STREAMLINE

WP3
Update user tools and administrative procedures

D3.1

Report on new access models

Expected date 14/11/2021

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

PROJECT DETAILS

PROJECT ACRONYM	PROJECT TITLE
STREAMLINE	**Sustainable research at micro and nano X-ray beamlines**
GRANT AGREEMENT NO:	THEME
870313	**H2020-INFRADEV-2018-2020 Development and long-term sustainability of new pan-European research infrastructures**
START DATE	
15/11/2019	

DELIVERABLE DETAILS

WORK PACKAGE ID	EXPECTED DATE
WP3	**14/11/2021**
WORK PACKAGE TITLE	DELIVERABLE TITLE
Update user tools and administrative procedures	**Report on new access models**
WORK PACKAGE LEADER	DELIVERABLE DESCRIPTION
Joanne McCarthy	**Report on new access models**
DELIVERABLE ID	
D3.1	PERSON RESPONSIBLE FOR THE DELIVERABLE
	Joanne McCarthy

NATURE

☒ **R- Report** ☐ **P - Prototype** ☐ **D - Demonstrator** ☐ **O - Other**

DISSEMINATION LEVEL

☒ P - Public
☐ PP- Restricted to other programme participants & EC:
☐ RE – Restricted to a group
☐ CO – Confidential, only for members of the consortium

REPORT DETAILS

VERSION	DATE	NUMBER OF PAGES
FINAL	**14/12/2021**	**13**
DELIVERABLE REPORT AUTHOR(S)	FOR MORE INFO PLEASE CONTACT	
Joanne McCarthy	**Joanne McCarthy**	

STATUS

☐ **Template**	☐ **Draft**
☒ **Final**	☒ **Released to the EC**

Contents

Introduction

This report describes the implementation of new access models at the ESRF, adapted to permit efficient access to the ESRF's facilities and optimise its EBS-enabled opportunities.

Entirely new methodologies are needed for the ESRF to function effectively as a user facility and to make the full power of the EBS available to diverse and demanding researcher communities. The challenges include increases in experiment turnover, user administration and experiment support, and quantity of data collected per sample.

The objective of Tasks 2.2 and 3.2 is to define and implement new and sustainable access models that optimise the use of the new ESRF-EBS source, allowing more impactful science to be carried out on the same time scale. Such access models, if proven successful, can be adopted by other European light sources planning major source upgrades and hence are beneficial to the European synchrotron research community as a whole.

The potential new access models considered, be they mail-in, grouped applications or long-term multi-annual access programmes, drew upon best practice from the existing BAG (Block Allocation Group) and rolling-access proposals and mail-in systems used for many years for academic access to structural biology (protein crystallography, bioSAXS and cryo-electron microscopy) and on existing Long-Term Project proposals. We have also looked at access systems in use at other facilities where some alternative modes of access are already operational, in particular for non-structural biology BAGs, but only on a relatively small scale.

The new access modes selected centre on "community access" and on remote access and mail-in services. For remote access, the arrival of the COVID-19 pandemic forced us to work intensely on this access mode in the first months of the STREAMLINE project, resulting in a very positive and giant leap forward for the most crucial elements of mail-in and remote access, and laying an excellent foundation for improvement and better integration of these solutions over the remaining years of the project. For community access, the ESRF has defined two new proposal types – HUBs and BAGs (for non-structural biology) - and have three very successful pilot projects running using these access modes. The work done so far and progress made will be summarised in this report.

Community access proposals

Introduction and motivation

With this new access mode, the ESRF is looking to facilitate access to the ESRF for researchers working in fields of important societal impact and willing to collaborate to produce more impactful science, but also to facilitate access for user communities if they can structure themselves in such a way as to efficiently use regular beamtime slots for the projects they consider to be of highest importance for the community. These community access proposals are intended to optimise the use of the new EBS X-ray beams that will allow faster and shorter experiments due to their unprecedented intensity and coherence by:

- encouraging user communities to agree together on the most important projects and samples for that community, and to assign priorities for a particular beamtime slot,
- ensuring regular access to ESRF beamtime to allow these priorities to be set and to allow a strategy for best use of the beamtime to be conceived within the community,

- reducing the lengthy set-up and take-down overhead time per project by fully utilising the useful beamtime in between to measure data on a maximum number of samples and projects,
- creating scientific synergy within the community to develop tools for data acquisition, analysis and interpretation.

