Case Study 1: Data and simulation driven understanding of catalytic activity

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1 Introduction

This case study is intended to show how the combination of existing data repositories can enable research reproducibility (and validation), reuse of data, reuse of processing tools and implementation of advanced data processing (Workflows, Machine Learning, Artificial Intelligence).

Researchers have been using different platforms to preserve research data. For instance, the facilities provided repositories (STFC eData), institutional repositories (Cardiff Research Poral), publisher repositories (ACS, RSC), specialised databases (CCDC), and general purpose repositories (Zenodo, Figshare, GitHub). Any infrastructure which aims to support data management need to operate in this environment. The UKCH has proposed the creation of a specialised catalogue linking data objects to publications, providing context information which can enable reproduction, reuse, and extension of results.

1.1 Context

Experimental and computational simulation techniques developed to understand the nature of materials and their practical applications in catalysis research rely on the use of data for building and validating complex models. The UK Catalysis Hub (UKCH) enables cutting-edge research in catalytic science, by facilitating access to state-of-the-art resources and expertise. UKCH provides access to well-equipped laboratories, sponsors access to facilities provided by the Science and Technology Facilities Council (STFC) and offers expert advice for processing and analysis of the data produced from experiments and theoretical models.

1.2 UK Catalysis Hub Data Management and Processing

The UK Catalysis Hub (UKCH) is designing two platforms to support the management and further use of catalysis research data: the Catalysis Data Infrastructure [8] and the Catalysis Research Workbench [9]. The Catalysis Data Interface will facilitate the localization of publications and research data objects in an array of distributed repositories. The Catalysis Research Workbench will facilitate access to processing tools for established processing and analysis tasks.

The CDI is proposed as an infrastructure to facilitate the management of research data produced by researchers. The CDI is proposed to encompass the presentation of research outputs (publications and data) in a digital repository that brings together an array of heterogeneous data types. The CDI is designed to hold references to research outputs, maintains links between them and promotes publishing and sharing of data.

The UKCH aims to support data processing through the design, development and deployment of the Catalysis Research Workbench. The Catalysis Research Workbench (CRW) will bring together tools and resources for analysis and processing of research data, supporting further exploitation of UKCH data assets. In the design phase, we started by implementing a workflow demonstrator for showcasing and evaluating tools which can support processing and analysing larger datasets. The first workflow implemented is an XAS-Data processing and analysis workflow.

This case study describes how these platforms are being designed to complement each other, while also working with existing and future infrastructures. The case focuses on the use of XAS data to illustrate these points.

2 Use Case Scenario

The development of the CDI and CRW considers the existing infrastructure which researchers are already using. For instance, large-scale facilities like Diamond Light Source, ISIS Muon and Neutron Source and the Central Laser Facility, have an operational framework to support their Data Management Policies supported by advanced catalogue systems that combine Laboratory Information Management System and Data Management System functionalities. These systems contain complementary data for each experiment like proposal, PI, Experimenter, Grant(s), device(s), experiment metadata and experiment results. Similarly, researchers also store data in institutional repositories, publishers' repositories, and specialised databases. As such, the CDI and CRW must align and work with existing operational workflows (Figure 1).

