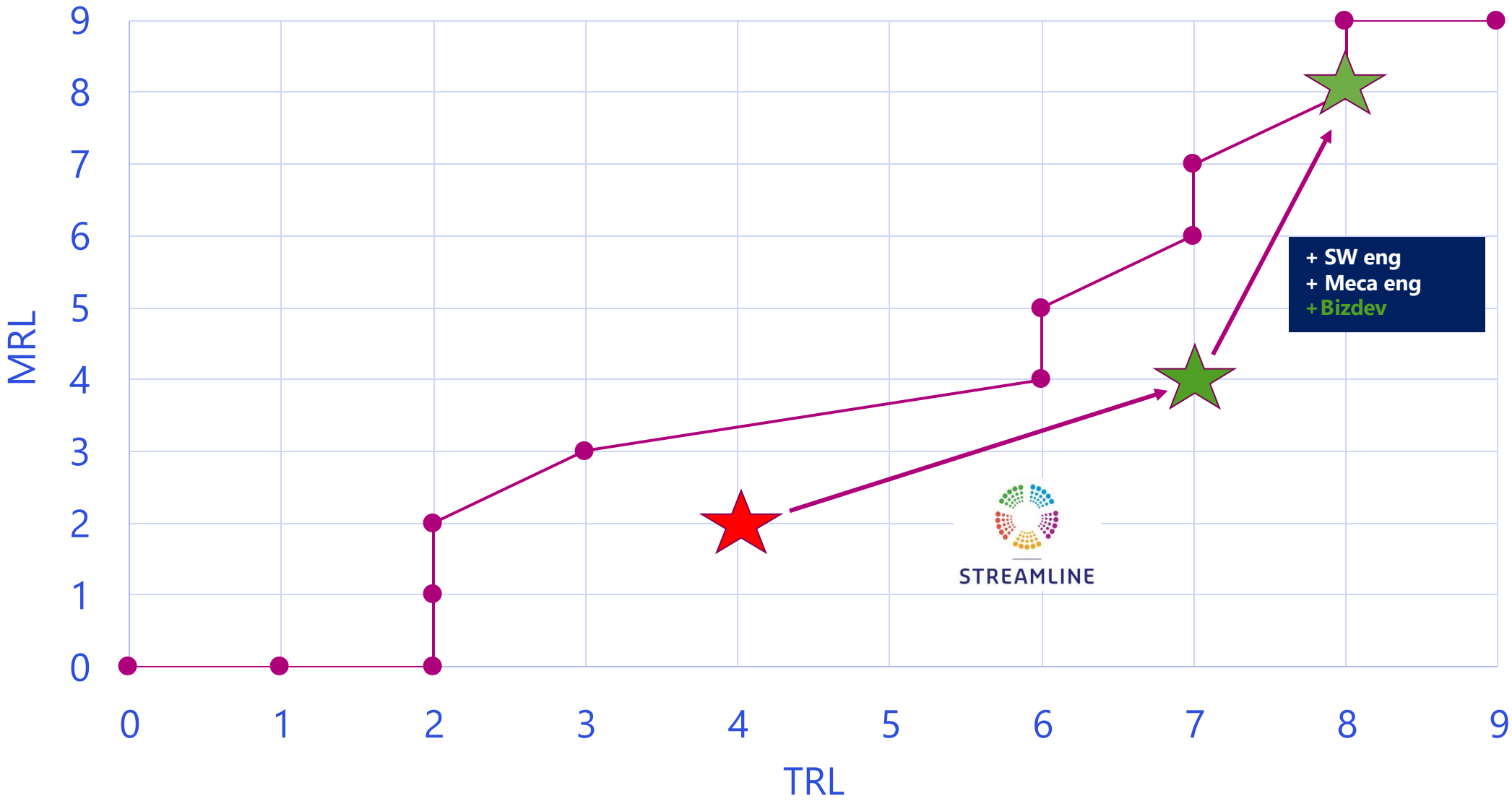
HT services developed in STREAMLINE - XRPD & XRF



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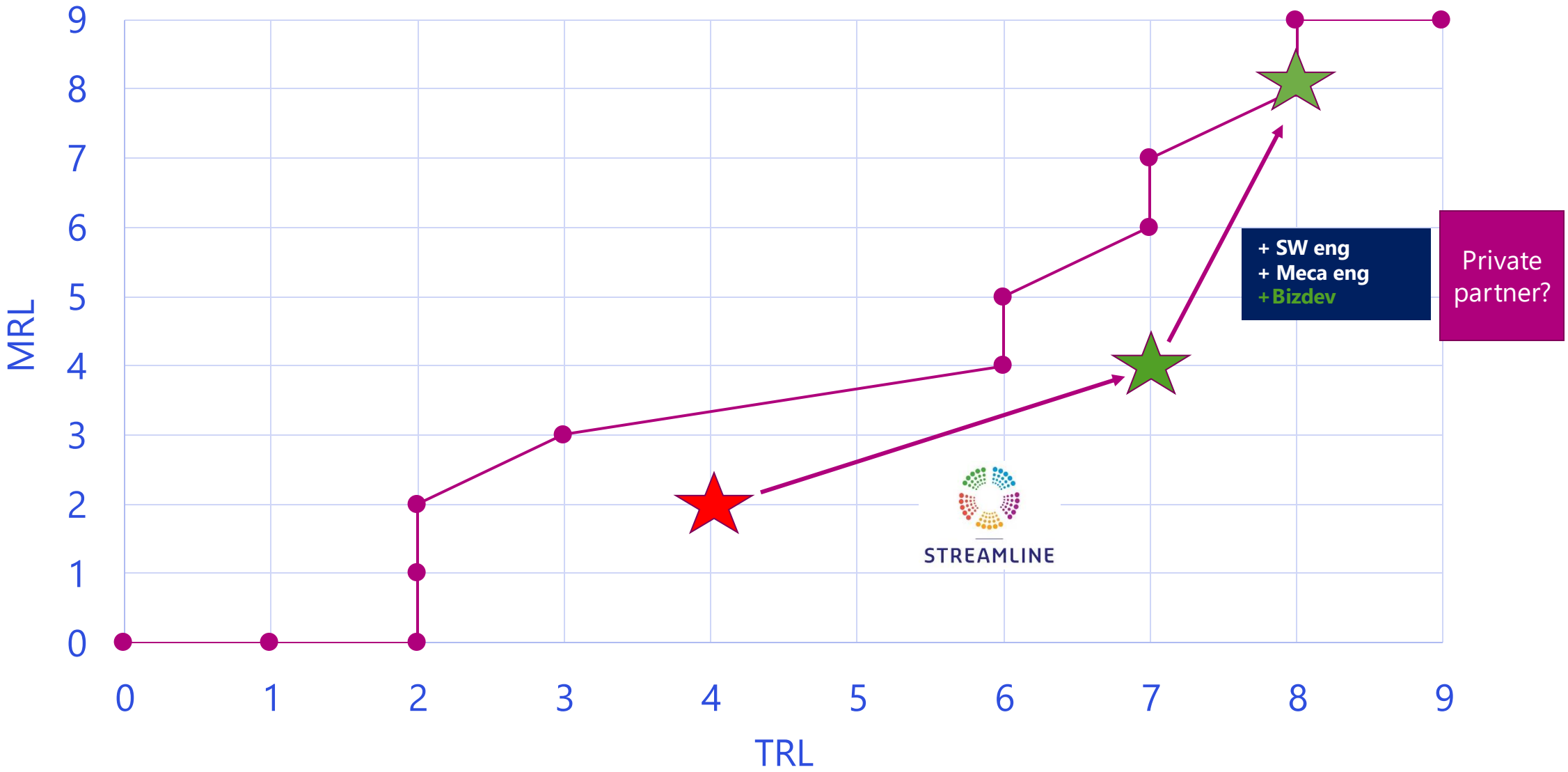

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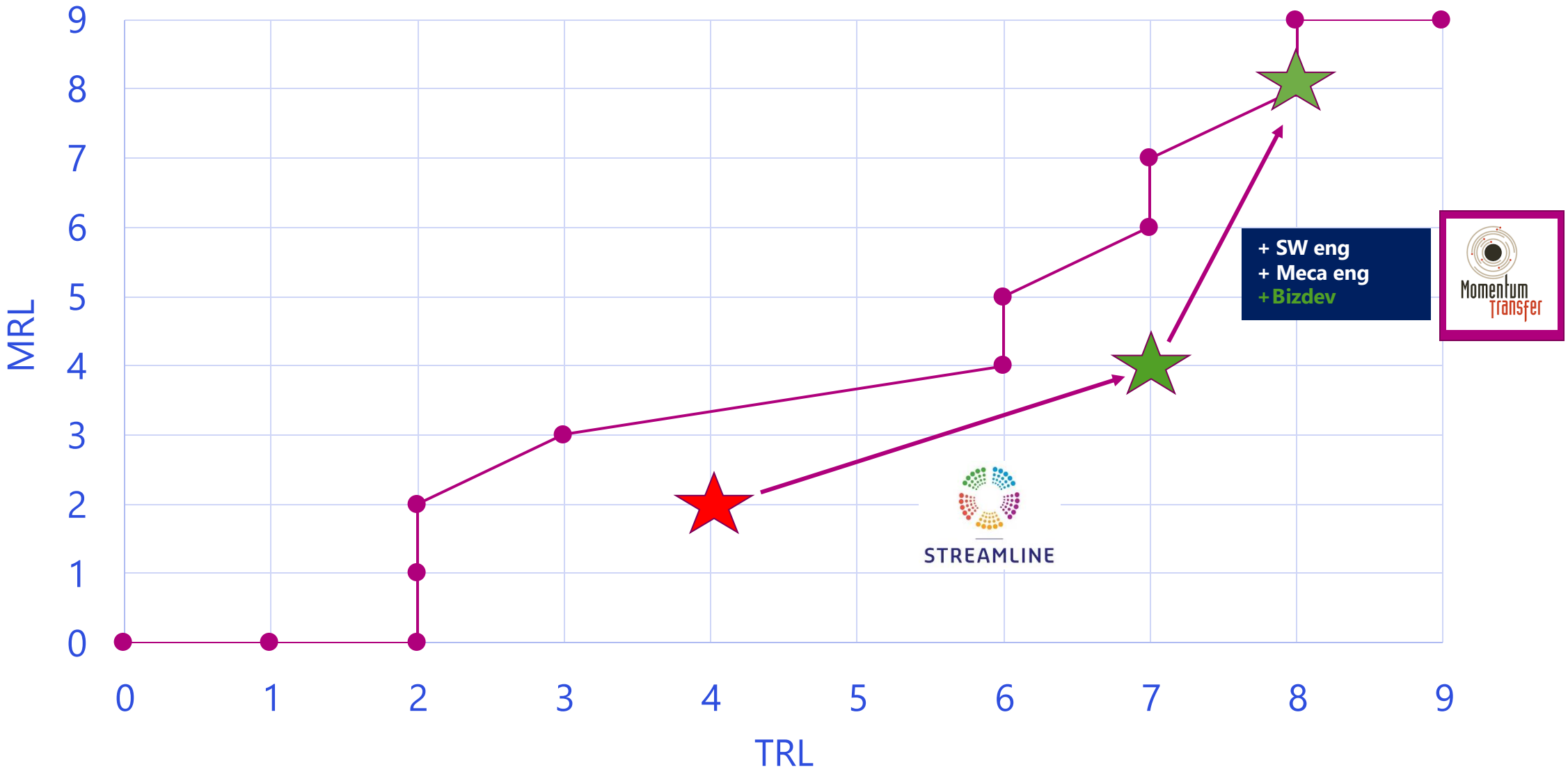

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Why high throughput characterisation is so important?

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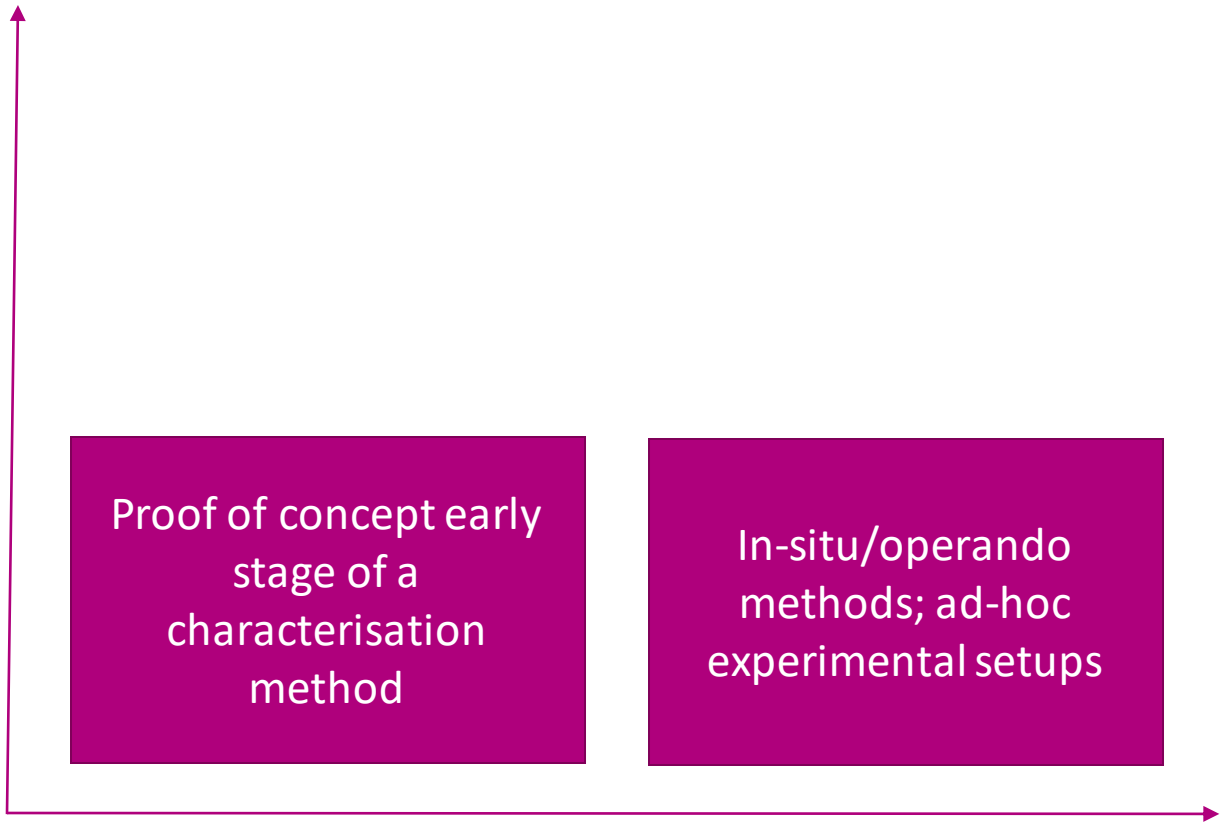

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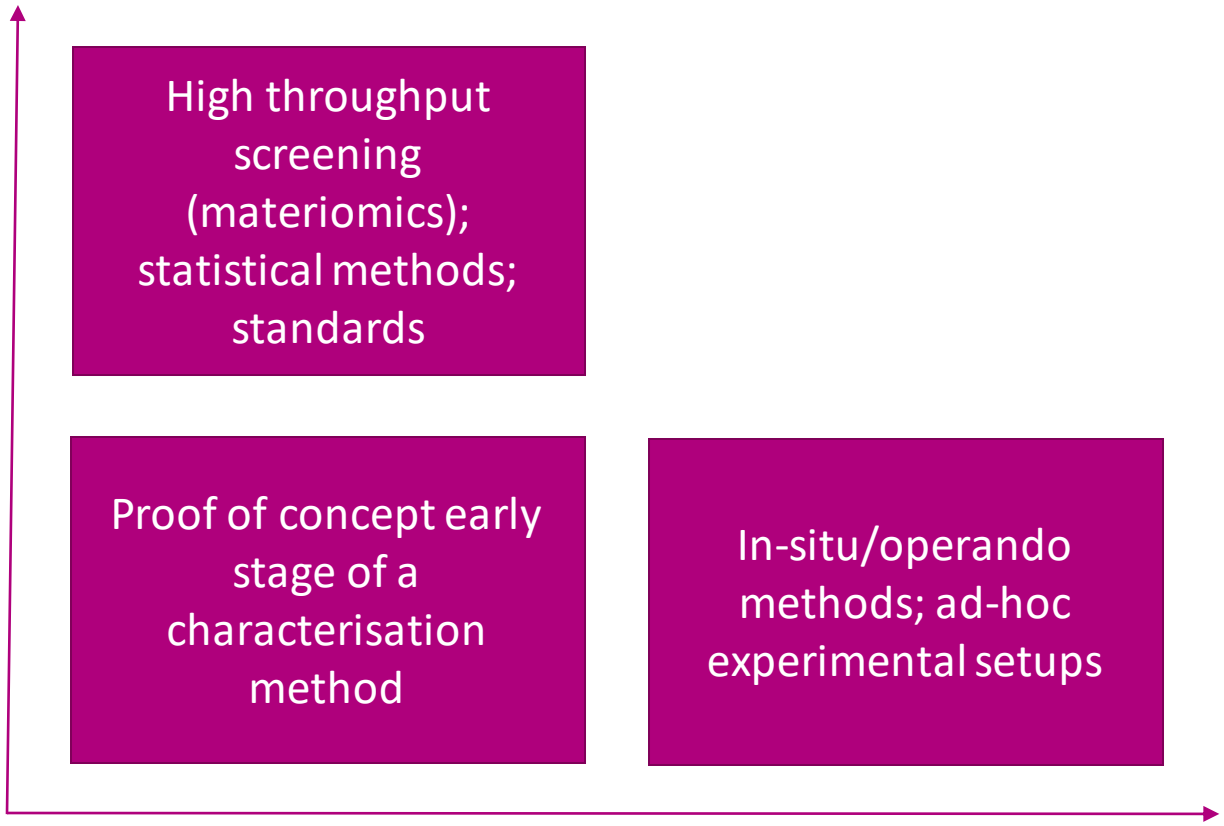

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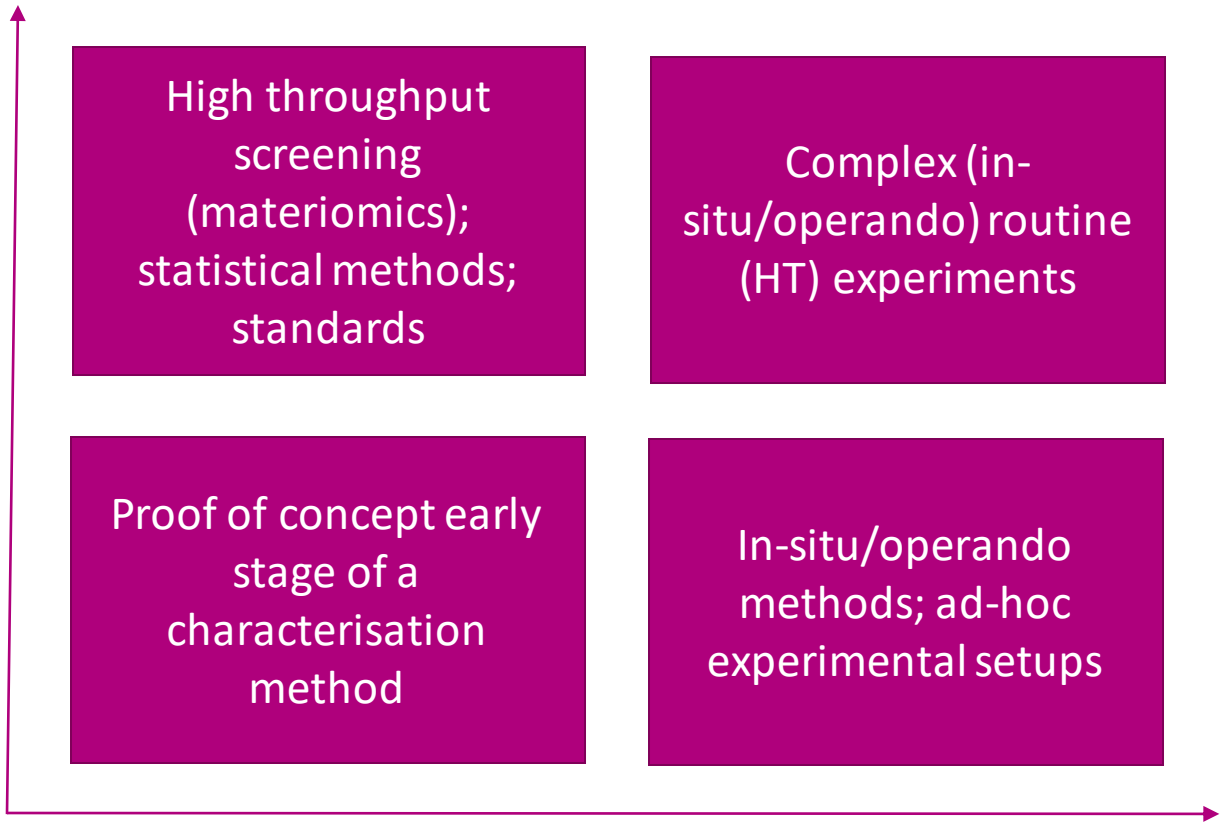

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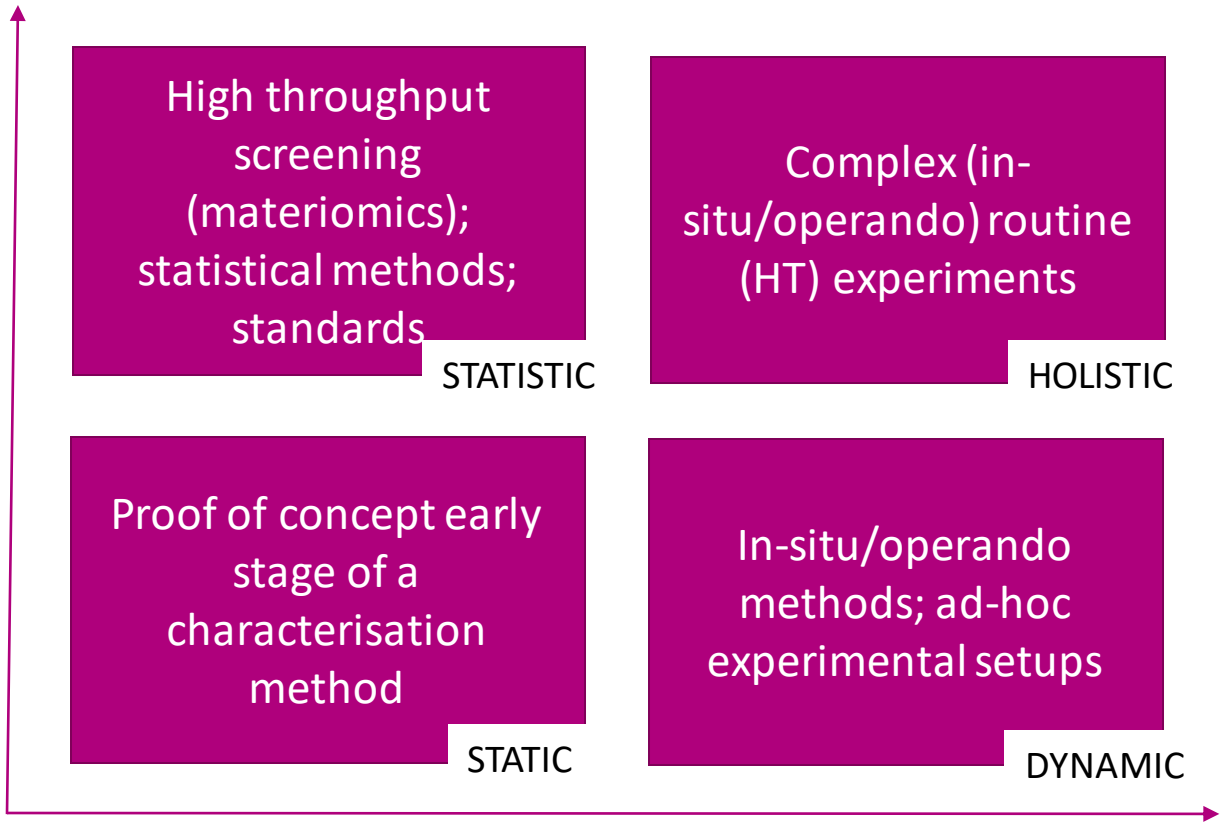

