



Wf4Ever: Advanced Workflow Preservation Technologies for Enhanced Science

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D2.2v2 Design, implementation and deployment of workflow lifecycle management components - Phase II

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This deliverable describes the second phase of delivery of workflow lifecycle management components. It includes a description of the Research Object Model, which facilitates interoperation between components; the RO Manager command line tool; the Research Object Digital Library; the RO-enabled myExperiment; and a definition of models for workflow abstraction and indexation.

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Executive Summary

This deliverable describes the second phase of delivery of workflow lifecycle management components. These components are focused around the Wf4Ever Research Object Model (RO Model), which provides descriptions of workflow-centric ROs – aggregations of content. This model is used to structure and describe ROs which are then stored and manipulated by the components of the Wf4Ever Toolkit.

The RO Model provides a framework for describing aggregations of content along with annotations of the aggregated resources, a vocabulary for describing workflows, and a vocabulary for describing provenance. The application of the model within the project has not resulted any significant changes, suggesting that the model captures user requirement adequately and has reached a level of maturity. We provide here a description of the RO model. We also present the components developed for creating and managing Research Objects: the RO Manager – the Research Object Digital Library.

One of the main developments in the last year consists in incorporating Research Objects within the myExperiment environment to allow scientists who already use myExperiment to create, share and reuse Research Objects. We discuss the efforts that went into this task, and show how myExperiment is using Research Object Digital Library as a back-end for storing and archiving Research Objects.

We describe advanced management functions that we developed for abstracting and indexing workflows, with the aim of supporting the discovery and reuse of workflows. We present an ontology that we developed for abstracting workflows using motifs that characterize data manipulation and transformation patterns. We also report on a solution that we developed for indexing workflows based on the services (processes) that they use.

This deliverable should be read in tandem with D1.3v2 (Wf4Ever Architecture – Phase II), D1.4v2 (Reference Wf4Ever Implementation – Phase II), D1.2v3 (Wf4Ever Sandbox – Phase III), D3.2v2 (Design, implementation and deployment of Workflow Evolution, Sharing and Collaboration components – Phase II) and D4.2v2 (Design, implementation and deployment of Workflow Integrity and Authenticity Maintenance components – Phase II) in order to provide a complete picture of the state of the Wf4Ever Phase II components.

This deliverable supersedes D2.2v1, and can be read as a standalone document.

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List of Ontologies

1. RO ontology: <http://purl.org/wf4ever/ro#>
2. Wfdesc ontology: <http://purl.org/wf4ever/wfdesc#>
3. Wfprov ontology: <http://purl.org/wf4ever/wfprov#>
4. ROEvo ontology: <http://purl.org/wf4ever/roevo#>

1 Introduction

This deliverable describes Phase II of the design, implementation and deployment of the Wf4Ever components that will support workflow lifecycle management. The document should be read in tandem with other Month 32 deliverables, in particular D3.2v2 (Design, implementation and deployment of Workflow Evolution, Sharing and Collaboration components – Phase II) [GC⁺13b] and D4.2v2 (Design, implementation and deployment of Workflow Integrity and Authenticity Maintenance components – Phase II) [GC⁺13a] which address complementary aspects of the overall wf4ver architecture and components. This deliverable supersedes D2.2v1, and can be read as a standalone document.

According to the Description of Work, *This prototype will include the following functionalities: new versions of the Research Object model and ontology network, advanced management functions (filtering, clustering, etc.), playback functionalities for reproducibility, and workflow classification, indexing and explanation techniques.*

These requirements are addressed in the following way:

Section 2 presents the Research Object Model defined within Wf4Ever. Specifically, we present a family of ontologies for specifying Research Objects and their associated resources, e.g., workflow, workflow runs, etc.

Section 3 presents the tools that we have developed for assisting users in creating and managing Research Objects. More specifically, Section 3.1 presents the Research Object Manager (RO Manager), a command line tool for creating, displaying and manipulating Research Objects. Section 3.2 shows how the myExperiment virtual environment [RGS09], was extended to allow end-users, who are not necessarily information technology experts, to create, share, publish and curate Research Objects.

Section 4 presents the Research Object Digital Library (RODL), which acts as a full-fledged back-end not only for scientists but also for librarians.

Section 5 presents the motif ontology that we developed for abstracting scientific workflows, and illustrates how it has been used to document workflows. It then goes on to present a solution that we developed for indexing workflows based on the processes (steps) they are composed of, with the purpose of assisting users in discovering workflows that are of interest to them.

2 The Research Object Model

The design of the Research Object model was informed by a systematic analysis of requirements expressed by scientists from the life sciences and astronomy fields¹. The application of the model within the project has not resulted any significant changes, suggesting that the model captures user requirement adequately and has reached a level of maturity. Figure 1 gives an overview of the abstract model of the Research Object model, distinguishing between core and extended requirements. There are three core requirements that have been identified, namely a mechanism for uniquely identifying Research Objects, a means for aggregating resources within a Research Object, and the ability to annotate the Research Object, its constituent resources and their relationships. The extended requirements highlight the need for specifying workflows (experiments), provenance traces of their executions, the evolution of a Research object over time, as well as mechanisms for expressing their dependencies.

As illustrated in Figure 1, we have realized the Research Object abstract model using a family of ontologies, which we will present in the rest of this section. Notice that we do not define ontologies for specifying dependencies, investigations, components and studies, since there exist ontologies that implement these aspects, e.g., the Dublin Core ontology² provide the means for specifying dependencies, and the ISA model³ provides concepts for specifying investigations and studies.

¹<http://www.wf4ever-project.org/wiki/display/docs/User+Requirements>

²<http://dublincore.org>

³<http://www.isa-tools.org>

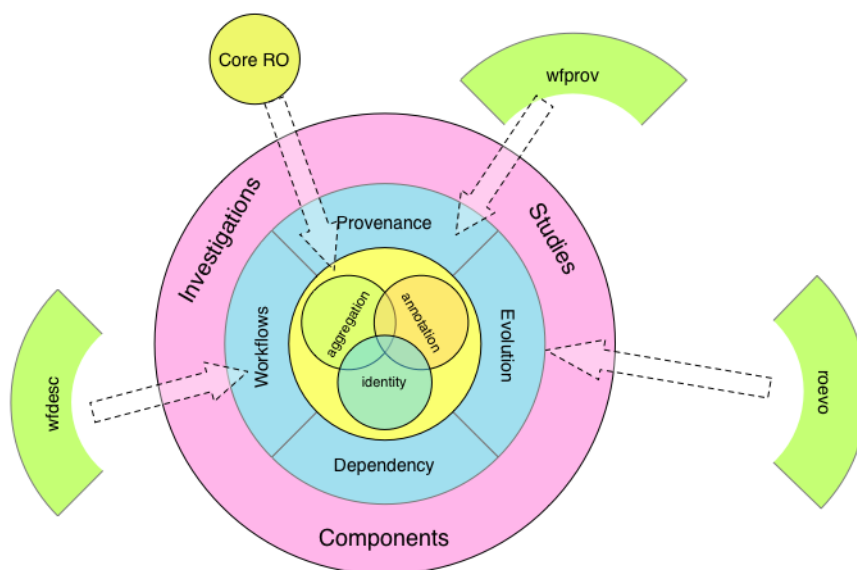


Figure 1: The Abstract Model of Research Objects, and the Ontologies that Realize it

2.1 Research Object Core Ontology

The Core Research Object Ontology (Core RO) provides the minimum terms that are essential to the specification of Research Objects. Specifically, it caters for two main requirements⁴ by providing a container structure that can be used by the scientists to bundle the resources and material relevant for their investigation, and by enabling annotations of such a container, its resources, as well as the relationships between resources thereby making the Research Object interpretable and reusable.

To cater for the specification of aggregation structures, we built the Research Object Core Ontology upon the popular ORE vocabulary⁵. ORE defines standards for the description and exchange of aggregations of Web resources. Figure 2 illustrates the main terms that constitute the Research Object Core Ontology, which we describe in what follows.

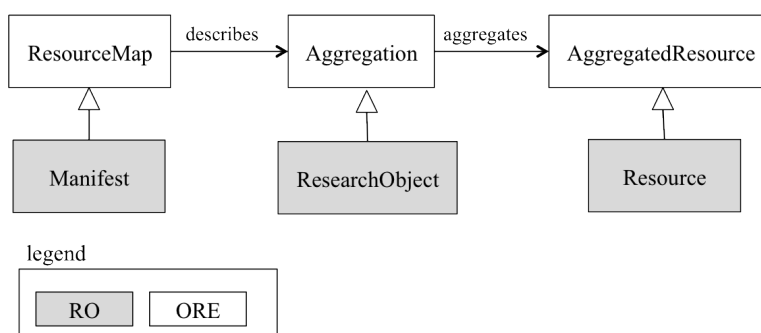


Figure 2: RO as an ORE aggregation.

- `ro:ResearchObject`⁶, represents an aggregation of resources. It is a sub-class of `ore:Aggregation` and acts as an entry point to the Research Object.