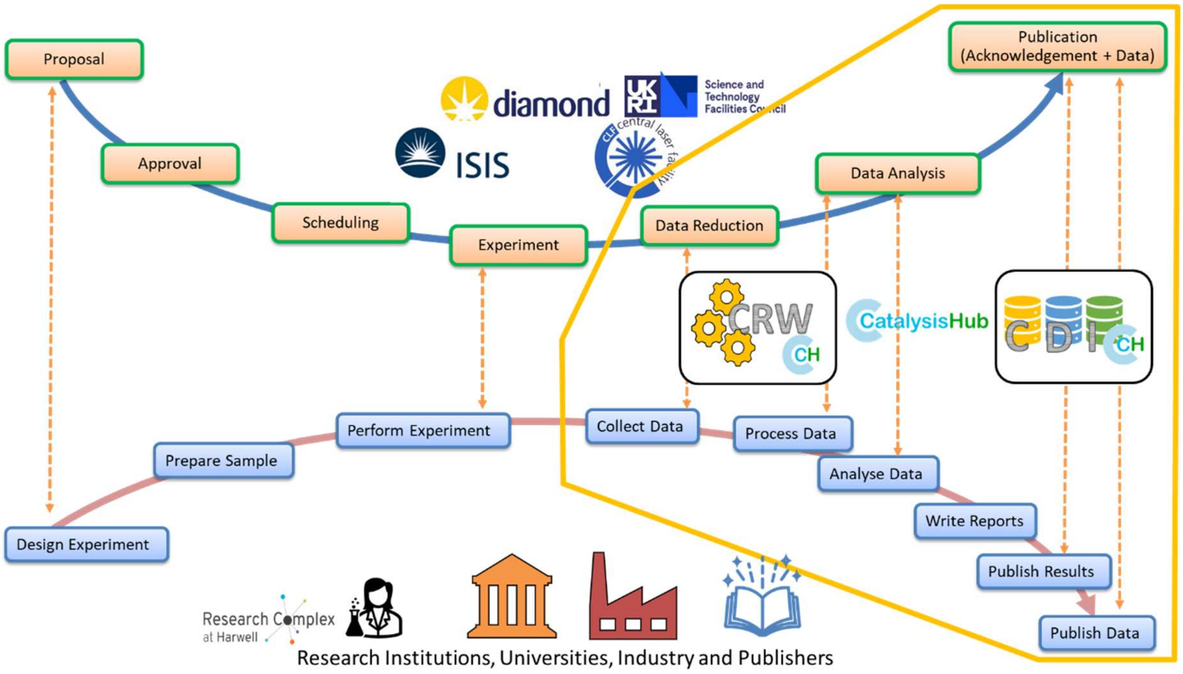

Figure 1 Integration of UK Catalysis Hub Platforms with existing operational workflows

Integrating the CDI and CRW in this research ecosystem is expected to encourage the reuse of data, processing, and analysis methods in novel ways. The combination of these platforms is expected to enable reproducibility, reuse of data, reuse of processing tools and implementation of advanced processing tools. The process of building the XAS workflow illustrates these points. The following subsections illustrate elaborate on these activities.

2.1 Reproducing Results

A scientist using the UKCH CDI can look at published articles with its source data and analysis process (including software used). The scientist should then be able to follow and reproduce all the steps of the analysis using tools indexed/hosted by the CRW. This can support training efforts and evaluation of results. The diagram in Figure 2 illustrates this process in this case the publication is linked to its data and processing tools, enabling reproduction of published results. To support this, each published result should be traceable to its source data, with a clear path of intermediate results and processing tools. This can be archived if the provenance information is made available.

