

Data Curation Framework for Facilities Science

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Abstract: The trend in research data management practice is that the role of large facilities represented by particle accelerators, neutron sources and other scientific instruments of scale extends beyond providing capabilities for the raw data collection and its initial processing. Managing data and publications catalogues, shared software repositories and sophisticated data archives have become common responsibilities of the research facilities. We suggest that facilities can further move from managing data to curating them which implies meaningful data enrichment, annotation and linkage according to the best practices which have emerged in the facilities science itself or have been borrowed elsewhere. We discuss the challenges and opportunities that are the drivers for this role transformation, and suggest a data curation framework harmonized with the research lifecycle in facilities science.

1 INTRODUCTION

The growth of research complexity, the increased costs of the advanced scientific instruments, and the internationalization of science have led to the emergence of research facilities that can be thought of as well-equipped hubs where research teams come to perform their experiments, often associated with other experiments in the same or other research centres.

The research facility core is typically represented by a unique scientific instrument: a particle accelerator, a neutron source, a powerful laser, a telescope, or a supercomputer that allows detailed simulation of natural phenomena, or by a few such instruments that offer researchers different experimental techniques. Examples would include the Diamond Synchrotron Light Source (www.diamond.ac.uk), ISIS neutron source (www.isis.stfc.ac.uk) or the future Square Kilometre Array (www.skatelescope.org). The exact boundary between basic and applied research on such facilities may be ill-defined, e.g. the same electron synchrotron may be used part time to explore the fundamental effects of particle collisions and part time as the source of synchrotron radiation for materials science, biology and pharmaceuticals. For the sake of clarity, we use the term “facilities

science” for the research performed on large-scale scientific instruments by visitor teams or individual researchers who obtain, via the application process, access to the common facility resource in order to conduct their experiments or observations, and to collect the resulting data.

The instruments and experimental techniques may be different between facilities; the purpose of research may be more inclined to scientific inquiry, or more practical in view of industrial applications. What is common across facilities science is a business model for servicing the facility users (researchers); the users’ social habits, e.g. the accepted modes of managing research output, are less definitive but also important. These commonalities lay a foundation for a generic data lifecycle in facilities science, as well as for common metadata models and information systems architecture.

Our modelling and implementation effort in respect to supporting the facilities’ data lifecycle is mentioned in this paper but we concentrate on challenges and opportunities that the facilities science business model and the researchers’ social attitudes present for data curators and technologists; we then discuss a framework that should address these challenges and opportunities.

2 CHANGING LANDSCAPE OF FACILITIES SCIENCE

The evolving changes in business model, technology and facilities users' behaviour are all interrelated and result in new challenges and new opportunities for the facility science stakeholders, specifically for data curators and IT specialists.

2.1 Changes in Business Model, Technology, and user Behaviour

A business model for user research on large facilities that emerged more than 50 years ago has been influenced by a few recent developments. Instrumentation and data analysis have become more user friendly than in early days of facilities science. This has led, among other effects, to a lesser significance of the instrumentation "gurus" with a current trend of not including them as the authors of research papers; the estimate e.g. for biology papers is that about half of them do not now include any facility staff members as co-authors (Mesot, 2012).

The advances of instrumentation and Internet have also led to the emergence of specific services for research and industry such as the UK National Crystallography Service (Coles and Gale, 2012) that allows users to send their samples for remote investigation according to one of the service plans. The sample exposure on a large facility like synchrotron radiation source may be just one of the experimental techniques included in the service plan so that users have got a "seamless" interface for the multi-aspect investigation of a crystal substance submitted. The service provider then collects all the experimental data and supplies them to the user in pre-agreed formats. The facilities themselves have also started offering this sort of "express" service with the user presence not required for the conduct of experiment.

The users' attitude towards research may also have a significant influence on the research lifecycle and services in support of it. The user monitoring exercise performed by PaNdata initiative showed that about seven thousand of visitor researchers across Europe, or 22 per cent of them have used more than one neutron or synchrotron radiation facility for their investigations (<http://wiki.pan-data.eu/CountingUsers>). The reasons for this substantial level of facilities sharing are often of a research nature as the characteristics of the experimental environment are different between facilities. The facilities sharing is a strong incentive for having a common infrastructure for data

management and user management which is now a focus of PaNdata Open Data Infrastructure project (see under <http://pan-data.eu/>).

