Wf4Ever: Advanced Workflow Preservation Technologies for Enhanced Science

STREP FP7-ICT-2007-6 270192

Objective: ICT-2009.4.1b — "Advanced preservation scenarios"

D2.2v1 Design, implementation and deployment of workflow lifecycle management components - Phase I

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This deliverable describes the first phase of delivery of workflow lifecycle management components. It includes a description of the Research Object Model, which facilitates interoperation between components; an initial Research Object Storage and Retrieval Service; RO Manager command line tool; and a definition of a model for workflow abstraction.

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0.2	17-07-2012	Sean Bechhofer	Updates and Examples
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Executive Summary

This deliverable describes the first 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. We provide here a summary of the RO Model and its accompanying documentation (the RO Primer), and highlight components developed for creating and managing Research Objects: the Research Object Storage and Retrieval API (implemented as part of the Research Object Digital Library (RODL)) and a command line tool – the RO Manager. These components and services are also discussed in D1.2v2 (Wf4Ever Sandbox – Phase II), D1.3v1 (Wf4Ever Architecture – Phase I) and D1.4v1 (Reference Wf4Ever Implementation – Phase I).

We also discuss preliminary work in defining a model for workflow abstraction, with the aim of supporting reuse of workflows (or their constituent parts), and present an initial characterisation of workflow decay, identifying causes of workflow decay based on an analysis of existing workflows in the myExperiment repository.

This deliverable should be read in tandem with D1.3v1 (Wf4Ever Architecture – Phase I), D1.4v1 (Reference Wf4Ever Implementation – Phase I), D1.2v2 (Wf4Ever Sandbox – Phase II), D3.2v1 (Design, implementation and deployment of Workflow Evolution, Sharing and Collaboration components – Phase I) and D4.2v1 (Design, implementation and deployment of Workflow Integrity and Authenticity Maintenance components – Phase I) in order to provide a complete picture of the state of the Wf4Ever Phase I components.

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1 Introduction

This deliverable describes Phase I 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 20 deliverables, in particular D3.2v1 (Design, implementation and deployment of Workflow Evolution, Sharing and Collaboration components – Phase I) [GC12b] and D4.2v1 (Design, implementation and deployment of Workflow Integrity and Authenticity Maintenance components – Phase I) [GC12a] which address complementary aspects of the overall wf4ver architecture and components.

According to the Description of Work, *This prototype will include the following functionalities: an initial Research Object Model (RO Model), implemented by means of an ontology network, and basic management functions (storage and access), validation functionalities based on RO provenance, and definition of semantic overlays and workflow provenance matching techniques for abstraction.*.

These requirements are addressed in the following way:

Sections 2, 3 and 4 discuss the Research Object Model defined within Wf4Ever along with a Primer document providing an introduction to that model and a collection of example Research Objects.

Sections 5 and 6 describe the initial Research Object Storage and Retrieval API and Command Line Manager. Both of these tools use the Research Object Model to structure the objects that they produce and consume. The RO Model is thus the "glue" that joins together the components and enables interoperation.

Section 7 discusses an initial model for workflow abstraction, while Section 8 presents a characterisation of workflow decay.

Note that this document represents the results from Phase I of the project – as a result, some areas are not yet complete and we expect updates, changes and extensions to be reported in Phase II of the project, due for completion in M32. For example, we expect that RO models reported here will be subject to change following further usage and experience, both within and outside the project.

2 The Research Object Model

The Wf4Ever Research Object model defines vocabularies that describe Workflow-centric Research Objects within Wf4Ever. The concept of Research Object is described in [B^{+}11] and further refined in [BCG^{+}12]. A complete, functional RO based ecosystem also requires a number of different services for creation, storage, manipulation, recommendation, visualisation etc. of Research Objects. These services are not considered as part of the model (although implemented services are described in this deliverable in Sections 5 and 6). Nor does the core model describe the evolution of Research Objects – this is discussed in D3.2v1 (Design, implementation and deployment of Workflow Evolution, Sharing and Collaboration components – Phase I) [GC12b].

