Deliverables

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Authors	J. Mc Carthy (ESRF), A. Chebre (ESRF), C. Blasetti (ELETTRA)

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Executive Summary

The need for remote/mail-in experiments at LEAPS and LENS facilities was boosted by the COVID-19 pandemic restrictions requiring facilities to enhance or develop from scratch tools and procedures to allow continuous user operation.

Restrictions have since eased, but the level of remote/mail-in experiments has remained significantly higher than in pre-pandemic times.

Within the Digital LEAPS "STARS" (Surveying Technology for Advancing Remote Services) internal project, WP1.1 (MailSamp - Overview of procedures for mail-in sample handling) had the aim to provide an overview of the procedures existing across facilities today for management of remote/mail-in experiments and associated sample transport.

The key points resulting from this survey are listed below.

1. Overview

The survey responses showed that there is no obvious consensus in the management of remote access and sample mail-in procedures in place at the different facilities in terms of the tools used and internal procedures implemented. This may be due to the need to implement both of these on a large scale in an urgent way in order to continue user operation during the pandemic.

2. Remote services

- Remote services have been developed at almost all facilities but need to be used only where they give added value to the experiment and/or user experience. Individual remote user access is very beneficial when combined with onsite users: it reduces the number of users who need to travel (and thus their carbon footprint) to only those essential for the experiment other team members can follow online and have access to the data without needing to come onsite.
- Fully remote experiments should not become the standard way of using a facility but can be a great opportunity for the user community in some specific cases: facilities can support scientists from countries who could have never physically attended experiments, thus becoming much more inclusive; researchers are now joining from South America and Africa and that is a very positive outcome. Other cases include: Macromolecular Crystallography (MX) experiments, standard setup measurements, sample feasibility and test measurements, short experiments to complete a project and allow publication.
- Fully remote access is not a preferred facility standard access route due to the lack of
 interaction between user teams and facility experts, loss of hands-on training
 opportunities that are needed in particular to prepare the next generation of young
 scientists and the potential decrease of researchers' networking capabilities. These
 points appear to result in a lower quality of the experiments outcomes, and a higher
 number of non-expert users in few years from now.
- Beamline staff should be the primary people to decide on whether an experiment can
 or should be carried out remotely, according to the best or easiest way of ensuring a
 successful experiment in the most efficient way.

3. Staffing

- The workforce of facilities is not adapted to an increased level of fully remote access, in particular at level of the beamlines, safety and UO staff.
 The increased level of remote access experienced already today has resulted in the need to manage two parallel access routes at all times: onsite vs remote user workflows. The survey confirms that facilities are struggling to maintain the flexibility required for user experiments while coping with the increased volume of samples and users to be supported, also resulting in more restrictive deadlines to be respected.
- Facilities need to take into account this shift towards an increased level of reception
 and return of user samples, by ensuring that staff who are experts in logistics,
 international customs issues, (dangerous) goods declaration, import/export, legal
 aspects, etc are directly assigned to the support of these activities, rather than reliyng
 on non-experts on beamlines and in User Offices to deal with these critical issues.

4. Sample / parcel tracking

• Tracking of user samples at the shipment or parcel level is desired and is something that would benefit from standardized solutions. At present, only 4 facilities have electronic solutions in place¹; most facilities expressed the desire to have such a solution, but they do not have available resources in the mid-term to develop it. Electronic tracking tools require specifications from a wide range of facility services including beamline staff, Safety, Stores, Logistics, User Offices, Financing, etc.

5. Update in Spring 2024

 Facilities welcome users in person again. Developments boosted during the pandemic benefit specific beamlines and communities (e.g. MX). Hybrid access mode allows participation of larger user groups.

¹ 3 ISPyB (ALBA, DLS, ESRF), 1 ICAT (ESRF), 1 VUO (ELETTRA).

Methodology

Since the overview of information on sample mail-in practices is being made in the context of the many different levels of remote access that now exist at the different facilities, we took this opportunity to also attempt to obtain an overview of the different type of experiments being currently offered, involving remote use of the facilities.

The survey was therefore split into 2 parts:

- Part A: Experiment types offered and remote services
- Part B: Mailing Samples

The survey comprised 7 Sections for each Part² and a total of 65 questions, the majority of which also allowed for free text comments; this was meant to allow facilities to share details in a collaborative spirit.

The survey was distributed as a Word document to the LEAPS and LENS members as well as to the LEAPS Associated Partner SESAME, requesting only one response per legal entity (e.g. grouping PETRA III and FLASH under DESY answers). The survey is available as a .pdf in Annex 1 of this report.

We received 21 responses covering 15 LEAPS members³, 1 LEAPS Associate (SESAME) and 5 LENS members.

All the responses were collated into an excel file that is available in Annex 2 via a hyperlink to the DESY cloud repository; this initial file was the one used to produce the following report. However, to ensure that accurate and up-to-date information is available at any time for any facility to refer to, a copy was made that facilities are encouraged to update and enrich in order to maximise best-practices sharing.

The original STARS WP1.1 deliverable refers to the situation in Spring 2022. We decided to ask the LEAPS and LENS facilities four questions (see Annex 3), to gauge the current situation in Spring 2024, ensuring time coherence with the WP1.2 and WP1.3 reports and providing a useful addon.

² Section 1 of Part A was a specific Glossary of terms used in the survey.

³ All LEAPS members except PTB.

Survey Analysis

Part A – Experiment types offered and remote services

1. Available Experiment Types at Facilities

TOPIC	KEY MESSAGES
Experiment types available at the various facilities	 Most facilities can offer mixed onsite/remote experiment types
	Different level of control given to the remote users resulting in a range of experiment types Final designs an experiment type is desided by the
	 Final decision on experiment type is decided by the beamline responsible after discussion with the users

Due to the COVID-19 pandemic, all facilities are able to offer a level of remote access which allowed some, but not all, experiments to continue during the pandemic. However, fully remote user experiments are clearly not a preferred access route outside of emergency times, except for some specific beamline and experiments where the remote access can be beneficial. The development of enhanced remote access has allowed most facilities to provide some form of mixed onsite/remote experiments (with varying levels of control given to the remote users as illustrated in experiment types #2 to #6 of the survey). This means that only the essential team members need to travel to the facility and other team members can participate remotely.