With such proposals, the Research Infrastructure (RI) places itself in the role of a driver/facilitator for selected areas that are considered of scientific and/or societal importance, rather than in the traditional passive role as a simple supplier of beamtime. The strategic choice of the scientific and societal areas to support can easily link with the European priority areas (such as cancer, circular economy, green deal, etc.), missions and strategic partnerships, so that the RI pushes towards greater and more impactful advances in these chosen areas. It is important to note that the ESRF is already very active in the battery priority area with its academic and industrial user communities directly, and via European projects such as BIGMAP (https://www.big-map.eu/) and TeesMAT (https://www.teesmat.eu/).

What is a "community access proposal"?

Community access proposals group together scientists working on similar scientific topics or themes who apply together as a consortium for a regular allocation of beamtime at the ESRF to work on that topic or theme. If successful, the ESRF will grant the beamtime to the community who decide between themselves how best to distribute the beamtime within the community and for which projects in order to produce the most impactful science in that field. In addition to the existing structural biology (SB) Block Allocation Group (BAG) proposals, the ESRF is also implementing

1. HUB proposals, and
2. BAG proposals for non-structural biology topics.

The essential difference between a BAG and a HUB is that a BAG groups together a number of independent Principal Investigators (PIs) working on similar scientific or technical projects, who share beam time and decide on measurement priorities. Apart from collaborating to share beamtime, they will generally work independently and do not necessarily share results, although they may if they wish. The HUB access mode is different in that it groups a number of PIs working on the same major scientific theme of significant societal importance, but who commit to collaborate and work together to coordinate the beamtime use and share results obtained in such a way that progress is faster and more impactful across the field, rather than made incrementally by the different PIs working separately. This necessitates that the HUB members share knowledge, beamtime data and results prior to publication.

The advantages of community access proposals in terms of proposal submission and evaluation and in terms of efficient beamtime use are illustrated in **Figures 1 and 2.**