Narrative text describing the model is published online[1] and the ontologies themselves also available[2]. We will not reproduce all this narrative text here, but provide an overview of the model and rationale.

A simple schematic of an RO is shown in Figure 1. The RO contains a workflow, input data and results along with a paper that presents the results and links to the investigators responsible. Annotations on each of the resources (and on the RO itself) provide additional information and characterise, e.g. the provenance of the results (the results were obtained by executing the workflow on the input data).

Research Objects play multiple roles. In the first case, they are *technical* objects. They provide access to the resources that are needed to support execution of investigations and record the provenance traces of those executions. They encapsulate dependencies between resources and maintain versioning information about the lineage and evolution of those resources.

At the same time, ROs are *social* objects. They encapsulate reusable protocols and know-how, record best practices and support reproducibility. They are citable artifacts that can be referred to and quoted, and record

[1] `http://wf4ever.github.com/ro/`
[2] `https://github.com/wf4ever/ro/`

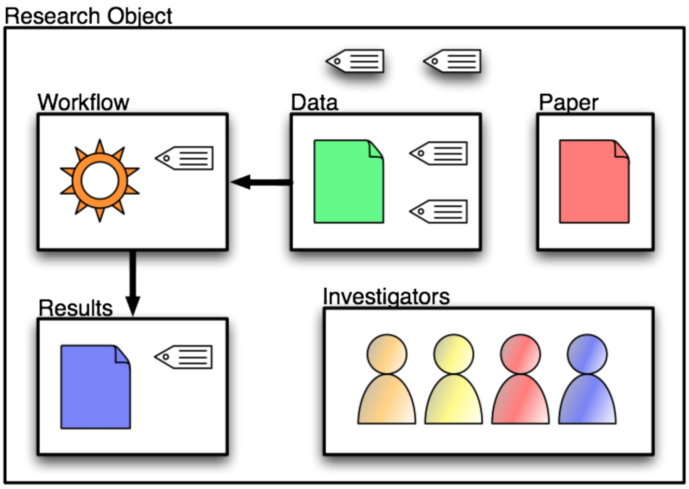


Figure 1: RO schematic.

and represent information about the people involved in investigations – those who create, use, extend and curate the objects.

These roles bring requirements on the representation structure and vocabularies used to describe Research Objects. The specification of the RO model focuses on the technical aspects and describes the core Wf4Ever Research Object vocabularies that provide container structures and vocabulary for describing workflow objects. Additional vocabularies covering evolution, lifecycle, versioning and other social aspects will be covered elsewhere (See D3.2v1 (Design, implementation and deployment of Workflow Evolution, Sharing and Collaboration components – Phase I) [GC12b] and D4.2v1 (Design, implementation and deployment of Workflow Integrity and Authenticity Maintenance components – Phase I) [GC12a]).

ROs allow for the aggregation of resources along with annotations on those resources concerning their provenance, use, characteristics etc. Aggregation is supported through the use of the OAI-ORE vocabulary[3] and annotation is supported through the use of the Annotation Ontology[4]. Re-use of these existing vocabulary will facilitate third party tools in understanding and processing Research Objects described using the model.

Finally, the RO Model provides a number of basic ontologies that are used within this aggregation/annotation framework to describe specifics of the Workflow-centric Research Objects. These are:

ro Provides basic structure for the description of aggregated resources and the annotations that are made on those resources.

wfdesc A vocabulary for the description of workflows. This provides an abstraction that can be mapped to different particular workflow systems. The ontology is intended as an upper ontology for more specific workflow definitions, and as a way to express abstract workflows, which could either be hand-crafted by users, or extracted from workflow definitions, for example Taverna's `t2flow` [MSRO+10] or Scufl2/footnote/urlhttp://dev.mygrid.org.uk/wiki/display/developer/SCUFL2 formats. A prototype service that transforms workflows into Research Objects, using the wfdesc ontologies has been developed (See D1.4v1 (Reference Wf4Ever Implementation – Phase I) [PH12]).

wfprov A vocabulary for the description of provenance information. This provides an abstraction that can be mapped to different provenance vocabularies, for example PROV-O[5] as developed by the W3C

[3] OAI-ORE is not a ratified standard produced by a body such as the W3C or IETF, but it is becoming widely used as a vocabulary for aggregation.