The example depicted in Fig.1 refers to the experiment type #7 in the survey where onsite users are mixed with remote users who can fully control the beamline and take data remotely. This experiment type is referred to by different names at different facilities, e.g. hybrid, semi-remote, etc. The advantages of mixing onsite users with remote users who can also control the experiment makes this type quite popular with both facilities and users.

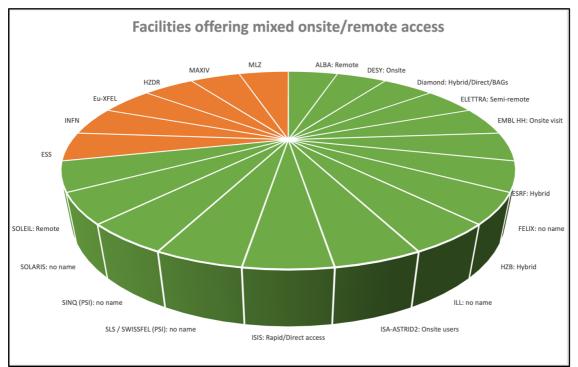


Figure 1: Facilities offering mixed onsite/remote access as defined in experiment type #7 of the survey where the remote users can control the beamline from home. When facilities offer this type of access (green), the name given to it is shown after the facility name. Facilities not offering it are shown in orange.

See Annex 2 - Expt Type Q3-5

2. Remote Users

TOPIC	KEY MESSAGES
Training for remote users	In most cases, no specific training is required
	Access to data for remote users is identical for onsite users

All but one facilities do not require a specific safety training for remote users. For the one, the training is mainly concerned with sending samples which is part of the standard user safety training in other facilities.

16 facilities have the option for users to follow the experiment remotely without being in control, and 13 have the capability of allowing the remote user to control the beamline. Most facilities impose some level of restriction on full remote control of the beamline by users, e.g. only for certain beamlines, local contact agreement, no physical movement of equipment, experienced users. Access to data for remote users is as for all other users, via metadata catalogues (e.g. ICAT, ISPyB), Globus, facility disks accessible for a fixed time. A small number of facilities (3) send the data to the users.

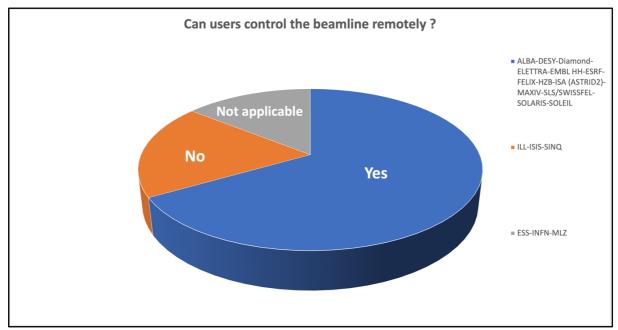


Figure 2: Facilities offering beamline remote control to users: list provided as picture legend.

See Annex 2, Remote Users Q6-8

3. Fully Remote Experiments

TOPIC	KEY MESSAGES
Fully remote experiments: present and future	 Not sustainable nor advisable for the future to the level of pandemic times, except for specific cases Requires exchange and agreement between local contact and user team prior, during and after the experiment Increased local contact responsibility in sample
	 Increased local contact responsibility in sample preparation and manipulation, as well as in reception and return of user samples

16 facilities allow fully remote experiments when the beamline and experiment are adapted for it, 1 facility plans to have this possibility and the remaining 3 consider that fully remote experiments were an exception that was required only to cope with the COVID-19 crisis.

There is no clear wish, indeed there is an opposition, to moving towards an operating scheme whereby fully remote measurements are the norm or done at a very high level. 19 facilities said they only had the staff capacity to support experiments without onsite users "to a certain extent" or "not at all". The majority of facilities have limits on the maximum number of fully remote experiments that can take place or on the hours during which these can take place. Several facilities commented that, except for the most automated experiments, fully remote experiments require significant extra workload and working hours.

Such experiments require increased responsibility on local contacts for sample preparation and manipulation, which would normally be done by the expert user team onsite. This is one of the major limits of fully remote experiments.

See Annex 2, Fully Remote Expts Q9-14

4. Financial support for experiments

TOPIC	KEY MESSAGES
Financial support for remote experiments	 Increased number of facilities offering financial support for sample shipment with respect to pre-pandemic times
	No financial gain from remote experiments as manpower and staff overheads outweighs travel budget savings

10 facilities offer payment of sample shipment instead of users, 6 facilities offer no financial support at all whilst 2 do so on a case by case basis. 3 facilities only pay for the return shipment of the samples.

The large majority of facilities that offer financial support see no financial gain from offering remote services as they require more investment in manpower and staff which outweighs any gain from the reduction in travel and accommodation expenses, also taking into account that transport of samples is paid for by many facilities.

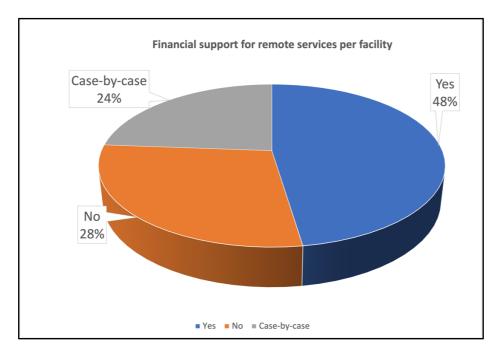


Figure 3: Overview of financial support for remote services. See Annex 2, Financial-Remote Q15-16

5. User Experience and Feedback

TOPIC	KEY MESSAGES
User experience and feedback	 Users appreciate the possibility to access the facility remotely when beneficial Onsite presence is still very much desired by the user community

The majority of facilities have noticed a recurring use of remote access from their users – trends show that recurring users are typically from outside the EU and from longer distances, or participants in short experiments (feasibility tests) and MX.

