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Putting the R into PlatfoRms

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Abstract

This paper looks at the question of how and why to bring about greater reusability of Research Platforms (variously called Virtual Laboratories, Virtual Research Environments, or Science Gateways). It begins with some context for the Australian Research Data Commons, where the authors are based. It then examines the infrastructure concerns that are driving the need for platforms to be created and remain sustainable, and the connection from this to reusability. The paper then proceeds to discuss the ways in which FAIR is being extended to a range of research objects and infrastructure elements, before reviewing the work of the FAIR4VREs WG. The core of the paper is an examination, with examples or case studies, of four different paradigms for platform reusability: accessing, adopting, adapting, and abstracting. The paper concludes by examining actions undertaken by the ARDC to increase the likelihood of reusability.

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Introduction

This paper will look at some aspects of applying the FAIR framework to what the ARDC calls Research Platforms. These are also variously called Virtual Laboratories, Virtual Research Environments, or Science Gateways, depending on the country and discipline norms, and there are some differences of nuance between these terms. Virtual Laboratories (Potkonjac et al, 2016) began as educational tools to enable students to learn techniques in a virtual setting. The Virtual Laboratory program begun by Nectar in Australia in 2012 used this term for a range of online environments funded from 2012 - 2019 that were mostly targeted at researchers. Virtual Research Environments (Allan, 2009) is a term mostly used in Europe and the UK to describe systems to enable researchers to carry out tasks that require access to a range of online resources. Science Gateways (Gesing, 2021) have as their goal to "make access to complex research infrastructures more user-friendly and to provide a platform for communities to share computational methods, data and knowledge" Note that although the name includes Science, the focus is not just on Science (as distinct from Humanities, Arts or Social Sciences) but all disciplines of research. Despite these differences of nuance, for the purposes of this paper they will be regarded as essentially equivalent.

The ARDC defines a **platform** as a set of shared interactive and persistent services, often with connections to specific data collections, that enables researchers to find and access, collect or generate, and analyse, combine or transform that data. In this way a platform is potentially an engine for enhancing the FAIRness (Findability, Accessibility, Interoperability, and Reusability) and value of data.

Whereas a platform may be initially developed to serve a specific purpose, it may be possible, and desirable, to re-use it for additional purposes and in ways not originally intended. This paper will identify a number of different platform re-use patterns, including case studies arising from investment programs run by the ARDC.

Background

Australian Research Data Commons

The Australian Research Data Commons (ARDC)¹ is a transformational initiative that enables the Australian research community and industry to gain access to nationally significant, leading edge data intensive eInfrastructure, platforms, skills and collections of high-quality data. As a national research infrastructure provider, the ARDC facilitates partnerships to develop a coherent research environment that enables researchers to find, access, contribute to and effectively use data-centric services in order to maximise research quality and impact. The stated purpose of the ARDC is to provide Australian researchers with competitive advantage through data.

In July 2018, the ARDC was formed under the Federal Government's National Collaborative Research Infrastructure Strategy (NCRIS) through the merger of three existing digital research infrastructure capabilities: the Australian National Data Service (ANDS), National eResearch Collaboration Tools and Resources (Nectar) and Research Data Services (RDS). In May 2019, the ARDC became a company limited by guarantee and is registered with the Australian Charities and Not-for-profits Commission. It currently has 20 members.

The ARDC strategy is delivered through four portfolios that together support the development of a national research data commons:

¹ http://ardc.edu.au/

- People and Policy connecting the ARDC to researchers, research institutions, industry, and government to enhance knowledge exchange and drive an effective national data skills ecosystem;
- Platforms and Software supporting an increase in high-quality, high-impact research through digital platforms and better research software practices;
- Data and Services providing competitive advantage to Australian researchers by improving the discoverability, accessibility, and usability of Australia's research data assets;
- Storage and Compute supporting Australia's data and research advantage through the provision of reliable and sustainable underpinning infrastructures.

ARDC Platforms program

One of the ARDC portfolio areas is a program of investment in platform infrastructure² over four years (2019-2023). The Platforms program seeks to enable transformative research using advanced software and platforms. It is doing this by:

- Enabling more researchers in more disciplines to have access to platforms that transform the way they do their research (both by increasing the speed of the research process, and the ability to do new kinds of research) through undertaking a series of Open Calls and subsequent investments;
- Identifying and promoting eResearch tools and services that can be shared or reused between platforms;
- Growing the community of platform developers and managers.