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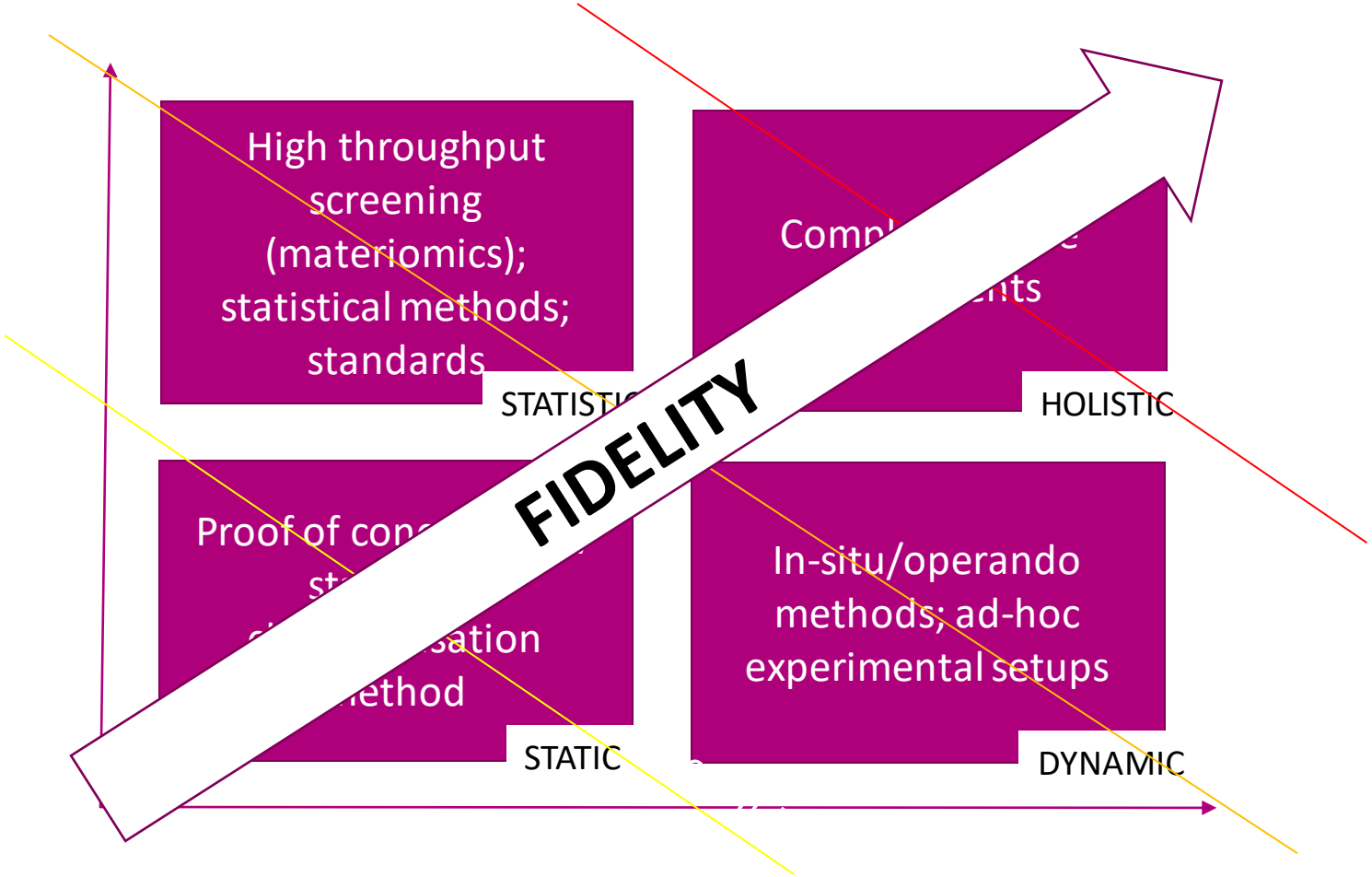

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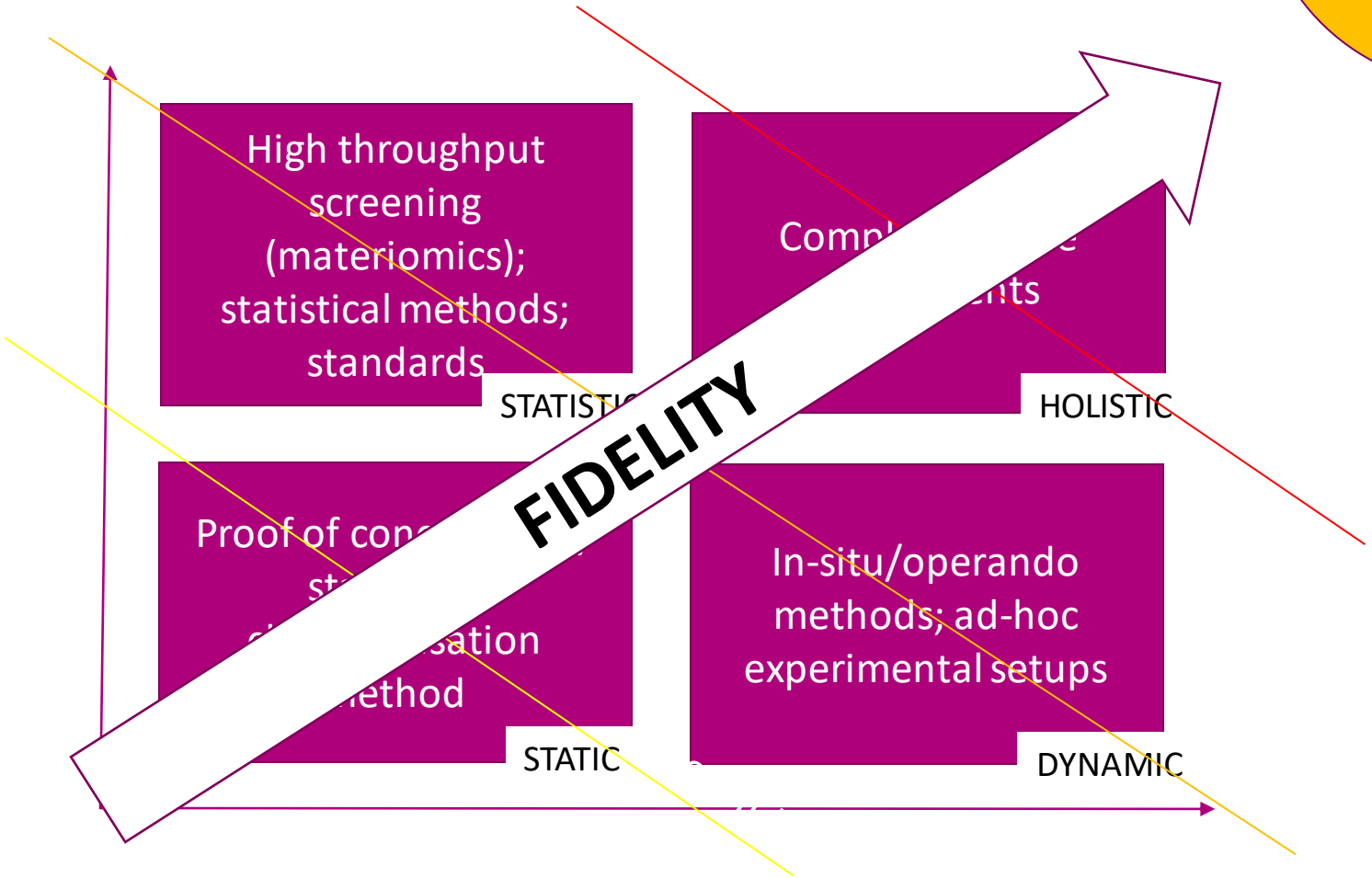
Advanced modeling + Digital twins



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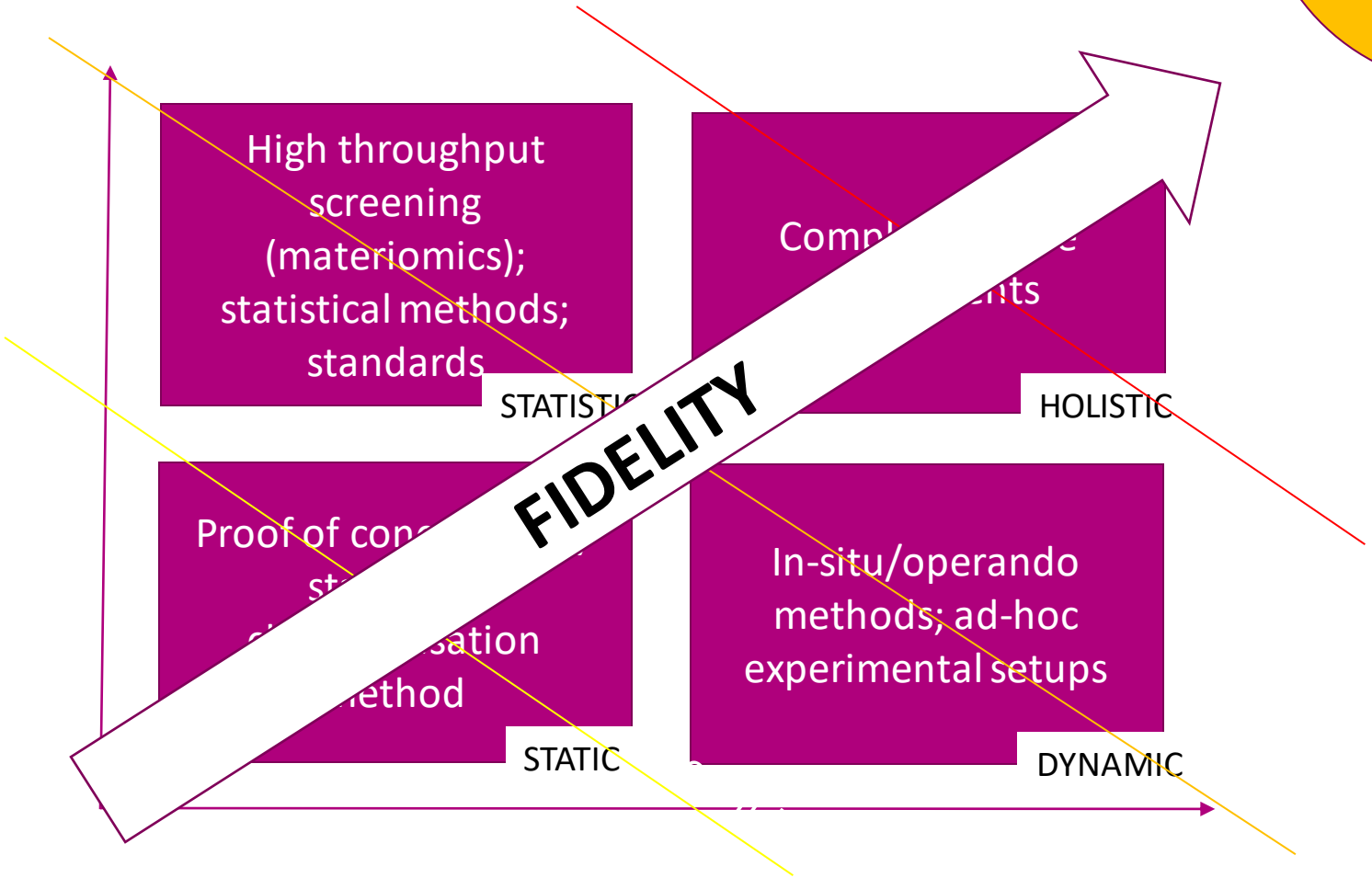
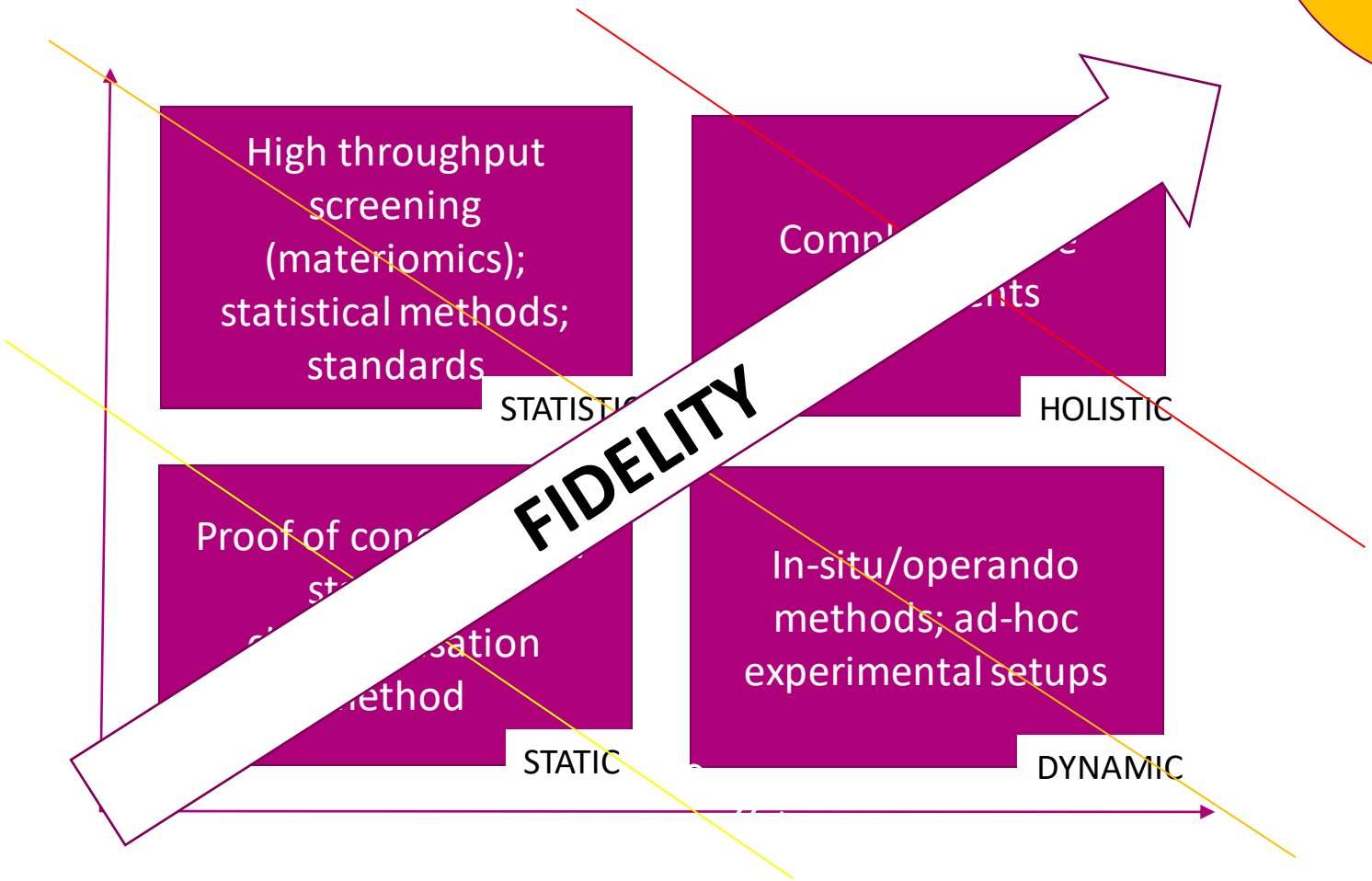
Advanced modeling + Digital twins



Artificial Intelligence

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N



Advanced modeling + Digital twins

ACCELERATED DISCOVERY

Artificial Intelligence

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Now that we told you WHY

let us tell you WHAT and HOW

Thanos the floor is yours…

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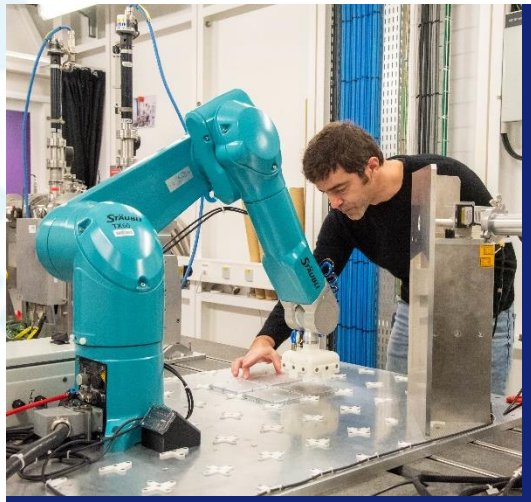
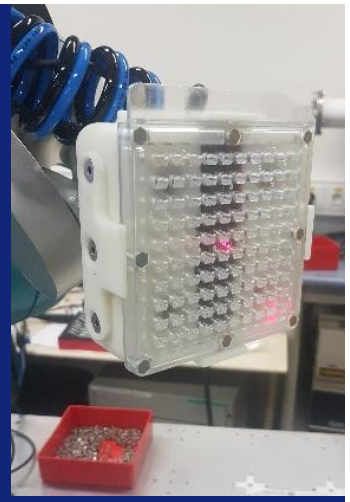
New High-throughput routine services at ESRF

High-Throughput X-ray Fluorescence





- Beamline: BM23
- Co-designed & co-developed with Univ. Montpellier
- Max. capacity 4000 samples
- Acquisition time: 30s
- 160 samples/hour
- 20.000 samples in 2 years

UNIVERSITÉ DE MONTPELLIER

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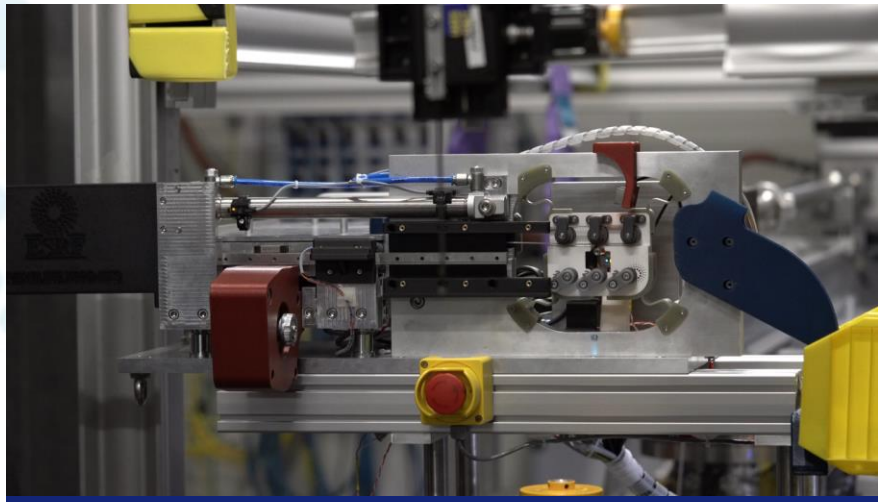
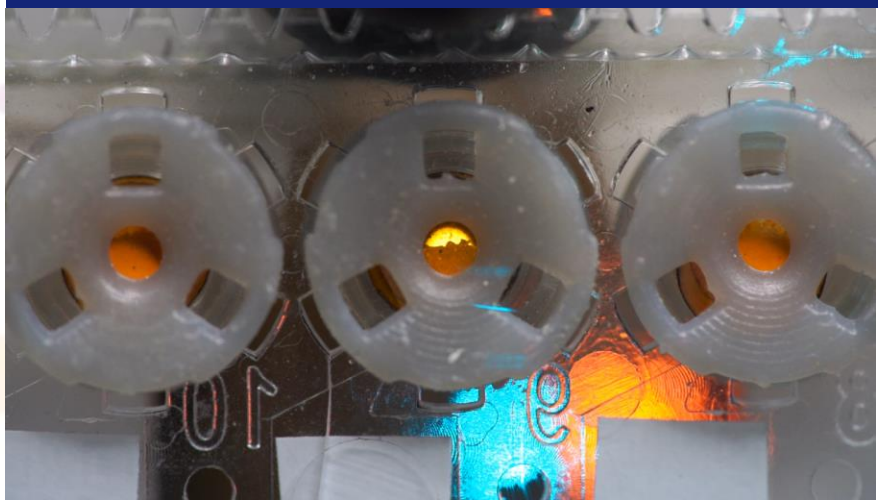
New High-throughput routine services at ESRF

High-Throughput X-ray Powder Diffraction





- Beamline: ID31
- Co-designed & co-developed with BASF
- Max. capacity 66 sample holders = 1056 samples
- Acquisition time: 1s – Currently: ~ 8s
- 300 – 400 samples/hour
- 9000 measurements the last 16 months
- 6 unique clients in 1.5 years
- Creation of a new start-up

BASF
We create chemistry

Momentum Transfer

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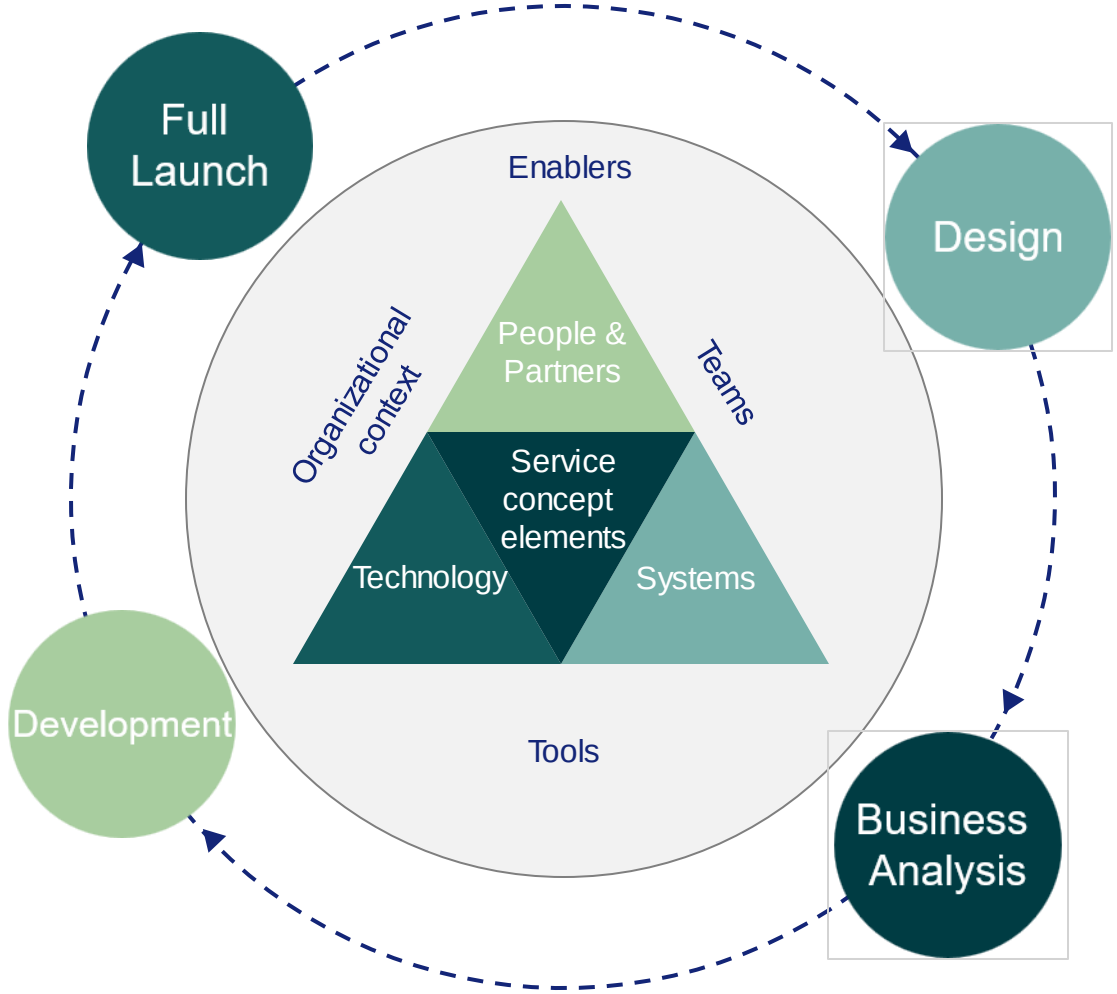
New service development process



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New service development process

Design

- Idea generation and motivation
- New services objective/strategy
- Definition of specifications
- Concept development, technical design and testing

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New service development process

Business Analysis

- Market research to identify customer needs, preferences and trends
- Analyse competitors and assess market demand for similar services

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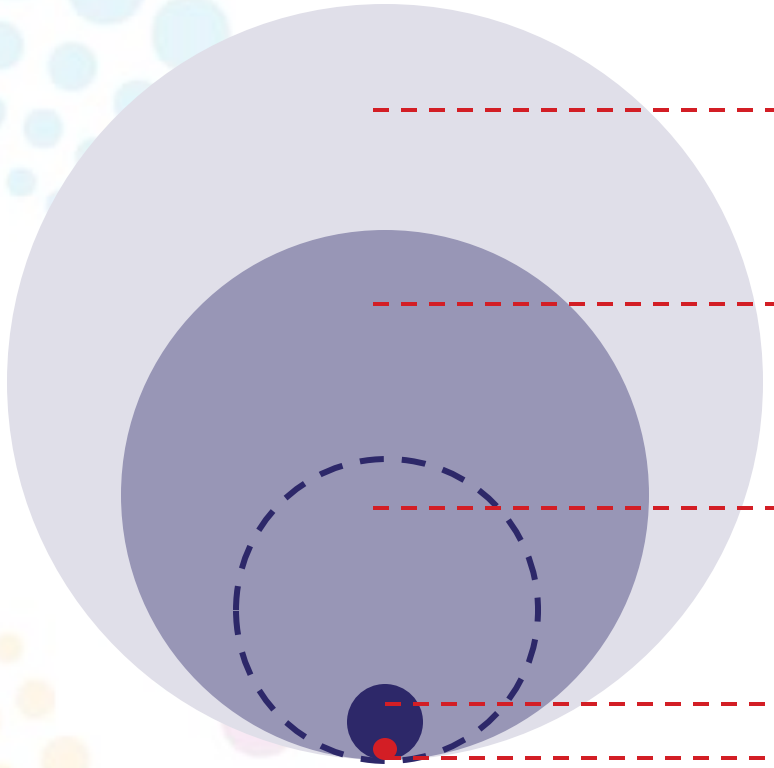
Market research and segmentation of HT-XRD

Market analysis



How big is the market.