Feedback indicates that users are very happy with the possibility to use remote services. Positive comments include: the opportunity for users to be able to perform an experiment and collect data during lockdown (8) and it has now evolved to the positive outcome of users not having to travel and therefore saving money (for those paying) and also time, especially for shorter experiments (7). Additionally, a faster turnaround for quick measurements (5), the benefits of staff engagement and therefore expertise (3) and the ability for more users to take part in the experiment remotely (2) were also listed as positive points.

Any complaints or negative feedback include: issues with shipment delays and customs (3 facilities), issues with connection stability and/or software instalment (4), lack of communication between staff and users and thus lack of training possibilities for PhDs (1), demand from users to be able to take more measurements (1) and transfer of workload from users to staff. 4 facilities have noted that users do notice the difference in experiment efficiency when one or more users are present onsite, and the inability to cover night shifts remotely was also listed as an issue as beamtime was lost by users in this regard.

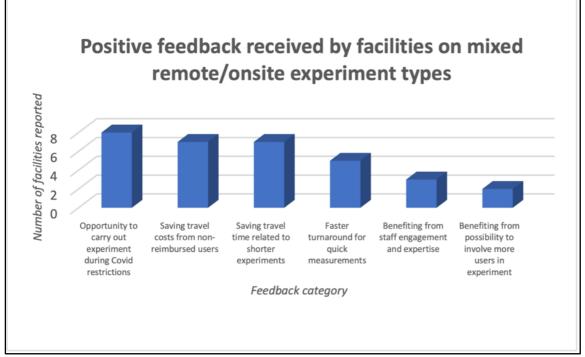


Figure 4a: Positive feedback comments received.

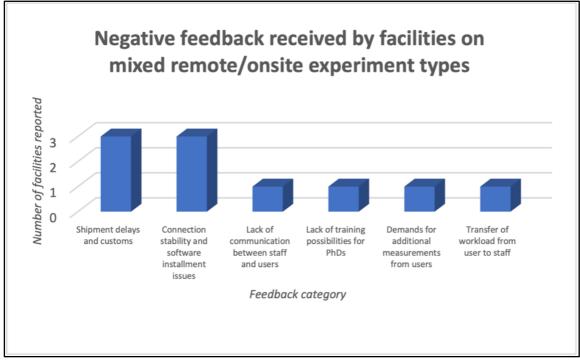


Figure 4b: Negative feedback reported about mixed onsite/remote experiment types.

See Annex 2, User Feedback Q17-20

6. Outlook

TOPIC	KEY MESSAGES
Future outlook	 Pandemic times workload not sustainable, need for more staff and users onsite whenever possible; mixed
	onsite/remote experiments best compromise

15 facilities are interested in increasing these services with an aim to reduce carbon emissions on the condition that it would not be detrimental for the experiments, the user experience or the staff's workload. Most facilities do not have a defined goal but several mentioned the need to increase automation and experiment standardisation in order to increase remote services in a significant way. 12 facilities developed their remote services because of the pandemic's constraints. In terms of satisfaction, the responses are mixed: some facilities (5) did recognize that these services added value as they allowed experiments to be carried out despite logistics restrictions and also led to the improvement of such systems already in place (5). It also met the users' request (1) and has led to users now being used to it and therefore being comfortable with the procedures (1). However, some facilities (4) think more development needs to be done on the systems and procedures in place to continue improving beyond the pandemic's restrictions, some also cited the additional workload on staff as a reason for increased remote access to not be a long-term solution (3) and some (2) were only partially satisfied and reiterated the loss of know-how for the future generation of scientists if such services remain popular amongst users.

See Annex 2, Outlook Q21-24

PART B - Mailing samples

7. Software and hardware tools

TOPIC	KEY MESSAGES
Software and hardware for	Few facilities have an electronic tracking system in place
managing samples	No obvious consensus on a common tracking system, but
	facilities would be interested if a standard solution could
	be made available

Only 4 facilities use a specific tracking system for parcels coming in and out of facilities, with another 3 using some other sort of system to keep records of it. Whilst 2 facilities track parcels manually, 4 facilities have electronic solutions in place: ELETTRA uses VUO, ALBA and DLS use ISPyB and ESRF uses both ICAT and ISPyB. 2 facilities use it to cover structural biology only whilst 5 use the tracking system for both structural biology and non-structural biology. 5 of these facilities say it does help with problem resolution when a sample is missing. Lastly, in 4 of these cases the tracking system is directly linked with the Digital User Office software.

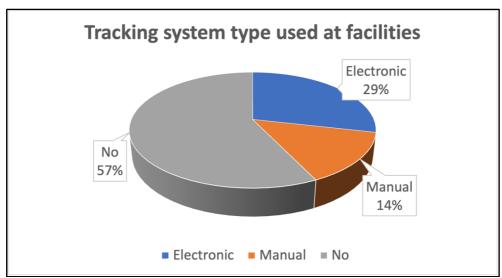


Figure 5: Overview of parcel tracking systems in use at the different facilities.

9 facilities are either looking to implement a tracking system or would be interested but with relatively low priority.

There appears to be no consensus towards a common favoured system – 3 facilities are interested in using ISPyB but its MX-specific nature makes it difficult to use for all samples.

In terms of labelling parcels, 5 facilities use systems which provide the option for printing specific labels from a software whilst 5 others strongly recommend to users to disclose all the information necessary for efficient tracking such as address, name of local contact, proposal number, beamline scientist, etc.

Only 3 facilities use barcode readers for tracking or identifying parcels/samples, and one facility provides auto-filling of courier documents thanks to an API between the courier management software and the facility software.

