STAP Report

Reflectometry Software April 2023

Andrew R. McCluskey*

European Spallation Source ERIC, Ole Maaløes vej 3, 2200 København N, DK

April 11, 2023

Following the late 2022 STAP, there was a request for a software update at every STAP meeting, rather than on the annual basis that existed previously. Here we detail some of the work conducted for reflectometry software since the last update. We specifically request feedback on the following aspects of the report (**the charge**):

- Are the service blueprints introduced here comprehensive (while remaining general)?
  - Are there any important interactions that the STAP feel should be highlighted/focused on?
- We are interested in extending the capability of the `scipp` reduction workflows to cover more of the operation modes of the ESTIA instrument. Do the STAP have relevant contacts that would be interested in collaborating (including themselves) to increase the operation mode coverage?
- The EasyReflectometry roadmap has been published online [1] Do the STAP feel any features are missing that should be considered?
- We ask the STAP members to download, install, and use the EasyReflectometry application (a new release will be available in the coming weeks) [2] and provide feedback on any aspect of the application. Note that the application for macOS is not yet signed and installation instructions can be found at `https://support.apple.com/en-gb/guide/mac-help/mh40616/mac`).
  - Please remember this project has thus far had a single person year of effort (one half of the IDS for two years) and is therefore still a beta product.

In this report, we cover work developing detailed plans for the interaction of different user types with the ESS computing staff and infrastructure (in the form of service blueprints), discuss the use of `scipp` to reduce data from the OFFSPEC instrument at ISIS (representing a second measurement mode of the ESTIA instrument), the latest developments and plans for the EasyReflectometry application and the work to integrate the metrology cart that will be installed at the ESTIA instrument. Over the past year, in addition to supporting the ESTIA instrument, the Instrument Data Scientist (Andrew R. McCluskey) has also served as the work package leader for WP8 (training materials and associated services) of the PaNOSC project as well as conducting independent research using statistical models to describe atomistic simulations (to use this to obtain a better comparison between simulation and neutron scattering data).

Service Blueprint

Contributors: Massimiliano Novelli (ESS).
In the STAP report from late 2021 [3], the anticipated analysis support for users was outlined. This involved the definition of different "user types" that are expected at ESS for the ESTIA and FREIA instruments and gave information about the support that they would be offered as part of an ESS experiment. The user types were defined as:

- new users to reflectometry that have no prior experience in reflectometry analysis;
- users with complex analysis requirements (e.g. constrained analysis of kinetic measurements);
- experienced reflectometry users with experience in reflectometry analysis; and
- users interested in the co-refinement of specular/off-specular/GISANS.

To prepare for user operation with this analysis support in place, there has been a focused effort within the DMSC to develop "service blueprints" that outline the interactions between users and ESS computing staff and infrastructure.

A service blueprint is a process chart that outlines how some **service** is delivered, from a user's perspective. In our context, the service is computing, i.e. reduction and analysis, support for users of the ESTIA and FREIA instruments at

*andrew.mccluskey@ess.eu

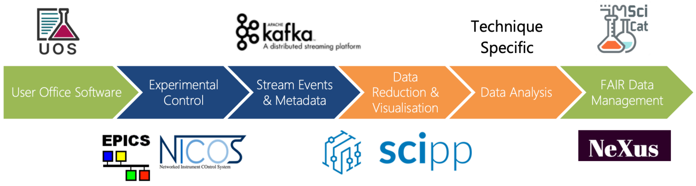

Figure 1: A diagram of the European Spallation Source data pipeline.

the European Spallation Source during user operation. Despite the focus on user operation, the exercise of defining this process will ensure that there is a clear understanding of the requirements throughout the ESS data pipeline, shown in Fig. 1.

A service blueprint defines interactions between the **user** and different **actors**, in this case, these actors include people (i.e. the Instrument Data Scientist), groups (i.e. the User Office), or software (i.e. `scipp`). The standard process for a service blueprint consists of four phases:

- **Aware**: how the user is made aware of the service;
- **Join**: once aware, the join process defines how the user is introduced to the service;
- **Use**: how the user interacts with the service (for our use case, we have broken this into two sub-phases; "Use - Beamtime" and "Use - Analysis" to reflect the continuing nature of the support after the beamtime is complete; and
- **Leave**: the process of the user leaving the service and how support is ended and tracked.