Another driver for change in data management and data curation is the emergence of new experimental techniques like neutron tomography, or using robots for manipulating multiple samples exposed to a synchrotron beam, or studies of dynamics of materials. The new techniques produce larger volumes of data making Big Data bigger than ever; they also raise potential opportunities for researchers to perform comparative and multi-aspect studies for the same samples using different experimental techniques, or using the same experimental technique for much wider variety of different samples. These trends appeal to providing a richer, well annotated and linked context for experimental data across different facilities, different experimental techniques and different sample types so that the mentioned research opportunities for comparative and multi-aspect studies could turn reality.

2.2 Challenges and Opportunities

The challenge of Big Data in terms of more processing power and more network bandwidth required is imminent and well understood. We will not detail it here apart from to note that addressing particular parts of the data files and archives for their inclusion in the research discourse, e.g. citing granular parts of the immense datasets, requires an adequate modelling of data, and scalability of data management.

The change of the instrumentalists' role who as we mentioned do not always receive a due credit for their job of preparing sophisticated experiments requires re-thinking of the attribution methods for research papers and other research outputs such as datasets. Facilities science may look at the developments such as role-based attribution in other fields of research (Marcos et al., 2012); this is just one example of how specialists in the facilities' information departments could explore the new information culture elsewhere, and promote the best practices of it across facilities science. This example also shows that data curation is in fact a responsibility of everyone involved in research lifecycle: the authors themselves, not any curation unit down the research results distribution road, should be able to add the structured description of roles according to a reasonable metadata standard.

Information departments then can be seen as hubs or centres of expertise which monitor, refine,

and communicate best practices of data curation for other stakeholders (research papers authors in the last example). The consistent and clearly formulated framework will make a collaborative data curation effort much better defined and communicated, and the best data curation practices more readily adopted by the research community. Supervision of various kinds of information through the research lifecycle will help then to create rich data aggregations and reproducible research workflows with contributions naturally made by different lifecycle stakeholders.

The next challenge and opportunity is presented by the emergence of research services such as the aforementioned UK National Crystallography Service. This trend raises questions on the user management, research proposals management and data management in facilities science. Just one example of that are the future role and the content of data management policies which some facilities tend to impose on their users as a pre-condition for getting a facility resource for research. The policy may ask users to agree with the public release of their experimental data after a period of exclusive access (typically a few years), or contain the requirement to submit the list of resulting publications back to the facility user office. This works well in a traditional business model of facilities science but does not take into account the emergence of the service intermediaries who may need to be a subject of the data management policy, too, so that it becomes a multilateral agreement.

The data management policy format which is now just plain text is also questionable as it is not interpretable without a human; this will be likely not enough for the automated research proposals management and data release management across different facilities. The development of licences for data re-use, or the adoption of suitable ones could alleviate the problem but licences might need a proper machine-oriented modelling for policy enforcement; the indication of what is possible in respect to structured modelling and automation of data licences can be seen in the recent formation of the Linked Content Coalition (www.linkedcontentcoalition.org) endorsed by the European Commission and some national governments. Again, information departments of large research facilities might consider borrowing the advanced practices and models of data licensing for their re-use in facilities science.

Another important consideration is the interoperability of metadata models and their actual implementations for different research facilities. The idealized metadata model for facilities science that

we call Core Scientific MetaData (CSMD) (Matthews et al., 2012) is derived from a generic research lifecycle in facilities science:

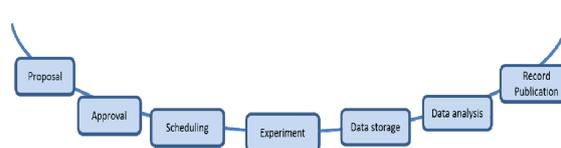


Figure 1: Generic research lifecycle in facilities science.

The different stages of research lifecycle produce data artefacts (research proposals, user records, datasets, publications etc.) that are similar across research facilities so having a common metadata model like CSMD seems sensible. However, it may be applied differently by different facilities; there are a few CSMD implementations in data catalogues across Europe by virtue of the ICAT platform (<http://code.google.com/p/icatproject/>) but the model, and the actual use of its elements may vary among implementations. This may result in extra design and implementation overheads when we consider federated services for a few facilities (even when based on the same software platform), also there is no guarantee that once we have the federated solution agreed and implemented, it will be not affected sooner or later by the diverging business needs of different participants. The common data curation framework for facilities science might help to have these needs permanently monitored, properly communicated and effectively reconciled thus serving as a well-structured business analysis wrapper for technology solutions.