7 facilities recommend standard types of sample transport container – all 7 mention standards for MX experiments (dewars, unipucks, etc), while only 3 mention non-MX standards such as powder diffraction, some liquid samples for specific beamlines, Peli boxes on spectroscopy BLs.

See Annex, Software-Hardware Q25-34

8. Financial support for mailing samples

TOPIC	KEY MESSAGES
Financial support for mail-in	13 facilities do cover expenses with varying rules
	Amounts spent on sample shipment vary greatly, from a
	few k€ up to 100k€/year

13 facilities cover the expenses linked to parcel shipment with varying reimbursement rules: some facilities (4) apply the eligibility for sample reimbursement by linking it to the eligibility of the session to have reimbursed users – one reimbursed dewar/parcel eligible per non-traveling reimbursed user. Others (3) only allow this on a case by case basis and allow for automatic reimbursement only if this was set up correctly via their systems (4). Finally, 4 facilities only pay for the return of the shipment to the home lab but not for its arrival at the facility which remains at the expense of the users. 8 facilities do track and monitor shipping expenses – 4 on a monthly basis, 2 on a quarterly basis and 1 annually (1 did not indicate the periodicity).

The amount spent on sample sending costs varies immensely between facilities, ranging from €5,000 or less per year to over €100,000 per year (DLS and ESRF).

No facility has received compensation from courier companies for damaged/delayed samples.

See Annex 2, Financial Samples Q35

9. Transport administration and customs

TOPIC	KEY MESSAGES
Transport and customs	Need for professionals to deal with logistics and custom issues
	Restrictions exist on the type of samples that can be mailed-in

More than half of the facilities share guidelines to the users in regard to the legal and safety requirements concerning the content of parcels. 7 facilities have restrictions in place for mailing in hazardous samples (gas, chemicals, radioactive and certain biological samples), 2 mentioned not accepting to receive live animals, 3 prefer not to handle and therefore receive samples requiring expertise to be handled. One did mention not accepting unique samples (such as samples of a cultural heritage nature).

Half of the facilities share guidelines/specific advice in regard to the administration formalities linked to customs: 8 facilities give safety and legal advice, 9 give advice on how to fill out the declaration form whilst a few give further advice on how to fill out courier related paperwork or how to pack the sample appropriately. The two main reasons cited were to prevent delays with courier and customs (7 facilities) and avoiding extra fees linked to priority shipping and customs fees (6 facilities). Some facilities have users declaring the real value of the sample while others ask users to declare a low value for customs purposes only and to avoid unnecessary high costs. This may depend on whether the user or the facility is paying for the cost of transport.

Most facilities mentioned destinations that are often linked to delays due to customs issues only: India 3 / Brazil 1 / Argentina 1 / Australia 1 / Norway 1 / UK 5 / US 3 / Spain 1 / Israel 2 / South Africa 2.

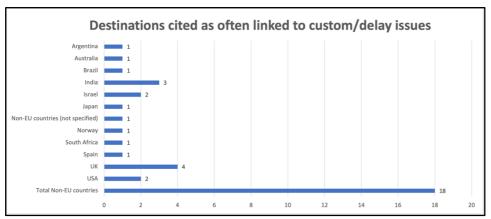


Figure 6: Overview of destinations to/from which customs/delay issues have been reported.

Some facilities (6) have indicated that cancelled experiments due to loss of samples simply are 'few' or between '10-20'. This was often linked to custom delays (6) which meant the dewars were warm by the time they had arrived or led to insufficient results. Finally, 7 facilities reported not having had to cancel an experiment at all.

11 facilities indicated that they have an export control specialist or similar position, though these are not full-time positions, while 4 do not. How much time is spent on user sample control within this position is not clear.

See Annex 2, Admin-Customs Q36-46

10. Courier

TOPIC	KEY MESSAGES
Couriers	12 facilities recommend specific companies to users but
	only 4 of them have a dedicated contract

12 facilities recommend specific companies/service providers to their users: GO! (1) / Fedex (8) / DHL (7) / TNT (3) / Jetpak (1) / Spedservice (1) / UPS (3) / Bartolini (1), but only 4 facilities (DESY, Diamond, ELETTRA, INFN) have a dedicated contract with a courier company/service provider. Reasons for not having a dedicated contract are: one facility mentioned the lack of time to arrange this, one mentioned that too few shipments were being sent for one, 4 facilities mentioned that users have their courier preferences or even contracts with home institutes rendering a facility-specific contract underused.

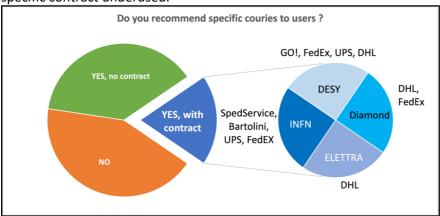


Figure 7: Share of facilities recommending specific couriers to users. For those 4 facilities that have a dedicated contract with a service provider / courier, companies are listed.

See Annex 2, Courier Q47-49

11. Reception and return of samples

TOPIC	KEY MESSAGES	
Sample reception and return	Transporting samples from central reception to	
	beamlines is carried out by beamline/lab staff for 10	
	facilities, and shared among User Offices, stores,	
	logistics, and third party providers' staff for the others	

15 facilities have a central facility for receiving and returning user samples, that is open during normal working hours (not evenings or weekends).

For 10 facilities, transporting the samples to the beamlines is the responsibility of the beamline/lab staff/local contact, for 4 of them the User Office takes care of this, stores/logistics staff do this in 2 facilities and according to 3 others this is handled either by a third party provider or the onsite transport company.

Upon reception, samples are stored in the central store/warehouse (8), in beamline/lab staff offices (5), or shelves/lockers close to beamlines/labs (5).

The local contact is informed about the delivery of the samples: 10 facilities use either email or phones upon reception, for 4 facilities this is done automatically via the tracking system notifications, 2 of them are contacted by the users directly and 1 facility has not yet defined a standard procedure for this.