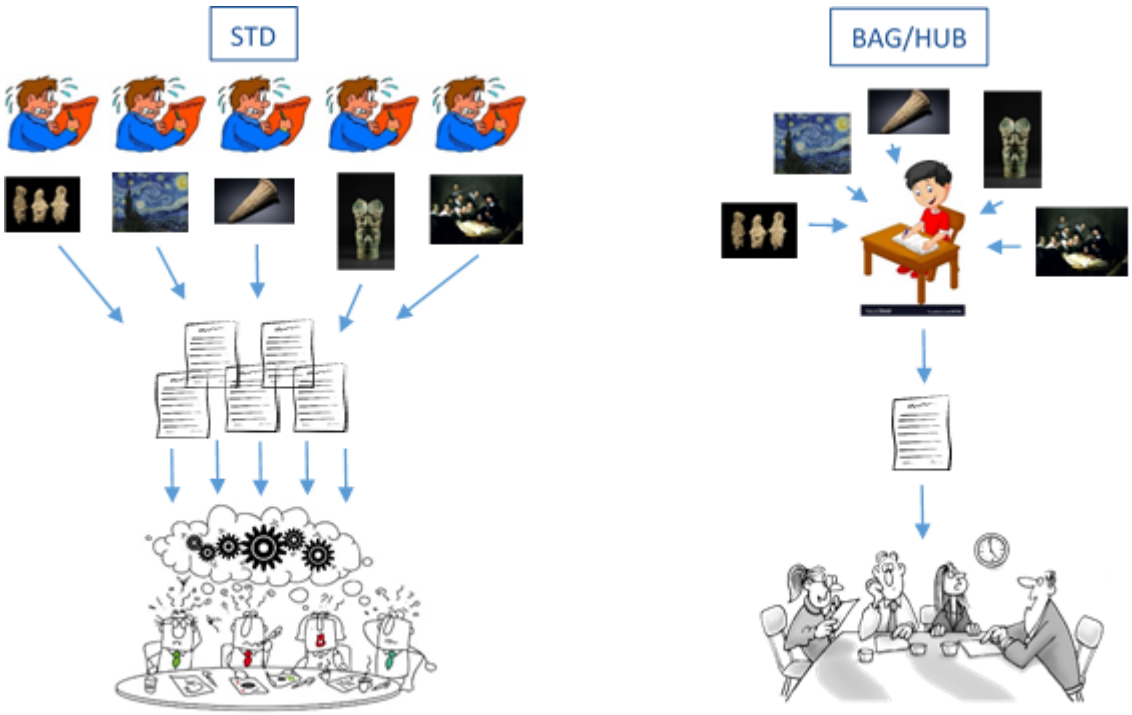

Figure 1: Community access proposals allow a single proposal for N users and N experiments.

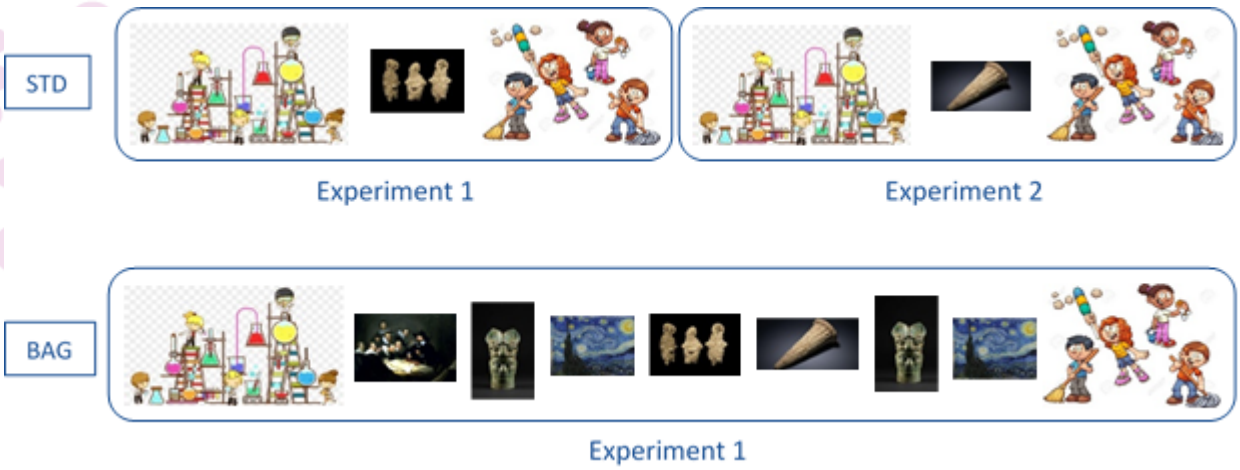

Figure 2: Community access proposals allow a single setup for N users and N samples/projects.

BAG and HUB pilot proposals

In late 2020, the ESRF SAC and Council approved the creation of pilot proposals to test these new access modes, and at the 1st March 2021 proposal deadline three pilot proposals for new community access proposals were solicited and submitted. These proposals are:

1. BAG Proposal – science driven
   HG-172 (Gonzalez): “Structural analysis of historical materials”
   Historical Materials BAG studying degradation of paintings, on ID13 and ID22

2. BAG proposal – technique driven
   MI-1397 (Eakins): “Shock BAG”
   For the study of materials under rapid and extreme loading, on ID19

3. HUB proposal
   MA-4929 (Lyonnard): “Multi-scale Multi-techniques investigations of Li-ion batteries: towards a European Battery Hub”
   Grenoble Battery Hub, on 19 different beamlines.