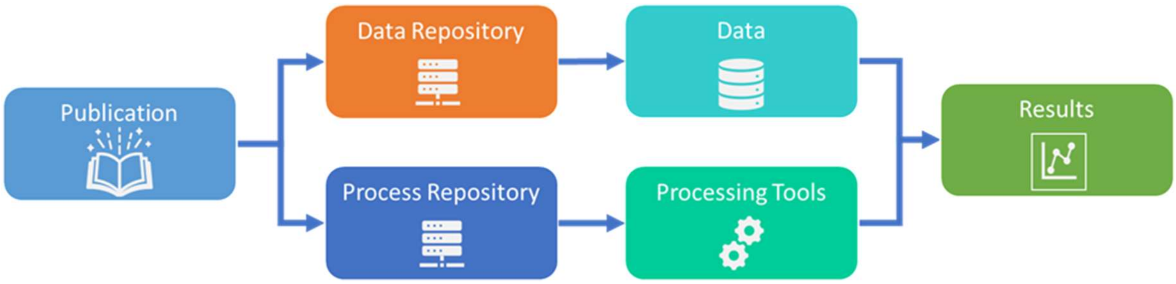

Figure 2 Reproduce results

2.2 Reuse Data

Reuse of data is enabled when publications are linked to supporting data. In this case, the scientist can obtain the published data and use alternative tools. This enables comparing the results produced by alternative processing tools, or extending the research by applying different analysis tools. The diagram in Figure 3 illustrates this process in this case the publication is linked to its data and the alternative processing tools are obtained a repository. To support this, each published result should include processable data in a format which can be used by more than one type of processing tool. This requires that the data formats are standardised or the development of mapping tools.

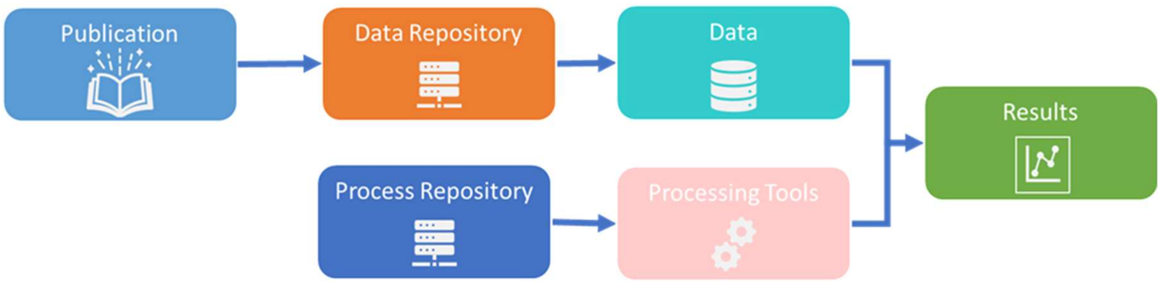

Figure 3 Reuse data

2.3 Reuse Processing Tools

Reuse of processing tools is enabled when publications are linked to their processing tools. In this case, a scientist can take existing processing tools and its corresponding results and gather different data to determine if the results are replicable. The diagram in Figure 4 highlights that processing tools linked to the publication can be recovered is linked to its data and used with different data. This requires standardised formats for data and provenance data.

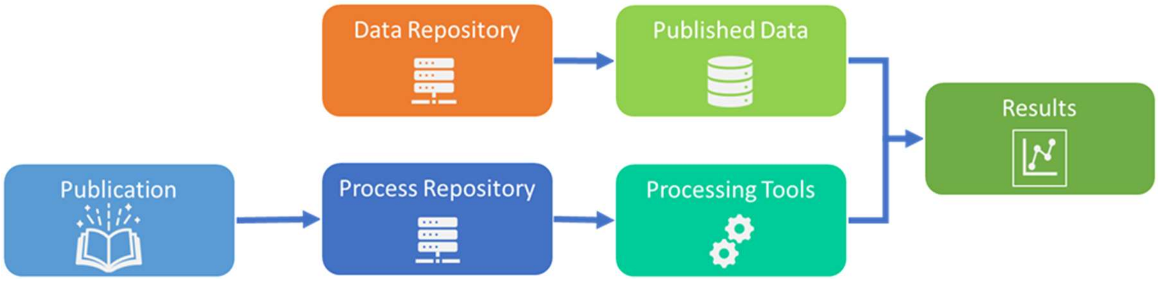

Figure 4 Reuse processing tools

2.4 Advanced Processing

The publishing of data is also required for designing processing and analysis experiments incorporating advanced techniques such as workflows, artificial intelligence, data mining or pattern matching. The diagram in Figure 5 highlights that data can be recombined with other data and alternative processing tools. This also requires standardised formats for data and provenance data.