One of the criteria for investment by the ARDC in any given platform was that the infrastructure be something available and supported at the national level. To support the broad collaborations required to achieve this aim, each of two open calls was run as a two stage process; a collaborative expression of interest (EOI) phase, and a competitive request for proposals (RFP). EOIs involved a lightweight application process and were published on the ARDC website to allow proposals to build on one another and encourage collaboration. ARDC encouraged and facilitated discussions between EOIs that proposed similar technological solutions or dealt with similar research problems. Following four weeks of brokered conversations, an RFP was issued, and these proposals were formally evaluated by an international panel of experts. The RFP required proposals to contain multiple partners (at least 3 organisations) and looked more favourably on those that had a geographical spread.

Ultimately, the ARDC invested AUD 21.7 million in total in 26 platform projects after the two open calls. This investment was matched by over AUD 35.97 million in investments from project partners. Although ARDC investment is usually the biggest single investment in each project, it is still a minority investor in the project overall. The ARDC believes that ensuring that the partners have 'skin in the game' via a substantial financial investment will contribute to the long-term sustainability of the projects.

The projects receiving investment covered the Australian National Science and Research Priorities³ and National Research Infrastructure Roadmap⁴ focus areas. This breadth of investment will ensure Australia's world class research system continues to improve productivity, create jobs, lift economic growth, and support a healthy environment.

² https://ardc.edu.au/collaborations/strategic-activities/platforms/

³ https://www.industry.gov.au/data-and-publications/science-and-research-priorities

⁴ https://www.dese.gov.au/national-research-infrastructure/2021-national-research-infrastructure-roadmap

Two other programs of activity delivered by other portfolios within the ARDC are particularly relevant to Platforms program projects.

The National Information Infrastructure program seeks to accelerate research and improve research integrity by providing services for the discovery, linkage and interoperability of data and other inputs/outputs of research. The services provided are frequently leveraged by the Platforms projects and include:

- A national research data discovery portal (Research Data Australia⁵);
- Different kinds of persistent identifiers (Datacite DOIs, Handles⁶);
- Support for different scientific terminology standards (Research Vocabularies Australia⁷).

The Research Cloud program seeks to enable the sustainable development and support of research data analysis and platform activities through the delivery of cost-effective, distributed and flexible national compute resources. This program is:

- Supporting a portfolio of eResearch tools and services for use by researchers and platform developers;
- Developing communities of practice and expertise in the delivery of cloud services for research;
- De-risking sector investment in innovative cloud infrastructure and services;
- Enabling interoperable application deployment across national (the Nectar Research Cloud), institutional and commercial cloud resources, as well as desktop and HPC.

Many of the Platforms in which the ARDC has invested are deployed on the ARDC Nectar Research Cloud⁸ which is managed by the Research Cloud program.

From FAIR data to FAIR platforms

The FAIR principles, at a high level, are intended to apply to all research objects (Wilkinson et al. 2016); including those used in research and those that form the outputs of research. Of course, digital objects such as data, software and workflows cannot be made FAIR in isolation - digital infrastructure is needed to store, manage, analyse and share the digital objects, and to make them discoverable.

When considering the application of the FAIR principles to platforms, there are two discrete aspects to be considered: how the platforms affect the fairness of data and other digital objects, and the fairness of the platforms themselves.

FAIRness pipelines

Platforms play a critical role in what could be called the FAIRness pipeline. A typical pipeline for research data begins with the collection or capture of data, its storage and analysis (often generating derivative or combined data subsets), and the sharing and publishing of the results. The infrastructure used at each stage in this pipeline has an impact on the FAIRness of the data generated. Ramezani (2021) characterised the impact of infrastructure on FAIRness as one of three possible outcomes:

⁵ https://ardc.edu.au/services/research-data-australia/

⁶ https://ardc.edu.au/services/identifier/

⁷ https://ardc.edu.au/services/research-vocabularies-australia/

⁸ https://ardc.edu.au/services/nectar-research-cloud/

- Enable (the service enables FAIR data by elevating the FAIRness of digital objects and/or supporting the FAIRification process);
- Respect (the service neither actively enables a particular FAIR principle nor interferes with it it can be said to respect the "FAIR-in-FAIR-out" principle);
- Reduce (The service makes data less FAIR at least for a particular principle for example by detaching metadata or a PID when it acts on a digital object).