⁴<http://www.wf4ever-project.org/wiki/display/docs/User+Requirements>

⁵www.openarchives.org/ore

⁶The namespace of the Research Object Core Ontology `ro` is <http://purl.org/net/wf4ever/ro#>

- `ro:Resource`, represents a resource that can be aggregated within a Research Object and is a sub-class of `ore:AggregatedResource`. A resource can be a Dataset, Paper, Software or Annotation. Typically, a `ro:ResearchObject` aggregates multiple `ro:Resource`, and this relationship is specified using the property `ore:aggregates`.
- `ro:Manifest`, a sub-class of `ore:ResourceMap`, represents a resource that is used to describe a `ro:ResearchObject`. It plays a similar role to the manifest in a JAR or a ZIP file, and is primarily used to list the resources that are aggregated within the Research Object.

The second core requirement that the Research Object Core Ontology caters for is the descriptions of the Research Object and its elements. We chose the Annotation Ontology (AO) release 2.0b2 [COC⁺11]. To annotate Research Objects, we make use of the following three Annotation Ontology terms `ao:Annotation`⁷, which represents the annotation itself; `ao:Target`, which is used to specify the `ro:Resource(s)` or `ro:ResearchObject(s)` subject to annotation; and `ao:Body`, which comprises a description of the target. In the case of Research Objects, we use annotations as a means for decorating a resource (or a set of resources) with metadata information. The body is specified in the form of a set of RDF statements, which can be used to, e.g., specify the date of creation of the target or its relationship with other resources or Research Objects. Also, annotations can be provided for human consumption (e.g. a description of a hypothesis that is tested by a workflow-based experiment), or for machine consumption (e.g. a structured description of the provenance of results generated by a workflow run). Both kinds of annotations are accommodated using Annotation Ontology structures.

2.2 RO Extension Ontologies

We present in this section two extensions to the core Research Object ontology. The first specializes the kinds of resources that the Research Object can aggregate. In particular, we present extensions to specify method and experiments and the traces of their executions. The second kind of extension shows how specific metadata information, describing the evolution of the Research Object over time, can be specified by specializing the Research Object core ontology.

Specifying Workflows To describe workflow Research Objects the workflow description vocabulary *wfdesc*⁸ defines several specific resources that are involved in a workflow specification. The choice of these resources was performed by examining the commonalities between major data driven workflows [Shi07], namely Taverna⁹, Wings¹⁰ and Galaxy¹¹.

Figure 3 illustrates the terms that compose the *wfdesc* ontology. Using this ontology, a workflow is described using the following three main terms:

- `wfdesc:Workflow` refers to a network in which the nodes are processes and the edges represent data links. It is defined as a subclass of the *Plan* concept from the PROV-O ontology, which represents a set of actions or steps intended by one or more agents to achieve some goals [LSM⁺13].
- `wfdesc:Process` is used to describe a class of actions that when enacted give rise to process runs. Processes specify the software component (e.g., web service) responsible for undertaking those actions.
- `wfdesc:DataLink` is used to encode the data dependencies between the processes that constitute a workflow. Specifically, a data link connects the output of a given process to the input of another process, specifying that the artifacts produced by the former are used to feed the latter.

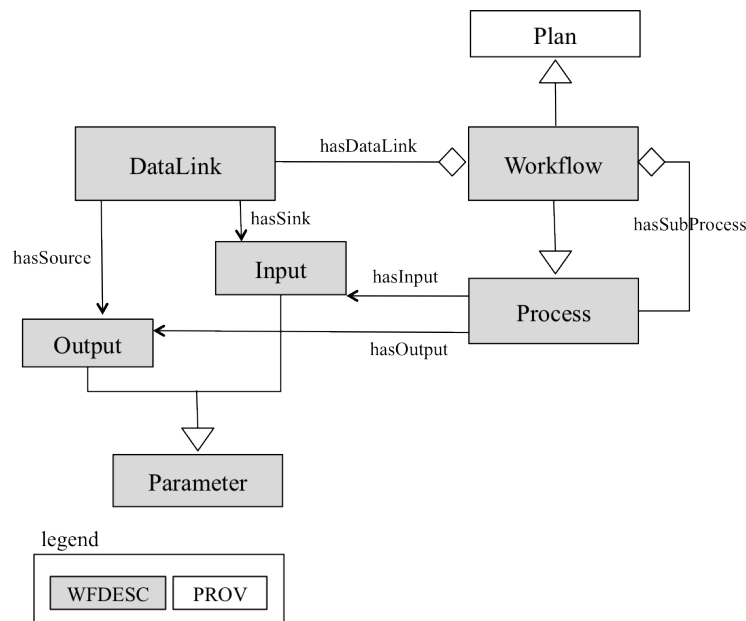
⁷The namespace of `ao` is <http://purl.org/ao/>

⁸The name space of *wfdesc* is <http://purl.org/wf4ever/wfdesc#>.

⁹<http://www.taverna.org.uk>

¹⁰<http://http://wings-workflows.org>

¹¹<http://galaxyproject.org>

Figure 3: The *wfdesc* ontology.

Describing Experimental Provenance using the *wfprov* Ontology The *wfprov* ontology is used to describe the provenance traces obtained by enacting workflows. It is defined as an extension to the ongoing W3C PROV standard ontology - PROV-O¹².

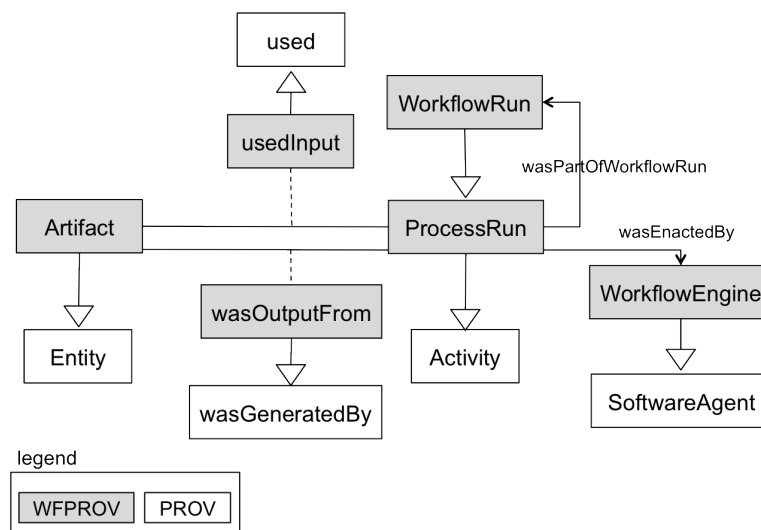
Figure 4: The *wfprov* ontology.

Figure 4 illustrates the structure of the *wfprov* ontology and its alignments with the W3C PROV-O ontology. A workflow run (*wfprov:WorkflowRun*) represents the enactment of a given workflow. It is composed of a set of process runs (*wfprov:ProcessRun*), each representing the enactment of a process. A process run may use some artifacts (*wfprov:Artifact*) as input and generate others as output. A process run is enacted by a workflow engine (*wfprov:WorkflowEngine*), which can be seen as a PROV software agent.

By chaining the usage and generation of artifact together, the *wfprov* ontology allows scientists to trace the lineage of workflow results. For example the user can identify the input artifacts that were used to feed the workflow run (as a whole) to obtain a given output that was generated by the workflow run.

¹²Note that the *wfprov* is reported in the W3C PROV Working Group implementation report.

Tracking Research Object Evolution using the *roevo* Ontology The *roevo* ontology is another extension to the minimal core ontology for describing an important aspect of Research Objects, its life cycle. To track the life cycle of a Research Object, we need to describe its changes at different levels of granularity about the Research Object as a whole and about the individual resources. Also, we want to provide sufficient details to track the changes in order to roll back to a particular version or to quality control changes. Therefore, we need to describe when the change took place, who performed the change, and dependency relationships between the changes. Change is closely related to the provenance of a particular version of a Research Object or a resource. A study of the latest PROV-O ontology shows that it indeed provides all the foundational information elements for us to build the evolution ontology.

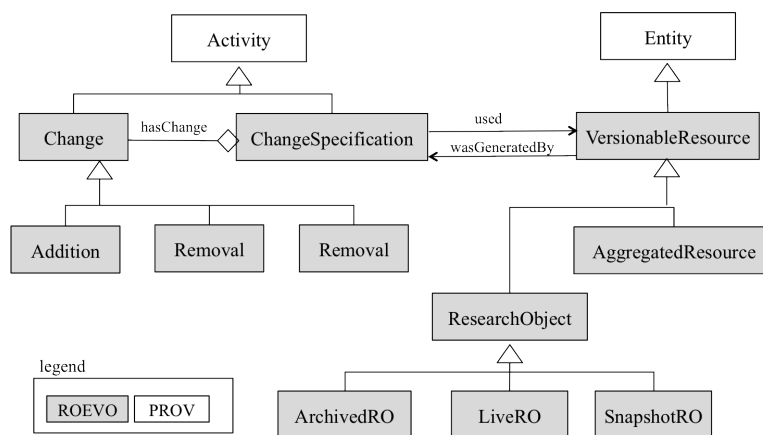


Figure 5: The *roevo* ontology extending PROV-O core terms.