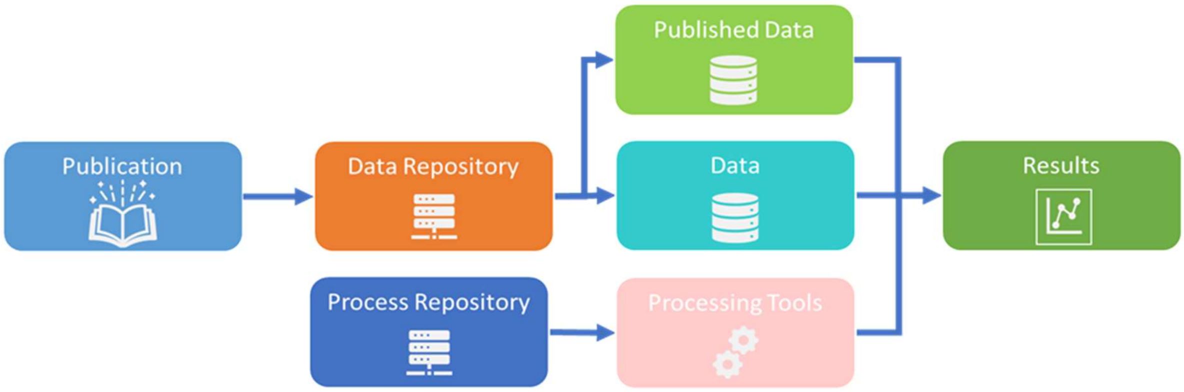

Figure 5 Advanced processing

3 Use Case Experiment

The process of design of the Catalysis Data Infrastructure (CDI) and the Catalysis Research Workbench (CRW) has reached a point in which we can start exploring the integration with existing infrastructures. Currently, the integration is loose and asynchronous. In this context, a researcher must access the CDI to look for publications, see if there are data objects linked to them, and then look for processing tools which can be used to reproduce the results. The experiment of this use case is designed to determine how easy is to perform these activities and what are the requirements to improve the current situation. The diagram in Figure 6 illustrates the five steps of the experiment.

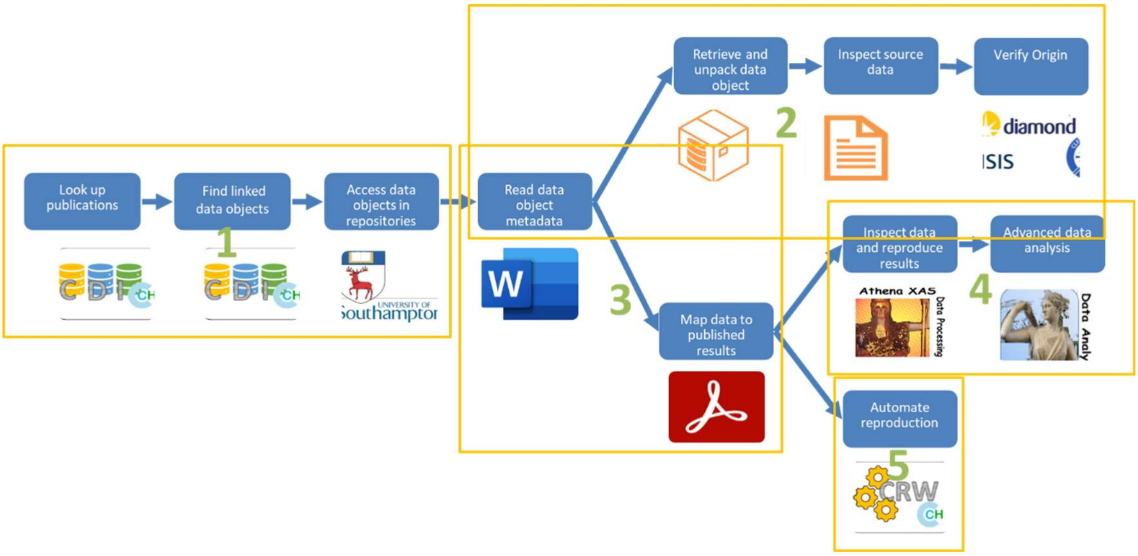

Figure 6 Proposed Experiment. 1 Find Linked Data Objects. 2. Track data provenance (verify where published data comes from). 3 Map published data to results. 4 Reproduce Results (learn how results were obtained). 5 Automate Reproduction and Use alternative software.