The local contact's roles vary depending on facilities, and can be responsible for: reception of samples (3), preparing the return (affix labels) (10), handling the paperwork linked to shipping (10), bringing to the User Office or logistics office for shipment (7), discussing return and informing users of arrival and return of parcels (7), disposing of samples (2).

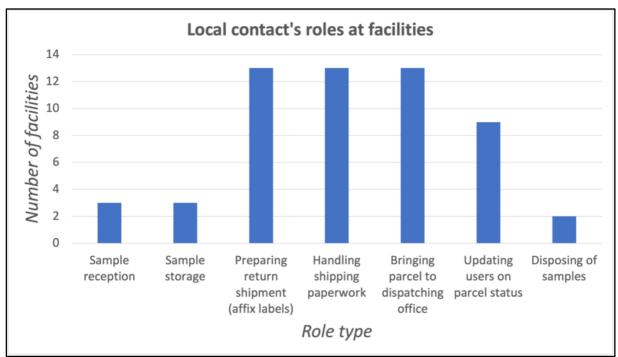


Figure 8: List of local contact roles for mailing samples.

In most cases the facility Safety Group does not play a role in reception of samples except for agreeing protocols for reception of dangerous goods. For most facilities, safety constraints approval is done either at the level of the proposal submission or experiment scheduling, via sample sheets.

See Annex 2, Reception-Return Q50-56

12. Staffing

TOPIC	KEY MESSAGES
Staffing	 7 facilities have a dedicated person or office to ensure fast resolution of issues; 9 indicate there is insufficient manpower Most issues require the involvement of several different services within the facility e.g. Stores, Safety, Software, Accountancy

Resolution of issues related to sample transport often involves 2 to 3 people from different departments across the facilities: beamline scientist and local contact (13), shipment/stores and customs expert (13), User Office (9), secretary/reception (2), Finance (2), Safety (5), ISPyB programmer (1).

7 facilities have a dedicated person/office for fast resolution of issues related to sample transport, 9 do not. In 4 facilities, it is a User Office staff member, in one facility the emphasis is on the teamwork of 3 staff (UO, Goods Handling and ISPyB engineer), in 2 others it is mostly the logistics/export control specialist handling these issues directly.

9 facilities indicate that there is insufficient manpower to handle the reception and return of samples – the main need would be for beamline staff given the increased workload remote access demands (3) then stores staff (2), safety staff (2) and a software engineer (1).

See Annex 2, Staffing Q57-61

13. User experience and feedback

TOPIC	KEY MESSAGES
User feedback	 Users mostly satisfied with the services offered but most
	still consider it as an alternative in specific circumstances,
	e.g. pandemic times

Generally users have been simply happy that the experiments could be performed at all during the pandemic. However, recurring customs problems and delays have been noted by some users who regularly transport samples and have faced more than one delay.

See Annex 2, User Feedback Q62-65

UPDATE - Spring 2024

Questions and summary of answers:

Please describe the evolution of remote / mail-in use of your facility since 2022? Please also comment on expected future trends.

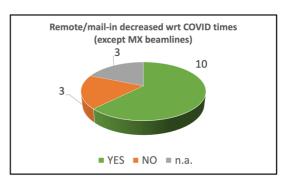
After the pandemic, there has been an overall decrease of both remote and mail-in access, except for MX (and some PXRD, SAXS) and tomography where exploitation and even development is continuing (example: from an average of 40% in 2021 to 10% in 2023, of which 90% is MX). Most facilities do encourage users to come back on-site. Hybrid access is however being exploited to foster participation of larger groups and communities. FELs: complexity of experiments is preventing remote access.

2. Has your facility implemented / planned new technologies for remote/mail-in? If yes, please give more details. If no, why?

In facilities where the number of MX / tomography users is high, developments are justified. Technologies exploited include: sample exchange robots, faster shipment procedures, online data acquisition and analysis tools, high-throughput pipelines (tomography).

3. Does your facility have a specific strategy concerning remote access, i.e. to encourage the return of users onsite or the opposite?

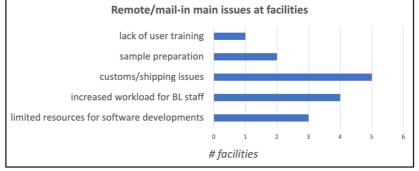
It is important to inform users about when it is feasible/desirable to perform an experiment remotely and when it is crucial to be onsite. Most facilities encourage users to come on-site, particularly after the pandemic times, to exchange knowledge and train future scientists. Fully remote access is encouraged only when beneficial for the scientific field, the user and the facility. Hybrid experiments are welcomed in most Synchrotrons. Among the developments for remote/mail-in, we can cite programs for in operando/in-situ and robotic arms for sample manipulation.



4. What are the main issues your facility is facing for the smooth and optimal use of remote / mail-in services?

Shipping issues – in particular customs delays, workload on BL staff, limited resources for software developments, sample preparation, lack of users training leading to inexperienced users.

For more details, see Annex 3.



Outlook

The survey responses and analysis were thoroughly discussed at a face-to-face workshop at HZB in Berlin in September 2022, as well as at the LEAPS Plenary Meeting at PSI in October 2022. The analysis and discussion have allowed the facilities to obtain a complete overview of the procedures existing today and the associated advantages and challenges.

By providing this database of available solutions and experiences, it is hoped that this may assist facilities who wish to enhance their user services or develop new procedures by adopting or improving procedures already in place elsewhere.

Suggesting to adopt standard solutions across all facilities was not the aim of this work package.

Consortium-based solutions, such as an agreed contract with the courier companies across all participating facilities, are desirable but are hindered due to country-specific and facility-specific constraints, e.g. import and export rules, the need to follow public calls for tender for courier services, etc.

The Horizon Europe EC funded eRImote⁴ project has been recently launched and is expected to seek solutions for digital and remote access provision across a variety of analytical facilities, including those of LEAPS and LENS. We are thus willing to share the knowledge gathered within this exercise if it is felt that this project could benefit from it.