An interesting development that *may* be considered a part of the emerging data curation framework but has exposed certain challenges, too, is the recent effort of minting Digital Object Identifiers for investigations performed on ISIS neutron facility (Wilson, 2012). Having permanent identifiers minted for particular investigations (experiments) should be enough for linking them to datasets and publications but in order to have a structured and linkable representation of a facility research environment, other parts of it such as scientific instruments, experimental techniques, people, organizations, software, derived data sets etc. need minting or borrowing identifiers for them, too. There is currently no sustainability model for this activity, as well as for the steady production and support of landing Web pages where the permanent identifiers (all kinds of them) should ideally resolve into. The different aspects – modelling, technological, operational – of the permanent identifiers management should be an important part

of the data curation framework for facilities science.

We should also mention organizational barriers to sharing the content and the context of the research discourse: grant applications, facilities beam time applications (research proposals), the raw data collected, the research outputs, the models and the software used for data analysis or long-term digital preservation – all these components tend to be managed and published under separate ownership but can and should be interlinked and navigable in order to get the most of the impressive resource spent on the preparation and the actual conduct of facilities research. Linked Data might help here, and it proved to be a productive methodology for processing Big Data in some important research fields with industrial output such as drug discovery (Dumontier and Wild, 2012). There are even more advanced data modelling techniques for sharing the reproducible research workflows that are well accepted in some research domains, e.g. biology (Bechhofer, 2013). However, these techniques typically cover only certain parts of the larger research lifecycle that are immediately related to research work, with the Researcher as a major target of data linkage and data sharing. The needs of other stakeholders residing in education, industry, research management and funding, or policy making are underrepresented and do not have a consistent framework where all of them, along with the researchers and intermediary services, could fit in.

In the absence of a structured data curation framework, the information departments of large facilities are often confined to supplying the technology solutions and IT services when their next role could be that of a conscious data curator helping to increase data value across the entire research data lifecycle for the variety of stakeholders (Wilson, 2012); information technologies and services would be then a very important means to underpin the data curation role but not the end in themselves.

In order to adopt this new role, the information departments of large research facilities cannot entirely rely on the existing organizational structure as their role and actual influence in a larger research context is inevitably limited. What they can do is devise and elaborate a common framework for sharing the existing best practices across different organizational units and collaborative projects; the framework will also serve to bring the best practices from elsewhere for the adaptation to the needs of facilities science. The projects, initiatives and working groups that the information departments are involved in will be a means to support certain “themes” in the common data curation framework.

This should result in better opportunities for the organizational units and collaborative projects to interoperate, to reconcile their priorities, and to set common (and commonly understandable) goals.

3 COMPONENTS OF DATA CURATION FRAMEWORK

We consider some aspects of a suitable data curation framework. It may take into account the actual content and the stance of the existing frameworks in the IT-relevant domains such as ITIL for service management (www.itil-officialsite.com), or the relevant project management frameworks. Those can be to a certain extent “role models” of what may constitute our own framework but there will be substantial differences, too, owing to the specifics of facilities science as business environment.

3.1 Data Curation Perspectives

The basis of the aforementioned mature frameworks is typically two-fold: generalization of best practices in the field and a consistent conceptual thinking often represented by the notion of re-usable “processes” and “functions” that reflect an importance of the operational perspective in the business world, and the functional nature of management style in many business projects and services. The framework for the research data curation should include the operational perspective and may develop a functional approach for certain domains, too, OAIS reference model for digital preservation (OAIS, 2012) being a good example of it. However, owing to the cooperative nature of scientific research (compared to the more direct governance in business world) and to the need for such a framework to be adaptive and comprehensive enough, it should include more perspectives:

- **Business Analysis Perspective**
The business case for data curation should be well formulated and permanently updated
- **Modelling Perspective**
Modelling may be applied to a variety of artefacts: to data or metadata, or to the policies and business processes
- **Technology Perspective**
Technology is important and should be consciously harnessed for data curation
- **Operation Perspective**
Data curator should always keep in mind the operational environment and issues that may

arise in it: scalability, sustainability etc.

- **Communication Perspective**
Structured communication with various data curation stakeholders should be a permanent activity accompanying all the others.

3.2 Data Curation Themes

The outlined Perspectives allow considering all the important aspects of a data curation problem or a data curation solution; in addition to them, the adaptive data curation framework will benefit from having permanent Themes. One or more Themes may be relevant to the scope of a particular project or initiative hence they are the tool for mapping the actual data curation effort (including development of new approaches and techniques) to the rest of the framework.

We list the Themes that are deemed important according to our own experience in data curation projects; as the framework evolves, they should be refined through discussions with a variety of stakeholders across different research facilities:

Table 1: Data curation themes.