A pipeline of steps thus might result in an increase in FAIRness, no change in FAIRness, or a reduction in FAIRness. In the same way that a chain is only as strong as its weakest link, any one step in the pipeline could degrade the overall FAIRness of the resulting outputs. Whether or not an Enable step in the pipeline would be sufficient to offset the impact of a Reduce step would need to carefully be evaluated on a case-by-case basis; a general answer is not possible.

How infrastructure elements such as platforms are designed and architected, and the functions they support, have a large impact on the (subsequent) FAIRness of the digital objects with which the platform interacts. The ARDC required the platforms it invested in to either enhance the FAIRness of the digital objects that they create or produce, or at the very least not make digital objects that they process less FAIR. For example, the format a platform outputs data in determines how interoperable the data are with other data and systems. Likewise, platforms can encourage findability by capturing and attaching descriptive metadata to the digital objects they create. Conversely, a platform could reduce the FAIRness of data by processing a raw dataset in an open, machine-readable format such as NetCDF, into a closed, proprietary format with bespoke semantic descriptors. As another example, if the data are only available via a bespoke (and usually undocumented) API they are effectively inaccessible.

FAIR platforms

As noted above, the initial applications of FAIR focussed on data use-cases. As FAIR has grown in popularity, people have sought to apply it to a wider range of research objects, including services (Koers 2020, Ramezani 2021) and software (Hong et al. 2021). The application of the FAIR principles is now also being considered for other areas, including workflows (Goble, 2020), machine learning (Katz, 2020), and artificial intelligence (Verma, 2021).

While some of the high-level FAIR principles as applied to data can be directly applied to platforms, others are not applicable. Although platforms depend on software, the recently developed FAIR Principles for Research Software (Hong et al. 2021) do not cover all the aspects of platforms, due in part to the complexity of a platform.

The authors believe that the FAIR principles should be applied to platforms due to their key role in the digital infrastructures that store, manage, analyse, and share other research objects:

- Continuity of the research record requires ongoing access to data, and the ability to reproduce research results;
- Given the increasing volume and complexity of data, access to software is essential to support access and reproducibility;
- This software often is deployed through platforms, both for ease of use and to provide access to enabling underpinning infrastructure;
- These platforms need to be sustained over the long term to meet the continuity driver.

It is worth noting that this sustaining can occur in two ways. One is the ongoing maintenance of platforms, so that they continue to meet the evolving needs of their target community of users. In this case, re-use of platforms and their components leads to less wheel-reinvention, greater use of shared or re-used code and thus more sustainable platforms. The

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other is where the platform is not necessarily kept available as a maintained running instance but is archived in a form (virtual machine image or container) that allows it to be "spun up" as needed, perhaps to reproduce results from a paper in the journal literature.

As a starting point, making platforms **themselves** FAIR (which is not the same as the way in which the platforms contribute to the FAIRness of the data they process), would require that:

- they are easily findable and accessible
- they should interoperate with other digital research infrastructures
- their technical architecture, components and services should be reusable
- where appropriate, they re-use existing elements.

The last two points will maximise the return on the investment made in building existing infrastructure and improve development efficiency by leveraging as much of what already is available as possible.

International Coordination

To explore these issues, the FAIR4VREs ⁹ Research Data Alliance working group began in late 2021 (NOTE: VREs was chosen for the name as the term most likely to work internationally). It will enable coordination between existing communities working with VREs, science gateways, platforms and virtual labs, to define what it means for VREs to be and enable FAIR, and provide guidance to VRE developers in achieving this. Specifically the working group is:

- Investigating how the existing application of the FAIR principles to data, software, workflows, computational notebooks, training materials, AI and machine learning enable VREs to enable FAIR digital objects, and themselves be FAIR, and identify any gaps in the existing work;
- Producing guidance on and examples of how VRES can and should be FAIR;
- Producing guidance on and examples of how VREs can and should enable FAIRness for other digital objects.

Reusability Patterns

The ultimate goal for the F, A, and I in FAIR, for all its various domains of application, is to enable the R: Reuse. So, how to ensure greater re-use of platform technologies in support of sustainable research infrastructure and more reusable research objects?

Before discussing re-use, it is necessary to reflect on the issue of the granularity of what is being re-used. Platforms present to the user as a single entity but are composed internally of a number of different elements: modules, workflows, integration frameworks, etc. Any discussion needs to be clear at what level the re-use is occurring. Additionally platform reuse can be considered from the perspective of three groups; the platform end-user, the platform builder, and the provider of the underlying infrastructure the platform depends on.