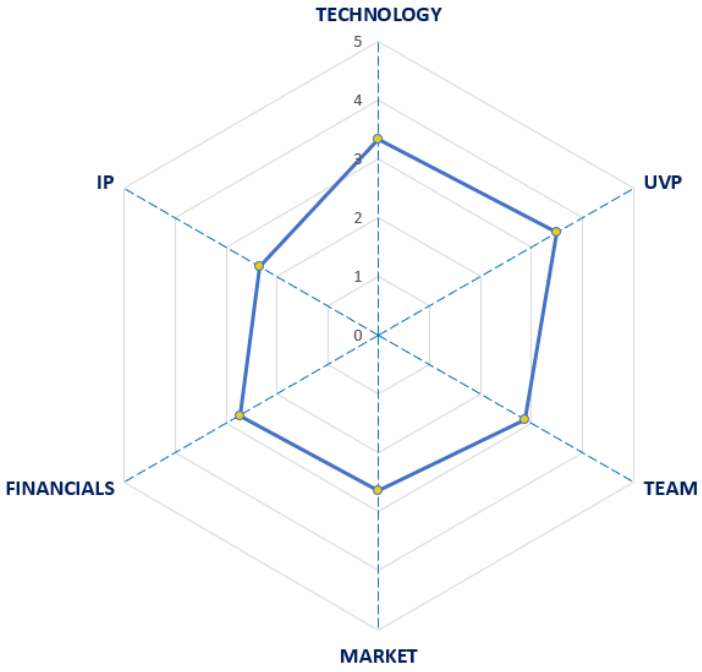
Market that fits us.

Market we could reach.

Our current capacity.

Our current clients/users.

Business opportunity self - assessment tool



- Measure the innovation maturity
- Understand strengths and weaknesses
- Measure the business opportunity potential

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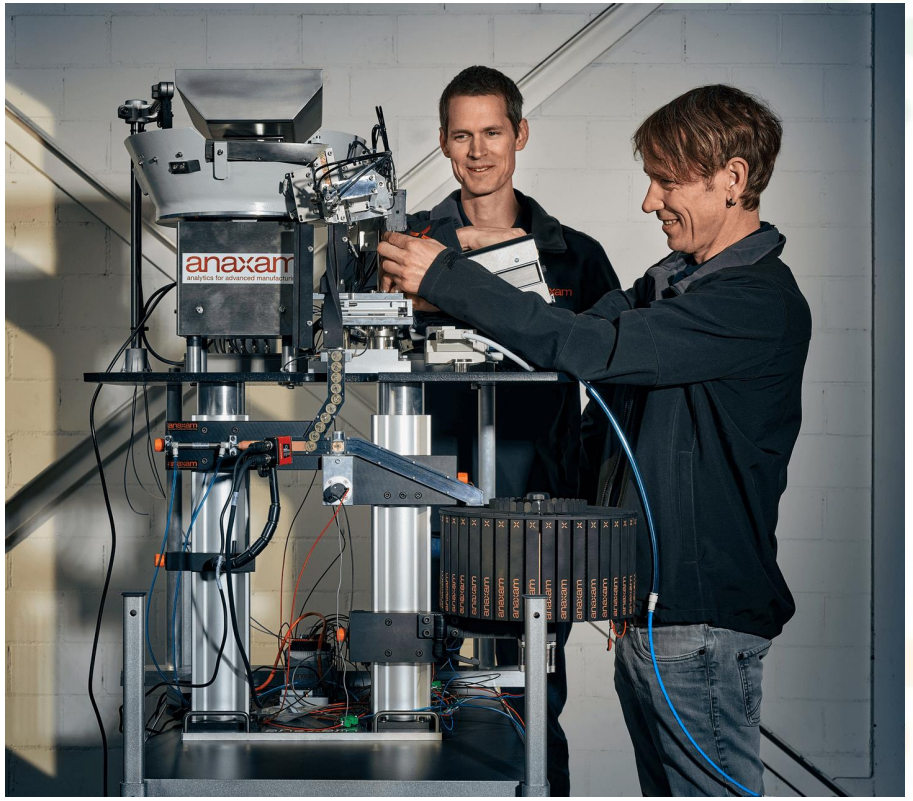
Do we have competitors?

HT-XRD systems worldwide

Currently both are at ESRF

ESRF

PSI



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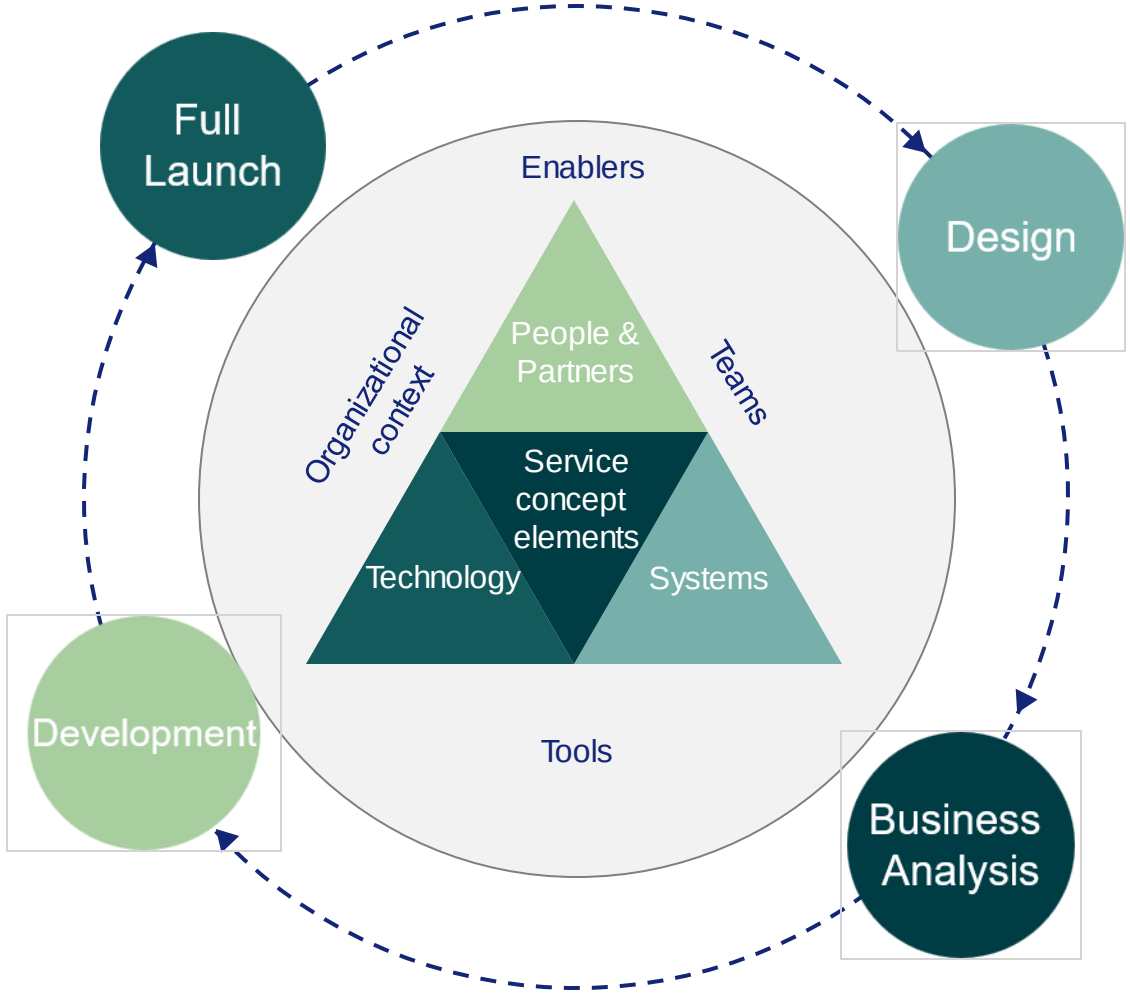
New service development process



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New service development process

Development

Service

- Clearly define the new service, delivery process, including infrastructure and technology.
- Determine pricing strategy based on market research and cost analysis.

Testing

- Create prototypes.
- Conduct pilot tests with small group of users.
- Incorporate feedback and make refinements to improve the service.
- Iterate on the design and functionality.

Promotion

- Develop comprehensive marketing strategy to promote the new service.
- Utilize various marketing channels.

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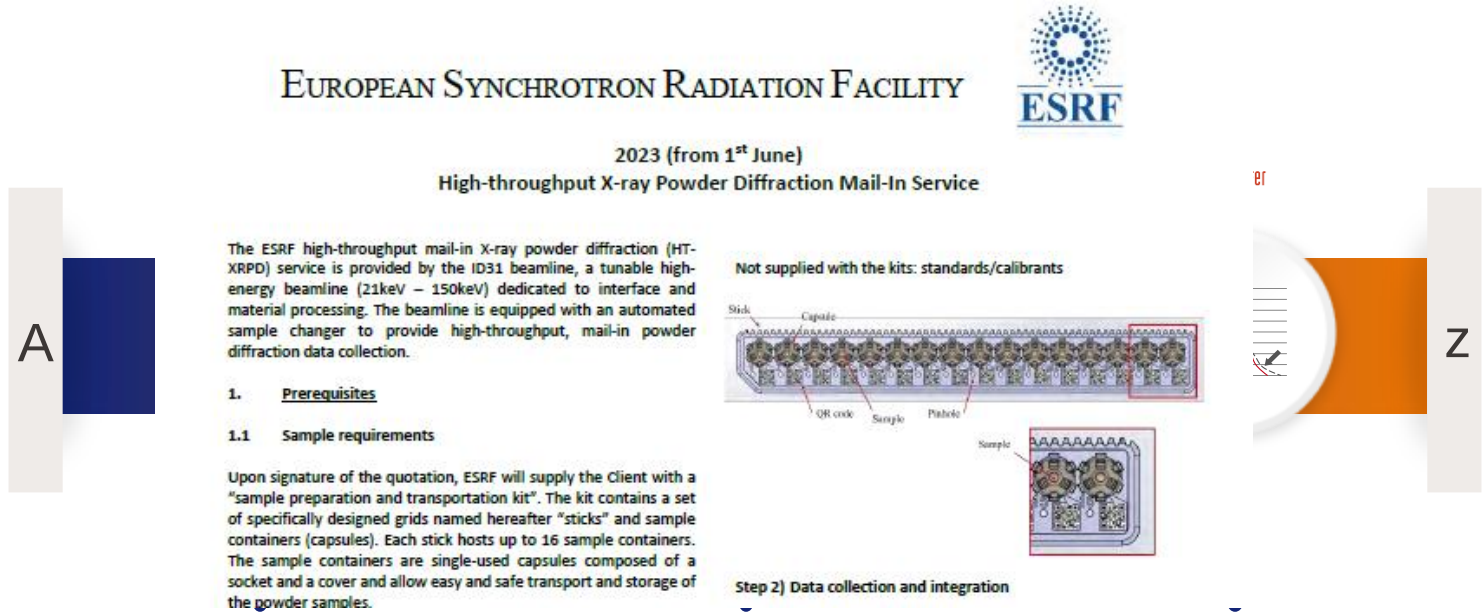
Which is our new service?

A



EUROPEAN SYNCHROTRON RADIATION FACILITY

2023 (from 1st June)

High-throughput X-ray Powder Diffraction Mail-In Service

The ESRF high-throughput mail-in X-ray powder diffraction (HT-XRPD) service is provided by the ID31 beamline, a tunable high-energy beamline (21keV – 150keV) dedicated to interface and material processing. The beamline is equipped with an automated sample changer to provide high-throughput, mail-in powder diffraction data collection.

1. Prerequisites

1.1 Sample requirements

Upon signature of the quotation, ESRF will supply the Client with a "sample preparation and transportation kit". The kit contains a set of specifically designed grids named hereafter "sticks" and sample containers (capsules). Each stick hosts up to 16 sample containers. The sample containers are single-used capsules composed of a socket and a cover and allow easy and safe transport and storage of the powder samples.

Not supplied with the kits: standards/calibrants

Step 2) Data collection and integration

Z

Sample preparation

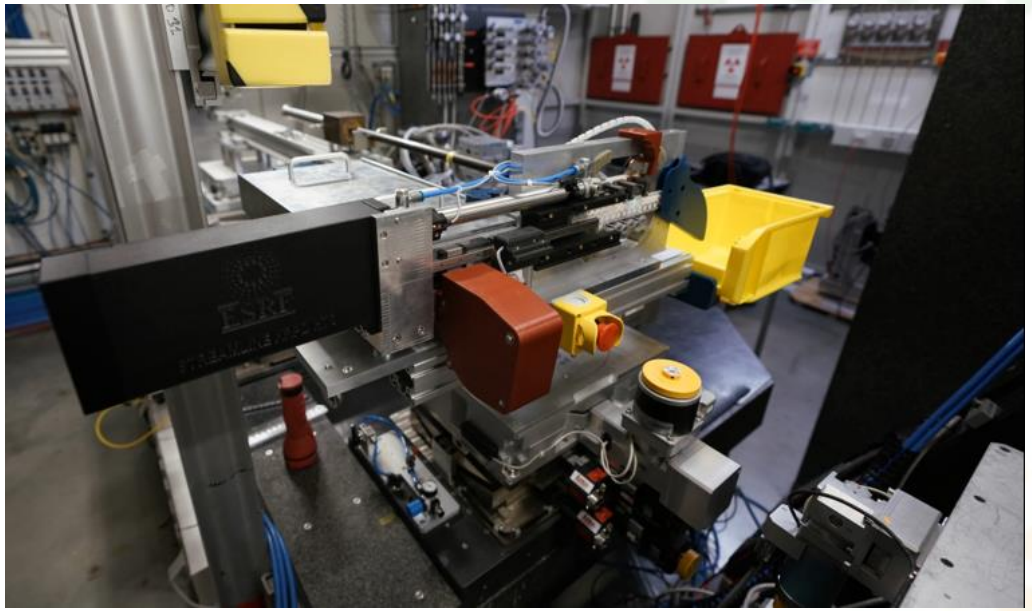
Data acquisition

Data analysis

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Prototypes, Testing & Refinements

The evolution!



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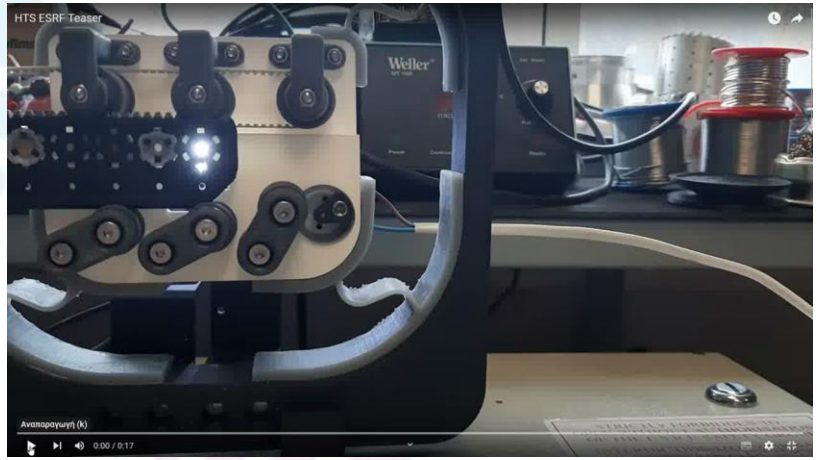
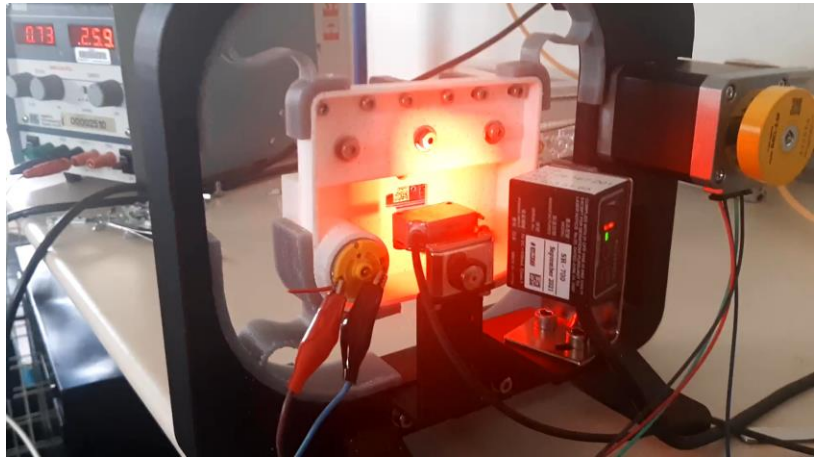
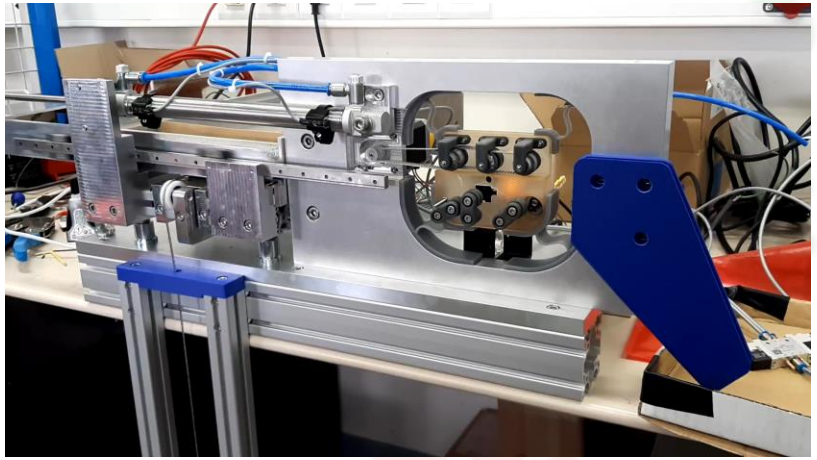
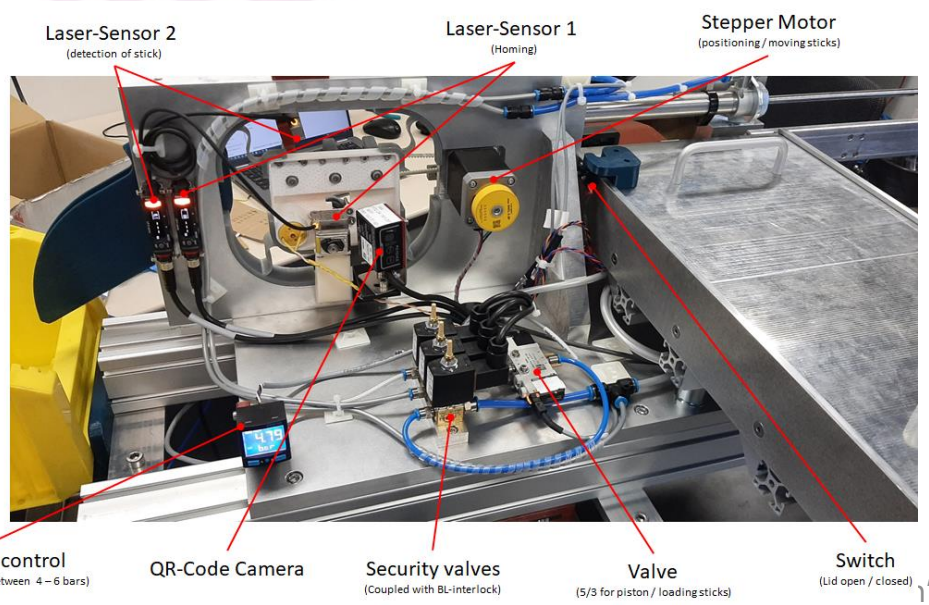
Prototypes, Testing & Refinements

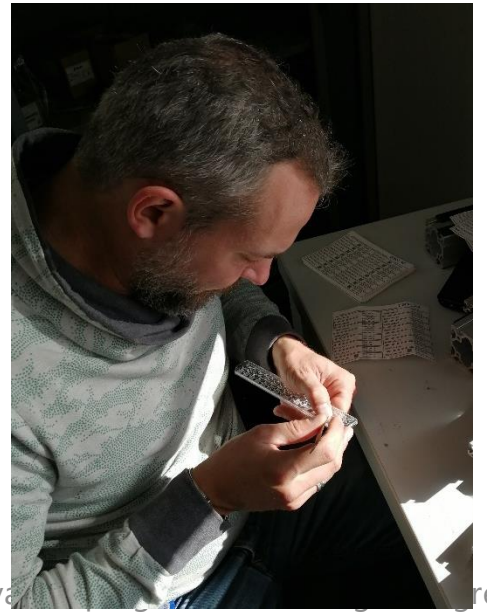
All parts are developed in-house!