The experiment was designed for XAS data processing because XAS analysis encompasses an array of a widely used techniques for the characterisation of catalysts in ex-situ, in-situ and operando conditions. XAS analysis relevance of for UKCH can be seen from the number of publications catalogued in the Catalysis Data Infrastructure that mention it (Figure 7). Additionally, the indexing of data objects in the CDI allows recovering data from existing platforms which researchers already use to preserve and publish catalysis research data such as STFC eData, ISIS TopCat, CCDC, and university research repositories. Therefore, the experiment was designed to look for data which may support reproduction of results, paying particular attention to the types of data published, the software required for reproducing results presented and the processing and analysis tools which can be leveraged to facilitate these activities.

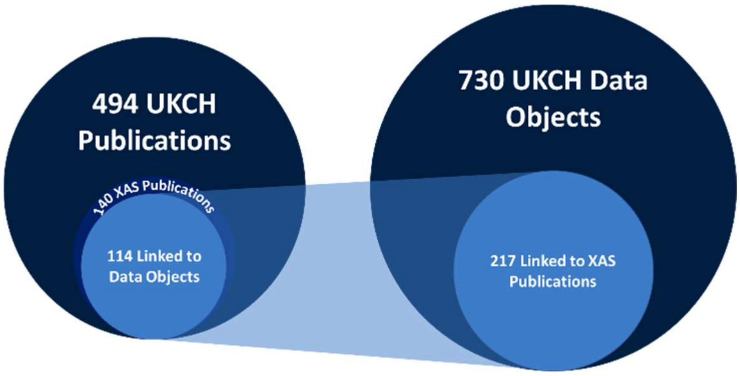

Figure 7 Proportion of XAS Publications and related Data Objects currently indexed on the Catalysis Data Infrastructure Prototype (Last updated Dec 2021).

3.1 Finding Data

Finding data should be a straightforward activity because publishers and founders require the publishing of supporting data. Additionally, a clear target of the type of data required, processable XAS data, also suggests a straightforward search. In practice, however, finding suitable data was not as simple. The main issue is that not all repositories offer suitable indexing/search functions which may allow locating the required data (including the current version of the CDI). Consequently, the search required data mining of publications indexed by CDI using a set of keywords associated to XAS experiments (X-Ray Absorption Spectroscopy, X-ray absorption near edge structure, Extended X-ray absorption fine structure) and their mnemonics (e.g. EXAFS, NEXAFS, XAFS, XANES, XAS). Applying the search to the 494 publications indexed by the CDI resulted in 140 publications that mention some XAS technique. 114 of these are in turn linked to 217 data objects. The next step required identifying which data objects may contain processable XAS data. 132 of these objects are documents (pdf, doc, txt or similar) while 85 are data sets, cif files, archive files, or raw data. After 33 of 85 data objects were further analysed to determine if they contained processable XAS data. This required accessing each data object's metadata and verifying the type of data. The metadata of 12 data objects indicated that they contain the required data. Three of the 12 data objects contained partial data (for reproducing plots only) or incorrectly labelled data (document format). This leaves 9 data objects containing some form of XAS processable data [1/H, 2/I, 3/B, 4/C, 5/D, 6/A, 10/E, 12/F, 14/G][1]. Table 1 summarises the filtering of data described and Table 2 summarises the characteristics of the retrieved data.

Table 1 Filtering of Data Objects

Data Object Filter	Count	%
All Data objects	730	100.00%
Linked to XAS publications	217	29.73%
Contain data (dataset, archive, raw data)	33	4.52%
Mention processable XAS data	12	1.64%
Contain processable XAS data	9	1.23%

The task of finding data took longer than expected, it took five days to get to the final set of nine data objects. Considering that data was already indexed and linked to publications. This indicates that the CDI may be improved by adding indexes to data to indicate the type of data, including experimental procedures and file formats. For repositories, it could be useful to add similar metadata to enable filtering.