Arising from the work of the FAIR4VREs¹⁰ group and informed by the experience of the ARDC Platforms program, this paper argues that there are four main patterns of platform reusability. These can be ranked in ascending order of difficulty from the perspective of those implementing the re-use of the platform.

⁹ https://www.rd-alliance.org/groups/fair-virtual-research-environments-wg

¹⁰ https://www.rd-alliance.org/groups/fair-virtual-research-environments-wg

Accessing

This re-use pattern applies in different ways to platform end-users and infrastructure builders. Accessing involves using existing infrastructure as is, and not needing to make any changes, beyond some configuration changes. In both cases, no changes are required to the code, and the re-users do not need to implement any new infrastructure. However, for the platform builder there will be resource costs (support channels, server instances, storage, network traffic) and a need to manage the additional platform end-users now accessing the platform.

Access for end-users involves using an existing running instance of a platform configured to meet their needs. OSF.IO ¹¹ and Zooniverse ¹² are good examples of this.

OSF.IO is geared towards supporting collaborative research projects with peers. It allows users to start a project and add collaborators, giving them access to protocols and other research materials. It also supports storing data, code, and other materials in OSF Storage, sharing papers in OSF Preprints or a community-based preprint provider, and searching across public projects to build on the work of others and find new collaborators. Because users are working on a hosted server instance, they do not need their own infrastructure or a server administrator.

Zooniverse is geared more towards what are sometimes called "citizen science" projects involving volunteers working with data of many different types. The Project Builder interface enables the project administrator to create a variety of role types, upload their data, define workflows, and choose the tasks they want their volunteers to carry out.

Access for platform builders involves using calls to modules in an existing platform via Application Programming Interfaces (APIs) to provide additional functionality to another platform running somewhere else. A popular approach for this is the Open Geospatial Consortium standards.¹³ This provides a rich set of APIs that are used by developers to build open interfaces and encodings into their products and services. As an example of their application to a project in which the ARDC is investing, the Ecocommons platform ¹⁴ provides an OGC Web Processing Service (WPS) API interface to each of the microservices it implements,¹⁵ allowing other platforms to call them as needed.

Adopting

This re-use pattern primarily applies to platform builders. Adopting a platform means taking a platform that was designed to be reconfigurable, redeploying it as a new instance, and making it available to a new community of users. Assuming the codebase is appropriately implemented with options defined using settings rather than hard-coded, the work required for the new setting may be significantly less than writing something from scratch. Of course, this will involve additional work for the original developers, but it does transfer to the adopters the resource costs of making the platform available to a new set of users. Conversely, it may mean that the platform might not be as well adapted to the specific requirements of the new setting (see Adapting below for a discussion of an alternative pattern in this case).

An example of this pattern is HubZero.¹⁶ As well as a hosted offering which users pay to access, the developers provide an open-source distribution at no cost which allows the adopters to modify the code themselves for hosting on their own infrastructure or via a third-party cloud provider.

¹¹ http://osf.io

¹² http://zooniverse.org

¹³ https://www.ogc.org/standards

¹⁴ https://www.ecocommons.org.au

¹⁵ https://www.ecocommons.org.au/wp-content/uploads/PUBLIC-EcoCommons-Solution-

Architecture_Published-Nov-20.pdf

¹⁶ http://hubzero.org

Adapting

A third re-use pattern also available to platform builders is to take an existing platform and adapt it to a different problem domain or set of requirements. This could either involve coordinated development between the two dev teams, or a fork of the codebase (in which case the adapters will need to ensure that they have access to ongoing enhancements in the original code, and the developers of that code will need to be aware that this is an issue).

Such an adaptation might involve some combination of the following:

- building connectors to different kinds of data sets
- supporting different kinds of analysis workflows
- providing different modelling tools
- offering domain-appropriate visualisation options
- connecting to specific underpinning resources (e.g. GPU clusters) as needed
- reskinning/rebranding to provide a unique look-and-feel

An example of this adaptation pattern is the Ecocommons platform (one of the ARDC Platforms investments). This came out of a series of earlier investments in a Biodiversity and Climate Change Virtual Laboratory (BCCVL) and an ecology-focussed cloud processing environment 'ecocloud'.¹⁷ The EcoCommons investment proposal to the ARDC in 2019 was to spend the first year of a three-year program in re-engineering their codebase to enable broader re-deployment. This was viewed by the ARDC as an attractive and strategic approach and the proposal was successful. In the 2020 Open Call for ARDC Platforms investment 12 of the 46 proposals proposed to take advantage of the re-engineered solution to partner with EcoCommons to apply their framework to a diverse range of challenges.