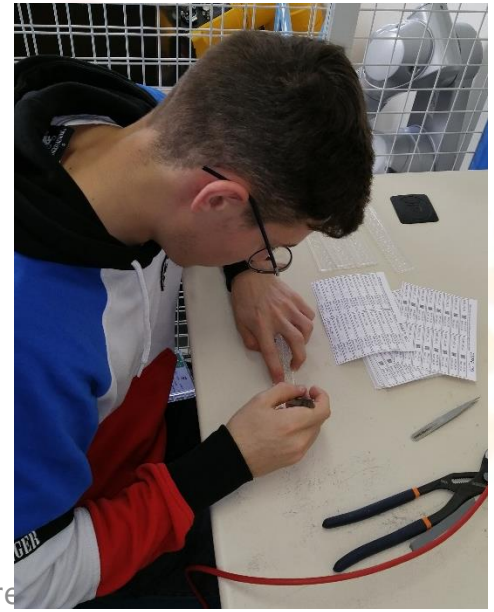




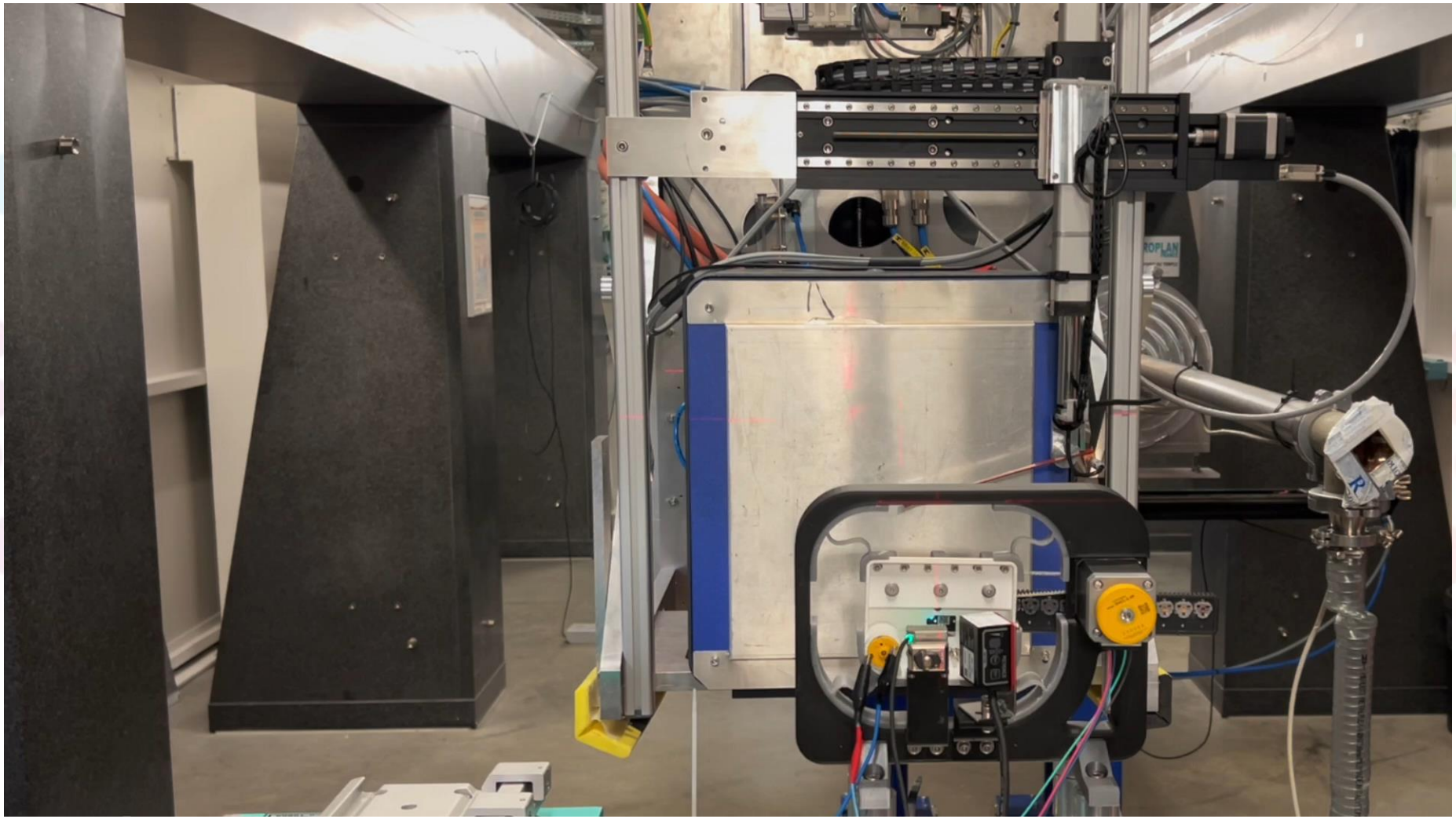








First commissioning on ID31



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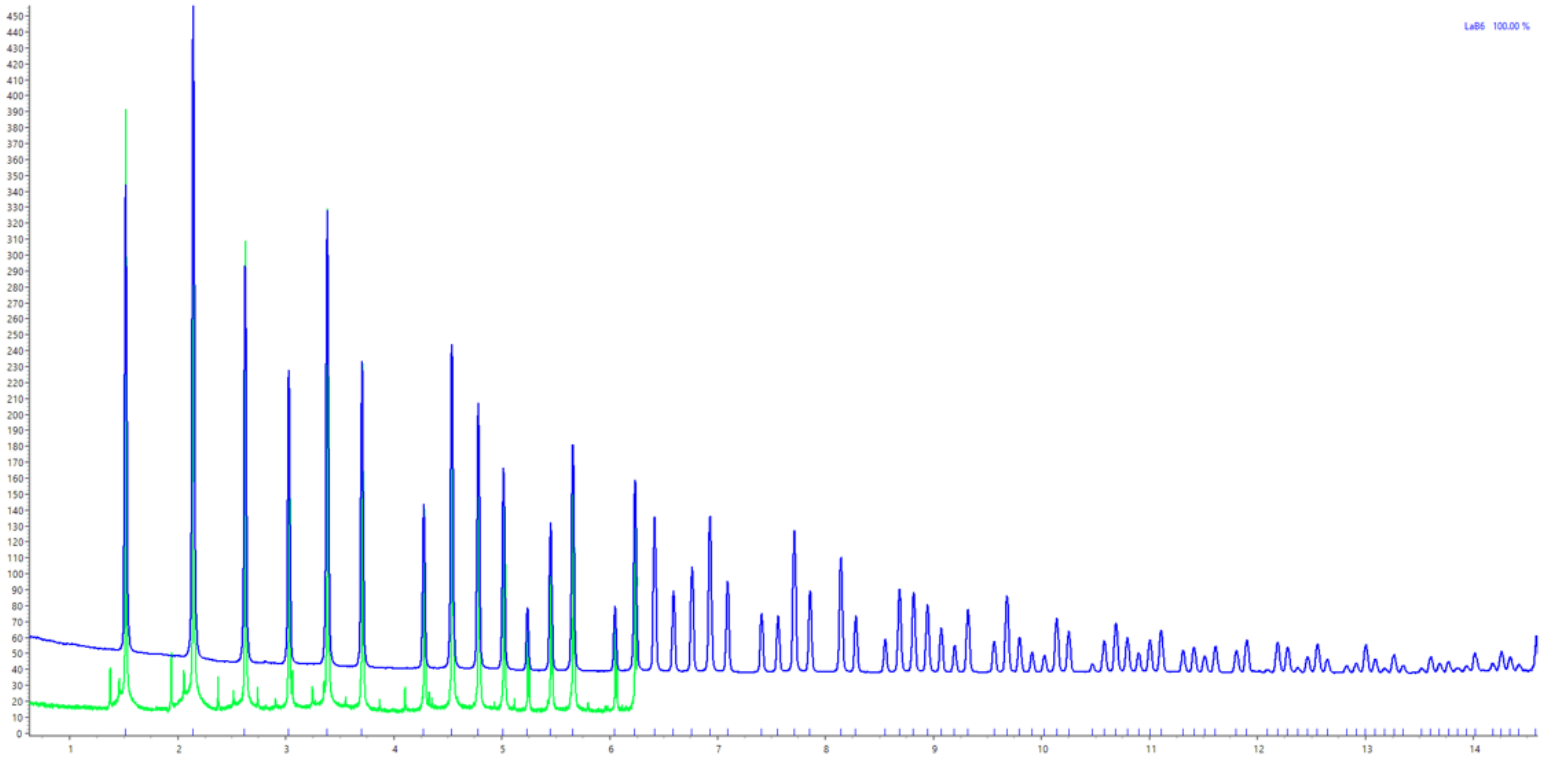
High-quality data

The Data: LaB6, ID31 vs. Laboratory (110° 2θ) CuK$\alpha_{1,2}$



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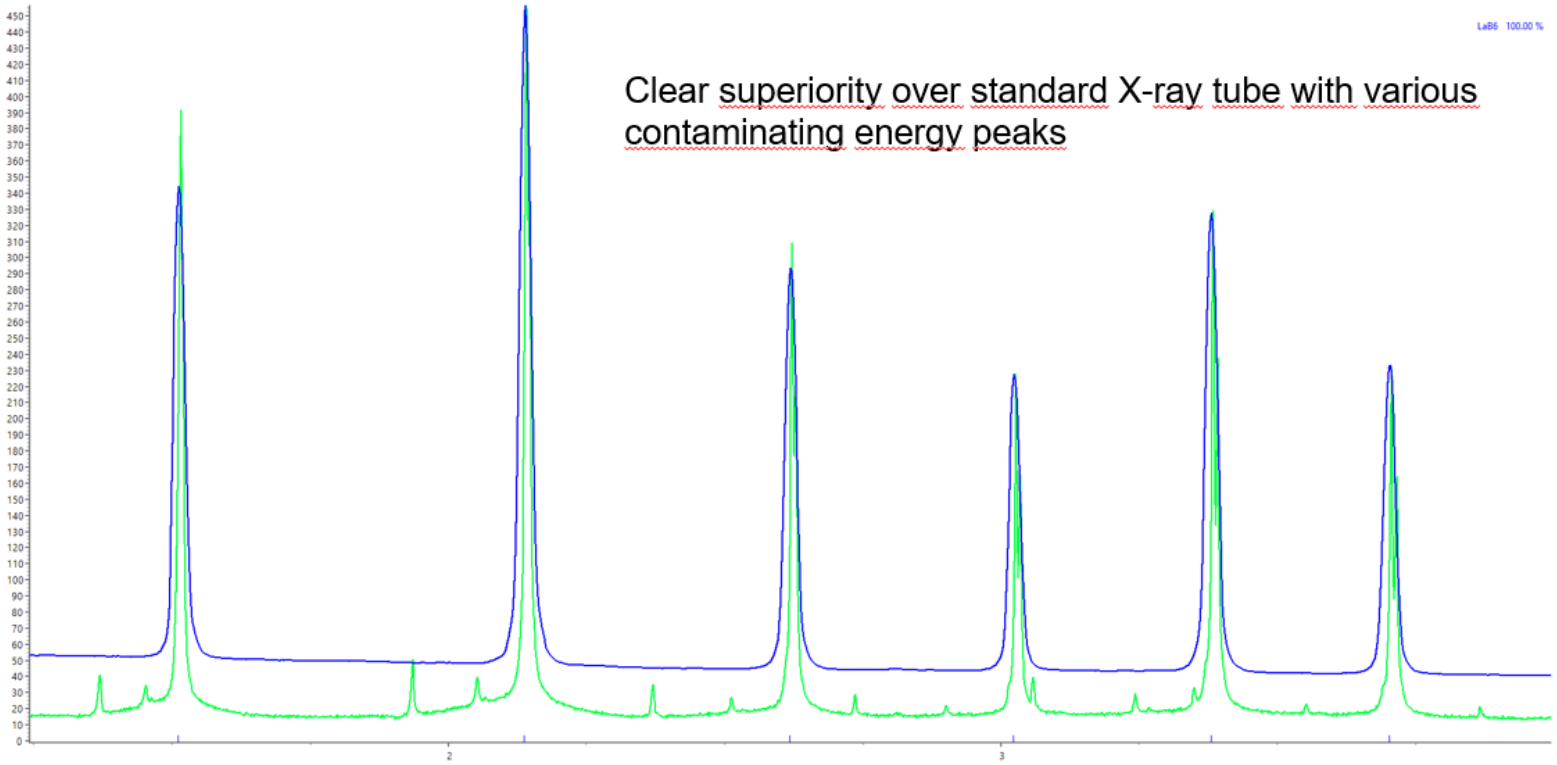

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New service development process

Development

Service

- Clearly define the new service, delivery process, including infrastructure and technology.
- Determine pricing strategy based on market research and cost analysis.

Testing

- Create prototypes.
- Conduct pilot tests with small group of users.
- Incorporate feedback and make refinements to improve the service.
- Iterate on the design and functionality.

Promotion

- Develop comprehensive marketing strategy to promote the new service.
- Utilize various marketing channels.

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Reaching out efforts

Events/initiatives

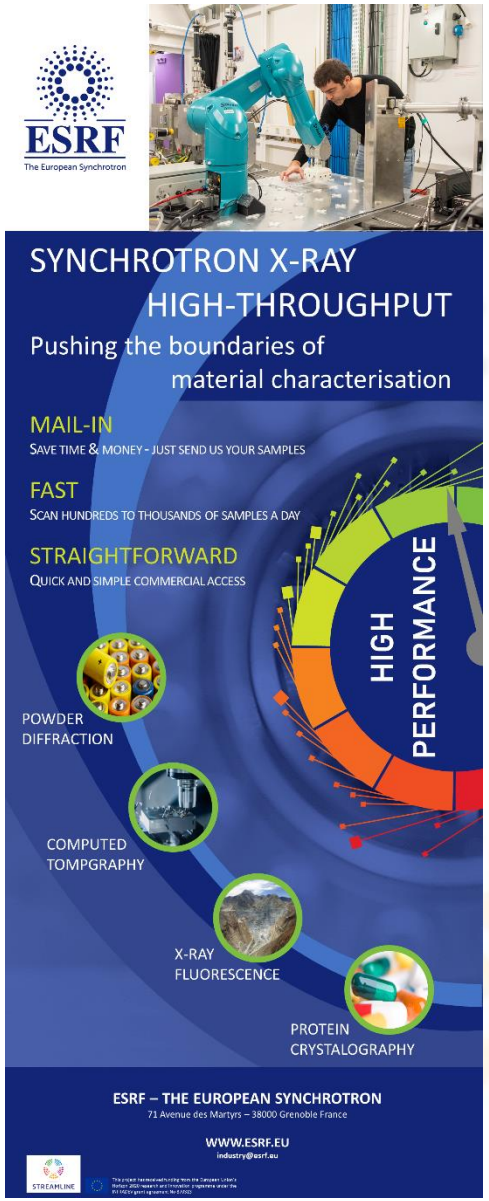
- Conferences
- B2B meetings
- On site visits
- Workshops
- Technical days
- Seminars & Webinars
- Training

Communication channels

- ESRF Website
- Social Media (such as Twitter, LinkedIn and YouTube)
- Streamline Website
- Newsflashes, Newsletter and cross-dissemination with other project channels (such as Giant, Lightsources.org & similar)

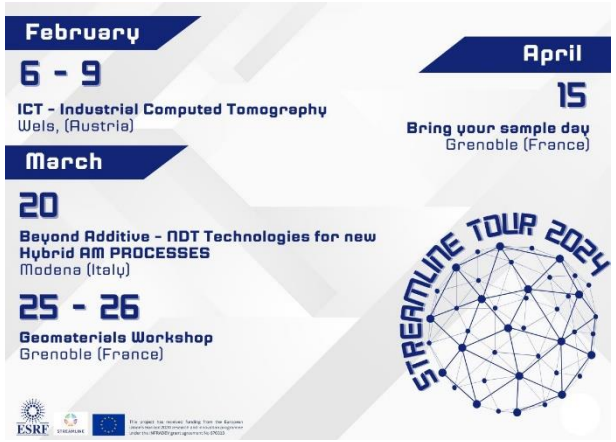
Marketing material

- Brochures
- Flyers
- Rollups
- Presentations
- Videos



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Streamline Tour



- 12 events
- 7 countries
- >150 new contacts

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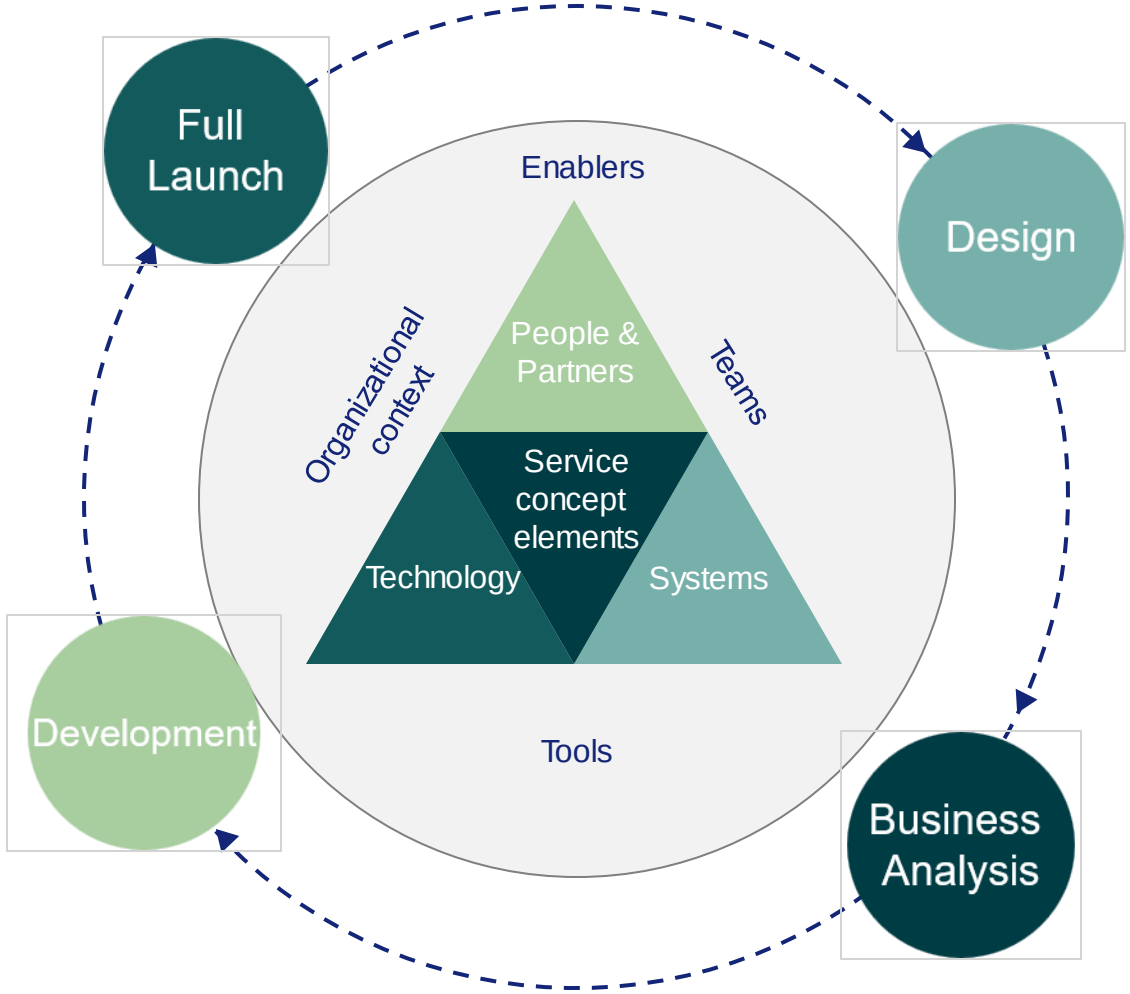
New service development process



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New service development process

Full Launch

- Official launch the new service with coordinated marketing campaign
- Monitor the launch closely and address any issues or challenges
- Gather insights from users for future improvements and iterations

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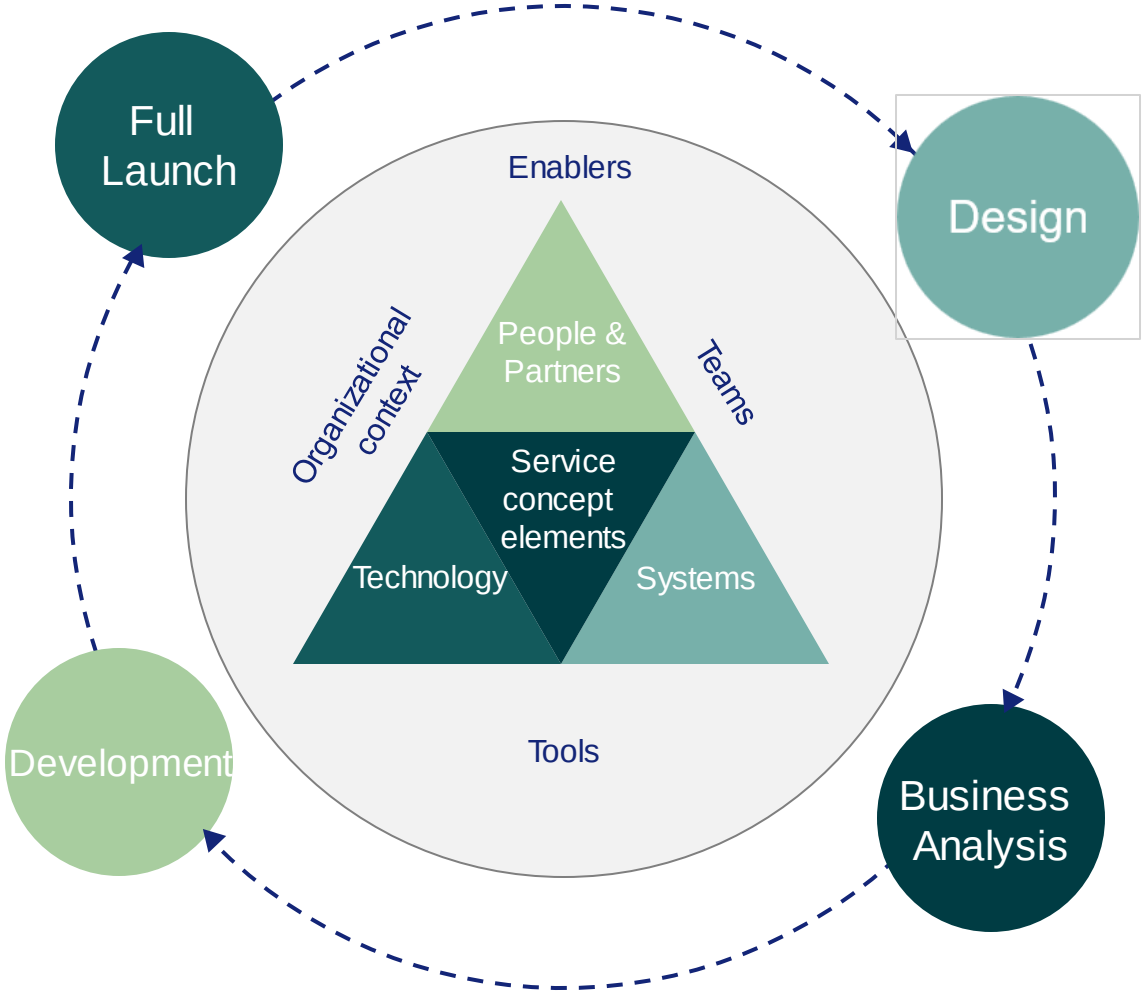
HT-XRD @ ESRF, Current situation and future steps

- Service available to academic and industrial users since 01/2023
- 1 shift dedicated to HT-XRD measurements every second week at ID31
- Collaboration agreement signed with BASF – ESRF owns the IPs
- Collaboration agreement with Momentum Transfer – under preparation
- ErUM – Transfer (BMBF) 3 years project, 2024-2027, is funded (DESY, BASF, ESRF)

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

New service development process



STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Thank you!

It’s teamwork!!!

STREAMLINE has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 870313.

STREAMLINE

ESRF
The European Synchrotron

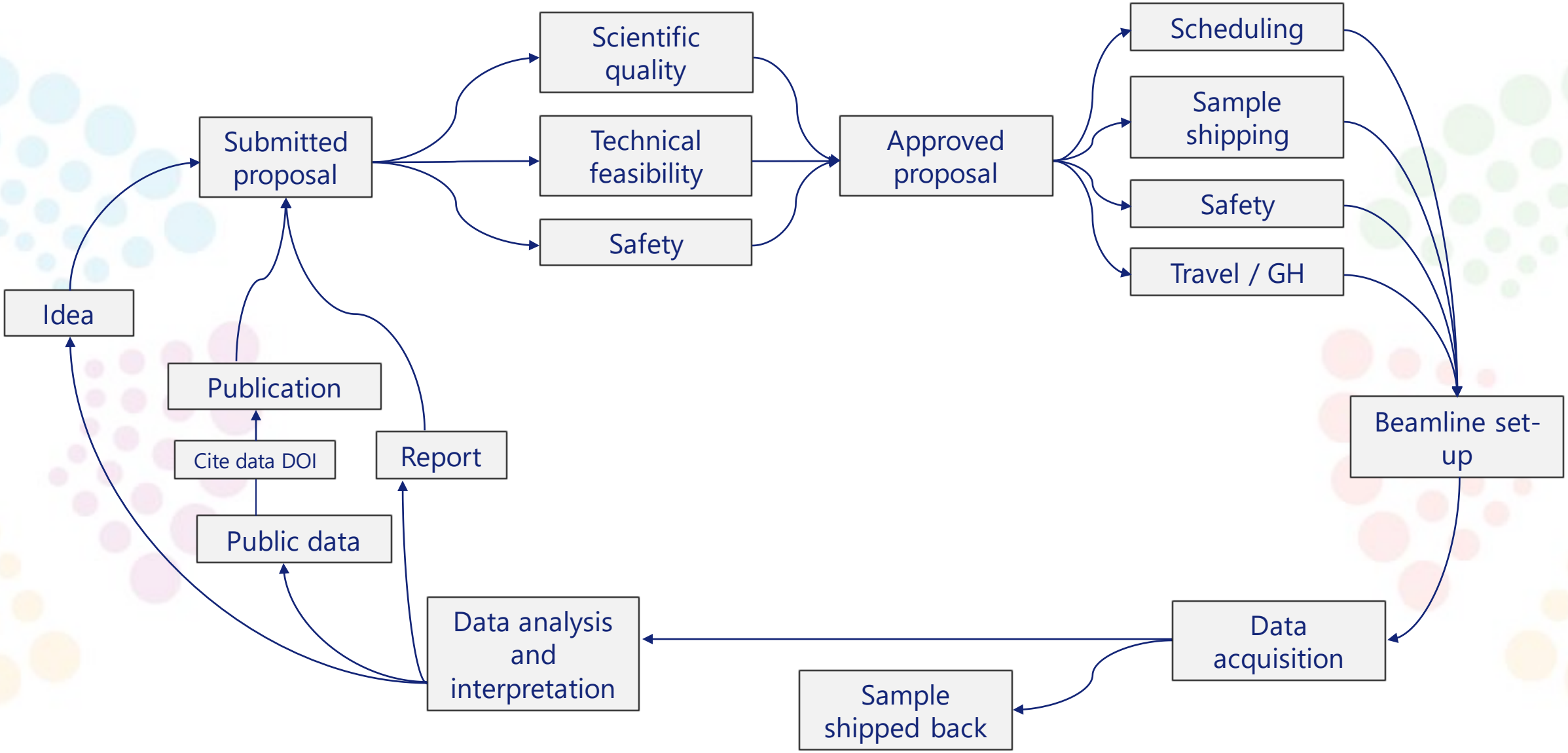
And NEXT UP we have…Novel Access to Large User Facilities

WP3: Update user tools and administrative procedures

Joanne McCarthy, Head of User Office

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

The Proposal & Experiment Cycle



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Motivation for new access models - some key figures

Most efficient way to carry out science and exploit the EBS?