Figure 5 illustrates the core concepts of this ontology and how it extends the PROV-O:

- To capture different status of a Research Object, depending on whether it is being edited, shared or archived, we created three sub-classes of `ro:ResearchObject`. The `roevo:LiveRO` is a Research Object that is being edited to capture research findings during a live investigation. The `roevo:ArchivedRO` can be regarded as a production Research Object to be preserved and archived, such as one describing findings published in an article, and it can no longer be changed. The `roevo:SnapshotRO` represents a live Research Object at a particular time, e.g., a Research Object that was submitted for a review before publication.
- Both a snapshot of a live Research Object and an archived Research Object can be regarded as a versioned Research Object, i.e. a `roevo:VersionableResource`. Because it is a sub-class of `prov:Entity`, we can reuse PROV-O properties to describe the provenance or changes of this entity, such as pointing to the activity leading to any of its changes, the source Research Object that it was derived from, and the agent involved in its change.
- A change is a `prov:Activity`, which means that it has a start time, an end time, an input entity and a resulting entity. Also a change leading to a new Research Object can constitute a series of changes. Therefore, we have a composite `roevo:ChangeSpecification` activity, which has a number of unit `roevo:Changes`. A unit change can be adding, removing or modifying a resource or a Research Object. But these different changes share the same pattern of taking an input entity and producing an output entity, which can all be nicely covered by properties from PROV-O.

As well as the above vocabularies, the Research Object model makes use of existing vocabularies, in particular, FOAF¹³, DCTerms¹⁴, CITO¹⁵, and SIOC¹⁶ to provide Research Objects designers with the means

¹³<http://xmlns.com/foaf/spec/>

¹⁴<http://dublincore.org/documents/dcmi-terms/>

¹⁵<http://vocab.ox.ac.uk/cito>

¹⁶<http://sioc-project.org/ontology>

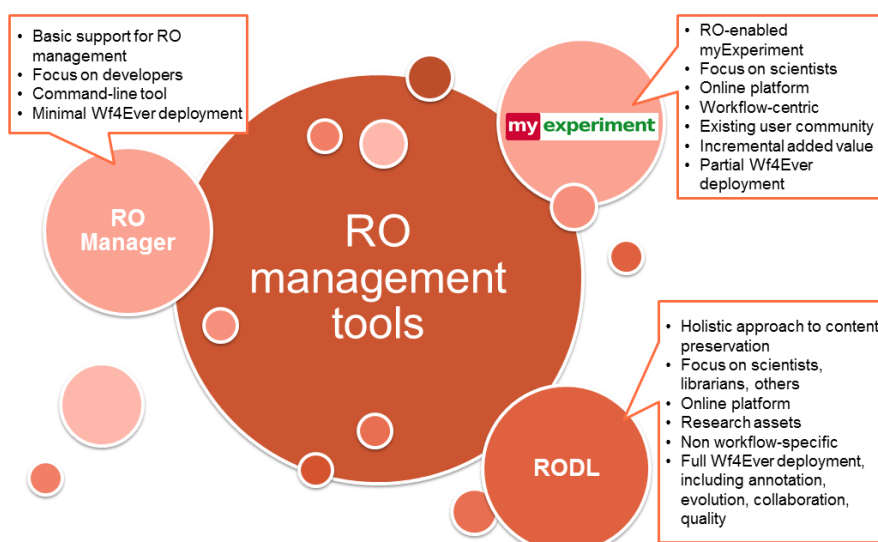


Figure 6: Research Object management tools.

to express aspects such as the people who were involved in the creation of a Research Object, its citation, as well as dependencies that the Research Object may have. For instance, we make use of the term `dc:requires` to specify that the execution of a workflow requires other resources, e.g., plugins, credential, or specific execution environment.

3 Research Object Management Tools

This section presents the tools developed for assisting users in creating and managing Research Objects. These tools are aimed towards different types of target users and their needs and represent different levels of deployment of Wf4Ever RO management capabilities according to such requirements. RO Manager, myExperiment, and RODL comprise our portfolio of RO management tools (see Figure 6). Details from the exploitation point of view about the portfolio will be given in the final exploitation plan (deliverable D8.5v2) of Wf4Ever's project results.

The Research Object Manager (RO Manager, Section 3.1) is a command line tool for creating, displaying and manipulating Research Objects, which incorporates the essential functionalities for RO management, especially by developers and in general a technically skilled audience used to working in a command-line environment. myExperiment (Section 3.2) has been extended [RGS09] to allow end-users, who are not necessarily information technology experts, to create, share, publish and curate workflow-centric Research Objects. The RO-enabled myExperiment incorporates a considerable amount of Wf4Ever's developments, especially the RO Model and Research Object management capabilities for end users. Finally, the Research Object Digital Library (RODL, Section 4) acts as a full-fledged back-end not only for scientists but also for librarians and potentially other communities interested in the aggregation of heterogeneous information sources with the rigor of digital libraries' best practices. RODL provides a holistic approach to the preservation of aggregated information sources and incorporates most of Wf4Ever's capabilities dealing with RO management, collaboration, versioning and evolution, and quality management.

3.1 Research Object Manager

The Research Object Manager (RO Manager) is a command line tool for creating, displaying and manipulating Research Objects. The RO Manager is complementary to RODL (see Section 4), in that it is primarily designed to support a user working with ROs in the host computer's local file system, with the intention being that the RODL and RO Manager can exchange ROs between them, using of the shared RO model and vocabularies. The RO Manager code base also includes the checklist evaluation functionality, described in D4.2 [GC⁺13a], which can be invoked using a command line or REST web interface.

Experience has shown that a simple command-line tool can provide developers and users with early access to functionality, and provide an opportunity to gather additional user feedback and requirements. RO Manager has also been used in conjunction with built-in operating system functionality for scripting prototype tool chains for more complex operations involving Research Objects.

The RO Manager allows users and developers to:

- Create local ROs;
- Add resources to an RO;
- Add annotations to an RO;
- Read and write ROs to the RODL;
- Perform checklist evaluation of an RO;
- Obtain a raw dump of Research Object metadata.

To illustrate how the user can interact with the RO manager to manipulate Research Objects, Figure 7 shows interactions for three RO Manager operations, `ro create`, `ro add` and `ro annotate`, which exemplify typical local RO management operations.

The four interacting elements presented are the user-issued command (`/user`), the RO Manager program (`/RO_Manager`), an internal RO metadata object (`/ro_metadata`) that manages the RO aggregation and annotation metadata, and the local file system (`/file_system`) where ROs are persistently stored and managed.

From this, it can be seen that:

- The `ro create` command initializes an RO structure by interacting directly with the file system.
- The `ro add` command uses the RO URI to initialize an `ro_metadata` object, and calls its `addAggregatedResources()` method to incorporate one or more files into the RO aggregation. The `ro_metadata` object updates the RO metadata structures in the file system through a series of read and write operations.
- The `ro annotate` command similarly uses the RO URI to initialize an `ro_metadata` object, and reads the existing annotations from disk. New annotations may be supplied as an attribute/value or attribute/link pair in which a case a new annotation graph is created in the file system. Otherwise the new annotation may already exist as a graph. In either case, the local copy of the RO manifest is updated to record the new annotation. The annotation may be applied to multiple resources in the RO. Eventually, the updated manifest is written to the file system by the `ro_metadata` object.

The RO manager is documented in a user guide that is available online¹⁷. An FAQ describing how to deal with various common operations using RO Manager is also accessible online¹⁸.