[4] Again, AO is not as yet a standardised vocabulary, but a W3C community group has been set up to oversee the drafting of a specification: `http://www.w3.org/community/openannotation/`

[5] `http://www.w3.org/TR/prov-o/`

Provenance Working Group.

All three ontologies, ro[6], wfdesc[7] and wfprov[8] are published online.

3 Research Objects Primer

The Research Object Ontologies and Vocabularies Primer is a document targeted at users, providing an accessible introduction to the Wf4Ever RO Model. This will enable readers to understand *what* the RO Model provides and *how* the RO Ontologies and Vocabularies can be used to describe an aggregation object that represents scientific experiments in a structured format.
The document is published online[9]

4 Research Object Examples

A number of exemplar Research Objects have been created. These provide illustrative examples of how the model may be used to describe aggregations of content.

4.1 Astrophysical Quantities

This RO collects together several resources including input and output datasets, scripts, web services and other documents. These relate to various tasks and stages of the experiment including *gathering*, *propagation* and *comparison* with intermediate results being passed from one stage to another.
A screenshot of the RO within the RODL is shown in Figure 2. This shows the conceptual view of the RO, with folders containing Workflow Runs expanded.
We can see here the relationships between a particular workflow run aggregated in the RO and its input, the workflow executed etc. These relationships are described using the RO model vocabulary, and the portal allows for export/publication of this metadata.
The RO is available in the RODL portal[10]

4.2 InterProScan

This is an example of an RO built around a workflow taken from myExperiment. The workflow performs an InterProScan analysis of a protein sequence using the EBI's[11] WSInterProScan service[12]. The workflow illustrates the issue of workflow *decay* as it can no longer be enacted. This is because the workflow involves EBI asynchronous services that were suspended as the EBI changed the way asynchronous services are handled.
Again, a snapshot of the RO in RODL is shown in Figure 3. Here, we can see annotation applied to the workflow within the RO, in particular a description discussing the problems with the workflow.
The RO is available in the RODL portal[13]

[6] `http://purl.org/wf4ever/ro`
[7] `http://purl.org/wf4ever/wfdesc`
[8] `http://purl.org/wf4ever/wfprov`
[9] `http://wf4ever.github.com/ro-primer/`
[10] `http://purl.org/net/wf4ever/ro/HyperLEDA_Luminosities`
[11] European Bioinformatics Institute
[12] `http://www.ebi.ac.uk/Tools/webservices/services/archive/pfa/wsinterproscan`
[13] `http://purl.org/net/wf4ever/ro/InterProScan_RO1`