We have prepared a service blueprint (see Fig. A.1) that defines the interaction with users that are **experienced neutron reflectometry users with no complex requirement needs and no interest in using EasyReflectometry for their analysis**. This blueprint will be used as the base from which all other blueprints grow, as this represents the most straightforward use case. We will outline the process that this service blueprint defines here.

The **aware** phase begins with the user being awarded their beamtime. Alongside the standard interaction with the local contact to arrange the practicalities of the experiment, the user will be made aware of the reduction and analysis support that is available. The user will be offered training in using EasyReflectometry and support in developing complex analyses (it is expected that the latter will be a collaboration between the IDS and the user that is reflected in the IDS receiving authorship on publications that result). For this example, we assume that the user rejects this additional support, opting for the base support; reduced data at beamtime and access to VISA for analysis. At this point, a repository will be created for the reduction scripts that will be used during their beamtime and link this with the `SciCat` entry associated with the experiment.

During the **join** phase, as the user prepares for their beamtime, the User Office will send out a reduction/analysis requirements survey. This will be a carefully prepared survey to help the IDS and instrument scientist to define the reduction workflow (and analysis, if desired) required for the given experiment (in consultation with the user). Once this is agreed with the user, the IDS or instrument scientist will define an automated `scipp` workflow, which will be used during the beamtime to reduce the data. Concurrent with this, the user will be required to define the samples that they will measure during their beamtime. This sample definition will be integrated into the `SciCat` metadata entry and these samples will be available in `NICOS` during the beamtime, such that the sample metadata is available in both the raw NeXus and reduced .ort file (the ORSO defined file format).

With all metadata and reduction workflows in place, (from the software side) the experiment is ready to take place (the **use** phase). When an experimental measurement is started, the user will be expected to select the appropriate sample such that this can be associated with the data. Once the measurement has started the event data will be streamed by Kafka and a remote server, with access to the reduction workflow, will reduce the data in real time. The live reduced data will be visible to the user as it is collected and updated at a set interval (for users interested in using EasyReflectometry there will be an effort to analyse this data on the fly using a predefined model). When a given experiment is stopped the **full** reduction will be triggered on the written raw NeXus file and the reduced .ort file will be written and associated with the `SciCat` entry. The visualisation of this reduced data will be available to the user, most likely through the `SciCat` web interface along with the available metadata, additionally, the user can tag the data in `SciCat`, for example, identifying "good" or "bad" data.

Once the data has been collected, the user beamtime will end. However, the interaction with the computing support will not end at this stage. The user will be invited to use the `VISA` portal for their data analysis, with common open-source analysis packages (i.e. `BornAgain`, `refnx` and `refl1d`) made available there (EasyReflectometry will also be available should the user want to use this). This allows the analysis to be performed on ESS compute infrastructure, removing the need for large datasets to be downloaded and enabling any analysis to be stored in the `SciCat` entry. Alternatively, the user can download their data from `SciCat` and perform the analysis, offline, on their local machine. During this stage, if the user has opted for additional analysis support, the IDS will be available for consultation regarding analysis (again, developing a collaboration with the user that is reflected in publication coauthorship).

The **leave** phase takes place after the data is analysed and either a publication is published or the data embargo period has lapsed, both of which may trigger the release of the dataset, with a DOI that can be cited. The inclusion of the metadata (such as sample information) in the `SciCat` entry means that the data will help to ensure that the dataset has been shared in a FAIR way.

Also available in Appendix A.I are the service blueprints for experienced users interested in using EasyReflectometry and users with no prior experience in neutron reflectometry (we do not discuss these in detail here). The service blueprint for the complex analysis use cases and those interested in off-specular/GISANS measurements are currently in preparation.

Reduction workflows for ESTIA

Contributors: Jan-Lukas Wynen (ESS), Neil Vaytet (ESS) & Simon Heybrock (ESS).
In preparation for commissioning, first science, and user operation, reduction workflows must be available for all operation modes of the ESTIA instrument. To this end, we identified eight operation modes that require different reduction workflows, which arise from three binary options in the instrument setup:

- Focusing mode;
- Polarisation; and
- Pulse skipping.