Idea

Submitted proposal

> 2500 proposals / year

Scientific quality

Technical feasibility

Safety

> 80 proposals / reviewer / year
125 reviewers

Approved proposal

Scheduling

Sample shipping

Safety

Travel / GH

> 100 000 samples / year

Travel budget 15% overspend

Beamline set-up

Data acquisition

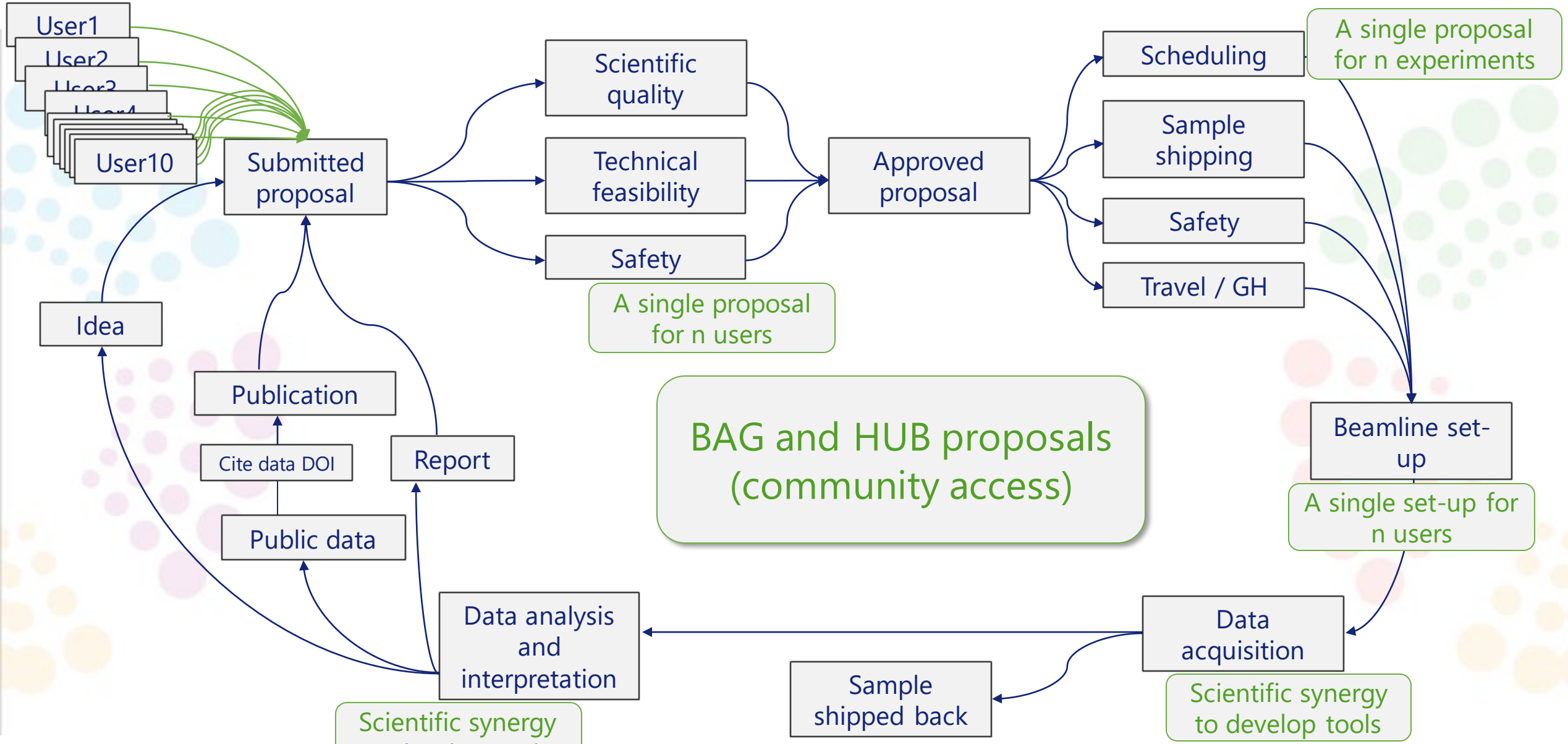
Speed x >10

Sample shipped back

Streamline WP3:
- optimize existing models
- create new models

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Enabling new access models – Community Access



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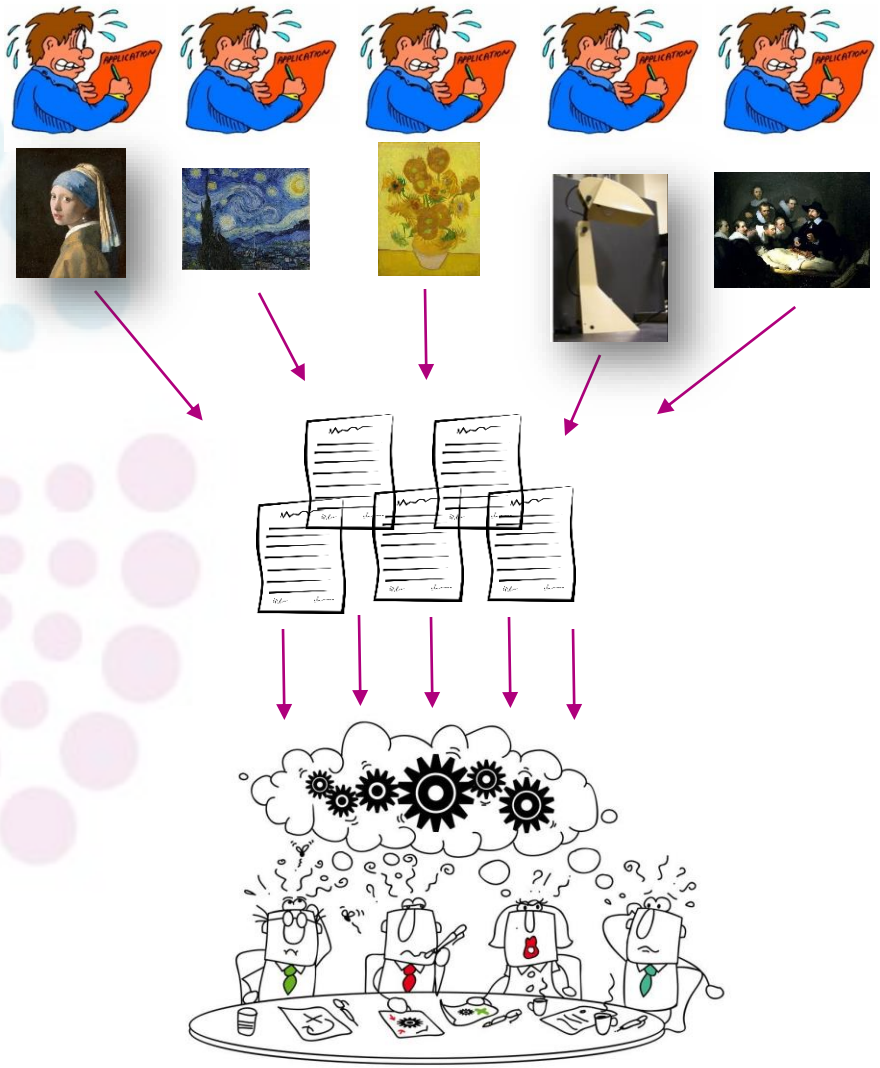
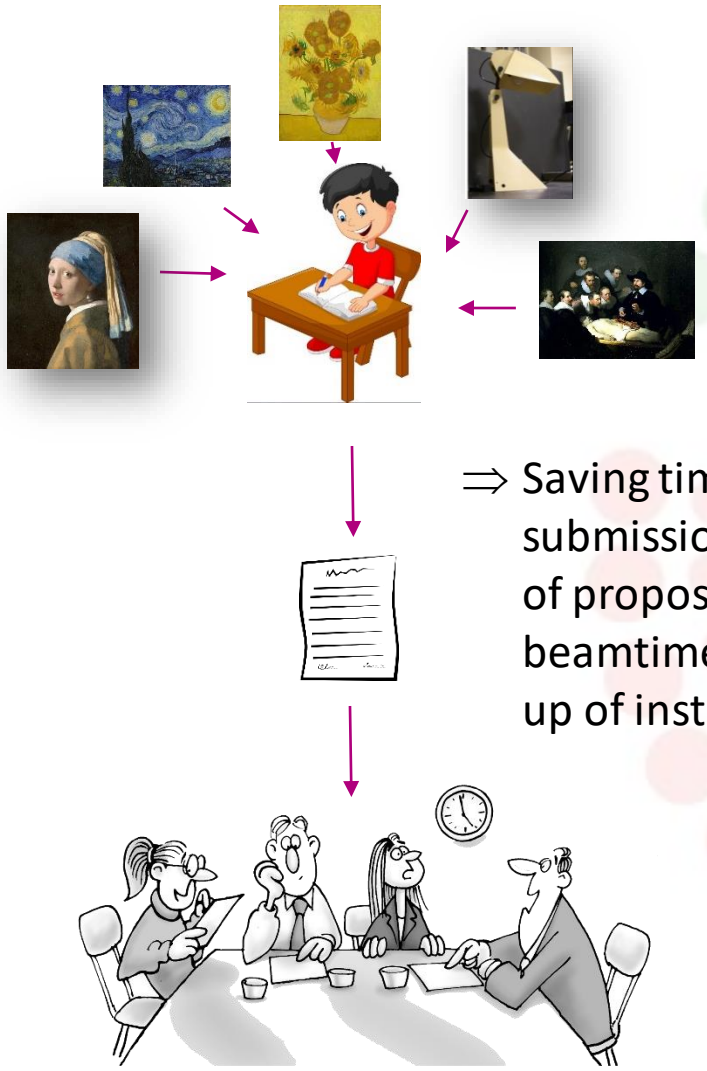
From standard access models to community access

Standard



BAG/HUB



⇒ Saving time in submission, evaluation of proposals, scheduling beamtime and setting-up of instruments

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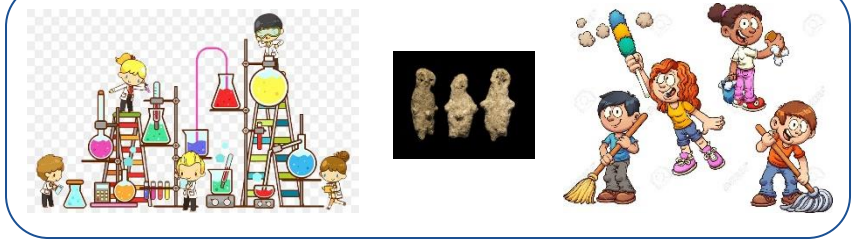
Community proposals – on the beamline

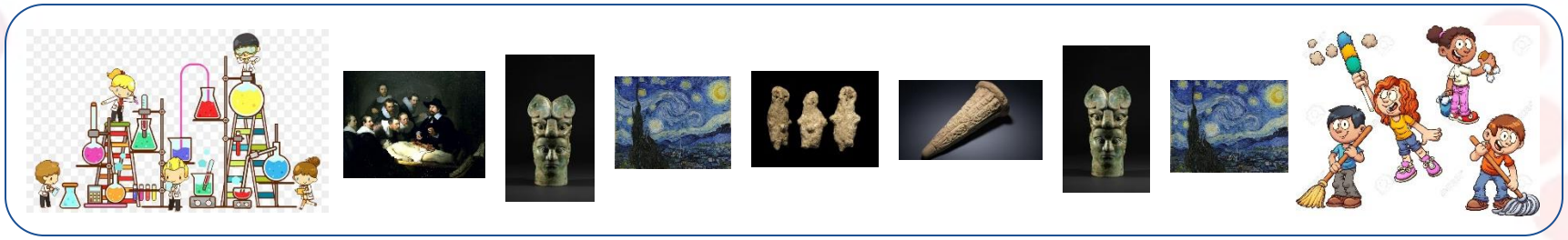
Standard



Experiment 1

Experiment 2

BAG/HUB



Experiment 1

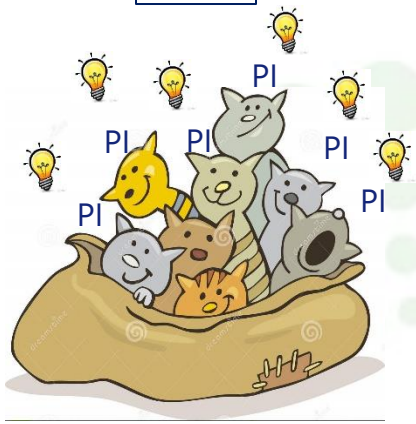
Community access proposals allow a single setup for N users and N samples/projects

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Enabling new access models – Community Access

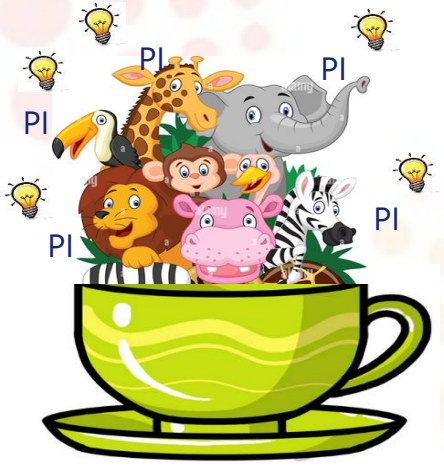
- increase ESRF responsiveness to societal challenges
- maximise impact of ESRF capabilities in specific areas
- provide new scientific opportunities
- expand ESRF role towards being an active facilitator for targeted communities
- group community request into single or few proposals
- guaranteed regular access – adjust goals, long-term plan to maximize impact
- users decide priorities for maximized output and impact

BAGS



Block **A**llocation **G**roups

HUBs



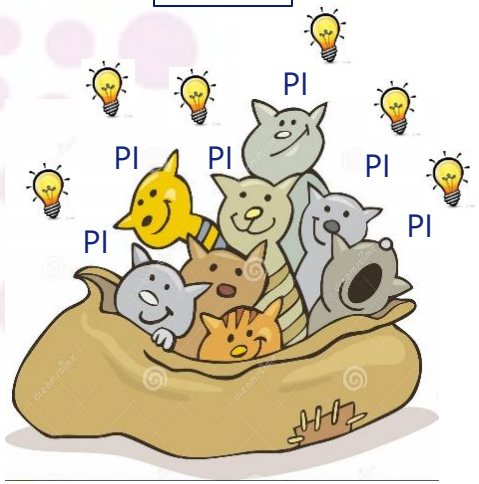
A hub of experts

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

BAGs and HUBs

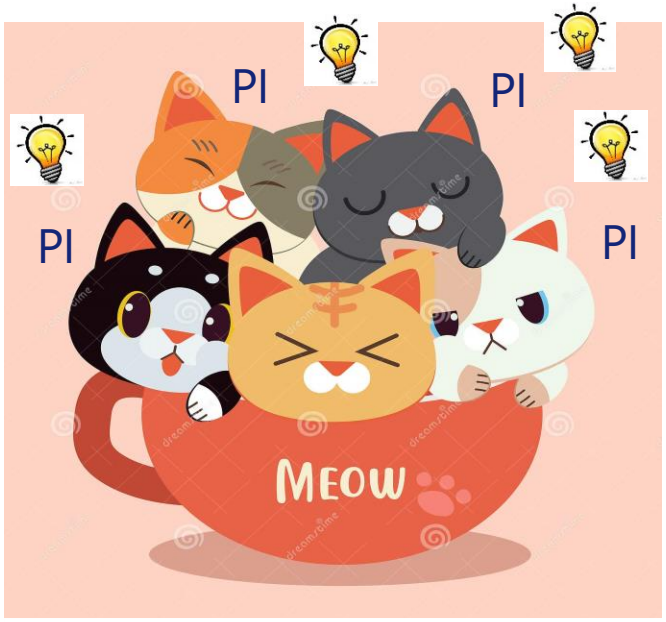
A **BAG** groups together a number of **independent** Principal Investigators (PIs) working in the **same scientific field** and sharing the **same synchrotron instrument need** (same beamline, same setup). They apply together as a consortium for a **regular allocation of beamtime** at the ESRF.
The aim is to produce the most impactful science in a specific field by allowing the community to share the beamtime and decide itself on measurement priorities, made easier by regular beamtime allocation.

BAGS



Block **A**llocation **G**roups

Comm**U**nity **P**roposals



- Community-driven technique-based BAGs
- Community-driven science-based BAGs
- ESRF as a science HUB in selected areas

A **HUB** groups together a number of **independent** Principal Investigators (PIs) working in the **same major scientific field of high societal relevance**, who commit to collaborate to **coordinate the beamtime use** and **share results obtained**. The aim is to create a **hub of researchers** of **differing expertise** working in the same major scientific field, who are willing to collaborate in order to produce greater advances and more impactful science in a shorter time frame.
This necessitates that HUB members share knowledge, technology, beamtime data and results prior to publication.

HUBs

A hub of experts

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HUB and BAG Implementation – Rules & Guidelines

Community Proposals - HUBs and BAGs

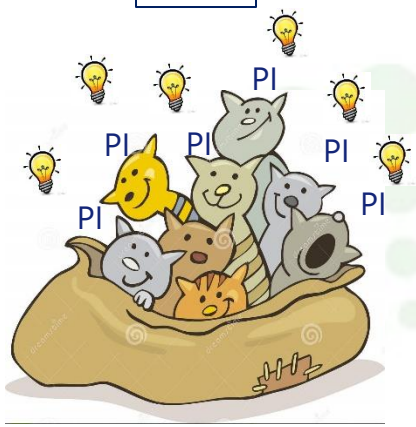
HUB PROPOSALS

Battery HUB

- Elaboration
- Consultation
- Documentation
- Web pages
- Announcement to User Community (4th October 2022)
- Integration in NEXT UP

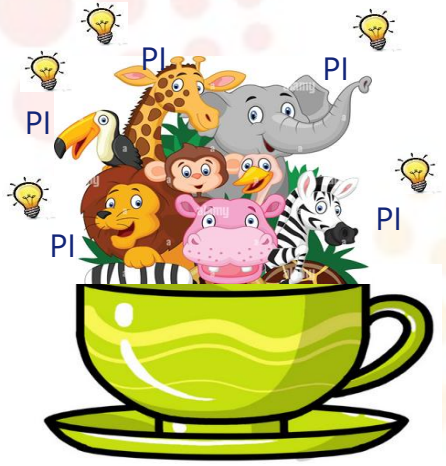
- What is a HUB Proposal?
- Submission and Duration of a HUB Proposal
- Governance
- Sharing of knowledge and data
- Proposers – who can apply?
- Evaluation procedure
- Reporting
- Instructions and templates for submitting a HUB proposal
- Instructions and templates for submitting a HUB report

BAGS



Block **A**llocation **G**roups

HUBs



A hub of experts

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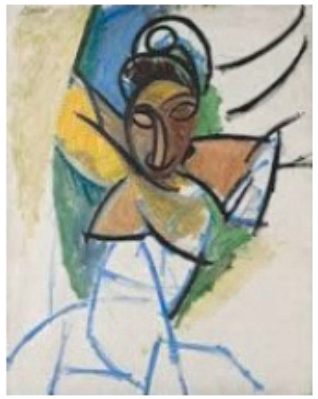
Enabling new access models – Community Access Pilot Proposals

Historical Materials BAG



The Courtauld · école normale supérieure paris-saclay · université PARIS-SACLAY · Universiteit Antwerpen · SCITEC · POLITECNICO MILANO 1863 · RIJKS MUSEUM · TU Delft · UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH · IRCP Institut de Recherche de Chimie Paris · MINISTÈRE DE LA CULTURE

molecules — MDPI

Article

The "Historical Materials BAG": A New Facilitated Access to Synchrotron X-ray Diffraction Analyses for Cultural Heritage Materials at the European Synchrotron Radiation Facility

Marine Cotte [1,2,*], Victor Gonzalez [3,*], Frederik Vanmeert [4,5,*], Letizia Monico [4,6,7,*], Catherine Dejoie [1], Manfred Burghammer [1], Loïc Huder [1], Wout de Nolf [1], Stuart Fisher [1], Ida Fazlic [1,8], Christelle Chauffeton [9,10,11], Gilles Wallez [9,11,12], Núria Jiménez [13], Francesc Albert-Tortosa [13], Nati Salvadó [13], Elena Possenti [14], Chiara Colombo [14], Marta Ghirardello [15], Daniela Comelli [15], Ermanno Avranovich Clerici [4,16], Riccardo Vivani [17], Aldo Romani [6,7], Claudio Costantino [6,7], Koen Janssens [4,8], Yoko Taniguchi [18], Joanne McCarthy [1], Harald Reichert [1] and Jean Susini [1,†]

Shock BAG

Imperial College London Institute of Shock Physics — William Proud, Simon Bland

cea — Arnaud Sollier

3SR — Pascal Forquin

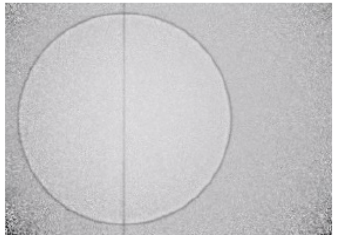
first light — Nick Hawker, Hugo Doyle

Department of Engineering Science, University of Oxford — Daniel Eakins, David Chapman, Clive Siviour

HZDR Helmholtz Zentrum Dresden Rossendorf — Dominik Kraus, Jörg Grenzer

University of Southampton — Fabrice Pierron

NRCN — Amitay Cohen, Arno Joshef-Hai, David Levi-H



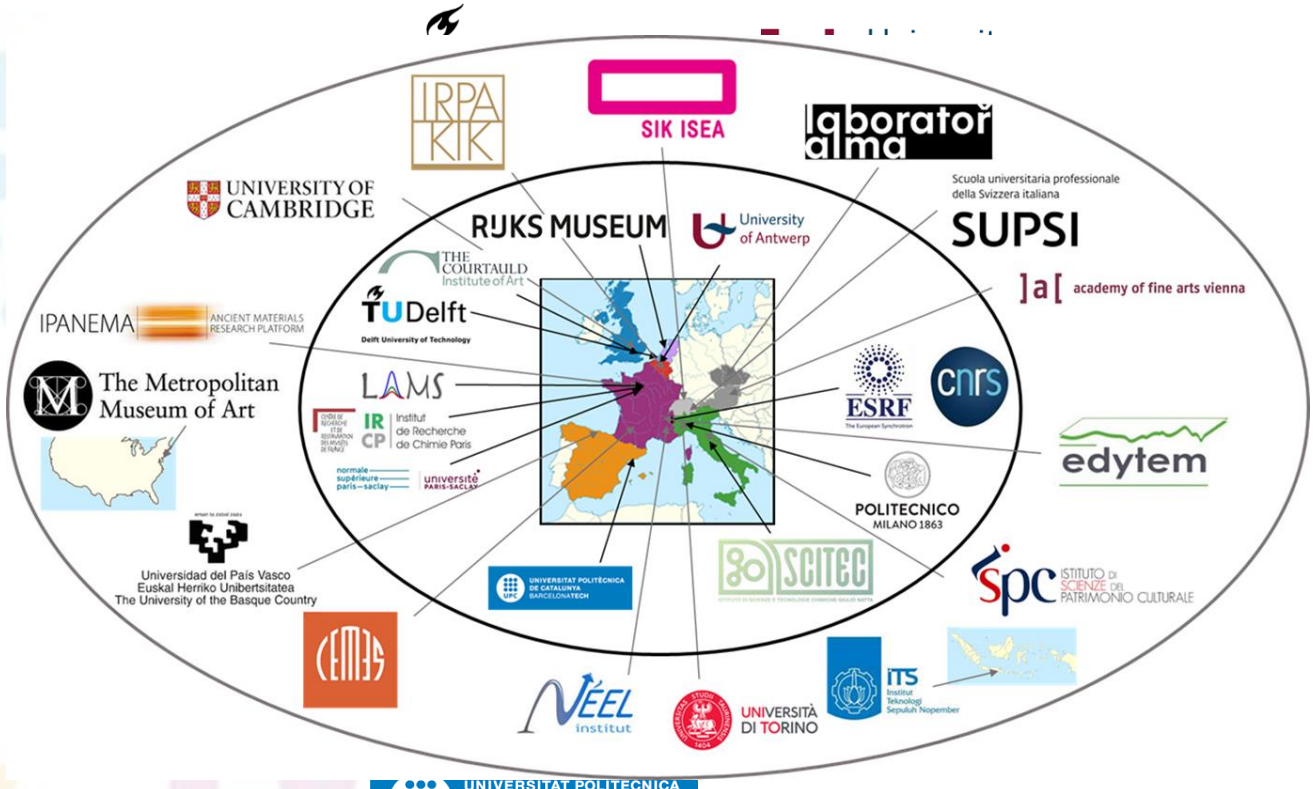
Collapse dynamics of spherical cavities in a solid under shock loading
Escauriza et al., Sci. Rep. May 2021
Time resolved radiography
ID19 - ESRF

Battery HUB

Accelerating Battery Characterization Using Neutron and Synchrotron Techniques: Toward a Multi-Modal and Multi-Scale Standardized Experimental Workflow.
D. Atkins *et al. Advanced Energy Materials*, 2021, 2102694.
DOI:10.1002/aenm.202102694

prizon 2020 research and innovation programme under grant agreement No. 870313.

The “historical materials” BAG



First ring: partners of the initial BAG proposal
Second ring: indirect partners through collaborations

11 European teams

- ENS Paris-Saclay (former Rijksmuseum): V. Gonzalez
- Rijksmuseum (former University of Antwerp, KIKIRPA): F. Vanmeert
- CNR-SCITEC: L. Monico
- ESRF: M. Cotte
- Courtauld Institute of Art: A. Nevin, A. Burnstock
- Politecnico di Milano: D. Comelli
- Rijksmuseum: K. Keune
- IRCP/C2RMF: I. Reiche
- Universitat Politècnica de Catalunya: N. Jiménez
- IRCP: G. Wallez
- TU Delft: M. Alfeld

https://www.esrf.fr/BAG/HG172

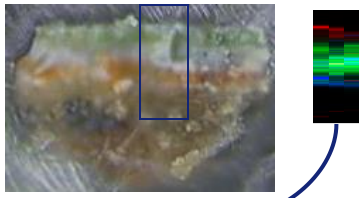
Heritage-bag@esrf.fr

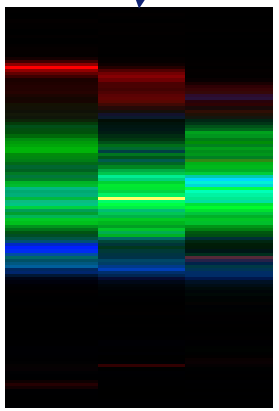
STREAMLINE has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 870313.