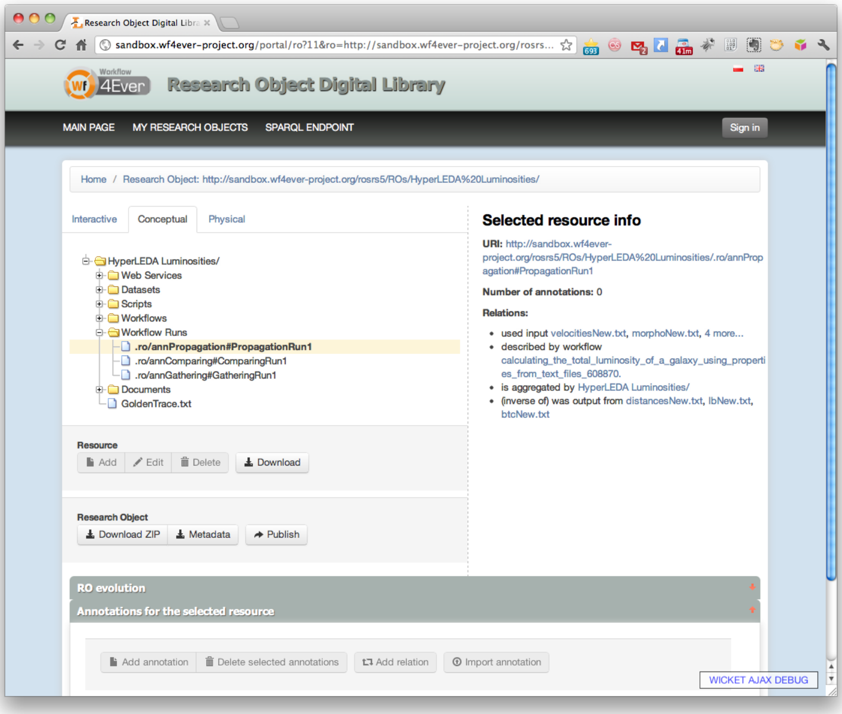


Figure 2: HyperLEDA luminosities example RO.

4.3 Repeatability and Reproducibility

Two example ROs illustrate how different levels of information can be recorded within the ROs in order to support a rerunning of an experiment. Figure 4 includes a workflow (along with its abstract description using the **wfdesc** ontology). In Figure 5, the RO also includes details of a workflow execution or run, using the **wfprov** ontology.

The ROs are available in the RODL portal[14]

5 Research Object Storage and Retrieval

The Research Object Storage and Retrieval API supports the creation, management and manipulation of Research Objects (ROs). The Research Object Digital Library provides an implementation of this functionality.

The ROSR API is provided as a RESTful interface, with the following functionality:

- Storing and retrieving research objects;
- Storing and retrieving resources aggregated within the research objects;
- Annotating the aggregated resources, including the research object itself.

The ROSR API uses the RO Model (as discussion in Section 2 to structure and describe the objects it creates.

Further information describing the details of the ROSR API are contained in D1.4v1 (Reference Wf4Ever Implementation – Phase I) [PH12].

[14] http://purl.org/net/wf4ever/ro/repeatability and http://purl.org/net/wf4ever/ro/reproducibility

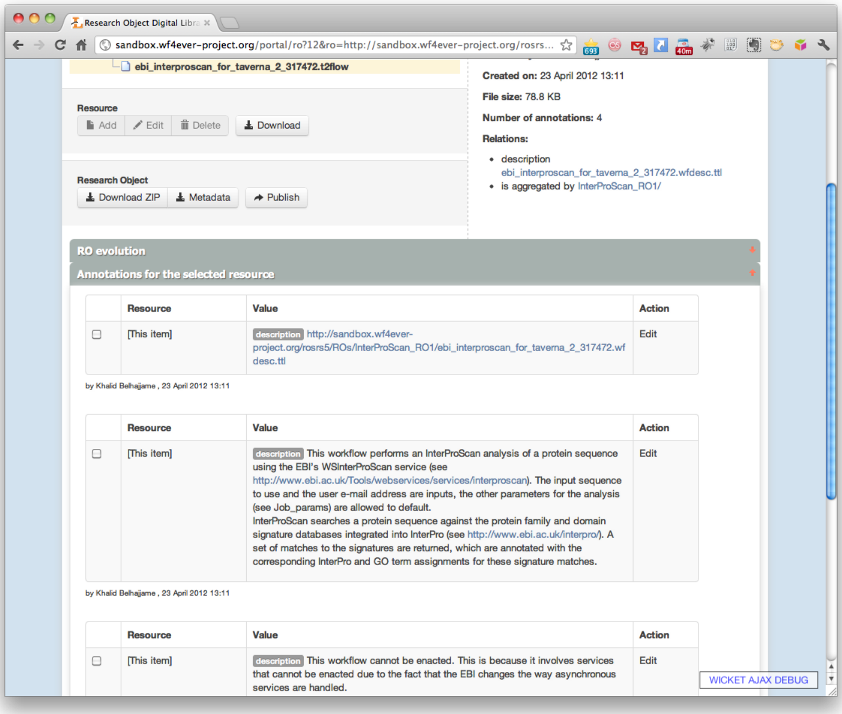


Figure 3: InterProScan example RO.

6 Research Object Manager

The Research Object Manager provides a command line tool for creating, displaying and manipulating Research Objects. The RO Manager functionality is complementary to that provided by the ROSR described in Section 5. In particular, the RO Manager is primarily designed to support a user working with ROs in the host computer's local file system, with the intention being that the ROSRS and RO Manager can exchange ROs between them – in part facilitated by the use of the shared RO vocabulary and model.