For simplicity, we will use a binary system for identifying the different operation modes, where the first digit is 0 for collimated and 1 for focusing, the second digit is 0 for non-polarised and 1 for polarised, and the third digits is 0 for non-pulse skipping and 1 for pulse skipping. Therefore the Amor reduction workflow available online [4] has the identifier of 100. Over the coming 18 months, we will endeavour to develop and document the eight reduction workflows for the ESTIA instrument. These will be developed using data from existing instruments with similar operation modes or McStas simulations.

Reduction and analysis of data from OFFSPEC

Contributors: Jan-Lukas Wynen (ESS), Neil Vaytet (ESS), Jos Cooper (ISIS) & Simon Heybrock (ESS).
Previously, the 100 reduction workflow was developed [4]. Building on this success, the 100 reduction workflow has been developed, in consultation with Jos Cooper (formerly one of the OFFSPEC instrument scientists). This `scipp` workflow has been developed to mirror the reduction process taken in Mantid, which is standard at the OFFSPEC instrument. We compare the `scipp` reduced data with that from Mantid in Fig. 2 and the full `scipp` notebook will be made available on the `ess` documentation pages [5] soon.

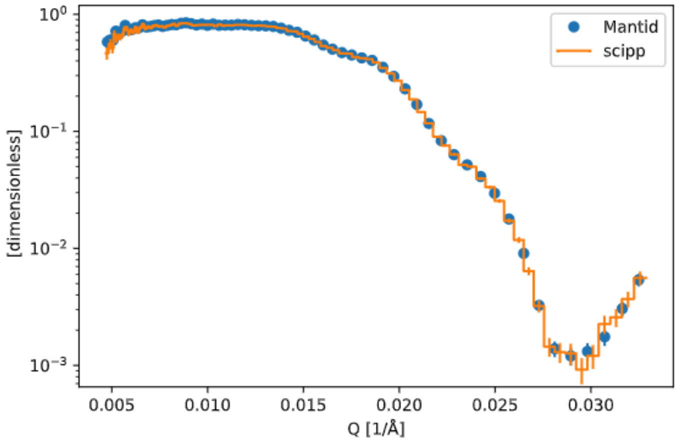

Figure 2: A comparison between the data reduced with `scipp` and that reduced with Mantid.

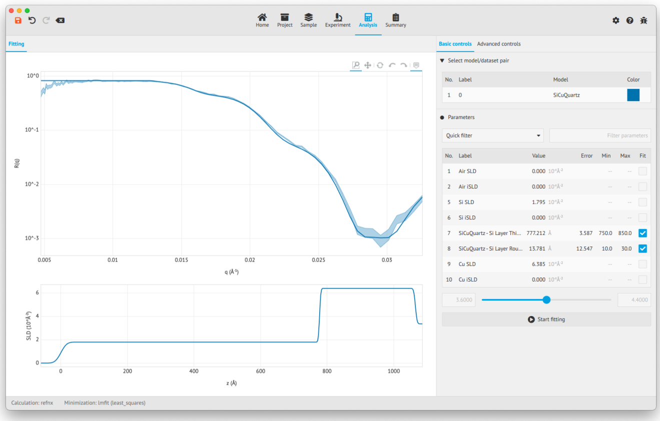

Figure 3: The reduced OFFSPEC data that has been read into EasyReflectometry.

The reduced data can be written into an ORSO-compliant .ort file (using the `orsopy` package), which can be read into the EasyReflectometry package (shown in Fig. 3) and analysed. The sample that was measured is one of quartz-copper-silicon at the solid-air interface, for which we were able to fit values similar to that found previously [6]. Currently, we only reduce a single-angle measurement, in the coming months this will be extended to include multi-angle support and the full dataset can be reduced and analysed.

Latest developments in EasyReflectometry

Contributors: Simon Ward (ESS), Piotr Rozyczko (ESS), Andrew Sazonov (ESS) & Jos Cooper (ISIS).

The EasyReflectometry project has been in development for nearly two years now with significant progress in this time. Already, EasyReflectometry is capable of analysing experimental reflectometry data using traditional minimisation approaches, matching existing software in this capability. The main development in the EasyReflectometry package since the early 2022 STAP meeting [7] has been in the fitting of multiple datasets in the graphical user interface. This can be performed using parameter constraints, meaning that this can be used for the constrained analysis of multiple isotopic contrasts or time-resolved measurements of thin film formation at interfaces. The current implementation of this is not the final version, it will continue to evolve to improve usability based on user feedback.