The Biosecurity Commons ¹⁸ was one of the successful projects that proposed to leverage EcoCommons. It is now taking the EcoCommons codebase and extending its functionality in two ways:

- Contributing new code that meets the needs of both EcoCommons and the Biosecurity Commons through merge requests back into the original code base, thus providing benefits to the original developers;
- Adding biosecurity specific modules for data handling and workflows (coloured red in Figure 1) to provide a biosecurity-focussed environment, powered by code re-use.

¹⁷ https://ecocloud.org.au/

¹⁸ https://www.biosecuritycommons.org.au/

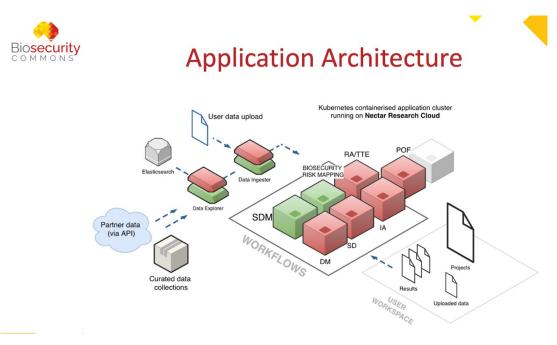


Figure 1: BioSecurity Commons Application Architecture

Abstracting

A fourth reuse pattern available to platform builders is to identify common elements and components that are used across multiple platforms and provide stand-alone deployments of these as shared research infrastructure. In this case research infrastructure providers may take on the operation of instances of these components, allowing platform builders to focus on the integration of these components into their platform, rather than needing to implement them from scratch.

The ARDC has done this both through the EOI process for our Platforms investments and by directly engaging with projects. In the first case, some of the EOI proposals were not for platforms *per se* but for services that made sense as part of a national research cloud offering. In the second case, ARDC staff identified multiple projects that could make use of the same services (either without changing their plans or with a small adjustment to their platform architectures).

The ARDC decided to invest in three services after testing the likely uptake with the intended users.

The first is a Virtual Desktop Interface running on the Nectar Research Cloud.¹⁹ Currently there are three desktops to choose from: Ubuntu 20.04, Centos 7 and Neurodesk (provided by AEDAPT ²⁰), and more desktops will become available over time. The default size of a Virtual Desktop is 4 virtual CPUs and 8GB RAM. Users will have the option to increase resources if the default is not sufficient for their computing needs. A single 50GB volume will be included for the Operating System and Working Storage. Transferring files to the desktop can be done via "drag and drop" to the desktop interface. Once users create a Virtual Desktop, it will be available for an initial 14 days. As well as direct invocation by users, this is also being made available to developers as a nationally provided and supported alternative to their own implementations.

Another abstracted service is the Australian Research Container Orchestration Service.²¹ This was originally an EOI proposal that was then welcomed as a candidate service by a number of the successful Platforms projects. It seeks to provide services and expertise to support the use of containers and Kubernetes in the Australian research community. The ARDC in

¹⁹ https://desktop.rc.nectar.org.au/about/

²⁰ https://ardc.edu.au/project/australian-electrophysiology-data-analytics-platform-aedapt/

²¹ https://arcos.ardc.edu.au/

conjunction with the national community is developing the requirements of ARCOS. At the time of writing ARCOS is coordinating a national team of experts in Kubernetes, including supporting related open source software for cloud native computing, engaging with the international Kubernetes and Cloud Native Computing communities, working with research communities and Platforms projects on understanding and supporting their requirements, establishing innovative and operational best practices amongst the national stakeholders, and cooperating on developing part of the national technical eResearch ecosystem.

The third abstracted service available for re-use is a JupyterHub package based on the JupyterHub installation developed for the re-engineered ecocloud component of the EcoCommons platform. This can now be deployed this on Nectar as a self-managed JupyterHub service. The package contains deployment scripts for how to set up a JupyterHub installation on a Kubernetes cluster provisioned by Nectar's Container Orchestration service, documentation with step-by-step instructions for a user to successfully create a running JupyterHub instance using their Nectar allocation, and documented examples on how to interact with the JupyterHub service. The ARDC has plans to use this distribution as the basis for a national JupyterHub service to support all Australian research users.