Table 2 Composition of XAS data objects downloaded

Description		Files
Selected and downloaded data objects		12
Not processable data objects		3
Processable XAS data objects		9
Downloaded Files (2.1 GB)		140
Processable data formats	athena files (prj)	37
	text data files (.dat)	1,006
	nexus files (nxs)	101

3.2 Verifying Provenance

Verifying provenance was partially successful. All the data objects selected indicate that they were produced at the Diamond Light Source Beamlines. The four objects [1/H, 2/I, 4/C, 5/D, 6/A]. which include text and nexus data contain metadata which indicates the beamline, instrument, and date of experiment. For the remaining five [1/H, 3/B, 10/E, 12/F, 14/G], provenance is partial as the included data is in the form of Athena project files, which do not contain metadata indicating where and when data was collected.

3.3 Mapping Data to Results

The large number of files, the variety of file formats and their relationships to data make require explicit metadata for mapping results to sources. The nine datasets include metadata that indicates which data objects correspond (support) published results. However, the metadata included is text data which needs to be interpreted by a human user. Explicit linking is required for speeding up linking.

[1] The references to publications and data objects are indicated by a number, and a letter separated by a slash (/), the number indicates the publication while the letter indicates the data object respectively.

3.4 Reproducing Results

The reproduction of results was possible in all cases. Figure 8 presents an example of the reproduction of results from [1/H]. However, reproduction of results was not completely successful, because three issues: missing data, proprietary files, and unreferenced data.

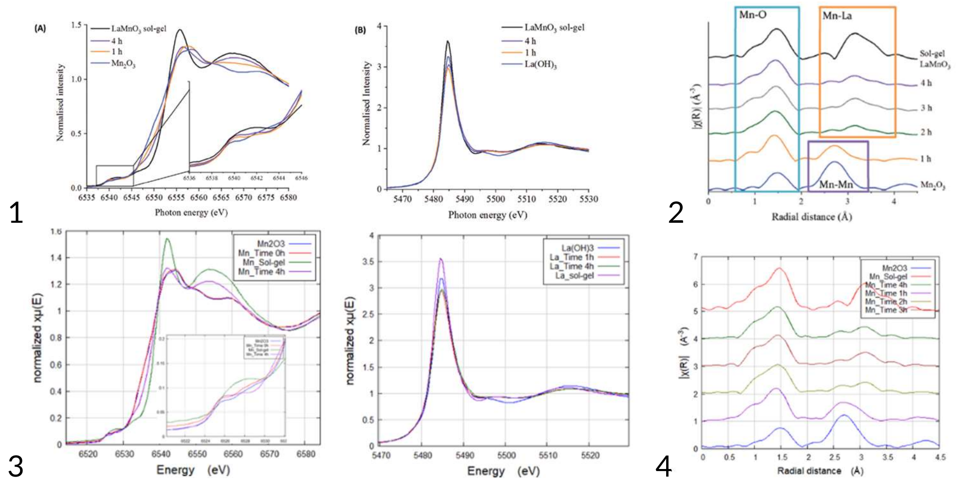

Figure 8 Reproduction of results: 1 and 2 correspond to Fig.2 and Fig3 respectively, from [1]; while 3 and 4 are their corresponding reproductions using the published data objects [H].

Missing and unreferenced data concern to parameters and standards used for fitting. In the case of parameters not all the parameters are included, so the effort of reproducing the results requires additional work to identify correctly which are the values used. Regarding standards, publications mention them in the text, but they are not included in the datasets or properly referenced. The issue with proprietary files is that even when these types of data are published, correctly interpreting it requires the use of licensed software for which there may not be open-source alternatives.