Alongside this major development, there have been smaller quality-of-life and sustainability developments, such as the ability to output simple plots of data and analytical models as PDFs and a complete rewriting of the continuous integration application-building process. Additionally, EasyReflectometry has received its first contributions from outside of ESS, namely Jos Cooper (ISIS) has contributed bug fixes and is looking to add functionality based on his work to develop experimental planning methods [8, 9]. There has also been preliminary work to design an interface for the analysis of polarised/magnetic reflectometry measurements (this will not be discussed in this report).

In addition to these functional developments, there have been administrative developments regarding the EasyReflectometry project. The first of these is that going forward EasyReflectometry will be supported by the EasyScience team as a whole, removing the sole developer role from Andrew R. McCluskey, which was identified as a single point of failure (however Andrew will still serve as product owner and lead developer). Additionally, as a component of the ESS planning exercises, a roadmap for the EasyReflectometry project has been developed [1], it is noted that this roadmap is not set in stone and may change both in terms of timescale and order of developments. For example, there was a suggestion that the Bayesian analysis work should be brought forward as a graphical reflectometry analysis package with access to Bayesian modelling would create a unique selling point for EasyReflectometry. As a result, a project has recently begun to integrate Bayesian methods into the EasyCore package (on which EasyReflectometry is built) making the functionality available across the EasyScience family (i.e. EasyDiffraction). This project is being led by Simon Ward (ESS) with input from Andrew R. McCluskey (ESS), an experienced user and developer of Bayesian methodology in reflectometry.

Metrology cart integration

Contributors: Artur Glavic (PSI).

The ESTIA guide system will be positioned and aligned using a custom metrology cart system. This cart will move up and down the Selene guides and is capable of moving the neutron mirror components within, using a screwdriver and interferometer. It is important that this process can be achieved in a reproducible way whenever it is performed. The cart has been discussed in detail at previous STAP meetings [10].

In the coming weeks, the metrology cart will be integrated and tested at the ESTIA beamline. At this time, the software developed by Artur Glavic to control the cart and drive the screwdrivers will be used. Following this initial operation test, the software will be handed off to the IDS to integrate the software into the `NICOS` interface for the ESTIA instrument and develop user (i.e. the instrument scientist) interfaces for interactions with this (following best practices for software development [11]). The final aim of this project will be to optimise the alignment of the Selene guide mirrors to obtain the best focusing of the neutron beam in a completely reproducible fashion.

References

[1] A. R. McCluskey, *EasyReflectometry-roadmap*, Available online at: https://github.com/easyScience/EasyReflectometryApp/blob/develop/ROADMAP.md, 2022-11.

[2] A. R. McCluskey et al., *EasyReflectometry-0.0.6rc*, Available online at: https://easyreflectometry.org, 2023-03.

[3] A. R. McCluskey, *Reflectometry STAP Report: Software*, Available online at: https://indico.esss.lu.se/event/2834/, 2021-10.

[4] A. R. McCluskey and N. Vaytet, *Divergent data reduction for Amor*, Available online at: https://scipp.github.io/ess/instruments/amor/amor_reduction.html, 2023-02.

[5] S. Developers, *Data reduction for ESS instrumentation*, Available online at: https://scipp.github.io/ess, 2023-03.

[6] J. H. Durant, `structure.py`, Available online at: https://github.com/James-Durant/fisher-information/blob/219c4b6ea087156ccb76474578261c7e1fc98a28/fisher-information/structures.py#L478, 2021-05.

[7] A. R. McCluskey, *Reflectometry STAP Report: Software*, Available online at: https://indico.esss.lu.se/event/2999/, 2022-05.

[8] J. H. Durant et al., “Determining the maximum information gain and optimizing experimental design in neutron reflectometry using the Fisher information”, J. Appl. Crystallogr. **54**, 1100 (2021).

[9] J. H. Durant, L. Wilkins, and J. F. K. Cooper, “Optimizing experimental design in neutron reflectometry”, J. Appl. Crystallogr. **55**, 769 (2022).