More details can be obtained about community access proposals and about each pilot proposal on the ESRF web site: https://www.esrf.fr/CommunityAccess. As well as testing the principle of these access modes, the pilot proposals are being used to identify the appropriate workflows required to handle properly proposals for community access in the future.

Governance, review and reporting

The principles, rules and guidelines for governance, review and selection, follow-up and reporting of community access proposals are currently being refined. A paper addressing all of these points was submitted to and endorsed by the ESRF Science Advisory Council at its 83rd meeting on 4-5 November 2021, and will now be submitted to the ESRF Council.

Beamtime use and feedback from pilot proposals

The 2 BAG and 1 HUB pilot proposals were submitted for the 1st March 2021 proposal deadline, and were awarded beamtime in the 2021-II scheduling period that runs from 16th August 2021 to 28th February 2022.

The “Historical Materials BAG” (HG-172) was awarded a total of 18 shifts (6 days) of beamtime: 12 shifts on ID13 (microfocus beamline) and 6 shifts on ID22 (high resolution powder diffraction beamline). They used 7 shifts on ID22 in late September 2021 and 12 shifts on ID13 at the end of November 2021. During these two experiment sessions, they were able to take data on more than 250 samples for 21 participating researchers/groups from six different countries, which is a much more efficient and productive use of one week of beamtime than if these same groups had applied individually through our standard access route.

This BAG already reports a growth of synergies between the different participants to ensure the most important projects are carried out and to improve data acquisition and data analysis tools and methodologies.

The “Shock BAG” (MI-1397) was awarded a total of 18 shifts (6 days) of beamtime on ID19 (microtomography beamline) and has four days of beamtime planned from 10-14 December 2021 for commissioning of a gas gun to be used by the team. This BAG gathers the European community of researchers working on the study of materials under rapid and extreme loading. It pools together shared equipment, personnel and expertise to underpin and enhance the science at the intersection of X-rays and dynamically-compressed matter. It is built upon the dedicated gas-gun, Hopkinson bar platforms, and multi-MHz X-ray imaging scheme, offering these proven tools and expertise to grow the high-rate and shock user community at ESRF. The equipment and techniques involved are complex, and the BAG allows equipment, knowledge and expertise to be pooled and shared to further this field.

The "Grenoble Battery HUB" (MA-4929) was awarded a total of 79 shifts (26 days) on 12 different beamlines in 2021-II, and in total will use 19 of the ESRF's 46 beamlines over the course of its first three years of existence. To date it has already carried out seven experiments on seven different beamlines, using a total of 60 shifts.

The creation of the concept of a battery HUB proposal at the ESRF has led directly to the creation of the "Grenoble Battery Hub", that was officially launched on 24th November 2021 via the signing of a Memorandum of Understanding (MOU) between the ESRF (the European Synchrotron), the ILL (Institut Laue Langevin), and the French Alternative Energies and Atomic Energy Commission (CEA) (see https://www.esrf.fr/home/news/general/content-news/general/launch-of-the-grenoble-battery-hub.html). The aim is to create a hub for research on sustainable electrical energy storage based on the use of cutting-edge neutron and X-ray techniques and instruments. The aim of this partnership is to accelerate Research & Innovation so that the next generation of batteries are more efficient, safer, cheaper and more sustainable. The Grenoble Battery Hub is linked to the European initiatives "BIGMAP", co-funded by the European Union's H2020 programme, and BATTERY 2030+. The next step for the Battery Hub is to open to the European battery R&D community to advance research in support of the European Green Deal, the UN Sustainable Development Goals and the European Action Plan on Batteries.

Launch of community access proposals for the user community

The aim is to open up the HUB and BAG access modes to the full ESRF community in 2023, after endorsement by the ESRF Council. Rules and guidelines for the creation and submission of HUB and BAG proposals, if approved, will be published in mid-2022, allowing user communities interested in community access to start discussions and preparations for proposal submission in 2023. Currently we plan one submission deadline for HUB proposals, on 15th January each year as for Long Term Project (LTP) proposals. We intend that BAG proposals may be submitted for the regular proposal deadlines of 1st March and 10th September each year.