Within the STARS project, work package 1.1 was dealing specifically with sample transport from the user facility to the research infrastructure, while WP1.3 (AutSamp - Automated Sample Handling) deals with persistent individual samples identification down to the single measurement level. This means that WP1.1 is concerned with parcel/shipment tracking while WP1.3 is concerned with individual sample tracking. WP1.2 (RemAcc - Overview of IT tools for remote access) aims to collect the information on the IT tools available to enable remote services.

During the final STARS face-to-face meeting (HZB, Berlin, February 2024), WP1.1 decided to collect a brief update from the LEAPS and LENS facilities, since the data collection of D1.1.1 referred to Spring 2022. In the meantime, the Canadian Light Source (CLS) also completed the main survey and participated into the update as well. The Excel file (See Annex 2) is a living document on the DESY Cloud, and future developments will be reported back to the community via the LEAPS Working Group 5 (User Services and Impact).

The current deliverable, that marks the end of STARS WP1.1, includes the outcome of the update collected in Spring 2024. The main message is that facilities are welcoming back physically present users, with a clear benefit for both the new generation of scientists and the facilities themselves. On the other hand, the IT tools boosted by the pandemic conditions are being exploited by specific (e.g. MX) beamlines but are also allowing "hybrid experiments", that are more inclusive and involve larger user groups.

⁴ https://erimote.eu/home

ANNEXES:

Annex 1: MailSamp Survey

Statement

The main aim of this survey is to obtain an overview of the practices in place at different facilities for allowing users to send their samples by mail to the facility and have them returned, rather than bringing them with them in the traditional way (Part B). Since such information is also being gathered in the context of the many different remote services that now exist at our different facilities, we also take this opportunity to try to obtain an overview of the different types of experiments now offered at your facilities involving remote use of the facility (Part A). The information gathered from the survey will be compiled so that its findings can be widely shared and be of use to all facilities who have, or wish to implement, such services. We hope that these actions will help facilities to share best practices and enhance the user experience.

Facility responses

Please note that we request ONE response per facility.

Please circulate this document to the relevant colleagues for completion, and return to us one consolidated response for your facility using the survey link that will be communicated to you in a few weeks.

General glossary of terms used in the survey

Sample: An entity which can be directly measured/studied/characterised on an instrument (beamline, cryoEM, support lab)

<u>Sample safety sheet:</u> A description of the sample composition, substances, or their main components used by the facility's safety team to evaluate the safety risks and recommendations associated with the study of the sample at the facility.

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PART A: EXPERIMENT TYPES OFFERED and REMOTE SERVICES

For this part of the survey, we will refer to the table of experiment types below in order to gather data based on criteria rather than defined terms and names (which differ greatly from facility to facility).

Expt Type	Users participate onsite ?	Users participate remotely?	Samples sent to the facility?	Users control beamline and take data?	BL staff run experiment and take data? *	Notes
#1	No	No	Yes, must be	No	Yes	Full service provided by BL staff - instructions provided beforehand by users.
#2	No	Yes, all	Yes, must be	Yes	No: (automation)	Implies level of automation, maybe samples loaded by BL staff.
#3	No	Yes, all	Yes, must be	Yes	No: (sample manip)	Significant sample preparation or manipulation by BL staff.
#4	No	Yes, all	Yes, must be	Yes	Yes	Control and data taking shared between user team and BL staff as required.
#5	No	Yes, all	Yes, must be	Partially	Yes	As above but users not given full control, some limitations applied.
#6	No	Yes, all	Yes, must be	No	Yes	Users only observe results (e.g. Zoom) and make decisions, no direct control.
#7	Yes, at least one	Yes, at least one	Can be	Yes	No	Users onsite and in charge but with some users participating remotely also.
#8	Yes, all	No, none	Can be	Yes	No	Users onsite and in charge - traditional.

^{*} More than the standard Local Contact role and duties



1. Specific glossary of terms used in the survey

From this point,

- The term "**remote user**" refers to a user who participates in the experiment but does not come physically onsite, i.e. he/she participates remotely from the home lab or elsewhere. It does <u>not</u> concern users who only access the data after the experiment has finished.
- the term "fully remote experiment" refers to all experiment types where no member of the user team is present onsite physically, i.e. types #1 to #6 and others that you may add where the answer to "Users participate remotely?" is "Yes, all".
- the term "remote services" refers to all experiment types where at least some users participate remotely in an experiment, and do not need to be physically present, i.e. types #1 to #7 (all except experiment type 8 that is the traditional fully onsite experiment (even if samples are sent)).

2. Available Experiment Types at Your Facility

1. Do you currently offer the experiment types above, and, if not, is your facility interested in developing them in the future? In each case please tell us the name given to this type of experiment at your facility and give any comments as necessary.

Expt Type	Currently available at your facility? Yes/No/NA	Name of this type at your facility	Wish to provide in the future? Yes/No/NA	Comments, including indication of BLs where this type is feasible.
#1				
#2				
#3				
#4				
#5				
#6		_		
#7		_		
#8				

2. Please describe any other experiment types that you offer, if not covered by the cases above. Please indicate the answers to the 5 criteria in each case, and give the name of this experiment type at your facility.