Past experience has suggested that lightweight, command line tools give users early access to functionality and provide an opportunity to gather additional feedback and requirements on that functionality. Command line tools can also be used with built in operating system functionalty as pipes and input/output redirection in order to quickly build prototype tool chains.

The RO Manager allows users to

- Create local ROs;
- Add resources to an RO;
- Add annotations to an RO;
- Read and write ROs to the RODL.

As with the ROSR, the RO Manager uses the RO Model to structure and describe the objects it creates.

Further information describing the details of the RO Manager are contained in D1.4v1 (Reference Wf4Ever Implementation – Phase I) [PH12] and D1.2v2 (Wf4Ever Sandbox – Phase II) [PHKG12].

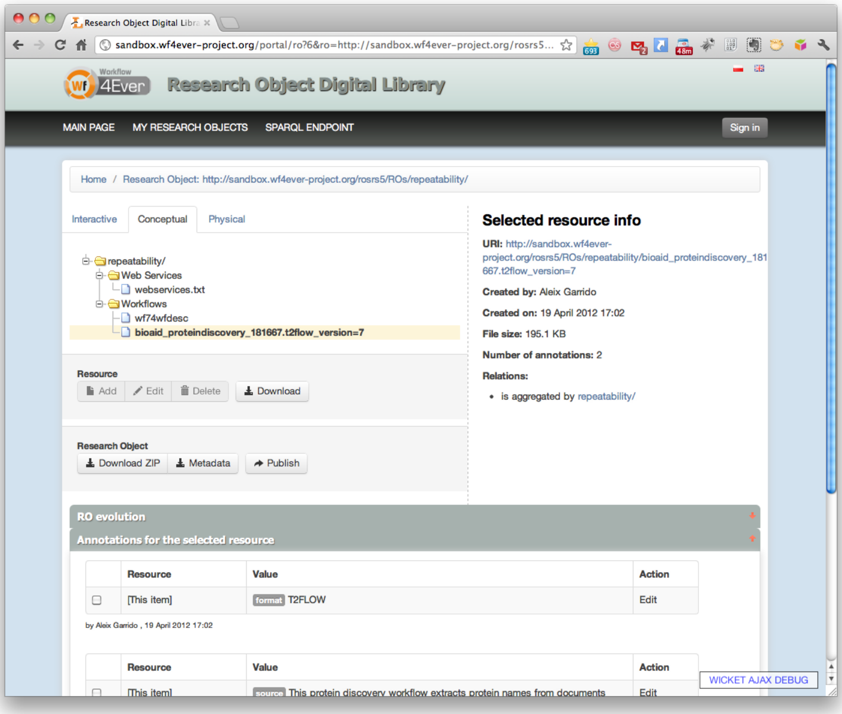


Figure 4: RO with workflow description.

7 Workflow Abstraction

The goal of specifying the abstraction of a workflow is to make workflows more reusable as a whole or some parts of it. In our work we define abstraction as the pattern that appears when a sequence of resources are executed together for a minimum number of times. This definition leads also to the concept of pattern or macro identification which applied to workflows leads to finding common sub-workflows. The work done so far for this purpose has focused on the creation of a trie structure [Knu11], which captures the sequences of execution of a workflow and keeps track of their statistics.

7.1 Workflow abstraction discovery process

Figure 6 shows the overall discovery process introduced in this section. The inputs are obtained by using the provenance of workflow results[15] from Taverna[16] and WINGS[17]. That provenance is stored in a trie structure which captures the order of the executed resources and stores the frequencies of appearance. Then, that information can be used to obtain the most frequent set of ordered executed resources which we have called macros and are identified in the figure at the bottom by black squares. Afterwards these detected macros, which represent some common workflow structures, could be hand-annotated in order to tag them or could be annotated automatically for example by assigning to them the same tags as the workflows that they belong to. Finally a taxonomy which includes all the identified macros by membership (bigger macros contain the smaller ones) can be created for indexing.