The user community has already shown significant interest in community access proposals and the first new hub that would be created if this access mode is confirmed by the ESRF Council is the "human organ imaging hub". Based on highly successful initial research carried out by a user team led by University College London and ESRF staff to image the lung of a COVID-19 victim using Hierarchical Phase-Contrast Tomography (HiP-CT) (https://www.esrf.fr/home/news/general/content-news/general/ebs-x-rays-show-lung-vessels-altered-by-covid-19.html; Imaging intact human organs with local resolution of cellular structures using hierarchical phase-contrast tomography, C.L. Walsh *et al., Nature Methods* (2021); https://doi.org/10.1038/s41592-021-01317-x), this hub aims to measure and make publicly available high-resolution images and data of all the organs of the human body, both healthy and diseased. Within the short span of a year, this project has already rapidly expanded and now includes 22 PIs and is therefore the prime candidate for the formation of the first official hub. In addition, this activity has acquired a very high level of visibility and attracted several large blocks of external (private) funding. This has already changed the way science is being conducted at the ESRF as the data are of such high relevance that all data are made publicly accessible immediately after initial reconstruction (see https://human-organ-atlas.esrf.eu/). In that respect, STREAMLINE has already shown success beyond all expectations.

Dissemination and adoption of community access proposals within the European light sources community

Both BAG and HUB proposals can be used as a template for adoption of such community access by other interested European light sources. The information has been disseminated on our web pages (https://www.esrf.fr/CommunityAccess), in our newsletter (https://www.esrf.fr/Apache_files/Newsletter/2021/December/index.html#/page/6), within LEAPS via the WG5 working group meetings (of which the author, Joanne McCarthy, is a member) and via a LEAPS seminar given by the ESRF Director of Research Harald Reichert in November 2021 (https://leaps-initiative.eu/https-leaps-initiative-eu-events-passed-events/). It has also automatically disseminated via the members of our SAC, many of whom are members of the management or users of other European light sources. As a direct result of the creation of the HUB proposal concept, a Strategic Access Task Force has been created within LEAPS to discuss the possibility and benefits of implementing such HUB-style access on a European level among several partner facilities, reserving beamtime for research on topics of high societal impact such as battery/energy storage research, cancer research, etc. The ESRF Director of Research is a member of the LEAPS Strategic Access Task Force.

Dissemination and communication

More details can be obtained for community access proposals and for each pilot proposal on the ESRF web site: https://www.esrf.fr/CommunityAccess.

ESRF newsletter article on new access modes:
https://www.esrf.fr/Apache_files/Newsletter/2021/December/index.html#/page/6.

Grenoble Battery Hub inauguration:
https://www.esrf.fr/home/news/general/content-news/general/launch-of-the-grenoble-battery-hub.html.

LEAPS seminar entitled “Feedback from the new ESRF-EBS Synchrotron” by H Reichert, the first in a series of lectures entitled “Feedback from new DLSR sources“: https://leaps-initiative.eu/https-leaps-initiative-eu-events-passed-events/.

Mail-In services and remote access

Introduction and motivation

The traditional way of carrying out experiments at large research infrastructures is for the user team to be present onsite for the experiment. User presence is often essential since the user team provides the expertise required for the particular project and samples in question. However, for certain fields of research, or certain beamlines where a high level of automation can be implemented, the principle of “remote access” is one that is of great interest to user teams and research infrastructures alike.

Remote access implies that the user or user team does not travel to the synchrotron, but sends the samples to be measured and can control and follow the experiment remotely from the home laboratory. An enhanced level of remote access is a “mail-in” service, where samples are sent and data are collected for the user team by the onsite beamline staff. This mail-in service can even include a level of data reduction and analysis, when requested and appropriate.