Expt Type	Users participate onsite ?	Users participate remotely?	Samples sent to the facility?	Users control beamline and take data?	BL staff run experiment and take data? *	Name of this type at your facility + additional notes
#9						
#10						

^{*} More than the standard Local Contact role and duties

3. Who, in your facility, is responsible for making the decision about under which format the experiment will take place? (several choices possible)





	 Beam Line responsible 	☐ Yes ☐ No ☐ Not applicable
	Local Contact	☐ Yes ☐ No ☐ Not applicable
	• User	☐ Yes ☐ No ☐ Not applicable
	Beam Line staff and user agreement	ent □ Yes □ No □ Not applicable
	• Comments:	
L		
4.	How long in advance does the decision	n need to be made (in the ideal case)?
5.		t when making this decision, e.g. instructions amline, staff's decision-making power, any

3. Remote Users

6.	Are your remote users required to follow a specific safety training, different to that for onsite users?		
	☐ Yes ☐ No ☐ Not applicab	le	
>	If yes, please specify the format: information sheet only,	quiz?	
7.	How do your users have access to the data? Please descr	ibe.	
8.	Are your remote users allowed to control the beamline reexperiment remotely (e.g. via Zoom)? (several choices po		
	Can control the beamline remotely applicable	☐ Yes ☐ No ☐ Not	
	Can follow the experiment remotely with no control applicable	☐ Yes ☐ No ☐ Not	
	Is this beamline dependent? applicable	☐ Yes ☐ No ☐ Not	
	Please give comments as necessary.		

4. Fully Remote Experiments

9.	Please describe (if applicable) how you collect the information necessary for your facility to conduct the experiment according to the users' instructions? (i.e. Experiment form, individual contact, database.) Refer to the experiment type numbers as required.
	☐ Not applicable
10	. What is the local contact's role and duties for fully remote experiments? Please describe briefly and refer to the experiment type numbers as required.
11	. Are you aware of any difficulties experienced by local contacts (e.g. issues of communication with users, complex sample manipulation, etc)?
12	. Does your facility have the staff capacity to support experiments without users being present onsite?
	☐ Yes ☐ To a certain extent ☐ No ☐ Not applicable
>	If yes or to a certain extent, under what conditions (e.g. a limited number or % of experiments, only certain heamlines, reduced operating hours, etc.)?

all experiments?



of parcels instead of users, payment of all samples sent, type numbers as required.	, , ,
16. Compared to onsite user expenses, do you see a financia services? Please give an estimate.	al gain from offering remote

6. User Experience and Feedback

17.	Do you have recurring users of your remote services?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, is there a noticeable trend? (i.e. country of origin/type of experiment/subject matter of the experiment).
18.	Do you collect feedback from those users?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, in what form?
19.	Do you receive any complaints from the users of your remote services?
	☐ Yes ☐ No
>	If yes, is there a general theme to the complaints?
20.	Overall, are users satisfied with the service?
20.	☐ Yes ☐ No ☐ Not applicable
>	If yes, please list the main reasons for their satisfaction.

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7. Outlook

21.	Are you interested in increasing your remote services with the aim of reducing the carbon emissions linked to users traveling to your facility?
	☐ Yes ☐ No ☐ Not applicable
22.	Do you have a defined goal for the number of experiments you would like to offer via remote services? Please share more details.
23.	What do you think could be improved within the remote service experience, and how? Please explain in a brief paragraph.
24.	Have the lockdown measures linked to the COVID pandemic affected your facility? $\hfill\Box$ Yes $\hfill\Box$ No
>	If yes, did you develop your remote services due to the pandemic's unprecedented constraints? $\hfill Yes \hfill No$
>	If yes, are you satisfied with it? Please share more details.



PART B: MAILING SAMPLES

1. Software and Hardware Tools

	25. Do you have a tracking system in place for the parcels coming in and out of your facility?		
		☐ Yes ☐ No ☐ Not applicable	
>	If yes, • •	Is it electronic or manual? Is it also used to track samples brought onsite by the users? Yes No Not applicable Is anyone responsible for the tool when an issue arises? Please share details.	
	•	Does it cover Structural Biology experiments, Non-Structural Biology or both? ☐ Structural Biology ☐ Non-Structural Biology ☐ Both	
	•	Are you satisfied with the end result? ☐ Yes ☐ No ☐ Not applicable	
	•	Does it help with problem resolution when a parcel is missing? \Box Yes \Box No, please share some details.	
>	If no, are	you looking to implement one?	
	•	If yes, is there anything stopping you from doing so?	

Please give details.

 If yes, are you looking to use an already existing tool? Please specify which one.
26. Do you request that facility-specific labels are affixed to parcels before sending, either for tracking or to provide information as required? ☐ Yes ☐ No ☐ Not applicable
> If yes, please share some details:
27. Do you use barcode readers at your facility for tracking or identifying parcels/samples? ☐ Yes ☐ No ☐ Not applicable
□ res □ no □ not applicable
➤ If yes, please share some details.
28. Do you provide auto-filling of courier documents thanks to a link between the courier management software and your own facility management software? ☐ Yes ☐ No ☐ Not applicable
> If yes, please share some details.

29.	Do you provide help (instructions, hints, auto-filling) to users for filling out the courier-specific documentation?
>	If yes, please share some details.
30.	For the samples being manipulated directly by the facility's staff, is there a different sample safety sheet provided to the users than the standard one available to visiting users?
	☐ Yes ☐ No
31.	Is your tracking system directly linked with the Digital User Office (DUO, VUO, DOOR, GATE, UAS, etc) of your facility?
	☐ Yes ☐ No ☐ Not applicable
32.	In your tracking system, do users need to fill out a different sample safety sheet than the one from the Digital User Office? $ \qed$ Yes $ \qed$ No
>	If yes, where can the users find the instructions on how to do this?
	33. Are your users required to follow a specific safety training if they wish to send samples?
	\square Yes \square No \square Not applicable
	➤ If yes, is it the same as your remote user/remote access safety training?
	☐ Yes ☐ No ☐ Not applicable
34.	Do you recommend standard types of sample transport containers for ease of use at the synchrotron?



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	☐ Yes ☐ No ☐ Not applica	ble
> If yes, please list it	/them.	



2. Financial

35.	. Do you cover the expenses linked to parcel shipment for at least some types of experiments?
	☐ Yes ☐ No ☐ Not applicable
>	If yes to question #34
	What are your reimbursement rules for sample shipments?
	 Do you track and monitor the shipping expenses linked to the service?
	\square Yes \square No \square Not applicable
	If yes, how often?
	■ Do you have a budget limit? □ Yes □ No
	• How do you link invoices received with a particular experiment? $\hfill\Box$ Yes $\hfill\Box$ No
	Which tools do you use to do this?
	 How much does your facility spend per year on sample sending costs? Please give an approximate amount.