¹⁷<http://wf4ever.github.io/ro-manager/doc/RO-manager.html>

¹⁸<http://www.wf4ever-project.org/wiki/display/docs/RO+Manager+FAQ>

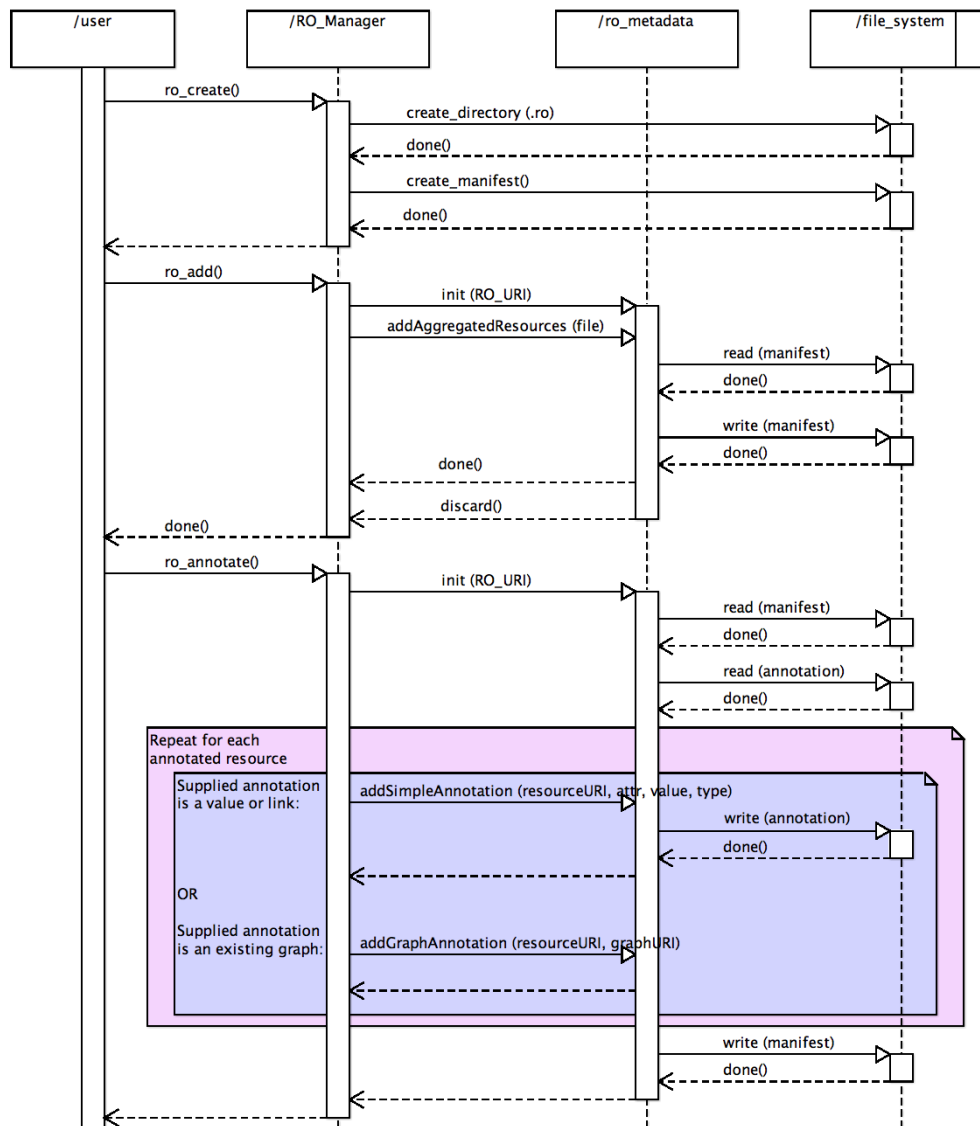


Figure 7: RO Manager sequence diagram illustrating interactions with the user.

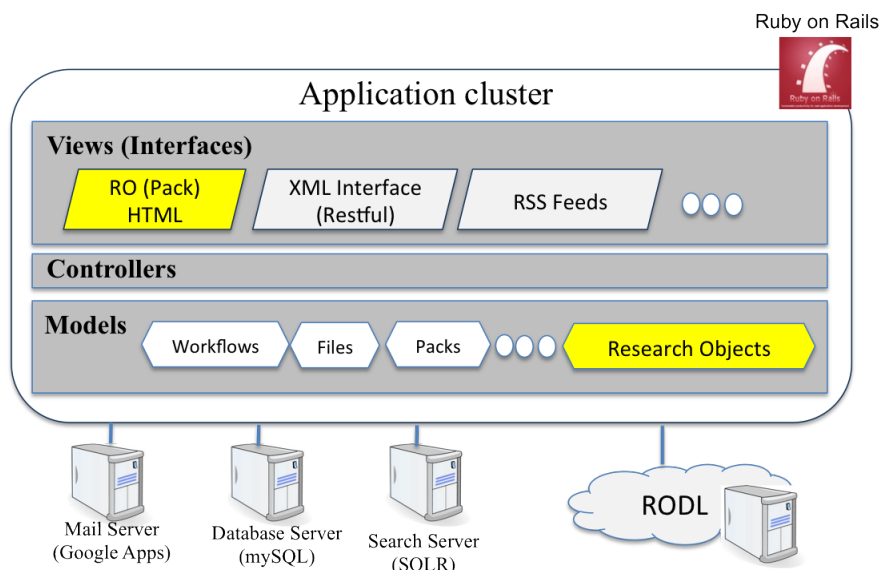


Figure 8: RO-enabled myExperiment (except RODL, the modules in the above figure belong to the myExperiment infrastructure).

The RO Manager is implemented in Python, and is available as an installable package through the Python Package Index (PyPI)¹⁹. The source code is maintained in the Wf4ever Github repository²⁰. The RO Manager is heavily dependent on RDFLib²¹, which provides RDF parsing, formatting and SPARQL Query capabilities. The RO Web service uses the Pyramid²² web framework, and uritemplate²³ for RFC 6570²⁴ template expansion.

3.2 Research Object-Enabled myExperiment

In this section, we describe how myExperiment [RGS09] was extended in order to cater for the sharing, publication and curation of Research Objects. myExperiment is a virtual research environment targeted towards collaborations for sharing and publishing workflows (and experiments). It provides the functionalities necessary for sharing workflows within and across multiple communities. In doing so, myExperiment adopts a social web approach, which is adapted to the need of scientists. The workflows that are shared using myExperiment do not need to be specified in a particular workflow management system. For example, we find on myExperiment workflows that have been specified using Galaxy [G⁺05], Taverna [WHF⁺13], Kepler [LAB⁺06] and Vistrails [CFS⁺06a].

While initially targeted towards workflows, the creators of myExperiment were aware that scientists want to share more than just workflows and experiments. Because of this, myExperiment was extended to support the sharing of artifacts known as Packs. A pack can be seen as a basic aggregation of resources, which can be workflows, but also files, presentations, papers, or links to external resources. The notion of packs has been widely adopted by scientists. At the time of writing, myExperiment had 337 packs. Just like a workflow, using myExperiment a pack can be annotated and shared.

In order to support complex forms of sharing, reuse and preservation, we have worked during the last year on incorporating the notion of Research Objects (which can be seen as advanced packs) into the development

¹⁹<https://pypi.python.org/pypi/ro-manager>

²⁰<https://github.com/wf4ever/ro-manager>

²¹<https://github.com/RDFLib>

²²<http://docs.pylonsproject.org/projects/pyramid/>

²³<http://code.google.com/p/uri-templates/>

²⁴<http://tools.ietf.org/html/rfc6570>

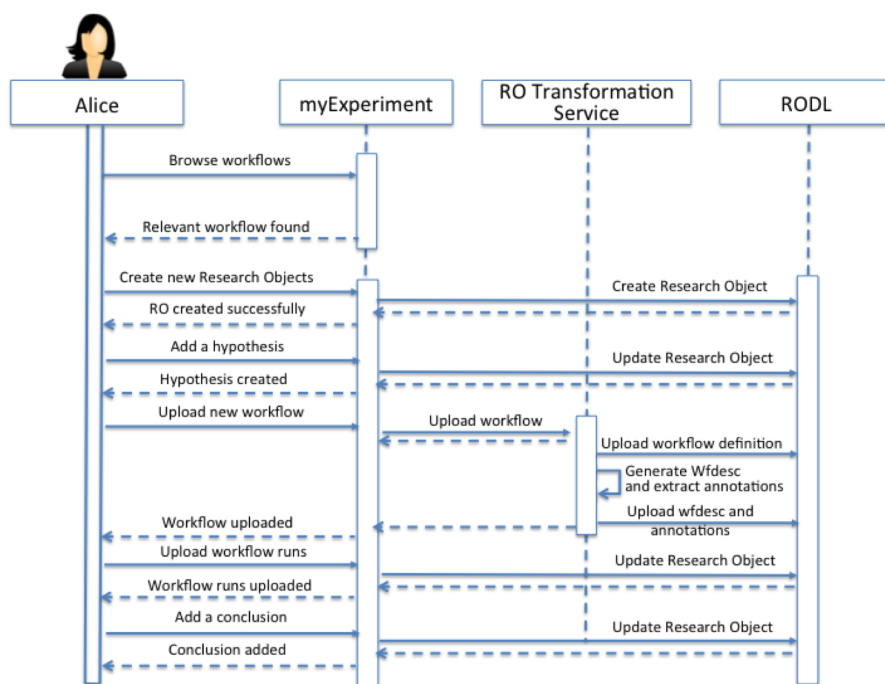


Figure 9: A Sequence diagram illustrating how myExperiment can be used to create Research Objects.

version of myExperiment²⁵. In addition to the basic aggregation supported by packs, alpha myExperiment²⁶ provides the mechanisms for specifying metadata that describes the relationships between the resources within the aggregation. Moreover, the structure and the types of the resources that compose a pack are now inline with those that have been identified thanks to the Research Object model. For example, a user is able to specify that a given file within a pack specifies the hypothesis, that another file specifies the workflow run obtained by enacting a given workflow, or that a given file states the conclusions drawn by the scientists after analyzing the workflow run.

Figure 8 illustrates a high-level architecture of alpha myExperiment, the development version of myExperiment into which the Research Objects capabilities were incorporated. As illustrated in the figure, at the level of the Rails²⁷ model, data structures that represent the Research Object and associated resources have been incorporated. To manipulate such data structures, the controller layer has been extended, and to provide non-information technology users with the ability to create and manage Research Objects, the view layer has been extended with the necessary HTML Web pages.

To illustrate how myExperiment can be used for managing Research Objects, Figure 9 depicts a sequence UML diagram illustrating a typical sequence of interactions that the user undergoes to create and share a Research Object. Alice (the user) first browses myExperiment to identify a workflow that is of interest to her investigation. Once she identified a relevant workflow, she downloads the workflow, modifies and re-purposes it for her investigation. Once she is happy with the *new* workflow, Alice decides to create a Research Object. In doing so, she specifies the hypothesis within a file, which is stored within RODL. RODL acts as a back-end for myExperiment to store the information about Research Objects. Alice then uploads her workflow to myExperiment. As a result, myExperiment sends a request to the RO transformation service, which uploads the workflow definition to RODL, transforms the workflow definition into wfdesc, and extracts the annotations that are bundled within the workflow definition. These elements, i.e., wfdesc specification and annotations, are then uploaded to the Research Object in RODL. Alice also uploads the

²⁵<http://alpha.myexperiment.org/packs/>

²⁶It is worth noting that once the development in the myExperiment alpha is judged mature, the new functionalities will be staged to the production version of myExperiment.