Remote access and mail-in services have existed for some time for the structural biology community and for clients purchasing beamtime to carry out proprietary research. These access modes have been particularly popular with the industrial community who are not subsidised financially for travel to the ESRF for proprietary beamtime and for whom the service aspect is attractive. They have also been used, although to a lesser extent, by the academic structural biology community who can benefit from combining remote access with the automated data pipelines that exist on the SB beamlines.

It was always the intention of the ESRF to extend remote access and mail-in services to other fields that could benefit from such access. Communities and techniques that may potentially largely benefit from remote access due to the automated equipment available (e.g. sample changing robots) or repetitive nature of measurements are powder diffraction, X-ray fluorescence spectroscopy, tomography, topography, SAXS and residual stress measurements (we are pursuing the first two in the context of STREAMLINE WP4; the others are either already in place or tackled via the IRT Nanoelec or the H2020 project EASI-STRESS). However, the arrival of the COVID-19 pandemic and the drastic restrictions this imposed on social interaction and international travel accelerated the need to implement remote access to user facilities on a grand scale, for all beamlines and all experiments.

Implementation of remote access and "staff-assisted" experiments in 2020

Within STREAMLINE, implementation of mail-in and remote access services is split across sub-tasks in two different work packages: WP3 (sub-task 3.1.2) deals with "sample declaration, tracking, handling and safety considerations", and WP4 (T4.3) deals with "LIMS for new mail-in services".

One of the major new developments required to implement large scale remote access was the creation of a sample tracking tool. The ESRF has implemented a Laboratory Information Management System (LIMS) using ICAT (https://www.esrf.eu/ICAT), an open source metadata management system designed for large facilities and provided by PaNdata (consortium of all photon and neutron sources in Europe, dedicated to sharing good practices of data management). ICAT enables the collection, storage and searching of generic metadata of experiments along with corresponding raw data and electronic logbooks, therefore enabling their reuse at a later stage. Since beamline data and metadata are stored in ICAT, implementing the sample tracking module in ICAT paves the way for user-friendly features linking users' samples, experiments and data.

The new sample tracking system has been in place since August 2020 and has been successfully used to track samples for both remote and onsite experiments on non-MX beamlines (note that sample tracking for MX beamlines has been using ISPyB for many years and so is not included in the scope of STREAMLINE activity and this report). Since then the developments of the sample tracking system have been focused on extending it with tools that allow the status of parcels and samples to be monitored in real time and by providing useful statistics for reporting, as shown in **Figure 3**. The general statistics help to understand how the tool is being used and also to understand the nature of items that are being sent.