[15] http://wf4ever.github.com/ro-primer/
[16] http://www.taverna.org.uk/
[17] http://wings.isi.edu/

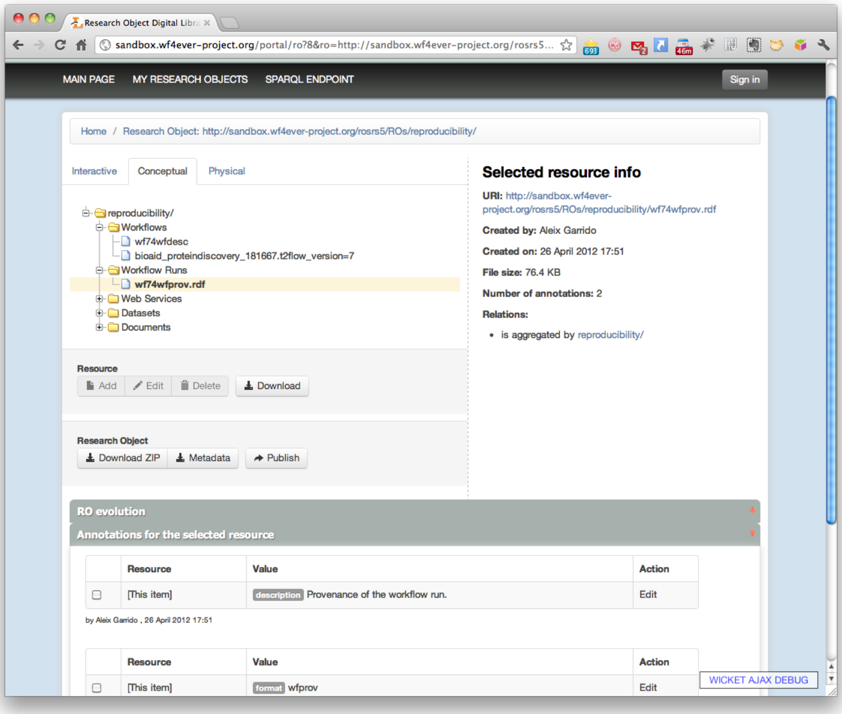


Figure 5: RO with workflow provenance.

7.2 Trie structure to store the provenance of workflow results

As introduced above we have used a trie for storing the workflow execution in an ordered way by including at different levels of depth the different inputs, processes and outputs (resources) which have been executed. A trie is defined as an ordered tree that stores a dynamic set of keys which are allocated at the leafs and the different internal nodes are the gateways. Therefore all the descendants of a node have a common prefix of the resource associated with that node. This is very useful for detecting common parts of different workflows because we can easily keep track of the number of times that a specific sequence of resources has been executed.

Therefore, the presented work is a bottom-up approach in order to study the actual provenance of workflow results (which represents the dataflow of an executed workflow as described in D4.2v1 [GC12a]) from a set of available workflows at Taverna and WINGS created for this purpose. The **wfprov** ontology[18] is publicly available, and some examples that have been created for this work and are part of the RO testbed[19]. The provenance of the workflow results of the different workflows examples have been used as inputs for creating the trie structure introduced above. Every resource executed and captured by the **wfprov** of a RO is then associated with a node in the trie structure and its frequency updated by increasing the number of times that it has appeared. Afterwards an analysis of the trie is done to obtain the most common set of resources which are going to identify the pursued abstract macros.

Although this is still a preliminary work and more examples are needed in order to be able to extract relevant macros, once a set of macros have been identified it would be possible to categorize them (manually or automatically e.g. by using workflow tags) and then build the associated taxonomy by using the trie membership relations. The code developed for the creation and maintenance of the trie structure and for accessing to the provenance of the workflow results repository is available[20]. It provides the following functionalities:

[18] `http://purl.org/wf4ever/wfprov`
[19] `http://www.wf4ever-project.org/wiki/display/docs/RO+testbed`
[20] `https://github.com/wf4ever/wf-abstraction`