Ebs in practice : a smaller and brighter beam

Dec 2006
map size: 150 × 60 µm²
pixel size: 1 × 20 µm²
15s / pixel
1h52 for 450 pixels

Nov 2021
map size: 800 × 370 µm²
pixel size: 1 × 1 µm²
0.016s / pixel
1h18 for 296 000 pixels

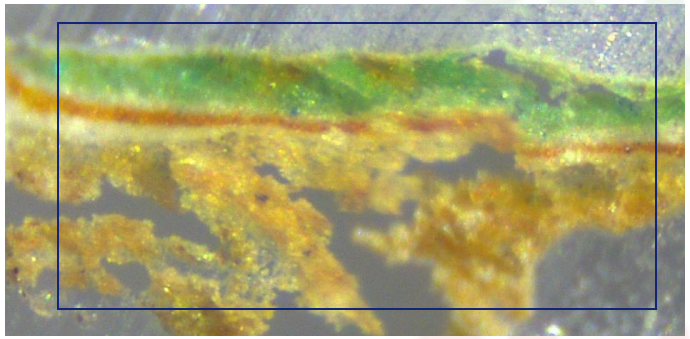


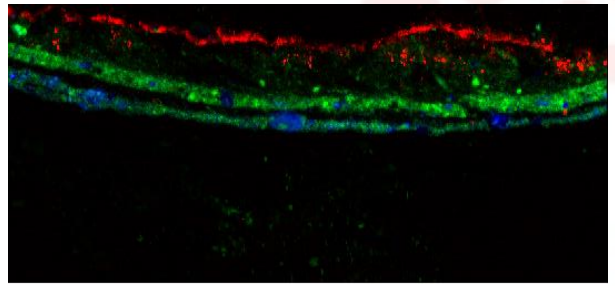


100µm

palmierite hydrocerussite

cerussite





Courtesy: Marine Cotte

- More samples
- Larger fields of view
- Higher resolution
- Better statistics

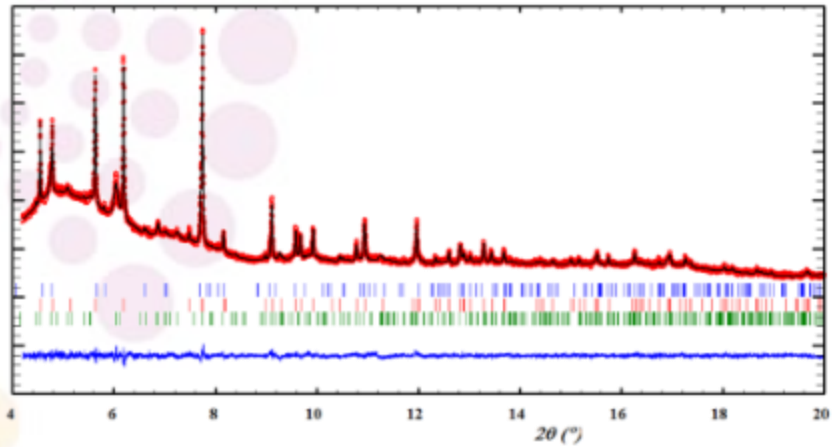
om the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

The historical bag beamlines

ID22 : High angular resolution XRD

- Energy: ~35 keV
- Scan range 2θ: 3 – 20°
- Analysis time: ~20 min/powder;~2 h/historical sample
- Instrumental function 2θ (FWHM of (111) Si peak) ~ 0.0027°
- Samples in capillaries

⇒ **precise and sensitive detection of crystalline phases, their identification, and the characterization of their microstructural and structural properties**



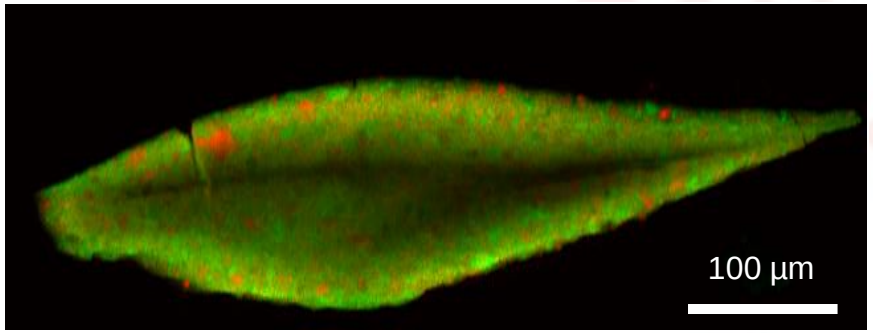
2 days every 6 months
Local contact : Catherine Dejoie
catherine.dejoie@esrf.fr

ID13 : High lateral resolution XRD

- Energy: ~13 keV
- Analysis time: ~10 min -2 h/map (15ms/ pixel)
- Beam size ~ 2×2μm²
- Samples as thin sections (preferable) or cross-sections

⇒ **stratigraphical distribution of crystalline phases at the micrometer scale**

Courtesy: Marine Cotte

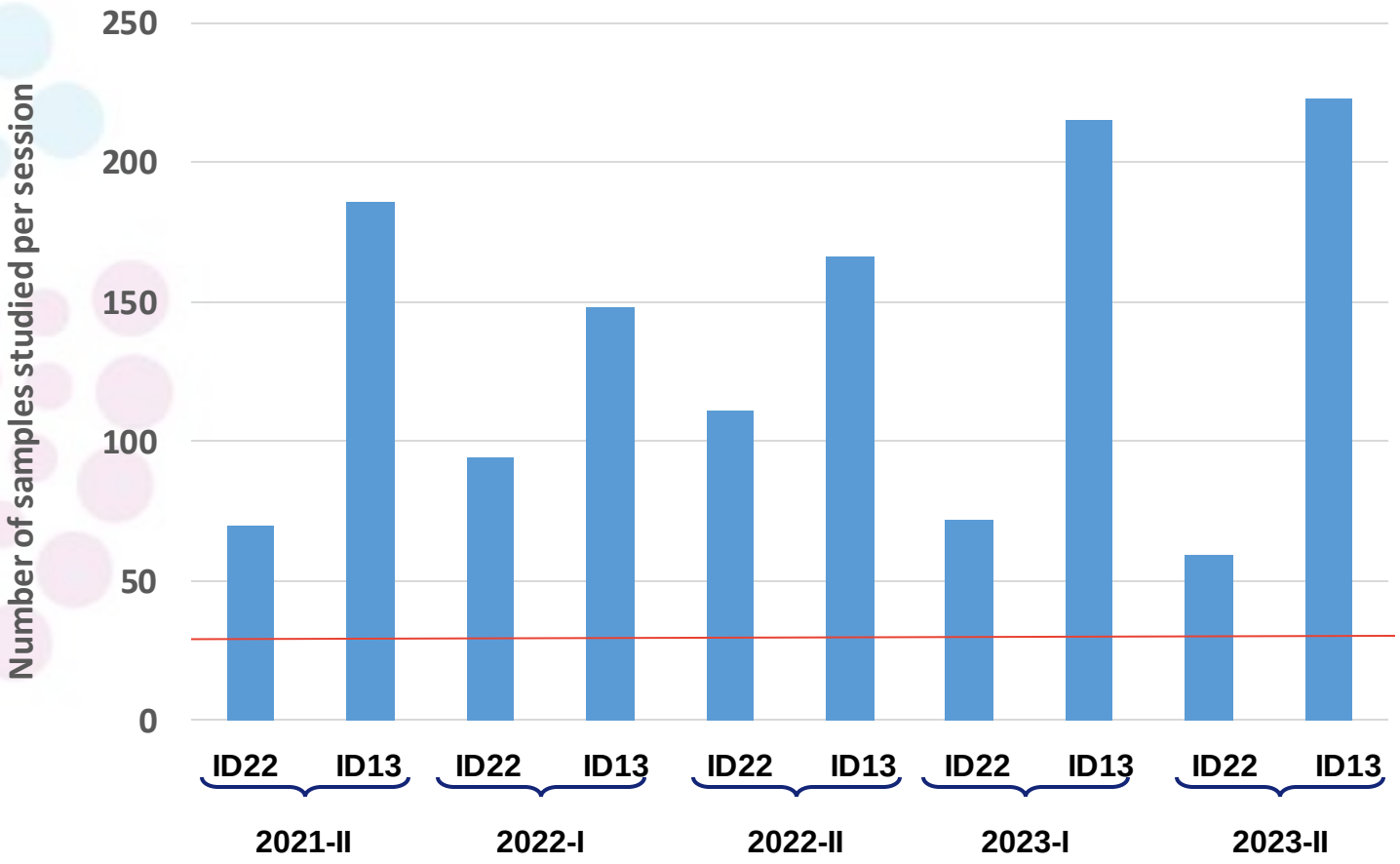


4 days every 6 months
Local contact : Manfred Burghammer
burgham@esrf.fr

s Horizon 2020 rese

The “historical materials” block allocation group: a high throughput!

The success of the BAG relies on the capacity to analyze tens of samples per experiment.



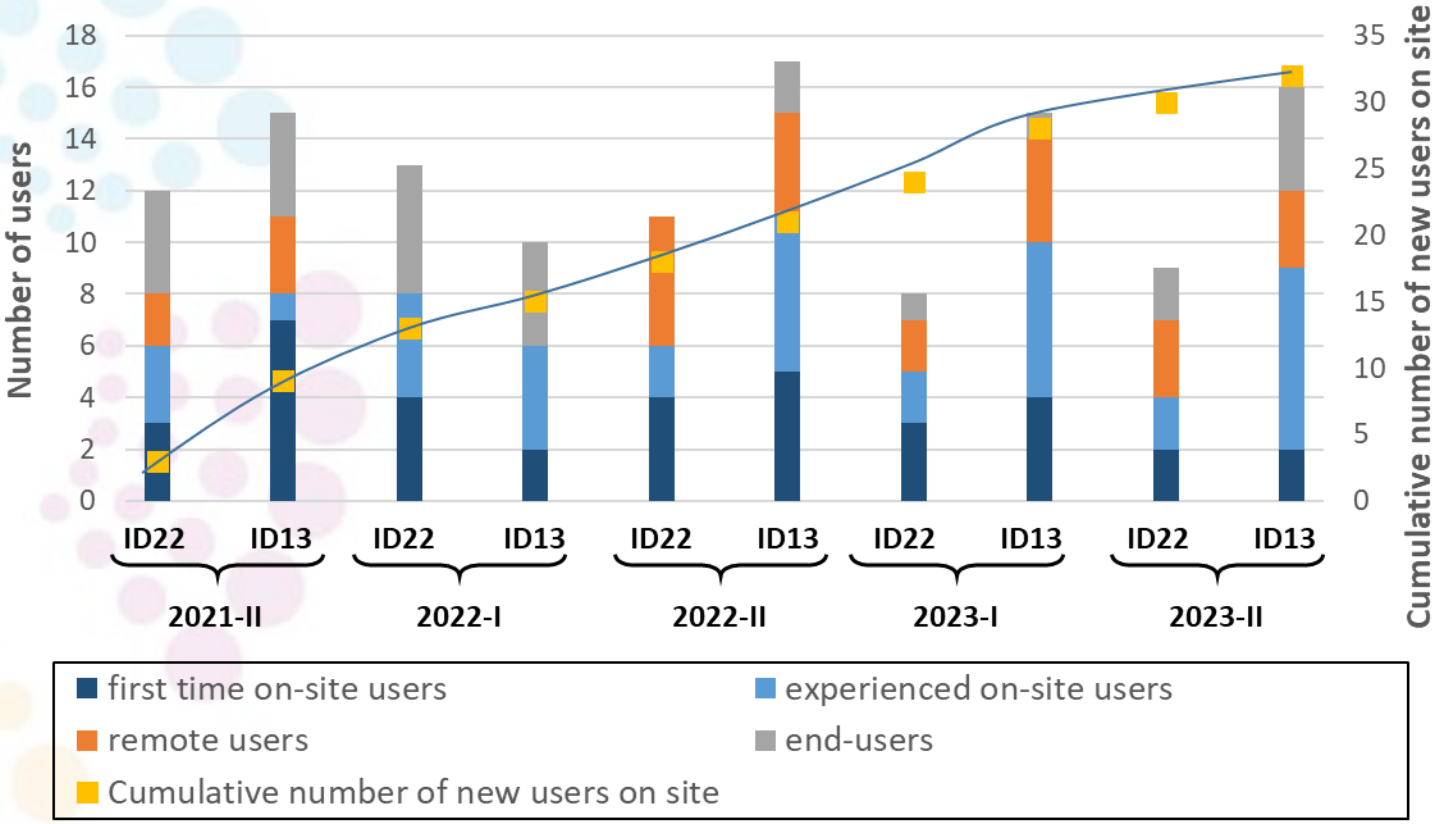
Courtesy: Marine Cotte

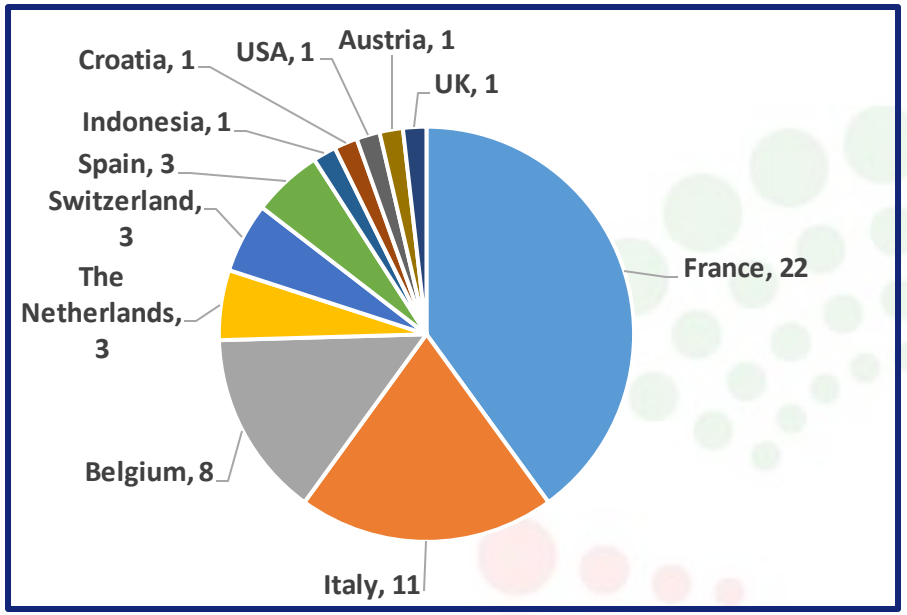
Before BAG or with standard proposal:
~<30 samples/ experiment

STREAMLINE has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 870313.

The “historical materials” block allocation group: a very efficient way to train new users

BAG gives an easy access to beamtime, in particular to **new users**, who can be trained by working with expert users

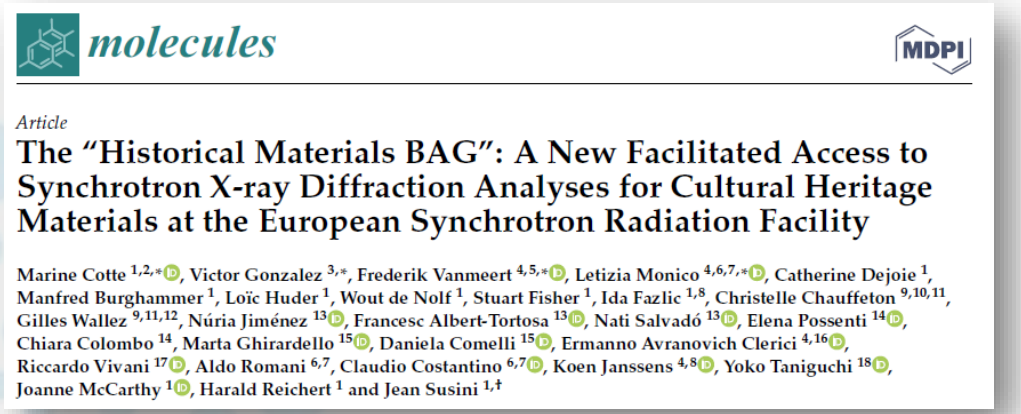




Courtesy: Marine Cotte

STREAMLINE has received funding from the European Union’s Horizon 2020 research and innovation pr

Some recent outcomes of the Historical materials bag


molecules

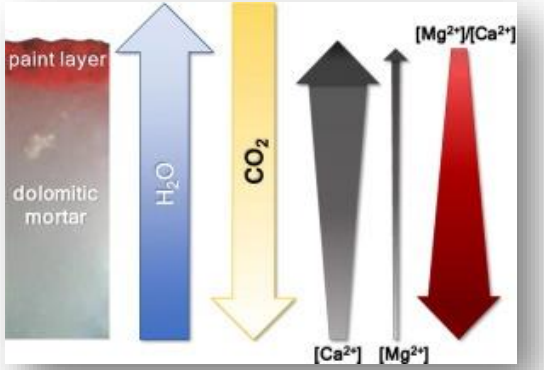
MDPI

Article

The "Historical Materials BAG": A New Facilitated Access to Synchrotron X-ray Diffraction Analyses for Cultural Heritage Materials at the European Synchrotron Radiation Facility

Marine Cotte [1,2,*], Victor Gonzalez [3,*], Frederik Vanmeert [4,5,*], Letizia Monico [4,6,7,*], Catherine Dejoie [1], Manfred Burghammer [1], Loïc Huder [1], Wout de Nolf [1], Stuart Fisher [1], Ida Fazlic [1,8], Christelle Chauffeton [9,10,11], Gilles Wallez [9,11,12], Núria Jiménez [13], Francesc Albert-Tortosa [13], Nati Salvadó [13], Elena Possenti [14], Chiara Colombo [14], Marta Ghirardello [15], Daniela Comelli [15], Ermanno Avranovich Clerici [4,16], Riccardo Vivani [17], Aldo Romani [6,7], Claudio Costantino [6,7], Koen Janssens [4,8], Yoko Taniguchi [18], Joanne McCarthy [1], Harald Reichert [1] and Jean Susini [1,†]

Picasso's *Femmes*
M. Ghirardello, *Microscopy and micro analysis*



Carbonation of fresco paintings, N. Oriols, *Cement and Concrete Research*

Cadmium yellow degradation in Miro's paintings, N. Gomez Lobon, *Heritage Science*

Black stains on the passepartout of Codex Atlanticus Folio 843 by Leonardo da Vinci, N. Guarnieri, *Scientific Reports*

Architectural Bricks from Khorsabad and Susa Sites: Characterization of Black Glazes, E. Beauvoit, *Heritage*

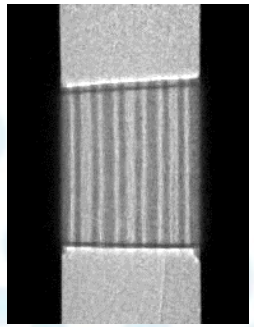
Since first beamtime in 2020-II:

- 14 publications
- 25 oral presentations
- 15 posters

Courtesy: Marine Cotte

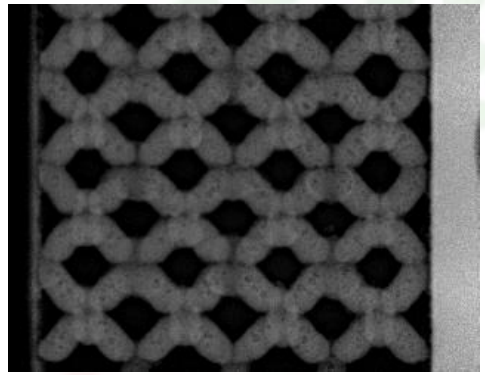
nding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

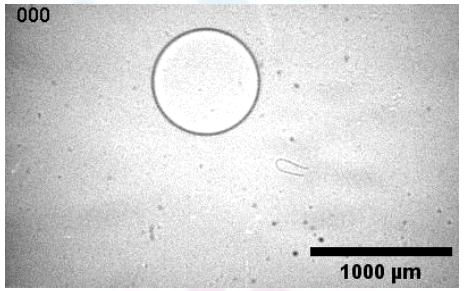
THE “SHOCK” BAG



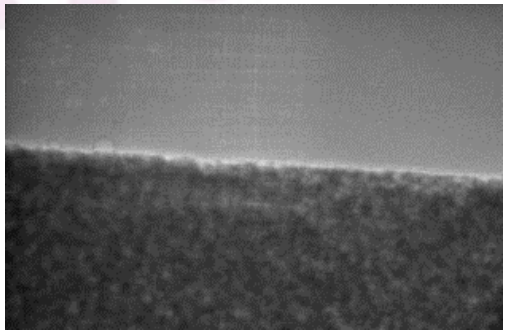
The Shock BAG coordinates and promotes access to high-resolution X-ray imaging for the study of **materials under rapid and extreme loading**. The BAG pools together shared equipment, personnel and expertise to underpin and enhance the science at the intersection of **X-rays and dynamically-compressed matter**.

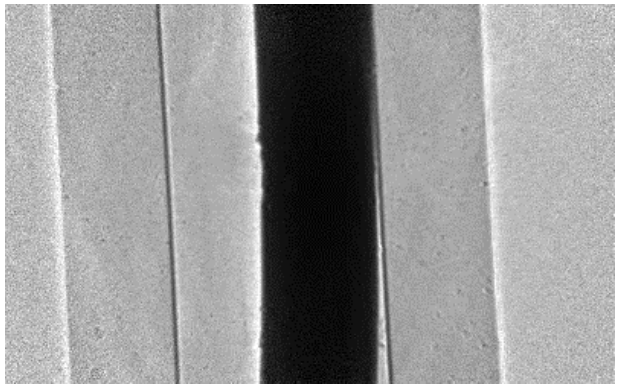
Courtesy: Alexander Rack

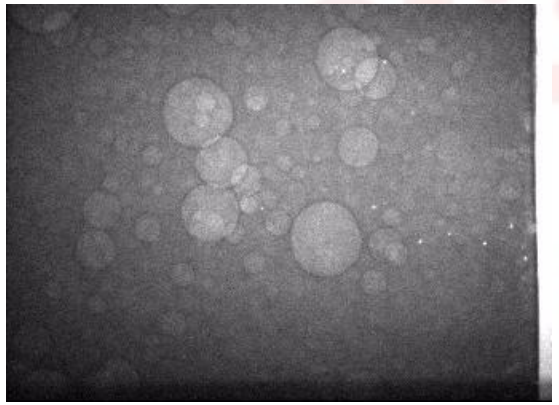




The combination of the research tools grouped in the BAG will enable us to generate and probe the **properties of matter at extreme conditions**, from damage in composites panels, to the physics of earthquakes, to the formation of asteroids in the early solar system.







STREAMLINE has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 870313.