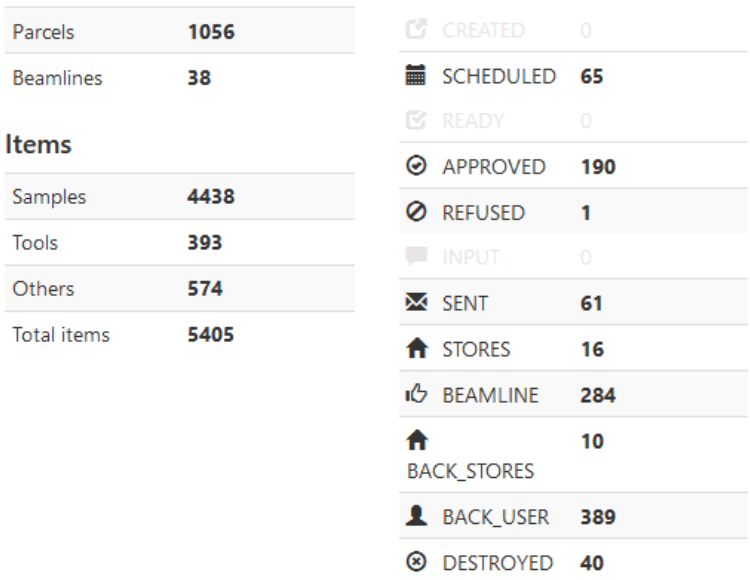

Figure 3: Parcel statistics since August 2020

In addition to the work in ICAT, developments were also implemented in the ESRF User Portal (our Scientific Management Information System) and in the overall workflow as shown in **Figure 4**. The remote and mail-in safety training module for users was rewritten, combining previous separate modules for remote access and for mail-in and updated to include non-MX experiment considerations. This new module is linked so that all users who use mail-in services and all remote participants in experiments have to carry out the training before being accepted on the experiment registration form. The existing sample sheets for declaring samples were updated to be usable for all experiment and sample types, and the mandatory creation of sample sheets for all accepted proposals was introduced. Finally, a protocol for remote and mail-in experiments was created, to be agreed between the user team and beamline personnel. The ESRF User Office provides support for problems and questions related to sample transport and tracking via the implementation of a JIRA trouble ticket platform, allowing users to open a ticket for any problems related to transport and customs, safety concerns, and the ICAT and ISPyB tools.

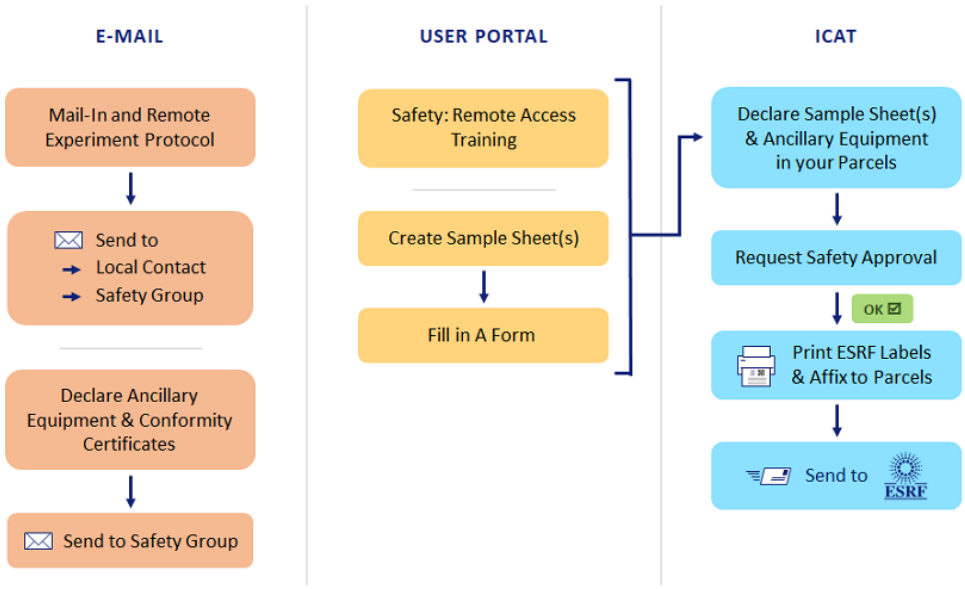

Figure 4: "Before the experiment" workflow for remote experiments on non-MX beamlines.

Remote use of the ESRF in 2020 and 2021

When the ESRF restarted after the EBS upgrade on 25th August 2020, all experiments had to be carried out remotely for the first six months or so due to the COVID-related restrictions in place. Users sent their samples using the newly developed sample tracking software, allowing ESRF safety and beamline staff to keep track of the samples that are onsite and their location. The remote access tools were used for beamtime at public, proprietary research and private CRG (Collaborating Research Group) beamlines. In the 2020 operation year, the ESRF was able to carry out 1082 experiments of which 803 (74%) were carried out fully remotely with no member of the user team onsite and a further 132 (12%) carried out with only one member of the user team onsite when this was allowed. 79% of all user visits were remote, meaning that the user registered on the experiment did not travel to the ESRF but stayed at home carrying out the experiment remotely. In 2021 the situation has improved, allowing more users to come onsite for their experiment. The comparative numbers are shown in Table 1.