²⁷<http://rubyonrails.org>

workflow runs obtained as a result of enacting her workflow, and specifies the conclusion she comes to at the end of her investigation.

Using myExperiment, Alice now has a Research Object, compliant with the models from Section 2, viewable and manipulable as a pack through myExperiment, and enriched with a hypothesis and conclusions that can assist other users in understanding and possibly reusing and re-purposing her research results.

4 Research Object Digital Library

The foundational service to preserve workflow-centric Research Objects is the Research Object Digital Library (RODL), which realizes the Storage and Lifecycle functionalities prescribed by Wf4Ever Architecture [DRHPP13]. RODL is a software system which collects, manages and preserves aggregations of scientific workflows and related objects and annotations, packed into Research Objects. RODL is a back-end service that does not directly provide a user interface, but rather system level interfaces through which client software can interact with RODL and provide different user interfaces as tailored to needs. This section presents the interfaces supported by RODL, and describes their implementations.

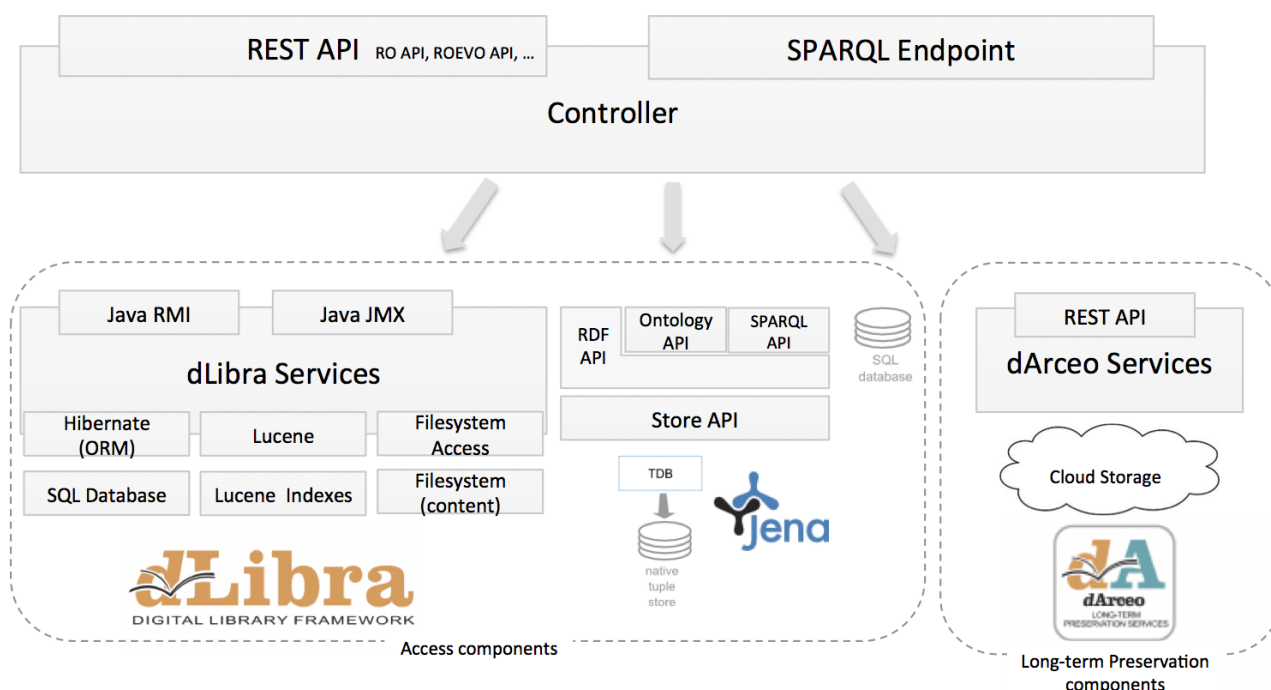


Figure 10: Research Objects Digital Library internal component diagram

4.1 The interfaces

The main system level interface of RODL is a set of REST APIs, including the RO API²⁸ and the RO Evolution API²⁹.

The RO API, also called the RO Storage and Retrieval API, defines the formats and links used to create and maintain Research Objects in the digital library. It is aligned with the Research Object model that is used to define Research Objects, and so it recognizes concepts such as aggregations, annotations and folders. The Research Object model ontology (see Section 2) is used to specify relations between different resources.

²⁸<http://wf4ever-project.org/wiki/display/docs/RO+API+6>

²⁹<http://wf4ever-project.org/wiki/display/docs/RO+evolution+API>

Given that the semantic metadata is an important component of a Research Object, the RODL supports content negotiation for the metadata resources, including formats such as RDF/XML, Turtle and TriG.

The RO Evolution API defines the formats and links used to change the lifecycle stage of a Research Object, most importantly to create an immutable snapshot or archive from a mutable live Research Object, as well as to retrieve the evolution provenance of a Research Object. The API follows the Research Object evolution model (see Section 2), which is most visible in the evolution metadata that are generated for each state transition.

Additionally, RODL provides a SPARQL endpoint that allows performing SPARQL queries over HTTP to the metadata of all stored Research Objects. It also implements the Notification API³⁰, which defines links used to retrieve Atom feeds with notifications of events about any Research Object. For searching the contents of Research Objects a Solr REST API and the OpenSearch APIs are provided. Finally, RODL implements a custom User Management API³¹ for registering users and generating OAuth 2 access tokens, providing the option of extending it with an access control layer in the future.

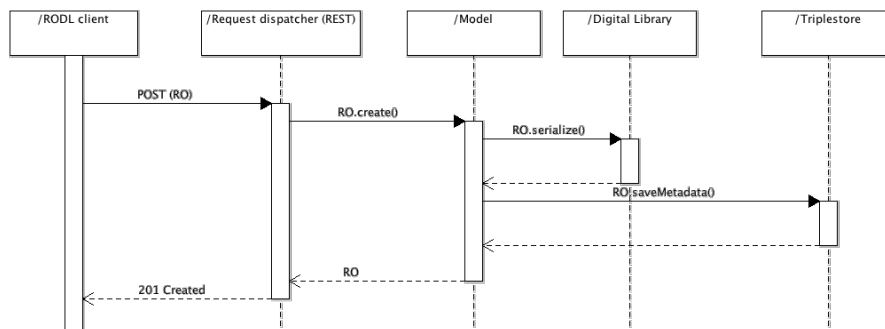


Figure 11: The sequence diagram for creating a Research Object in RODL

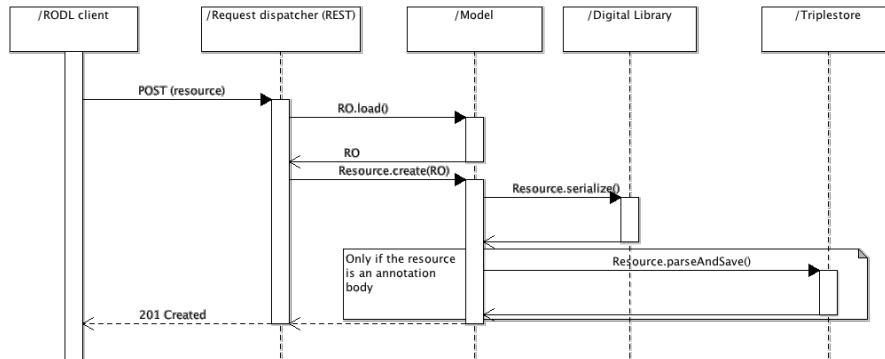


Figure 12: The sequence diagram for aggregating a new resource in a Research Object

4.2 The implementation

One of the main design challenges related to the implementation of RODL was the need to support both live, dynamically changing Research Objects as well as immutable snapshots that are intended for a long-term preservation. With this in mind, the RODL has a modular structure that comprises the access components, the long-term components and the controller that manages the flow of data (see figure 10). For immutable Research Objects, they are stored in the long-term preservation repository once they are created. The live Research Objects, on the other hand, are pushed asynchronously after every change or periodically, depending on the configuration.

³⁰<http://wf4ever-project.org/wiki/display/docs/Notification+API>

³¹<http://wf4ever-project.org/wiki/display/docs/User+Management+2>

The access components are the storage backend - dLibra³² - and the semantic metadata triplestore. dLibra provides file storage and retrieval functionalities, including file versioning and consistency checking. It has a built-in text search engine and it manages users and controls their access rights. It allows organizing stored objects into hierarchical structures and associating metadata at the level of object aggregations. It is also possible to use a built-in module for storing Research Objects directly in the filesystem.

The semantic metadata is additionally parsed and stored in the triplestore backed by Jena TDB³³. Jena TDB is an actively developed RDF store implementation, which provides good support for transactions, querying, caching and using named graphs. The use of a triplestore helps in RODL internal data processing and offers a standard query mechanism for RODL clients. It also provides a flexible mechanism for storing metadata about any component of a Research Object that is identifiable via a URI, which apart from workflows and other resources, may include parts of workflows or external resources (e.g. web services, data sources).