SHOCK BAG: Partners

Courtesy: Alexander Rack

Imperial College London – Institute of Shock Physics
William Proud, Simon Bland

cea
Arnaud Sollier

3SR
Pascal Forquin

cnrs – ACO-CHOCOLAS – Matériaux sous Hautes Vitesses de Déformation – Groupe de recherche cnrs
Thibault De Resseguier, Laurent Berthe

first light
Nick Hawker, Hugo Doyle

Department of Engineering Science – University of Oxford
Daniel Eakins, David Chapman, Clive Siviour

Univerzita Pardubice
Jiri Pachman

HZDR – Helmholtz Zentrum Dresden Rossendorf
Jörg Grenzer, Dominik Kraus

Universitas Osloensis MDCCCXI – UGA Université Grenoble Alpes
Francois Renard, Benoit Cordonnier

Manchester 1824 – The University of Manchester
Neil Bourne

Uni Freiburg – Fraunhofer EMI
Georg Ganzenmüller

University of Southampton
Fabrice Pierron

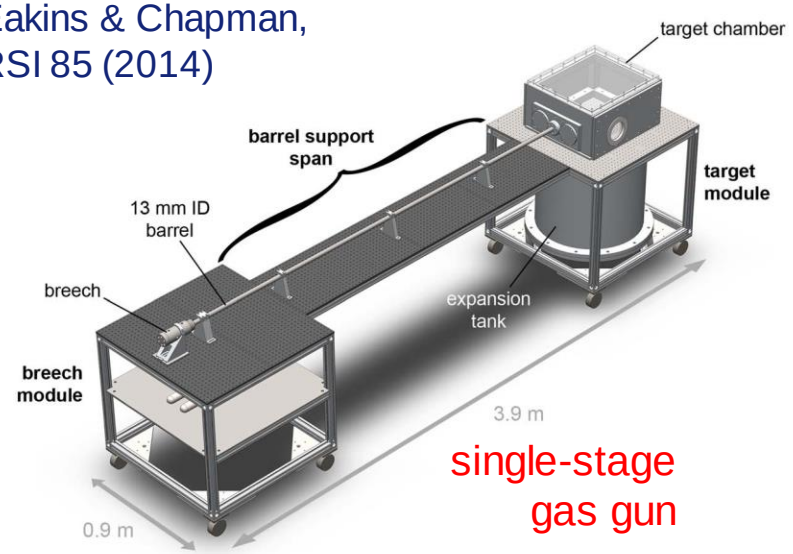
NRCN
Amitay Cohen
David Levi-Hevroni

Lawrence Livermore National Laboratory
Minta Akin

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

SHOCK BAG: Platforms *Courtesy: Alexander Rack*

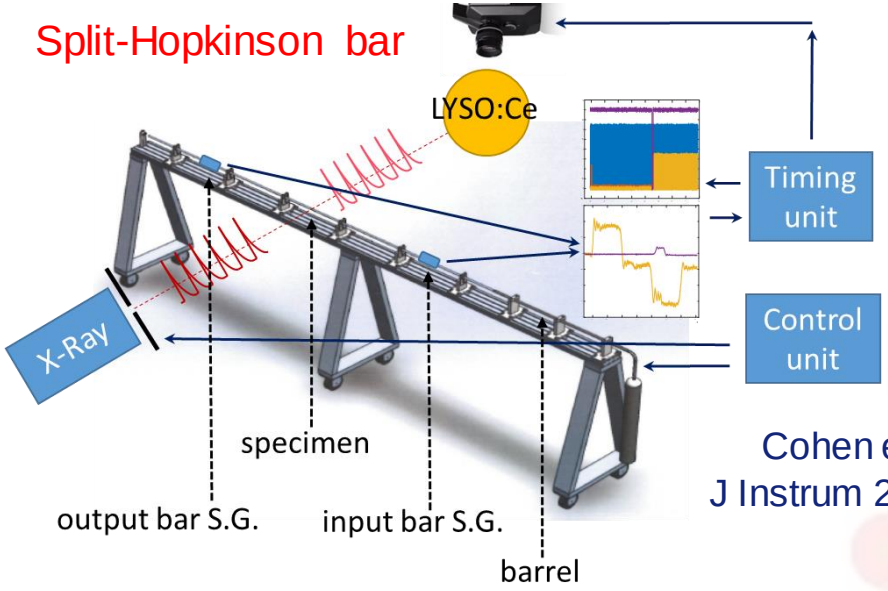
Eakins & Chapman,
RSI 85 (2014)



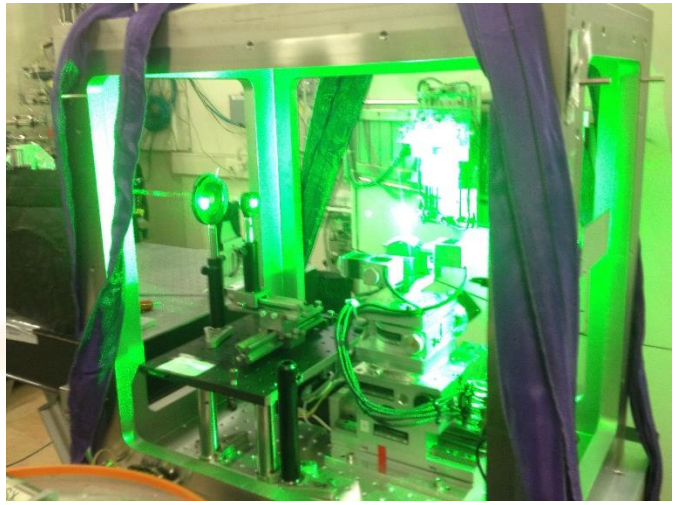
single-stage gas gun

Olbinado et al.,
J Phys D 2018

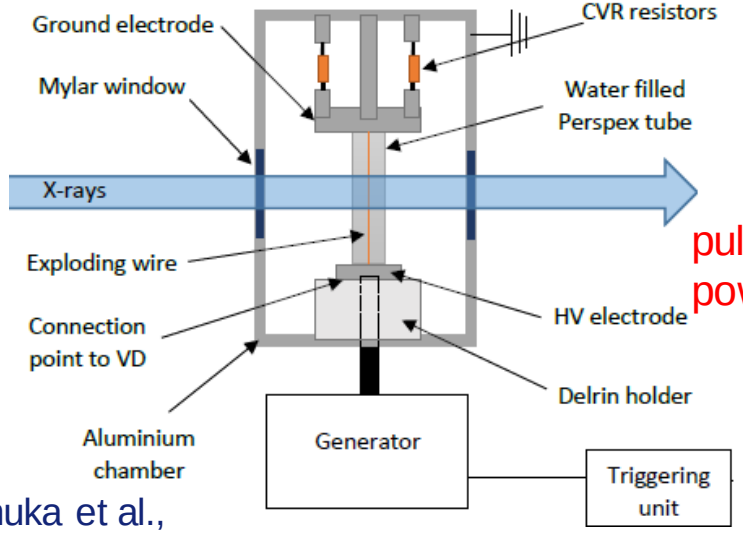
Split-Hopkinson bar



Cohen et al.
J Instrum 2018



pulsed laser



pulsed-power

Yanuka et al.,
J Appl Phys 2018

energetic materials

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SHOCK BAG @ ESRF and the EBS

"Video about the BAG: https://youtu.be/s3uDECwnFrw
#EBSstories New SHOCK Beamtime Allocation Group at the ESRF

"We have at ID19 now a unique combination of loading platforms which can be coupled to our high-speed X-ray imaging facility. Elsewhere in Europe there is nothing like that, and the BAG allows us to gather the corresponding user community to fully exploit these unique capabilities."

Alexander Rack (ID19)

"Research using this equipment ranges from finding how impact triggers earthquakes to improving materials for industrial applications. We work with a number of different industries, civil aerospace for example, or automotive….
What the Shock BAG allows us to do is to offer these platforms to the wider community so they don't have to build them, and also to provide expertise in the operation of those systems."

Daniel Eakins (Oxford, UK)

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

THE PILOT BATTERY HUB – MULTI-SCALE, MULTI-TECHNIQUE TO SEE THE INVISIBLE IN BATTERIES

BATTERY PILOT HUB

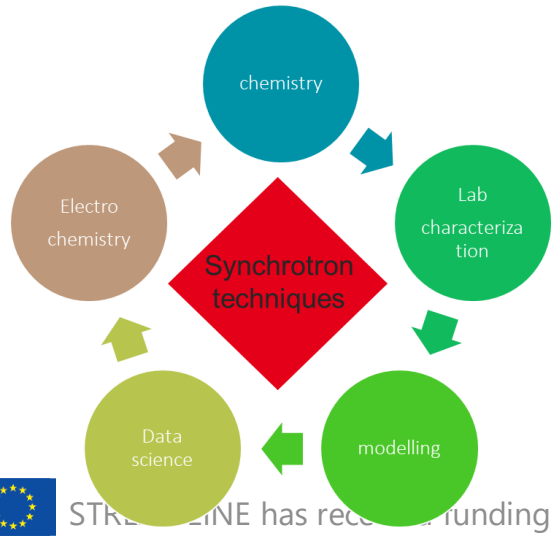
2021-2024 - 20 beamlines
8-10 experiments every 6 Months
70 researchers from CEA and partners
Phase 2 = a European consortium

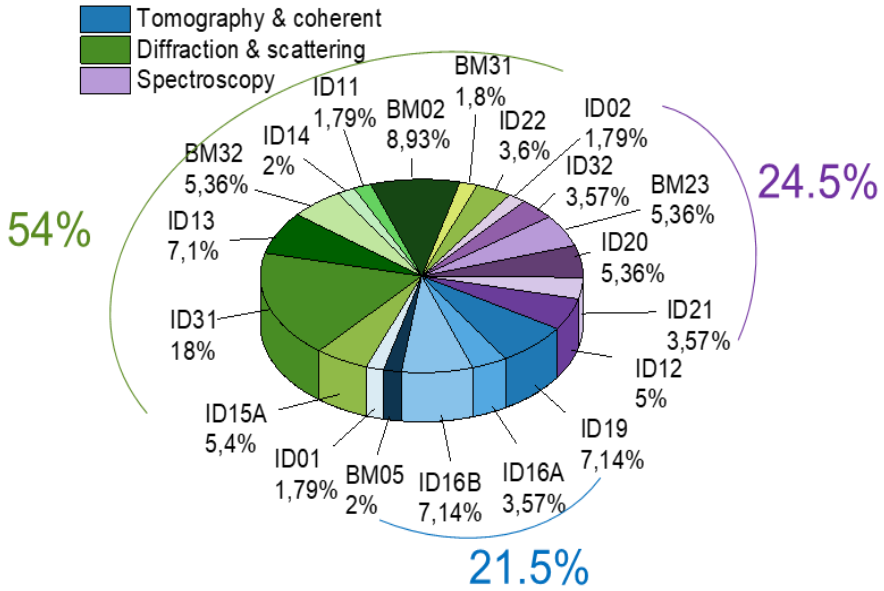
A 3-year program to accelerate battery research using synchrotron techniques and perform advanced characterization of chemistries & reactions at multiscales

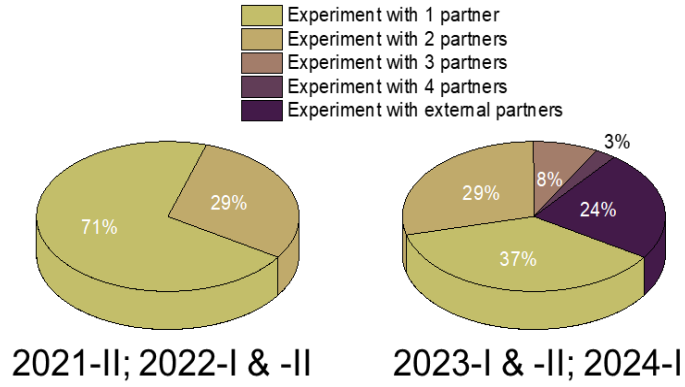
Goal : improve performance, durability and safety ; invent batteries of the future.

Courtesy: Sandrine Lyonnard

Correlative multimodal characterization techniques







STRE[illegible]LINE has rec[illegible] funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

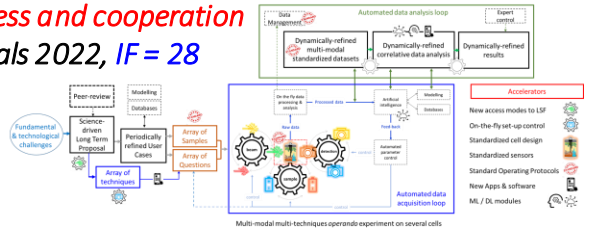
Courtesy: Sandrine Lyonnard

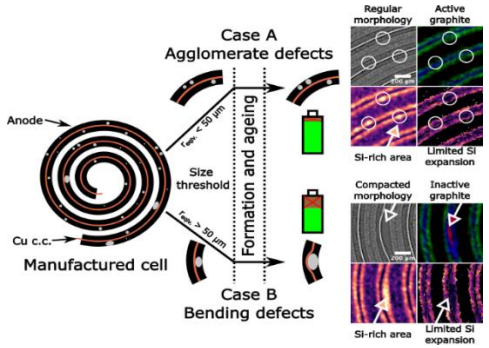
Scientific Highlights

Crucial information was obtained in the hub towards safer, cost-effective, higher energy density, and more sustainable batteries

- Degradation and safety studies
- Properties of new materials as solid state electrolytes
- Operando investigation of model and real (commercial) systems
- Studying batteries beyond Li-ion and current chemistries

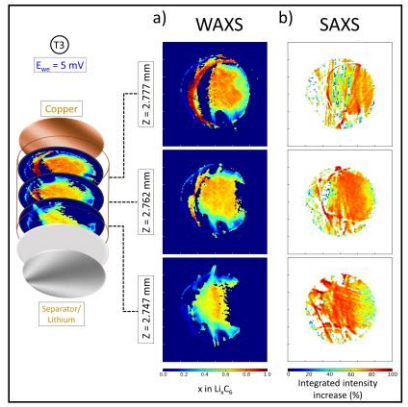
New modes of beam access and cooperation
Advanced Energy Materials 2022, IF = 28



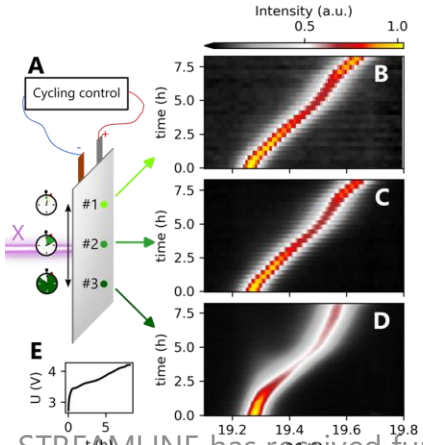


Where do defects come from in real cells
Energy & Environmental Science, 2024, IF = 32.5

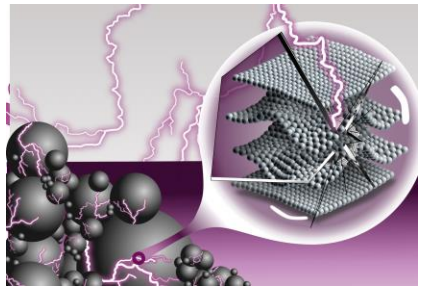
Charge dynamics in anodes during relaxations
Adv. Energy Materials 2023 (IF = 28)



Quantitative beam evaluation
ACS Energy Letters 2022, IF = 22



Unified structure of layered oxide cathodes
Energy & Environmental Science, 2024, IF = 32.5



Cover of the journal

Mean IF of HUB publications > 20

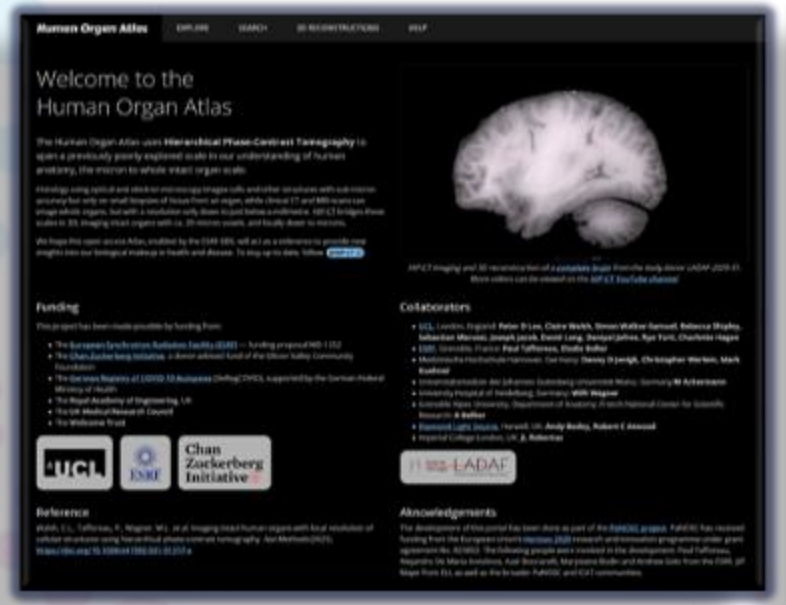
Publications	Number
Published	8
In review	7
To be submitted (in 3 M)	13
Many more in pipeline!	

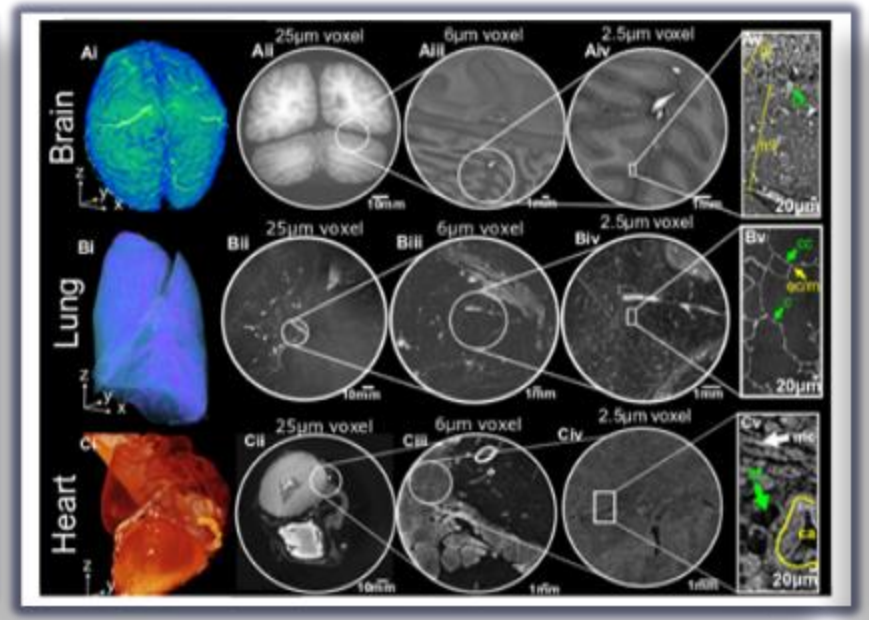
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme und

The Human Organ Atlas Hub (HOAHub)

GOALS

Creation of a physical and virtual Hub which uses HiP-CT to scan whole human organs with local cellular resolution, producing a ''***Human Organ Atlas in Health and Disease***''.



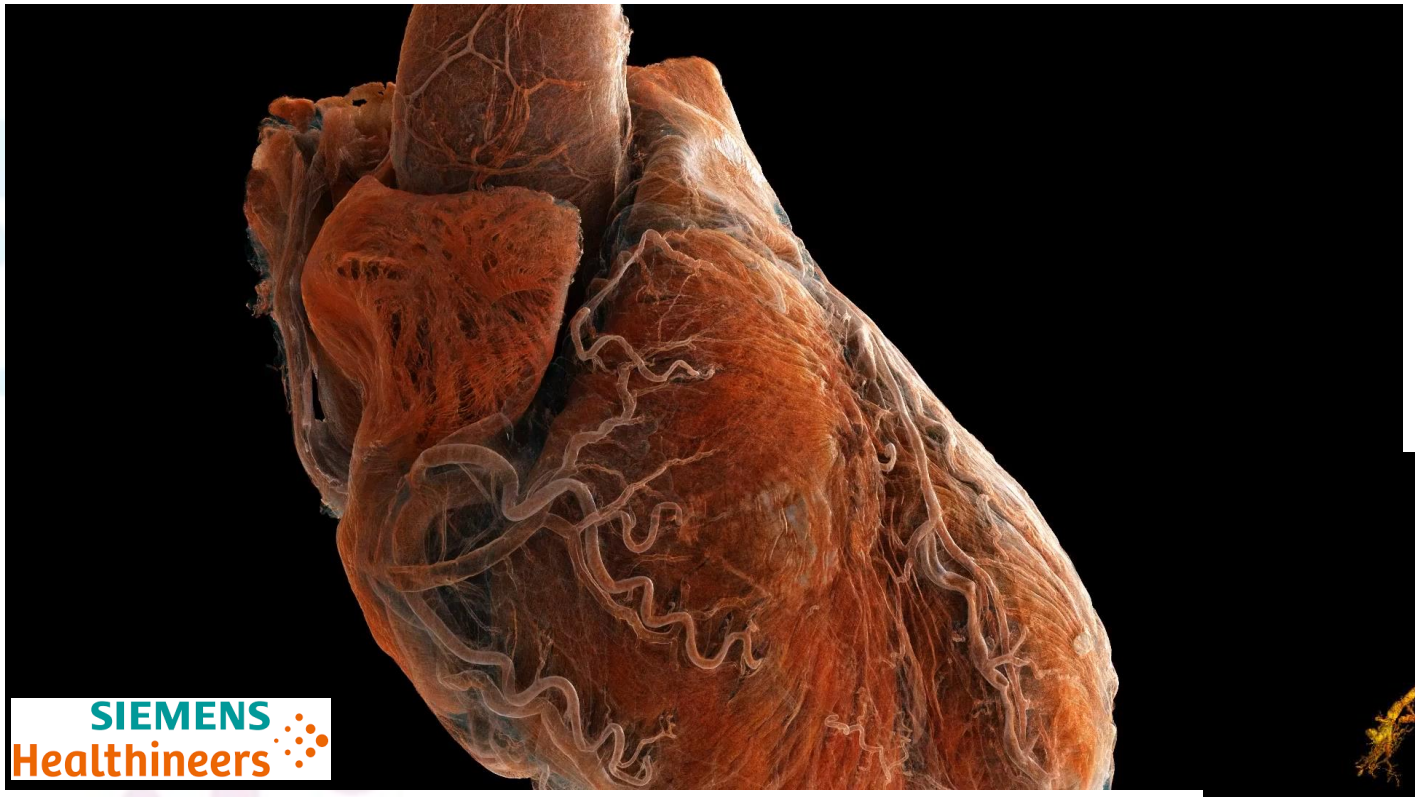


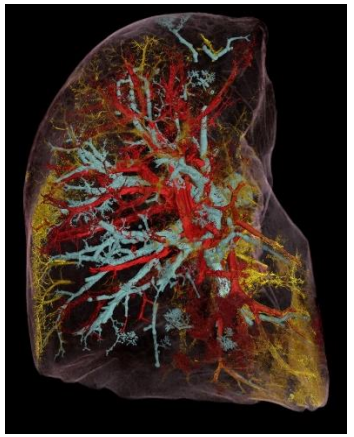
EXPECTED IMPACT

- Advance biological, medical and computational fields
- Provide anatomical training resources
- Set a new Gold Standard for validating CT, MRI and 3D histology
- Enable new clinical insights and potentially improved diagnosis
- Data re-use to support clinical AI/ML learning systems

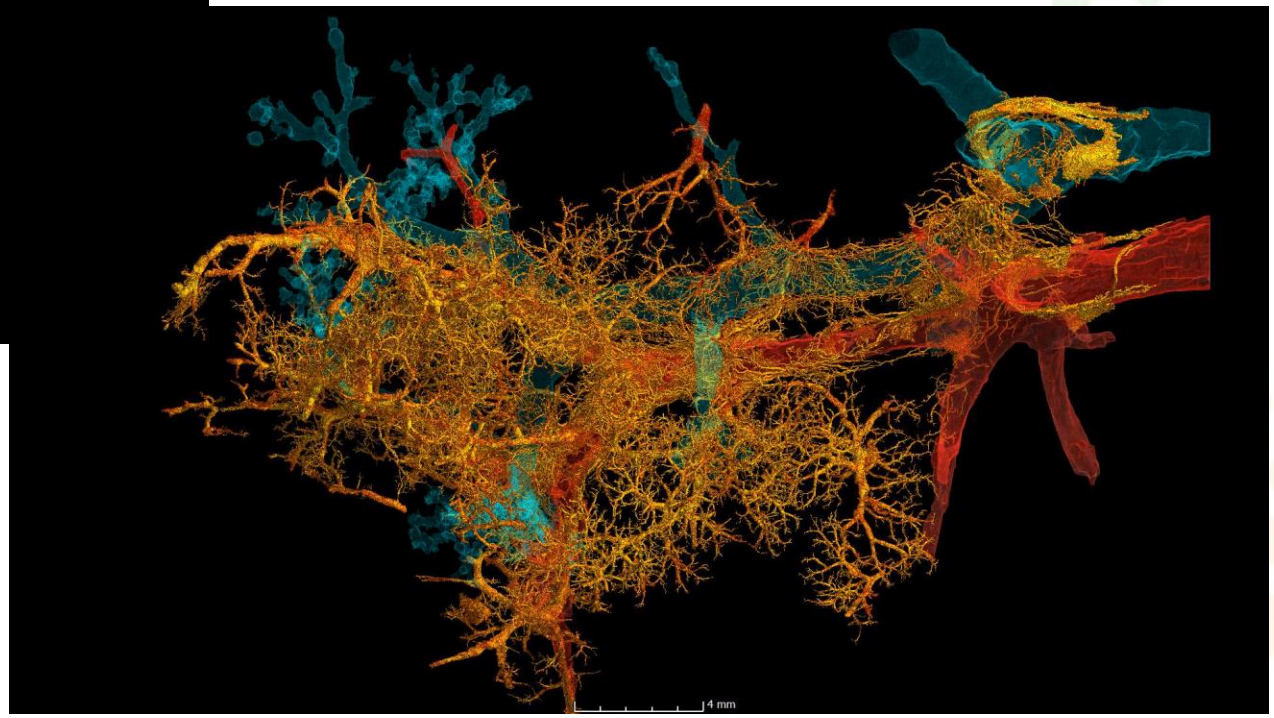
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

The Human Organ Atlas: a new insight into the human body





COVID-19 affected lung:
Blue: Airways
Red: Still functional blood vessels
Orange: Clotted blood vessels



HUMAN ORGANS ATLAS
Already over 40 groups worldwide collaborating to provide samples and utilise/share the results

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Courtesy: Peter Lee

What is the HOAHub?