Year	Total Experiments	Fully Remote Experiments	Single Onsite User Experiments	% Remote User Visits
2020 (1 March 2020 to 16 March 2021)	1082	803 (74%)	132 (12%)	79%
2021 (17 March to 31 December 2021)	1630	794 (49%)	127 (8%)	45%

Table 1: Remote user experiments in 2020 and 2021.

The implementation of tools for remote access at the ESRF was a huge success, allowing many user experiments to be carried out despite the pandemic-related travel and distancing restrictions. However, the vast majority of non-MX experiments were carried out through “staff-assisted experiments”. This means that although the user team joins the experiment remotely, presence of local staff scientist(s) was absolutely necessary as an annex to the remote user team to carry out the experiment successfully. This is the case for all beamlines, experiments and techniques where high levels of automation or repetitive measurements are not possible, or where significant sample preparation/manipulation is needed. Staff-assisted experiments are extremely intense in terms of workload for staff scientists and can generally not make optimal use of the 24/24h beam availability. They therefore cannot be considered as a viable way of running user experiments in the long term or on a grand scale, except in the case of emergency situations such as those we have had to deal with. Finally, it should be noted that many experiments absolutely require the full user team to be present at the beamline to carry out the experiment successfully, and around 30% of allocated proposals could not be carried out at all in 2020 due to restrictions in user travel and/or in allowed onsite user presence. These proposals were carried over into 2021.

Future developments for improving remote access services will therefore concentrate on those experiments, techniques and beamlines that could really benefit from such an access without any loss in the quality of the experiment carried out, where users can use automated routines and remote control to fully run the experiment from home with only limited support from local staff. The aim is to provide services appropriate for the X-ray techniques being offered and for the selection of high-throughput services to be developed in WP4. We will also build on our experience of using the sample tracking tool to improve this tool and implement additional features, as well as optimising the overall workflows to provide a fully integrated approach to sample declaration, transport and measurement.

Dissemination and communication

Instructions on carrying out non-structural biology remote experiments at the ESRF: https://www.esrf.fr/NonMX-RemoteExperiments.

Instructions for using the sample tracking tool in ICAT: https://www.esrf.fr/home/UsersAndScience/UserGuide/Preparing/ImportingEquipment/non-structural-biology-samples-how-to-create-a-shipment-icat.html.

Rapid/flexible access

Rolling access proposals exist already at the ESRF for the Structural Biology (SB) community, to be used by small groups who are not already members of a SB BAG. A rolling access proposal is one that may be submitted at any time during the year as soon as samples are available, so proposers do not have to wait for one of the two annual proposal submission deadlines (1 March and 10 September). However, rolling proposals are not adapted for implementation on a large scale since a) it is difficult to handle over-subscription correctly when reviewers cannot see and compare all proposals at the same time to decide which ones should be allocated in the limited time available, and b) the ESRF has an obligation to ensure a fair scientific return to our 21 member and associate member countries while protecting the quality of science carried out, and this is not possible without knowing what proposals will come in, when, and from which countries, and being able to directly compare them at a particular moment in time before allocating beamtime. Indeed, the beamtime used by SB rolling proposals constitutes less than 5% of all SB beamtime, and so is only a very small part of that activity.

Instead we consider that rapid and flexible access is a very positive direct side effect of community access proposals and remote access possibilities, as both allow beamtime to be allocated and used more flexibly and rapidly. An existing BAG or HUB that obtains a new sample to measure that is considered of highest priority does not have to write a proposal, wait for the next proposal deadline and wait a further 6-12 months for beamtime to be scheduled; the principal investigators can just agree between themselves that this sample should be measured during the next regularly allocated slot of beamtime. Remote access would also allow new samples to be sent for preliminary tests before allocating any large amount of beamtime. Therefore, we do not intend to extend the implementation of rolling access proposals beyond what already exists, but rather encourage the creation of community access proposals to achieve the desired flexible and rapid access.