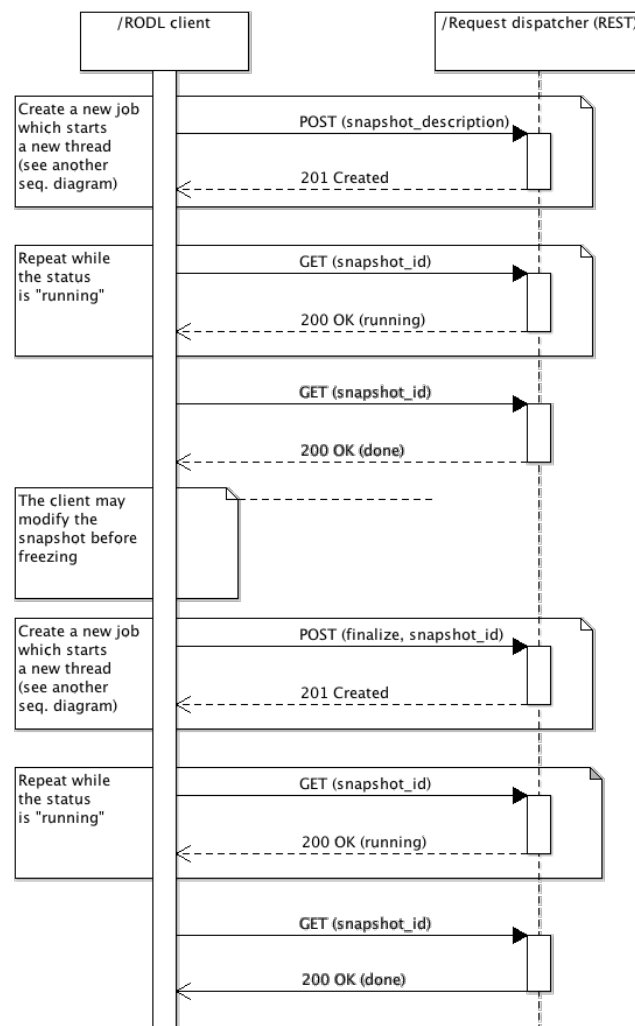


Figure 13: The sequence diagram for creating a snapshot or release from the RO Evolution API client perspective

The UML sequence diagrams (Figures 11,12) illustrate the interactions between the controller, the storage backend and the triplestore for the basic operations of creating a Research Object and aggregating resources to it. Creating immutable snapshots of Research Objects is a more complex process which involves copying the resources, recording their provenance, optional modifications by the user and finally releasing as a published, immutable object. Figure 13 shows how RODL clients can perform these steps via the RO Evolution

³²<http://dlib.psnc.pl/dlibra/>

³³<http://jena.apache.org/>

API. Figures 14,15 present the interaction between internal RODL components when performing the process of creating the snapshot.

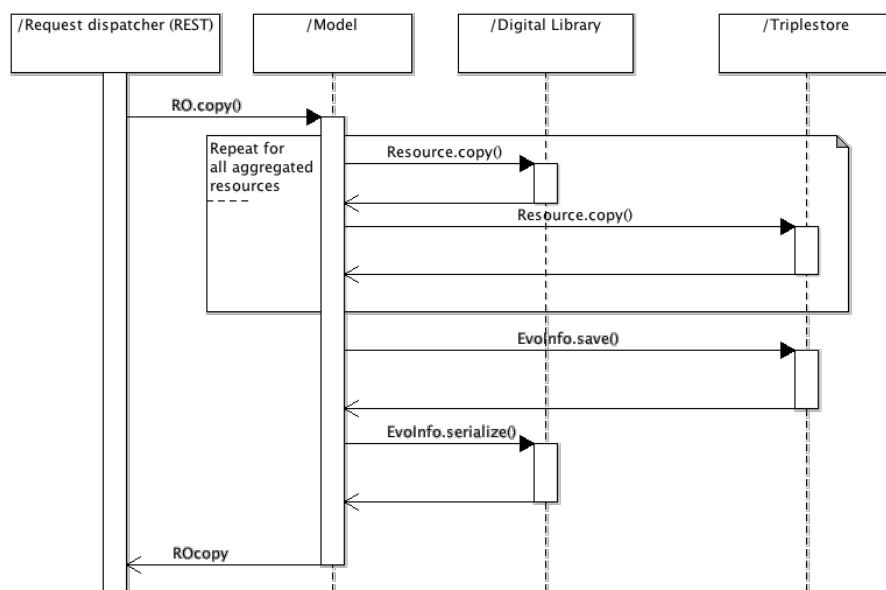


Figure 14: The sequence diagram for preparing the snapshot of a Research Object

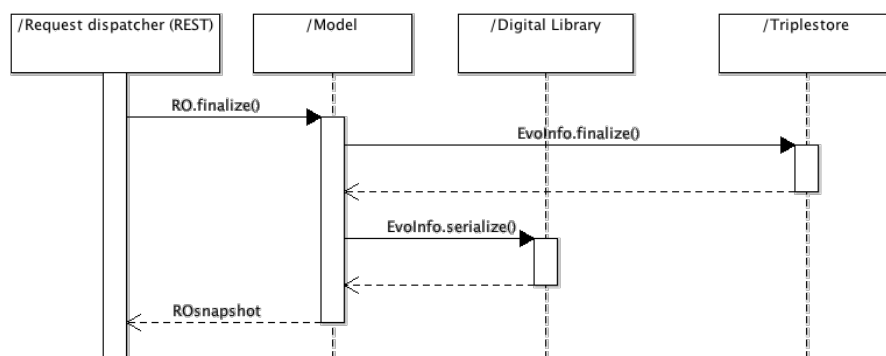


Figure 15: The sequence diagram for finalizing the snapshot and making it immutable

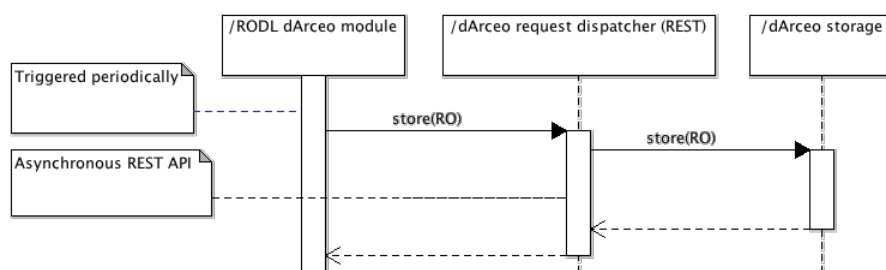


Figure 16: The sequence diagram for storing Research Objects in dArceo

The long-term preservation component is built on dArceo³⁴ - a system for long-term preservation of digital objects developed by PSNC. dArceo stores the objects and monitors their quality, alerting the administrators if necessary (see Figure 16). The standard monitoring activities include file format decay alerts and fixity checking but can be enhanced using a plugin mechanism. In case of RODL, dArceo periodically monitors

³⁴<http://dlab.psnc.pl/darceo/>

the quality of Research Objects by calling the Checklist Evaluation and Stability Services³⁵. If a change in quality is detected, notifications are generated as Atom feeds in compliance with the Notification API mentioned above. This helps detect and prevent workflow decay which occurs when an external resource or service used by the workflow becomes unavailable or is otherwise behaving differently.

dArceo gives the possibility to define migration plans that allow to perform a batch update of resources from one format to another, when necessary. In case of workflows, this may be applied for instance when a flat Taverna t2flow format should be converted to a complex scuff2 format (which, N.B. uses the Research Object model similarly to Research Objects). Another case could be a batch update of workflows that depend on a malfunctioning external resource.

Objects in dArceo can be stored on a range of backends, including specialized preservation repositories such as the Platon service³⁶, storing data in geographically distributed copies and guaranteeing their consistency. A running instance of the RODL is available for testing³⁷. At the moment of writing, it holds more than 1300 Research Objects.

4.3 RODL clients

The reference client of RODL is **the RO Portal**, developed alongside RODL to test new features and expose all available functionalities. It is running as a web application³⁸. Its main features are Research Object exploration and visualization; it also allows creating user accounts in RODL and generating access tokens for other clients. The RO Portal uses all APIs of RODL. The development version of **myExperiment** (see Section 3.2) uses RODL as a backend for storing packs. It uses the RO API. Finally, the **RO Manager** (see Section 3.1) is a command line tool that is primarily used to manage a Research Object stored on a local disk. It allows to push a Research Object to RODL via the RO API, as well as converting it into a snapshot in RODL.

5 Abstracting and Indexing Workflows

Using the research object model, one may use any vocabulary that fits their purpose. In this section, we provide two models that we developed for annotating workflows. The first one is aimed at abstracting workflows (Section 5.1), and the second at indexing workflows (Section 6).

5.1 Workflow Abstraction using Motifs

Workflows serve a dual function: first, as detailed documentation of the scientific method used for an experiment (i. e. the input sources and processing steps taken for the derivation of a certain data item), and second, as re-usable, executable artifacts for data-intensive analysis. Scientific workflows are composed of a variety of data manipulation activities such as Data Movement, Data Transformation, Data Analysis and Data Visualization to serve the goals of the scientific study. The composition is done through the constructs made available by the workflow system used, and is largely shaped by the function undertaken by the workflow and the environment in which the system operates.