Theme	Comment
Identification of the existing and emerging data curation stakeholders	Also monitoring their needs that may lead to the roles change
Facility user management practices and policies	Including comparative studies across facilities
Data curation practices and policies in facilities science	Analysing them for different stages of facilities research lifecycle
Data curation practices and policies elsewhere	To adopt the best of them in the facilities science
Permanent identifiers *	Minting or re-using them for instruments, techniques, samples, papers, datasets etc.
Data Context *	Modelling and managing various metadata and Linked Data; monitoring linkable data sources and services
Data mining *	Discovering data patterns; data indexing and classification
Data analysis and visualization *	Including those in collaborative environment ("virtual labs")
Data value and data cost	How to model, measure, and manage them
Standards and recommendations	Adoption of the best and opportunities to contribute

Star marked items may be considered particular techniques of data curation but we reserved dedicated Themes placeholders for them to emphasize their importance.

Some of the Themes may look specific to certain Perspectives but in fact, every Theme may require many Perspectives applied. As an example, when we consider minting DOIs we should employ the Operation Perspective that will advise on the feasibility and costs of exploiting the practice in a sustainable manner, and the Communication Perspective in order to educate stakeholders concerned, and to get their feedback for the practice improvement.

3.3 The Framework Application

The framework can be applied to the identified Problems, or to Solutions in order to evaluate their feasibility or quality. The recommended process can be outlined as follows:

1) For a particular project aimed at management or curation of facility science data, identify major Problems or Solutions that seem viable.

2) Identify where the Problem or the Solution applies in the facilities research lifecycle (see Figure 1); it may be one or a few stages.

3) Apply different Themes to the Problem or the Solution, and decide which ones are most relevant or most important in a particular case (prioritize Themes for each Problem or Solution).

4) Consider each prioritized Theme from each of the five Perspectives; decide which Perspectives are most relevant or most important in a particular case.

5) Elaborate the prioritized Themes and Perspectives against the Problem or Solution. If new Problems or Solutions emerge whilst applying the framework, apply it to them, too.

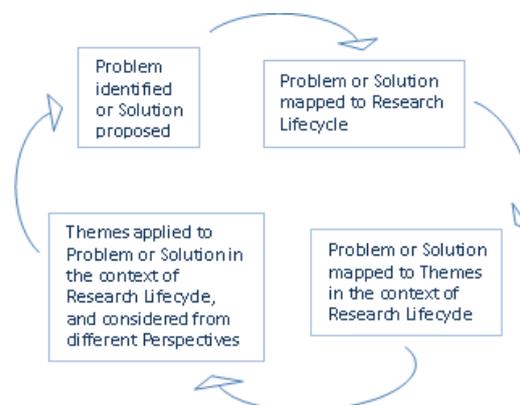


Figure 2: Data curation framework application.

As applying the framework will take into account the significance of Themes and Perspectives in each particular case, we expect that the entire number of aspects to be considered (that is a multiplication of the number of significant Themes by the number of significant Perspectives) should not exceed a dozen or so for a particular Problem or Solution. If this reasonable limit is going to be exceeded, the Problem or Solution should be decomposed, with the framework applied to the identified components. Applying the framework stops when all the Problems or Solutions have been considered from all significant Perspectives. The examples of particular outputs resulted from the framework application will be the IT solution quality assessment, or the data management plan.

3.4 Further Works and Reference Implementation

The core of the framework outlined in this paper should be discussed with a variety of data curation stakeholders in different research facilities, and elaborated accordingly; PanData consortium and its projects (www.pan-data.eu) will be a proper forum for that. The resulted framework can be applied then to a particular business case in the interests of a certain research facility, or a few.

The case we are willing to consider is the long-term digital preservation of the research outputs of neutron and photon facilities; specifically, the preservation of the more complex information aggregations than just raw datasets. This will require a more universal and multi-aspect approach than can be found in particular digital preservation projects that typically have their own specific agenda and use the data samples of facilities research output only for illustration purposes. One of the problems that as we hope the framework will help to address in digital preservation is the validated alignment of the system architecture and technology to the actual data preservation policies and procedures.

4 CONCLUSIONS

Large experimental facilities have a unique position in the research landscape that allow them to evolve from supplying the crude services (time slots and experimental environment) through various modes of managing research data to becoming the researchers' partners in meaningful data curation. Sharing and refining the best practices across organizational units and research centres should

result in birth and growth of a common data curation framework for facilities science that covers the entirety of the research lifecycle and takes into account the business analysis, modelling, technological, operational, and communication perspectives. Such a framework will give a common language for various case studies, system design and implementation effort of different organizational units and collaborative projects; it will be therefore a valuable aid to the consistent and sustainable data curation in large experimental facilities and collaborations of them.

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