3.5 Automate Reproduction

The final part of the experiment is intended to show the use of alternative software (reuse of data) and the implementation of advanced processing (implementing a scripted workflow). To illustrate automation, we created a scripted Perl-Demeter workflow which can read text (csv) input files which describe the inputs and the operations to be performed on those inputs. Then we recreated the same workflow using Python-Larch and Jupyter, reading the same data and files. Both examples are available from the UK Catalysis Hub GitHub page[2].

3.5.1 Experiment summary

The datasets selected for the use case allowed reproduction of results using the analysis tools defined in the papers using the openly available software for processing and analysis (Athena and Artemis [11]). Additionally, the data also support use of alternative software (Demeter and Larch) which supports both reuse of data, reuse of processing tools, extension for advanced use (automated reproduction through scripting).

Performing the experiment described in Figure 6, that is finding data, verifying provenance, mapping results, reproducing results, and automating reproduction were all possible, with some adjustments (see Table 3). Finding data, mapping data and automation of reproduction were possible in all cases. Verification of provenance was possible for four data objects [1/H, 2/I, 4/C,

[2] https://github.com/UK-Catalysis-Hub/XAS-Workflow-Demo/tree/main/PSDI_pilot

5/D, 6/A]. For the remaining five [1/H, 3/B, 10/E, 12/F, 14/G] provenance verification was not possible as the datasets only included intermediate results (in the form of Athena project files).

Reproducing results is the second activity with partial success because additional data was required in some instances and these data were not published or correctly referenced by the publications.

The types of data published are not always supportive of reproduction. The levels of published data vary considerably from additional tables and figures in document formats (supplementary data), to comprehensive data sets including raw data, intermediate results, and processed data. The exploration of the data indicates that most of the published data objects are supplementary data, while processable data is a small proportion of all published data. The breakdown of data is shown in Table 1. In the end, only 9 publications are linked to data objects that supported reproduction [1/H, 2/I, 3/B, 4/C, 5/D, 6/A, 10/E, 12/F, 14/G].

Table 3 results of proposed experiment for the nine publications-data objects

Pub/DO	Find Data	Verify provenance	Map to results	Reproduce Results	Automate Reproduction
[1/H]	OK	Partial	OK	Partial	OK
[2/I]	OK	OK	OK	Partial	OK
[3/B]	OK	Partial	OK	Partial	OK
[4/C]	OK	OK	OK	Partial	OK
[5/D]	OK	OK	OK	Partial	OK
[6/A]	OK	OK	OK	Partial	OK
[10/E]	OK	Partial	OK	Partial	OK
[12/F]	OK	Partial	OK	Partial	OK
[14/G]	OK	Partial	OK	OK	OK

4 Identification of requirements

The initial recommendation derived from the results of the experiment defined above led to three recommendations which were oriented towards ensuring the reproduction of results, reuse of data and software, and enabling advanced processing and analysis (Table 4). It is assumed that following these recommendations will facilitate performing actions such as those described in the experiment section above.

Table 4 Recommendations to improve reproducibility, reuse of data and software, and advanced processing

1. Publish and link (reference) raw and intermediate data
2. Publish metadata in structured form (XML, JSON) (in addition to document format), including:
    a. type of data published (.dat, .txt, .csv, .xlsx, .nxs, .opj, .opju, .pdf)
    b. software used to produce/read data
    c. link to additional data
    d. mapping of data to published results
3. Prefer open source software (some data cannot be processed without a licensed program e.g. Origin files (.opj/.opju))

4.1 Discussion with users and initial requirements

These recommendations were integrated in two posters to be discussed with researchers in two events: UK Catalysis Hub Winter Conference 2021 (December 2021 – UKCHWC 2021), ans UK Catalysis Conference (January 2022 – UKCC 2022).

The posters presented enabled discussion with researchers that raised several issues which prevent them from following the recommendations suggested above. These issues were summarised and classified in three groups: usability of repositories, management of provenance, data publishing guidance (Table 5).