HOAHub

Our Vision: To create a synergistic interdisciplinary group exchanging ideas, best practice, physical and software resources to make a highly efficient pipeline for HiP-CT, from autopsy to biomedical impact, solving some of the most relevant global biomedical questions


Peter Lee
Co-Chair/PI

Claire Walsh
Director/PI

Anastasia Yendiki
PI, Harvard Medical School

Danny Jonigk
PI, RWTH Aachen University

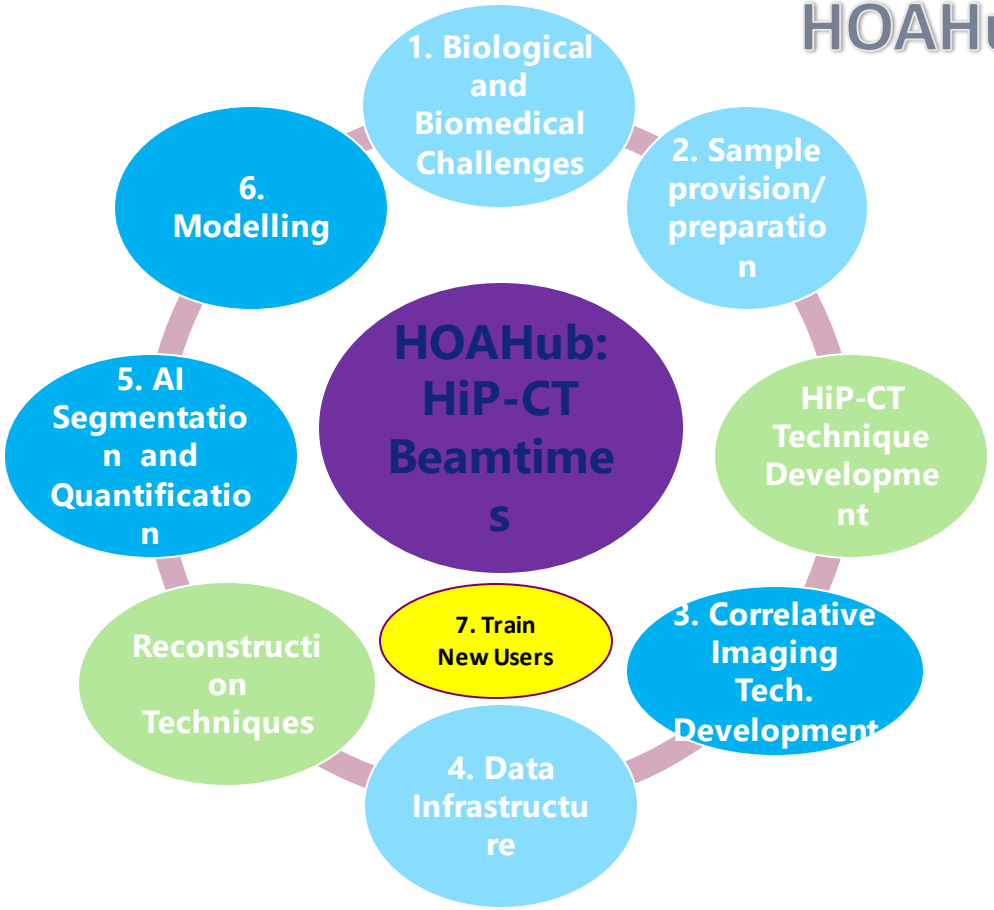
Max Ackermann
Co-Chair/PI
Johannes Gutenberg University Mainz

Stijn Verleden
PI, University of Antwerp

Alexandre Bellier
PI, Grenoble Alpes University and LADAF

Bernadette de Bakker
PI, Amsterdam UMC

https://mecheng.ucl.ac.uk/HOAHub/people/



Ca. 80 organs to date: 28 lung/lung lobes, 16 brains, 24 kidneys, 21 hearts, 2 livers, 2 spleens, 8 prostates, and hundreds of local cellular level resolution zooms …

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Were does all data go?

Courtesy: Peter Lee

HOAHub

Human Organ Atlas EXPLORE SEARCH ← BACK TO RESULTS

Complete heart from the body donor LADAF-2020-27

Description

Complete scan at 25.08um performed by HiP-CT on the beamline BM05 of the heart from the body donor LADAF-2020-27 using quarter-acquisition protocol.

DOI	
Users	Paul Tafforeau, Claire Walsh, Willi L. Wagner, Daniyal J. Jafree, Alexandre Bellier, Christopher Werlein, Mark P. Kuhnel, Elodie Boller, Simon Walker-Samuel, Jan Lukas Robertus, David A. Long, Joseph Jacob, Sebastian Marussi, Eeline Brown, Natalie Holroyd, Danny D. Jonigk, Maximilian Ackermann, Peter D. Lee
Technique	Hierachical Phase-Contrast Tomography
Instrument	BM05, ESRF

Patient

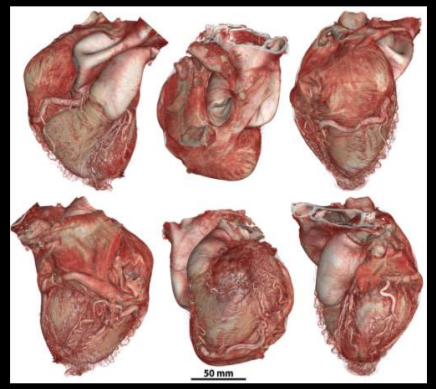
Institute	Laboratoire d'Anatomie des Alpes Francaises
Number	LADAF-2020-27
Age	94 yo
Sex	female
Weight	45 kg
Height	unknown
Medical info	right sylvian and right cerebellar stroke, cognitive disorders of vascular origin, depressive syndrome, atrial fibrillation and hypertensive heart disease, micro-crystalline arthritis (gout), right lung pneumopathy (3 before death), cataract of the left eye, squamous cell carcinoma of the skin (left temporal region)

Sample

TXT LADAF-2020-27_heart_25.08um

ZIP 25.08um_2020-27_heart_pag-0.24_0.41_jp2_

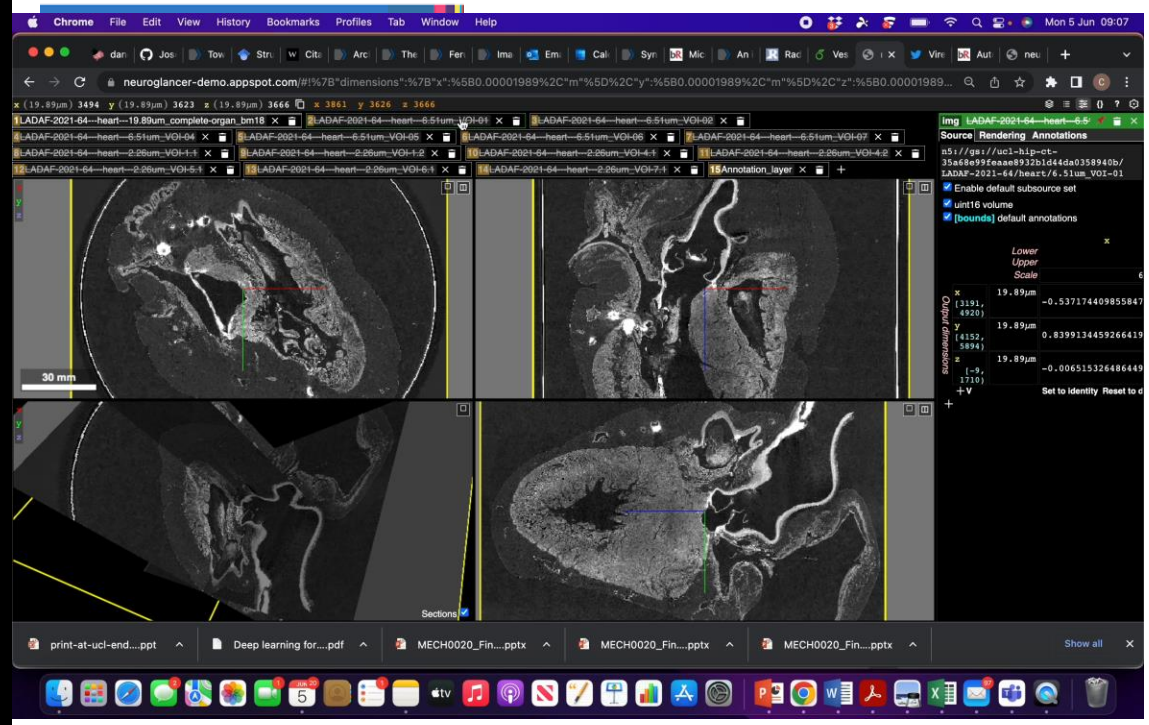
ZIP 50.16um_2020-27_heart_pag-0.24_0.41_jp2_



google/
neuroglancer

WebGL-based viewer for volumetric data

47 Contributors · 55 Used by · 2 Discussions · 847 Stars · 266 Forks



https://human-organ-atlas.esrf.eu/ : *An **open-access database** developed as part of the **EU project***

PaNOSC

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313

Enabling new access models – Fast Access

Idea
Submitted proposal
Scientific quality
Technical feasibility
Safety
Approved proposal
Scheduling
Sample shipping
Safety
Travel / GH
Beamline set-up
Data acquisition
Sample shipped back
Data analysis and interpretation
Report
Publication
Cite data DOI
Public data

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

Fast Access

Sample feasibility and short measurements	Hot topics	Standard measurements
• Assess experiment feasibility • Assess sample quality • Short measurement to complete publication or thesis • Short measurement not justifying STD proposal (<1 shift)	• Scientific projects of very high scientific or societal importance • Fast access primordial (societal importance (COVID), time pressure (Hayabusa), competition)	• Out-of-deadline call for measurements with fixed set-up • Maximise number of research groups that can be served by the facility • Optimise output vs beamtime • Samples for setup, rather than setup for samples

Challenging for an international facility with country balance obligations, but vital to maximise impact and output
Formalise existing solutions so they can be accounted for and reported properly

STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

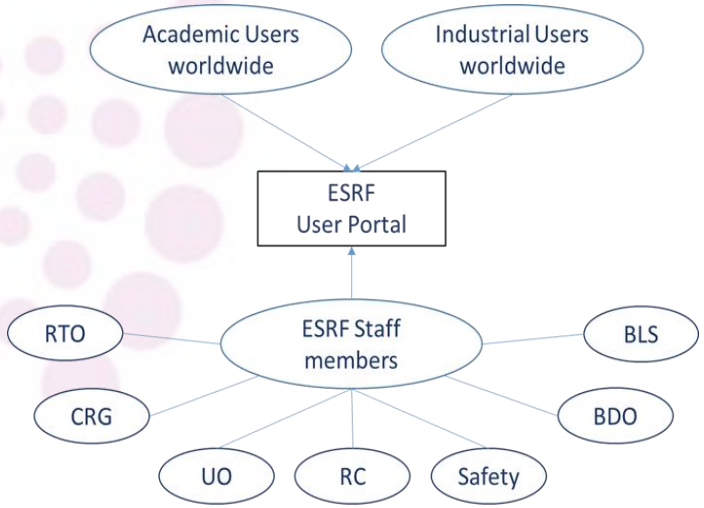
ENABLER: New EBS eXperiment Tool – User Portal "NEXT-UP"

Update of user administrative procedures

- Update existing workflows
- Integrate new workflows
- Facilitate and enhance user experience
- Manage higher throughput

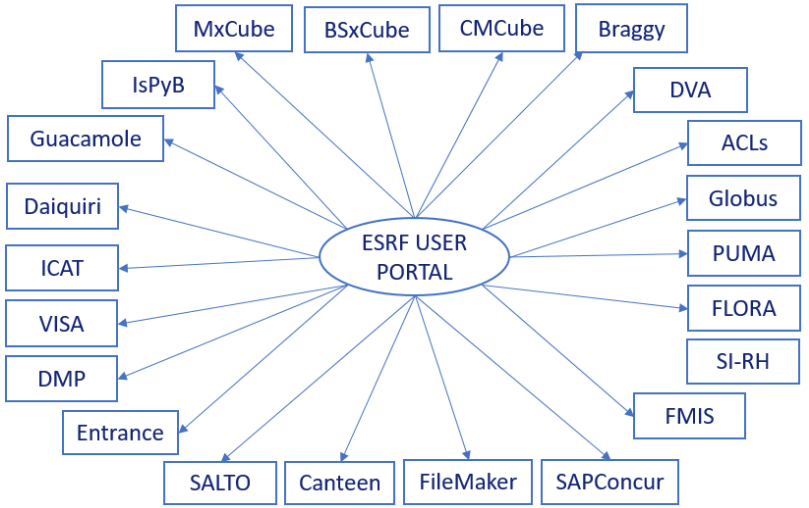
ESRF USER PORTAL replacement

- Modern and easy to use interface
- Change technology for future proofing
- Modularisation of functionalities
- Restructure of database architecture



Integrating all ESRF user processes for:

- **Modern needs**
- **Expectations**
- **Capacities**



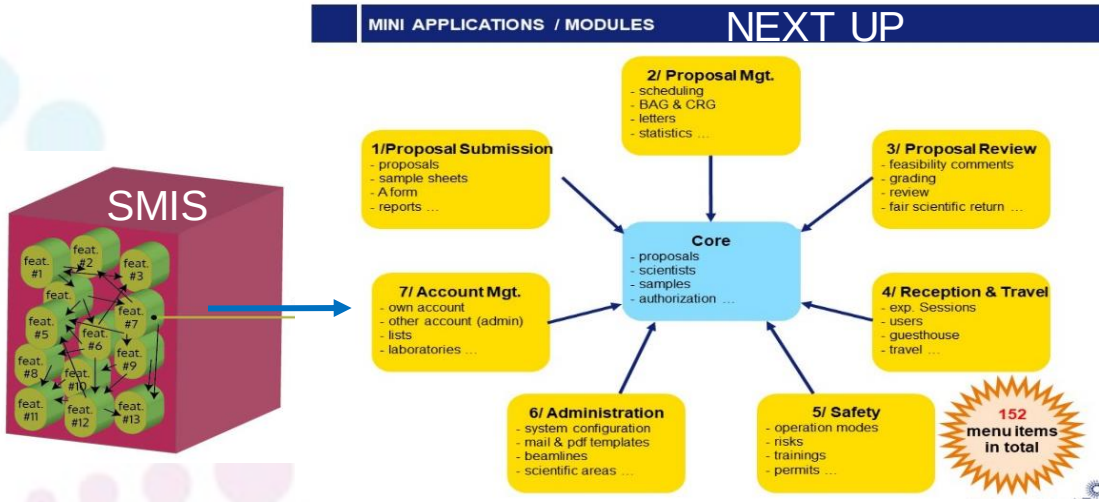
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

NEXT UP: Why and how are we changing the ESRF user portal

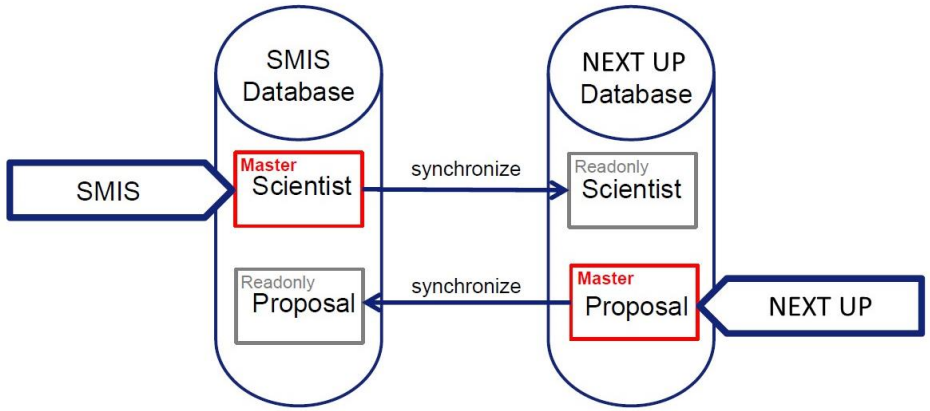
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313.

NEXT UP: Why and how are we changing the ESRF user portal

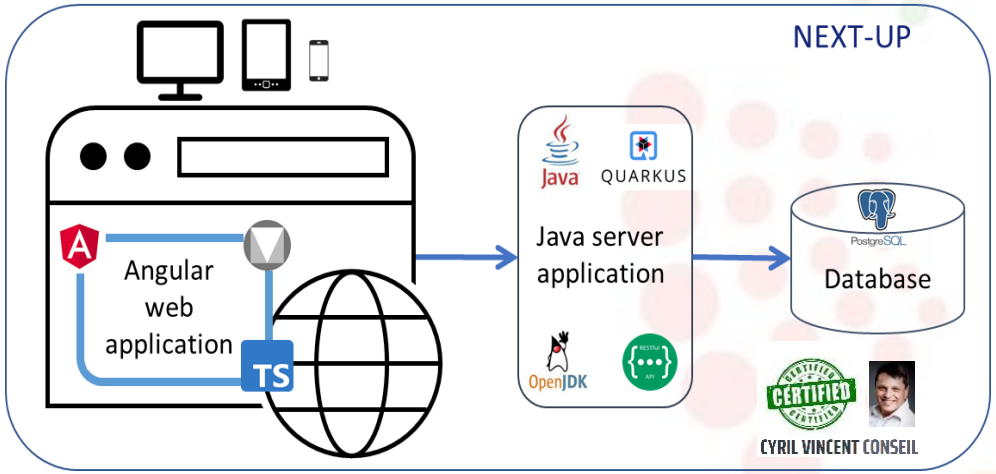
➔ Modularisation of the functionalities:



➔ Co-existence:



➔ Technologies:



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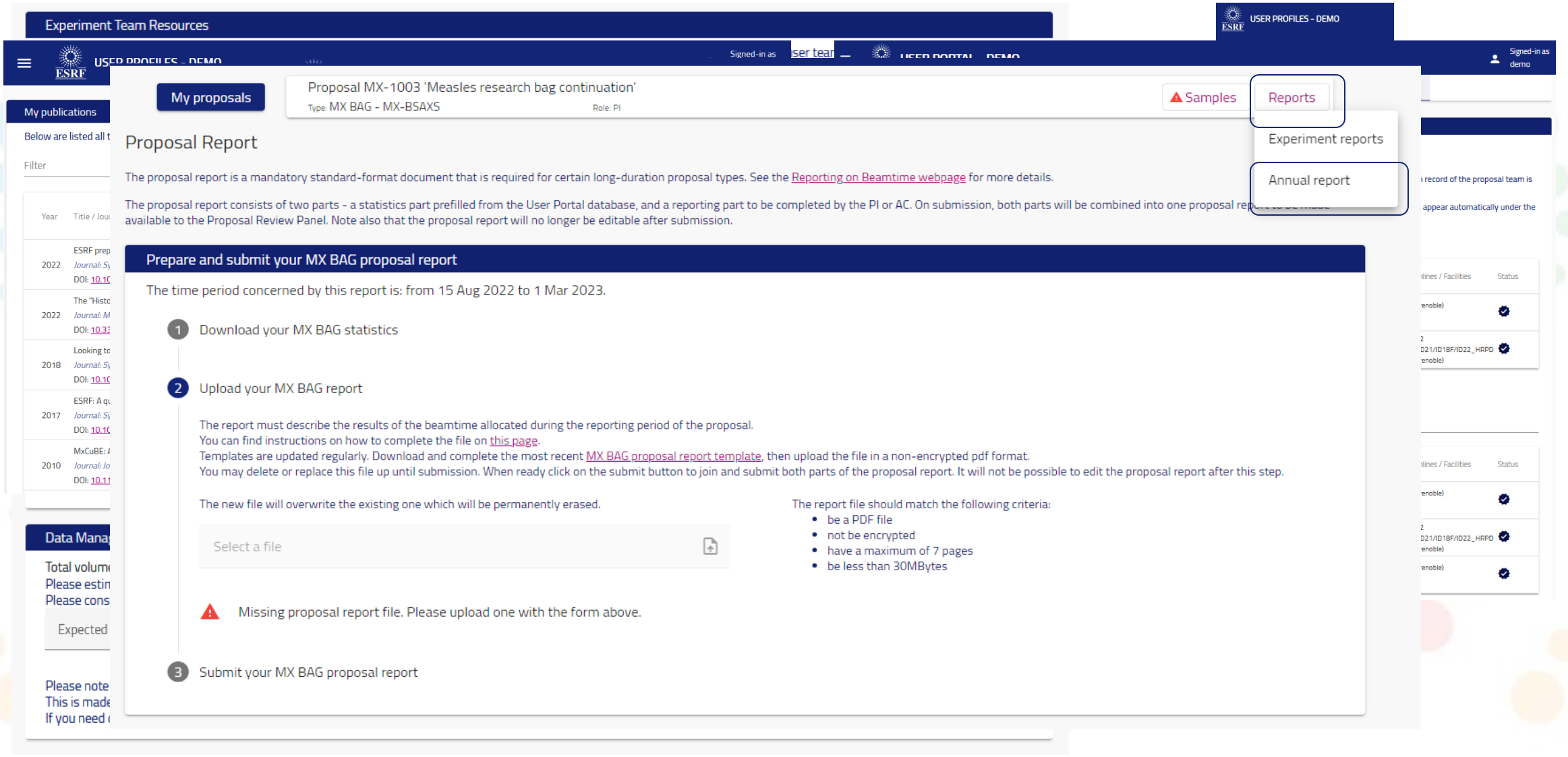
NEXT UP: New user experience



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NEXT-UP Release 1

Release 1 of the new platform on 24th May 2024

- Proposal submission of all proposal types
- Draft and submitted proposals lists
- New sample sheets for all proposals
- Proposal reports for MX BAGs
- User profile with “My Publications” list

- Real-time saving of data entered in web forms
- Multiple draft proposals
- Alternative Contact for proposals (same rights as the Principal Investigator)
- Correct labelling of new, continuation or resubmission proposals.
- Updated proposal form content, including new questions on user team resources.
- Updated sample sheets, including new questions.
- Past ESRF beamtime activity of proposer team, with status of experiment report submission.
- 'My Publications' tool to automatically populate the publications section of a proposal (publications must already be in the ESRF Library database)
- New MX BAG proposal & annual report submission workflows – simplified, stats provided to proposers from database (beamtime usage, participants, **publications**), report uploaded as pdf.

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Members of the Executive Team & Project Support Team: **Gary Admans, Patrick Bruno, Ennio Capria, Marine Cotte, Delphine Chenevier, Chiara Facoetti, Andy Götz, Gema Martinez Criado, Joanne McCarthy, Ed Mitchell, Stephanie Monaco, Annalisa Pastore, Eleonore Ryan, Anne Talucci**

All STREAMLINE participants

ESRF Senior Management

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Project Reviewers: **Lars Osten Christer Frojd, Axel Steuwer**

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STREAMLINE

THANK YOU FOR YOUR ATTENTION

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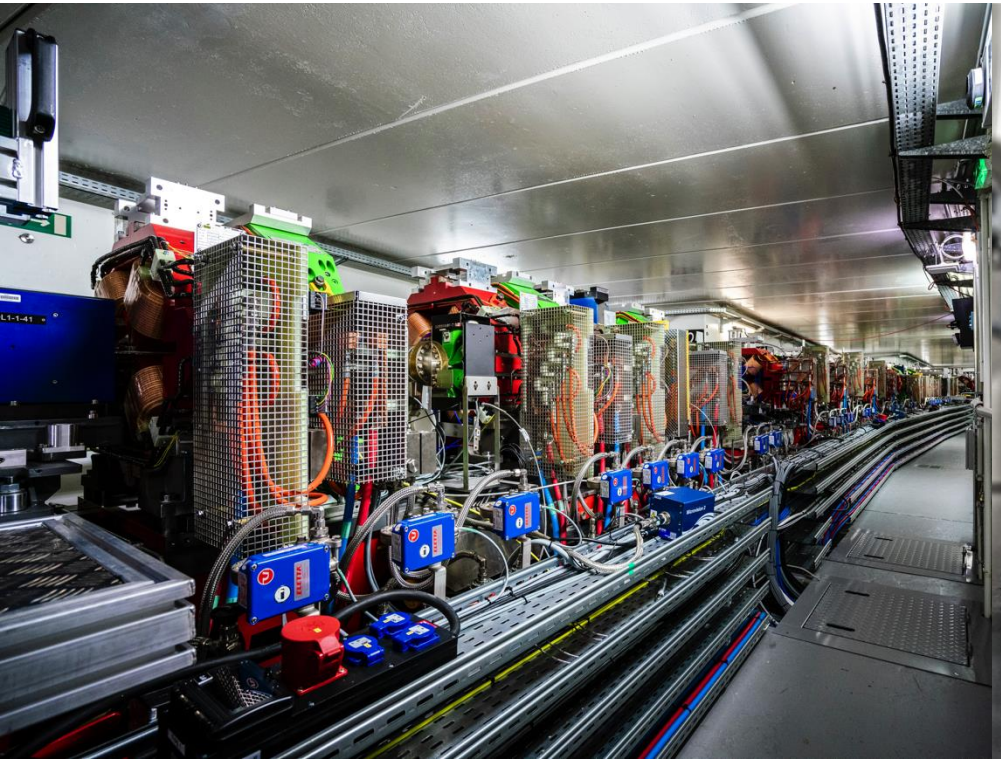
The European Synchrotron



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