[10] A. G. Glavic, *Prototype testing: Robotic Adjustment*, Available online at: `https://indico.esss.lu.se/event/1240/`, 2019-04.

[11] J. Wuttke et al., “Guidelines for collaborative development of sustainable data treatment software”, J. Neutron Res **24**, 33 (2022).

A.I. Service Blueprints

Fig. A.1 shows the service blueprint when the users are experienced in neutron reflectometry and have their own analysis preferences, Fig. A.2 shows the service blueprint for experienced users that are interested in using EasyReflectometry for analysis, and Fig. A.3 shows the service blueprint for users with no reflectometry experience.

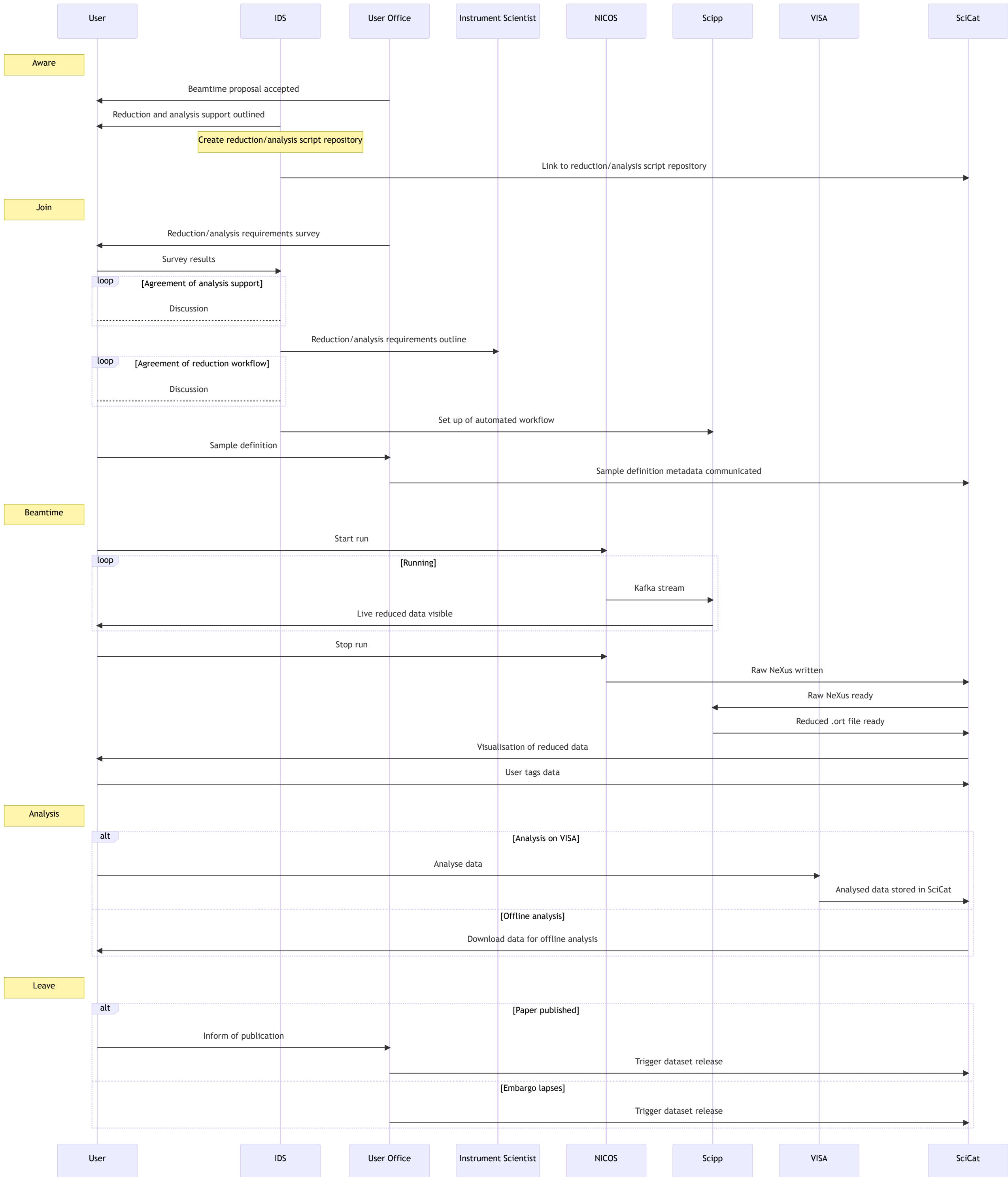

Figure A.1: The service blueprint for experience neutron reflectometry users that have their own analysis software preferences.