Encouraging Reusability

The ARDC sees benefits for a range of stakeholders in greater reusability of Platforms.

For the users, they get access to higher-quality and sustained platforms, where they are less likely to invest time in learning a system that might go away, and where they can be more confident of the enduring role of the platform in the ecosystem of scholarly outputs, including long-term reproducibility.

For the developers, they can draw on reusable components and architectures at reduced effort, as well as potentially attracting co-development activity to assist them.

For the investors, they derive greater impact from their investments by avoiding wheel reinvention, or investment in projects that only have a short life. Even if the platforms end up being replaced, some of their components may continue to be developed and re-used by other platforms.

To increase the likelihood of realising these benefits, the Platforms theme within the ARDC undertook two intentional steps to ensure greater reusability for the projects in which it invested.

Design of Open Calls

The Open Call process was intentionally designed to maximise reusability, and this came into play at multiple points. The EOI process made it clear that the ARDC had a strong bias towards Adopt or Adapt over new builds. Indeed, the development of a new platform from scratch was explicitly ruled out of scope. During the brokering phase, proponents were directed to look at existing solutions and encouraged to reuse them where possible. The assessment criteria (which in the 2020 Open Call were made public before submission of the RfPs) strongly encouraged reuse of existing platform technologies by scoring proposals higher that did so.

Architecture Assistance

The ARDC has also been actively driving re-use of infrastructure developed under the Platforms program through the analysis of platform architectures to identify potential applications of the re-use patterns described above. Given the spread of activities across the program's portfolio of twenty-six projects, there are many examples of functional requirements or project objectives that can be addressed by shared solutions. The ARDC is in a unique position to identify and act on these similarities through its insight across all these projects.

A key example, briefly mentioned above, is the JupyterHub on Kubernetes service abstracted from the EcoCommons platform and packaged for redeployment on the Nectar

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cloud. As a result of consultation with the AgReFed project on solution options for their needs, this distribution has already been picked up by the AgReFed platform and has substantially reduced the development effort that would have been required had they developed this capability from scratch.

The ARDC was also able to broker discussions between two major projects in the Platforms program, EcoCommons and the Australian Transport Research Cloud (ATRC), based on key similarities in purpose and structure in their respective architectures. Analysis of the recently developed ATRC platform architecture indicated the approach, and some solutions, employed by EcoCommons were both relevant to, and potential sources of guidance for the implementation of the ATRC design. EcoCommons had substantial experience in utilising a key third-party software component, and this provided valuable insight for the ATRC development team as to how they could best use this component to meet their own needs.

Platforms Community of Practice

The ARDC also facilitates the Platforms Community of Practice (PCoP) for the projects. Monthly virtual PCoP sessions provide a space for project teams from around Australia to share and learn from each other about both technical and non-technical aspects of platform development. New and emerging technologies being investigated by one project can be shared with the group, as can good software development practices.

Conclusion

The ARDC has invested in platforms to meet its stated objective to provide Australian researchers with competitive advantage through data. Platforms are an effective way to provide researchers with access to tools and underpinning resources to enable them to transform their research activity both in speed and kind.

The benefits of FAIRness that have been recognised for other research outputs have benefits for platforms as well, both for the platforms themselves and for their role in the FAIRness data transformation pipeline.

The work of the ARDC Platforms program has identified four different reusability patterns, each of which might be appropriate in different circumstances, and each of which has its own pros and cons. Platform adopters are encouraged to consider what might work best for them in the light of this analysis.

Reusability of platforms doesn't just happen. Before investing in any platforms infrastructure, the ARDC intentionally designed a number of elements into the Open Call process to improve the chances that reusable platforms and reuse would occur. After the investment decision had been made, the ARDC provided expert and careful assistance with architecture decisions to improve the chances that the resulting solutions would be reusable and reused.

This approach worked. As described above, the BioSecurity Commons is an adaptation of the EcoCommons platform for a different domain, in a way that strengthens both. Other platforms in which the ARDC has invested are now being assessed as elements of the final solution for two new Thematic Research Data Commons that are in preparation, one in the area of health and medical, and the other in the area of ecology and agriculture.²²

²² https://ardc.edu.au/news/designed-for-the-future-thematic-research-data-commons/

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