A major difficulty in understanding workflows is their complex nature. A workflow may contain several scientifically significant analysis steps, combined with other Data Preparation or result delivery activities, and in different implementation styles depending on the environment and context in which the workflow is executed. This difficulty in understanding stands in the way of reusing workflows.

³⁵<http://wf4ever-project.org/wiki/display/docs/RO+checklist+evaluation+API>,<http://wf4ever-project.org/wiki/display/docs/Stability+Evaluation+API>

³⁶<http://www.platon.pionier.net.pl/>

³⁷<http://sandbox.wf4ever-project.org/rodl/>

³⁸<http://sandbox.wf4ever-project.org/portal>

As a first step towards addressing this issue [GAB⁺12] describes a catalogue of domain independent conceptual abstractions for workflow steps called scientific Workflow Motifs. The catalogue was built based on an empirical analysis performed over 260 workflow descriptions from Taverna [WHF⁺13], Wings [GRK⁺11], Galaxy [GNT10] and Vistrails [CFS⁺06b]. Motifs are provided through i) a characterization of the kinds of data-oriented activities that are carried out within workflows, which are referred to as Data-Operation motifs, and ii) a characterization of the different manners in which those activity motifs are realized/implemented within workflows, referred to as Workflow-Oriented motifs. Figure 17 shows an example of a Taverna workflow with its motifs highlighted. The workflow transfers data files containing proteomics data to a remote server and augments several parameters for the invocation request. Then the workflow waits for job completion and inquires about the state of the submitted warping job. Once the inquiry call is returned the results are downloaded from the remote server.

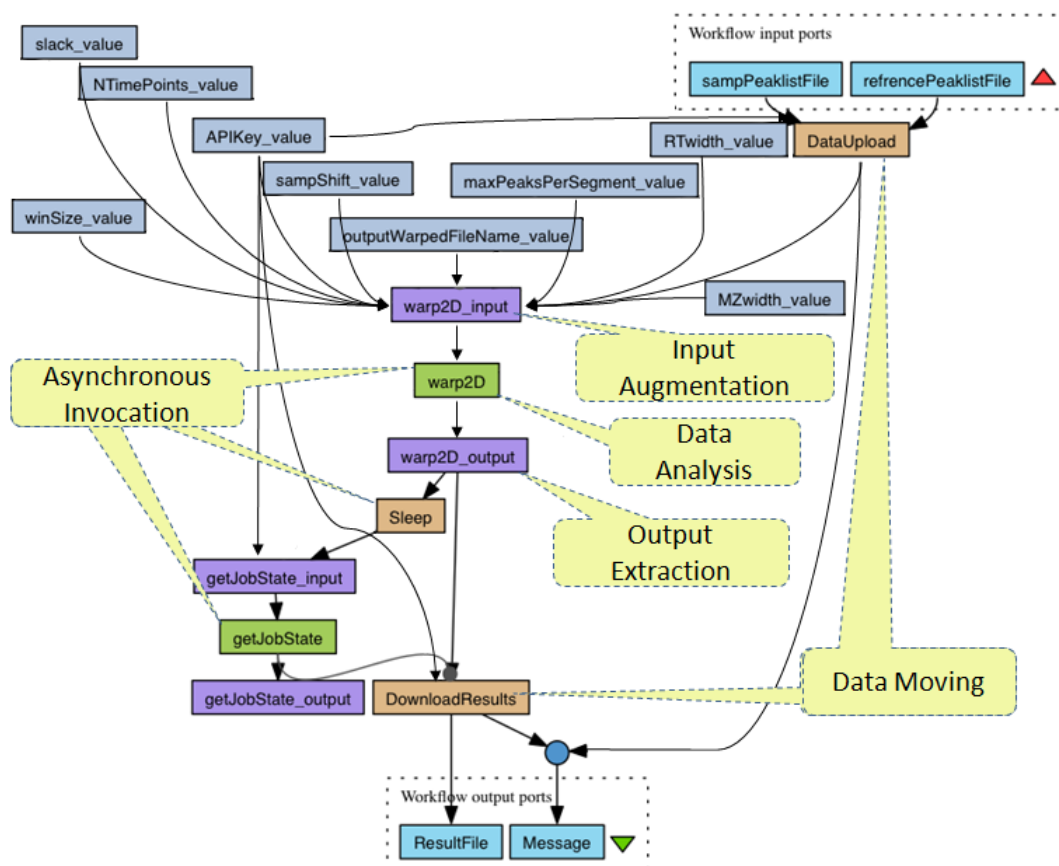


Figure 17: Sample motifs in a Taverna workflow for functional genomics.

This section describes the Workflow Motifs ontology³⁹, an OWL 2 encoding of the aforementioned motif catalogue. The goal of this ontology is to provide the means to annotate workflows and their steps with the motifs of the vocabulary, without setting any restriction on how the workflows are defined themselves.

5.1.1 Representing Motifs

Figure 18 shows an overview of the class taxonomy of the ontology. The class Motif represents the different classes of motifs identified in the catalog. This class is categorized into two specialized sub-classes DataOperationMotif and WorkflowMotif, which are sub-classed following the taxonomy represented in [GAB⁺12].

³⁹<http://purl.org/net/wf-motifs>



Figure 18: Diagram showing an overview of the class taxonomy of the motif OWL ontology.

The ontology provides three properties to link motifs to workflow specifications and their fragments. The `hasMotif` property associates workflows and their operations with their motifs. The properties `hasDataOperationMotif` and `hasWorkflowMotif` allow annotating workflows and their steps with more specificity. These properties have no domain specified, as different workflow models may use different vocabularies for describing workflows and their parts.

5.1.2 Representing Workflows and Workflow Steps

Workflows may be represented with different models and vocabularies like OPMW [GG11], P-Plan [GG12] or D-PROV [MDB⁺13]. While providing an abstract and consistent representation of the workflow is not a prerequisite to the usage of the Motif ontology, we consider it a best-practice to use a model that is independent from any specific workflow language or technology. An example of annotation using the `wfdesc` model is given in Figure 19 by showing the annotations of part of the Taverna workflow shown in Figure 17.

The annotations encoded using the Motif Ontology could be used in a variety of applications. By providing explicit semantics on the data processing characteristic and the implementation characteristic of the operations, annotations improve understandability and interpretation. Moreover, they can be used to facilitate workflow discovery. For example, the user can issue a query to identify workflows that implement a specific flow of

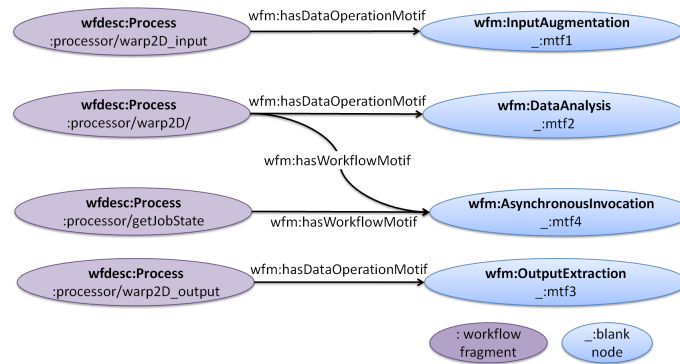


Figure 19: Subset of the annotations of the Taverna workflow shown in Figure 17 using the wfdesc model.

data manipulation and transformation (e.g., *return the workflows in which data reformatting is followed by data filtering and then data visualization*). Having information on characteristics of workflow operations allow for manipulation of workflows to generate summaries [ABGK13] of workflow descriptions or their execution traces.

6 Indexing Workflows

This section shows how workflows have been indexed using a generalized trie structure⁴⁰ and a serialization process. A workflow wf can be defined as a set of $Processes_{wf}$ and $Params_{wf} \mid wf = Processes_{wf} \cup Params_{wf}$ where the $Processes_{wf}$ are the definition of specific tasks to be executed and uses wfdesc:Process for its description, and $Params_{wf}$ defines the inputs and outputs of those tasks described by wfprov:Input and wfprov:Output which are subclasses of wfdesc:Parameter. On the other hand, a trie structure is an ordered tree data structure that allows to store dynamically a vector or an associative array where the keys are the values being stored itself. The main characteristic of this structure is absence of tree nodes being used for storing the key associated with that node but the position of the node within the tree defines the key. Another characteristic of this structure is that all the descendants of a node have a common prefix and therefore allows indexing simultaneously complete or partial paths to a specific node.

For our purposes of indexing a workflow, or generally speaking any DAG, by using a trie structure as a sequence of items which represents the DAG partially or completely for later accessing, a preprocessing of the set of workflows is needed as a first step. For accomplishing with this preprocessing goal of adapting a DAG to the trie indexing structure we have used one of the possible topological orders of a DAG. It is known that any DAG has at least one topological ordering which assures that if a vertex u is linked through an edge to vertex v , then after sorting it the vertex u will come before v in ordering. This topological ordering does not have to be unique and therefore a DAG could be defined by multiple topological sorts. Similarly to [MAYU03], in order to avoid the possibility of having similar workflows defined in different ways within the same indexing structure, we have chosen the lexicographical order of processes as common criteria to be applied. Therefore, the chosen overall used criteria for ordering the DAG sequentially has been both the topological and lexicographical orders.