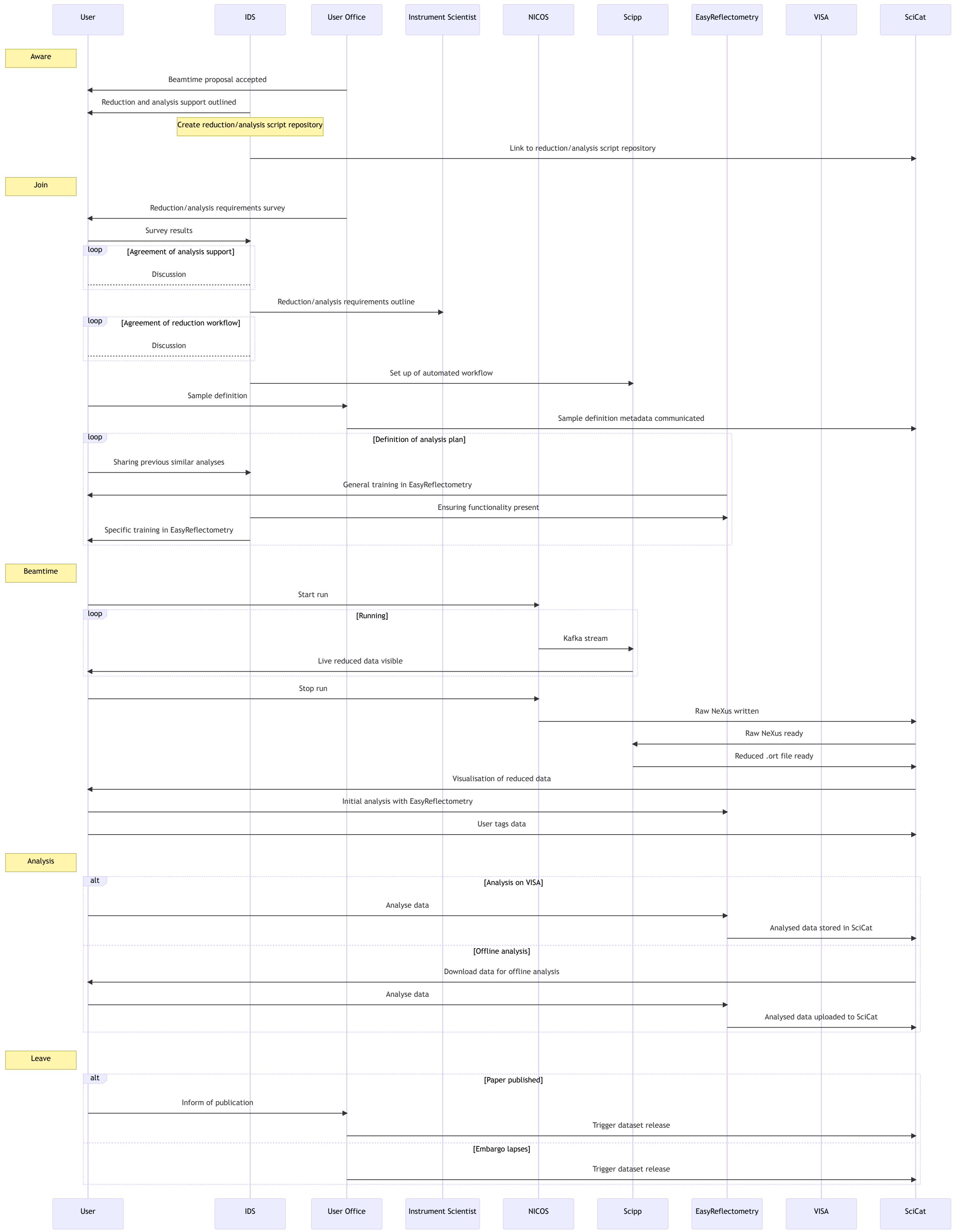

Figure A.2: The service blueprint for experience neutron reflectometry users that are interested in using EasyReflectometry.