Table 5 Problems reported during poster sessions

Problem 1: Usability of repositories. The difficulty of use of repositories was mentioned as a relevant issue. Users pointed out that the processes and tools which support data publication are hard to use and not intuitive, requiring users to know how to annotate, format, and curate the data.
Problem 2: Management of provenance. From collection at the lab or experimental facilities, trough processing and analysis, to finally formatting and publishing keeping track of provenance is a manual process. There are no current tools supporting it.
Problem 3: Data publishing guidance. Entities requiring publishing of data do not specify the kind of data to be published, consequently there is a wide range of data object types being published. Some authors are very thorough and publish raw, intermediate, and processing data and map it to published results; meanwhile, other authors just include additional (supplementary) data in the form of documents and figures.

In response to the issues described above, we identified four basic requirements for the data processing tools and the data publishing platforms. These four requirements are detailed in Table 6.

Table 6 Initial requirements

Requirement 1 Generate Provenance. Processing tools could be adapted to generate provenance metadata to enable tracing each result presented. This could be a modification of existing logging features, aligning them with standards like PROV-O.
Requirement 2 Generate Metadata. Processing and analysis tools could be modified to produce outputs ready for publishing (with metadata and provenance data ready). Experiment management systems already encode metadata about experiments. Processing and analysis tools could take provenance and setup data to produce new links in the provenance chain and additionally produce metadata for publishing
Requirement 3 Simplify the deposition of data. The publishing of data should be integrated as part of the existing processing and analysis workflows and transparent to users. The tools outlined above, could produce outputs which if fed to deposition systems could simplify data curations and publishing tasks.
Requirement 4 Annotation tools. Data annotation tools which can produce metadata are needed to facilitate mapping (linking) results to source objects. These tools should be integrated into the data publishing facilities to support the publication of data with prefilled formats and recommendations to support deposition.

4.2 Validation of initial requirements and further issues

The initial requirements were taken into consideration for preparing two presentations to enable validation and refinement. These presentations were discussed with researchers in two events: PSDI Consultation (March 2022 – PSDIC 2022) and UK Catalysis Hub Core Science Meeting (March 2022 UKCHCSM 2022). The consensus was that the issues and proposed and the initial set of requirements presented a viable path for improving the data publishing practices.

During the presentations, various colleagues raised additional concerns. These concerns were again grouped in three categories: data ownership, manual lab books, and programmatic access to repositories (Table 7).

Table 7 Issues raised during presentations

Problem 4: Data Ownership. Issues about the ownership of data were also raised, this is related to clear data management policies and use agreements. Most times this has been addressed by licencing agreements.

Problem 5 Manual lab books. Facilities and laboratories still rely on manual input of information on lab notebooks. Information in those is harder to retrieve.

Problem 6 Programmatic access to repositories. Repositories provide mainly manual interface for accessing data. This prevents use of high throughput methods. Future improvements to repositories should include the implementation of programmatic access to repositories (API, web services).

5 Conclusions

This case study offers view of the support required for effectively preserving data so that it can be later discovered and reused. As such, it has direct links to the last three phases of the JISC research data lifecycle (Figure 9)[3] (4) Manage, Store & Preserve, (2) Share & Publish, and (3) Discover, Reuse & Cite. However, the support and modifications outlined in the initial requirements affect all stages of the research data lifecycle.

Figure 9 JISC ResearchData Lifecycle Model

Modern requirements engineering processes need to be interwoven into the software lifecycle from design and planning through to development, deployment, and decommissioning [7, 13]. The interweaving addresses changes in technology and changes in the nature of requirements. Consequently, we expect that addressing these additional issues and integrating them into the design of the PSDI will form part of the follow up design and implementation phases. A continuous requirements process would also allow greater participation of the user community, addressing their concerns and integrating them into the final design products.

[3] https://www.jisc.ac.uk/guides/rdm-toolkit

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