The figure 20 shows how the "Extract proteins using a gi - output as fasta file"⁴¹ example which was obtained from ProvBench data set [BZG⁺13], is sorted by applying our criteria. One of the main advantages of this approach is that after transforming the DAG workflow into a sequential linked set of resources it can be indexed almost instantaneously and the time for searching and exact matching is linear with the size of the

⁴⁰Trie comes from the word **reTrieval** indicating the process of information accessing but it is also called suffix tree.

⁴¹<http://www.myexperiment.org/workflows/1182.html>

tree which is also directly related to the vocabulary size of the domain.

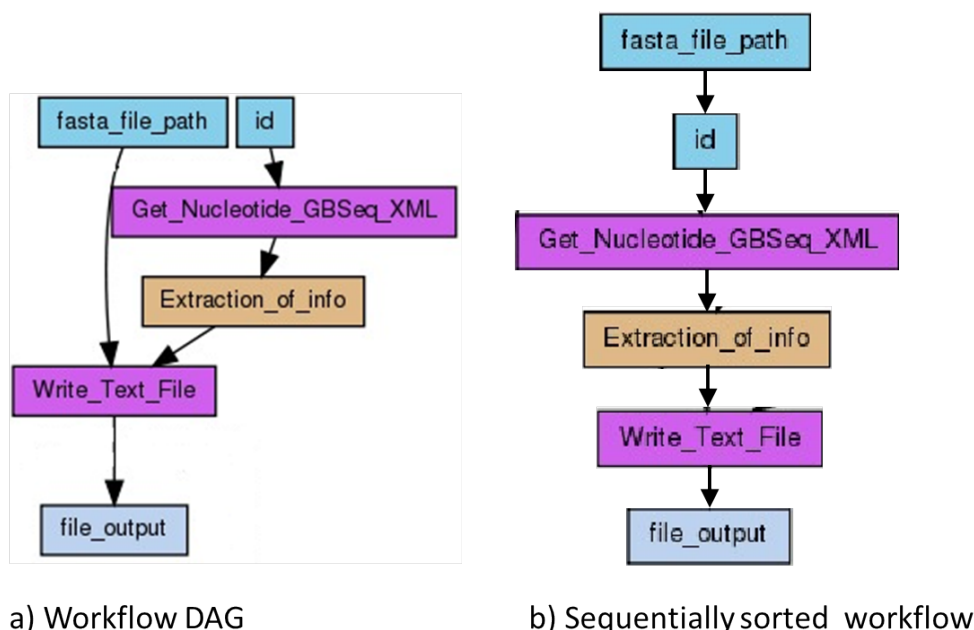


Figure 20: Sorting the "Extract proteins using a gi - output as fasta file" example obtained from ProvBench

6.1 Applications and Implementation

In order to provide scientists with searching and design capabilities we have implemented two different web services which makes use of the above introduced indexing structure for accessing to workflows and recommend next steps given the previous ones. It is worth highlighting that the implemented indexing structure could be also used for other purposes as the discovery of frequent patterns by using the collected statistical information and mining the semantic trie structure which would take full advantage of the intrinsic sequential ordering of the trie structure.

The implementation of both services (searching and next step recommendation) has been done applying the guidelines of the Wf4Ever project and using the wfprov and wfdesc ontologies. Both services are REST and can be called by an HTTP GET method which upon on ACCEPT headers may return XML or JSON formats. Also for implementation purposes we have encapsulated the trie indexing structured in order to provided the above presented services. The interaction between the mentioned components can be seen at Figure 21.

6.1.1 Searching

This service⁴² searches for those workflows which contain a specific sequence of processes providing on real time a list including all of them. The service accepts an array of processes' names as input parameter process[] (e.g. process?=p1&p2&p3). Therefore the general call would be of the form⁴³:

The output is an XML or JSON structure with the following attributes:

- **Process_id**: is the name of the process or processes used in the query.
- **freq**: is the number of times that the sequence of processes appears in other workflows.
- **URIs**: are the ROs' URIs which contain workflows where the requested sequence appears.

⁴²<http://sandbox.wf4ever-project.org/wfabstraction/rest/search>

⁴³[http://sandbox.wf4ever-project.org/wfabstraction/rest/search{?process\[\]}](http://sandbox.wf4ever-project.org/wfabstraction/rest/search{?process[]})

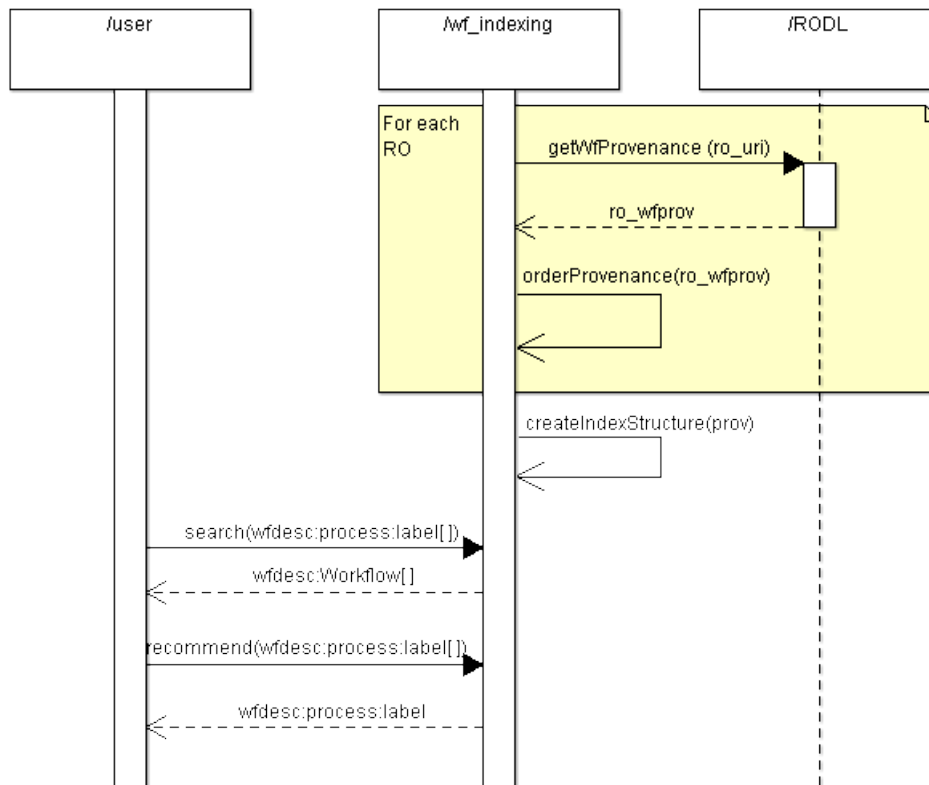


Figure 21: Sequence diagram for workflows indexing, searching, and recommending next step processes.

6.1.2 Next step recommendation

The proposed trie structure captures the provenance of workflows execution associated to scientific experiments allowing their indexation based on the temporal information that they contain. The trie structure is also updated to gather the needed statistics for mining the execution of workflows and provide the recommended next process based on how frequent a pattern of use occurs. So far we collected the number of times a process occurs in the dataset and also the probability associated to that pattern given the set of patterns of the same size. The fact that the exact matching searching is linear with the size of the tree (which is dependent of the use vocabulary, in our case the domain has been restricted to the set of processes included in ProvBench [BZG⁺13]) makes it very suitable for this type of applications. The implemented service⁴⁴ accepts an array of processes' names as input parameter process[] (e.g. process?=p1&p2&p3) and its general call would be of the form⁴⁵:

The output is an XML or JSON structure with different attributes:

- **Id**: is the name of the recommended process for that input query.
- **freq**: is the number of times that it appears in different workflows.
- **prob**: is the probability of the given recommendation taking into account the whole set of possible next steps.

⁴⁴<http://sandbox.wf4ever-project.org/wfabstraction/rest/recommend>

⁴⁵[http://sandbox.wf4ever-project.org/wfabstraction/rest/recommend{?process\[\]}](http://sandbox.wf4ever-project.org/wfabstraction/rest/recommend{?process[]})

7 Summary

We have presented in this deliverable the final version Research Object model defined within Wf4Ever, as a family of ontologies. We also presented the tools that were built on the model in order to facilitate the creation, curation and sharing of Research Objects, namely, the Research Object Manager (RO Manager), a command line tool for creating, displaying and manipulating Research Objects, RODL, which acts as a back-end, with two storage alternatives: a digital repository to keep the content, as a triple store to manage the metadata content, and the myExperiment virtual research environment, which was extended to allow end-users to create, upload, share and curate Research Objects. We also presented two models that can be used for annotating workflows with the objective to abstract and index them.

Our ongoing and future work aims to advertise and disseminate the Research Object model and the tools developed around it. In this respect, it is worth mentioning that we have launched a website dedicated to Research Objects⁴⁶, with examples that assist prospective adopters in understanding the model usage and benefits.

⁴⁶<http://www.researchobject.org/>

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