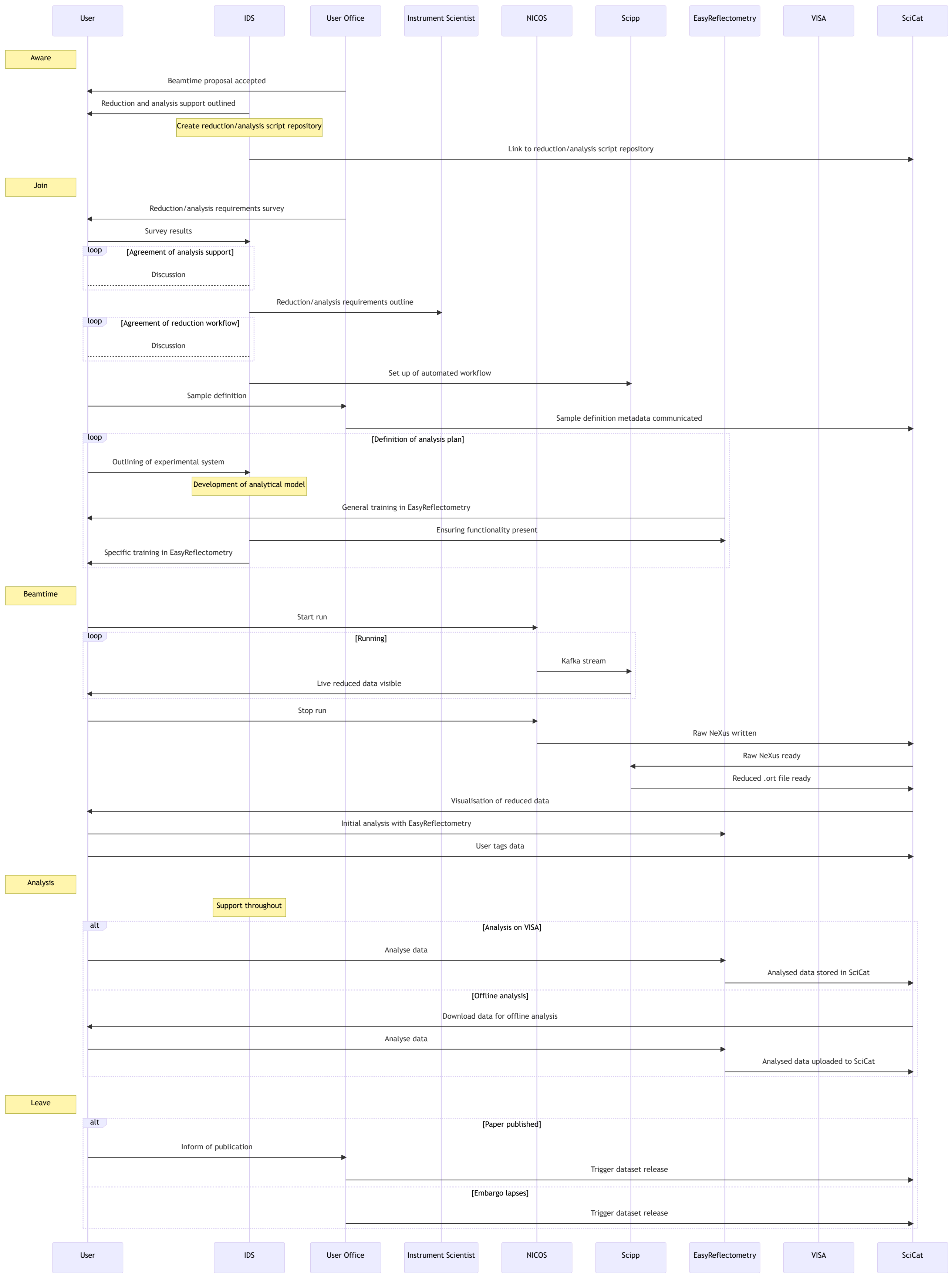

Figure A.3: The service blueprint for users with no experience in neutron reflectometry.