•	Do you often receive compensation from courier companies for
	damaged/delayed samples resulting in cancelled experiments/irreversible delays
	in research?

•	If so, by which courier?	

3. Transport administration and customs

re	o you share any guidelines to your users in regard to the legal and safety equirements of your facility or your country in relation to the content of the parcels ou receive for remote experiments? Yes No Not applicable
<i>></i>	If yes, are there any goods you forbid from sending to the facility? (i.e. unique samples/dangerous/voluminous or extremely expensive materials/artefacts).
	re there any samples that you would prefer the facility not be responsible or handling and therefore only allow in-person experiments for?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, please list them by category.
	o you share any guidelines/specific advice in regard to the administration ormalities linked to customs?
	☐ Yes ☐ No ☐ Not applicable
	yes, please list them and the reasons for this advice (i.e. prevent further delays, roblems with insurance, etc.).
39. D	o your users declare the real value of the sample on the custom declaration?
	☐ Yes ☐ No ☐ Not applicable
40 D	o you find that some samples cannot be sent from certain destinations?



	☐ Yes ☐ No ☐ Not applicable
	> If yes, please list the type of samples and country of origin/destination.
41.	Are there any destinations, which are often linked to delays due to custom issues only?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, please list them.
42.	Do you have a specific system in place for a small number of countries based on previous bad experiences? Yes No Not applicable
>	If yes, please list them and add a brief explanation.
43.	Are there any countries (where the samples would be sent from) which you now refuse to work with?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, please list them and give a main reason.



44. Are there any samples you do not trust the courier companies with?

>	If so, please list them.
45	. How many experiments have been cancelled since the beginning of the pandemic (since 1st March 2020) due to the loss of a unique set of samples?
46	. Does your facility have an export control specialist or a similar position within its ranks?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, how much time is spent on sample control within this position?



4. Courier

47. Do you have dedicated contracts with couriers or do you recommend specific ones to your users?
\square Yes \square No \square Not applicable
➤ If yes,
Which ones?
Are you satisfied by their service?
 Do you have a dedicated contact at those couriers which allows for fast resolutions?
> If no, why not?

48. Which courier do you get the most complaints about? Please list them.



49. Are there couriers you have stopped using due to recurring problems?If so, which ones and please explain why?	

5. Reception and return of samples

50.	Do you have a central facility, e.g. reception department/stores, for receiving/returning user samples?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, is it adapted to handle/manage this service? Please describe briefly.
>	If yes, who brings the samples to the experimental station?
51.	Are there times when deliveries cannot be received either because the reception department is closed or because access to the facility or contact person is restricted?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, please list them.
52.	Where do you store the samples you receive? Please briefly describe.
	☐ Yes ☐ No ☐ Not applicable

53. Do you have enough space for storing them?





☐ Yes ☐ No ☐ Not applicable
54. How is the local contact informed about the delivery of samples/equipment?
55. What is the local contact's role in reception and return of user samples (e.g. returning samples to central facility, affixing return labels, informing users, etc.) ?
56. Is your safety group adapted to the reception of samples by courier?
☐ Yes ☐ No ☐ Not applicable
Please list any issues you may be encountering.

6. Staffing

57. Do you need to provide additional training to users and/or to staff when samples are

If yes, please describe the main additional topics of training required.
How many people within your facility are usually involved in the resolution of issues elated to sample transport? (e.g., customs, legal, safety, damaged) Please list them roles, not individual names).
Oo you find that the communication between those departments is sufficiently efficient?
\square Yes \square No \square Not applicable
Oo you have a dedicated person/office for fast resolutions of issues related to sample ransport, relaying information between all the concerned departments?
\square Yes \square No \square Not applicable
yes, please describe the function and job title?
l er





61. In general, do you have enough manpower for handling the current level of reception and return of user samples at your facility?
□ Yes □ No
> If no, please describe the main areas where more staffing would be required.

7. User Experience and Feedback

62	experiments or remote-style experiments)?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, is there a noticeable trend? (i.e. country of origin/type of experiment/subject matter of the experiment).
63	. Do you collect feedback from those users on this service?
>	\square Yes \square No \square Not applicable If yes, in what form?
64	. Do you receive any complaints from the users about your sample mailing service or procedures? ☐ Yes ☐ No
>	If yes, is there a general theme to the complaints?





65	. Overall, are users satisfied with the service?
	☐ Yes ☐ No ☐ Not applicable
>	If yes, please list the main reasons for their satisfaction.
>	If no, please list the main reasons of their dissatisfaction.

Annex 2: MailSamp Survey Compiled original answers from facilities

The answers to the survey were compiled into an Excel sheet which is available through the following link on the DESY cloud:

https://desycloud.desy.de/index.php/s/GwMJZmtFzdqks5M/download

This version of the file is locked from editing so that the original answers to the survey can be reviewed as reference to the report but an editable version is also available on the cloud for facilities to update and use as a working document.

Annex 3: MailSamp UPDATE questions – Spring 2024

- 1. Please describe the evolution of remote / mail-in use of your facility since 2022? Please also comment on expected future trends.
- 2. Has your facility implemented / planned new technologies for remote/mail-in? If yes, please give more details. If no, why?
- 3. Does your facility have a specific strategy concerning remote access, i.e. to encourage the return of users onsite or the opposite?
- 4. What are the main issues your facility is facing for the smooth and optimal use of remote / mail-in services?

The answers to the survey were compiled into an Excel sheet which is available through the following link on the DESY cloud:

https://syncandshare.desy.de/index.php/s/BJAQi66JaF6b8aN?dir=undefined&path=%2FReports%20%26%20Dissemination&openfile=643836117