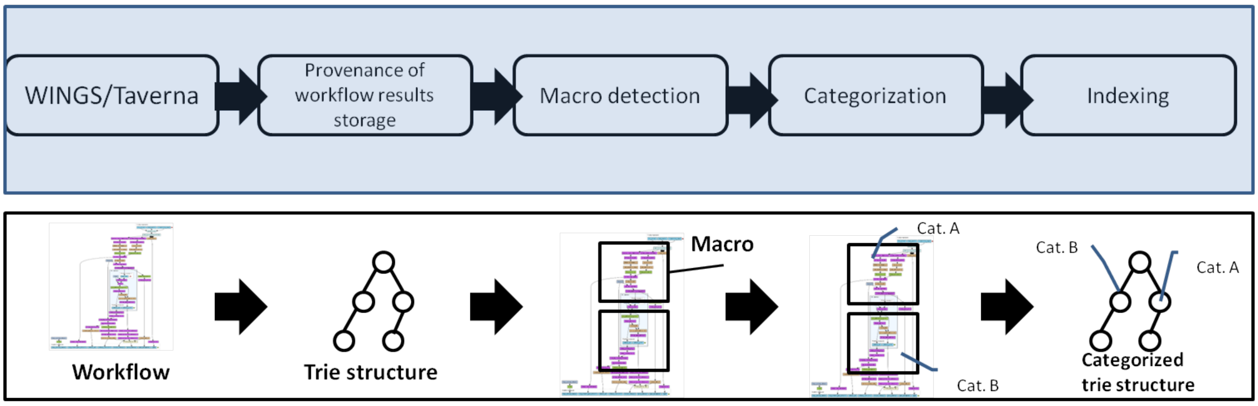


Figure 6: Workflow abstraction discovery process.

- It stores the provenance of the workflow results in an ordered way together with the appearance frequency of their resources.
- It calculates relative frequencies at different levels of the trie.
- It provides different modes to traverse the structure (pre-ordered/level-ordered)
- It provides an output XML structure with relative frequencies per level and per process (an output example is available[21]).

8 Characterising Workflow Decay

The main impediment to workflow preservation is workflow decay. Indeed, our experience with scientific workflows suggests that a large proportion of workflows suffer from decay [Bel07], which decreases their value over time. For example, the RO example presented in Section 4.2 contains a workflow that suffers from decay.

Broadly speaking, we can distinguish two forms of decay. i)- **Inability to re-execute the workflow**: due to many factors, including the unavailability of third party resources that are responsible for executing the tasks that compose the workflows, we may not be able to re-execute a given workflow. ii)- **Inability to reproduce workflow results**: a less severe, yet relevant, form of decay, is the inability to obtain the same (or similar) results when re-executing the workflow. Reproducing previous results can be primordial in reinforcing trust in scientific results and can be used in peer-reviewing as a mechanism to validate the results claimed by given scientists [FBS11, GRB12].

The above discussion raises the following question. *What are the causes of workflow decay?* To identify and characterise the causes of workflow decay, we adopted a bottom-up approach, whereby we manually analyzed 92 Taverna workflows from the myExperiment repository. We chose Taverna workflows because they form the largest available workflow collection (more than half of the workflows in myExperiment are Taverna workflows at the time of writing), and Taverna workflows have been published on myExperiment since its launch in 2007, therefore providing a good insight into decay over those years.

To base our analysis on a sample of workflows that is representative of the set of workflows in myExperiment, we selected workflows using the following three criteria:

- The year of creation of the workflow: we believe that the decay of workflows could be directly impacted by the year of their creation, hence we tried to make an even coverage of Taverna 1 workflows [OAF^{+}04] and Taverna 2 workflows [MSRO^{+}10] between the years 2007 and 2012.

[21] https://github.com/wf4ever/wf-abstraction/blob/master/outputExample.xml

- The creator of the workflow: in order to reduce possible bias introduced by specific workflow creators, we avoided choosing workflows created by the same person in the same year.
- The domain of the workflow: our workflow selection also had a good coverage of domains, covering 18 different scientific (such as life sciences, astronomy and cheminformatics) and non-scientific domains (such as testing of Grid services). Figures 7 illustrates the domains of the workflows that we selected for decay analysis.

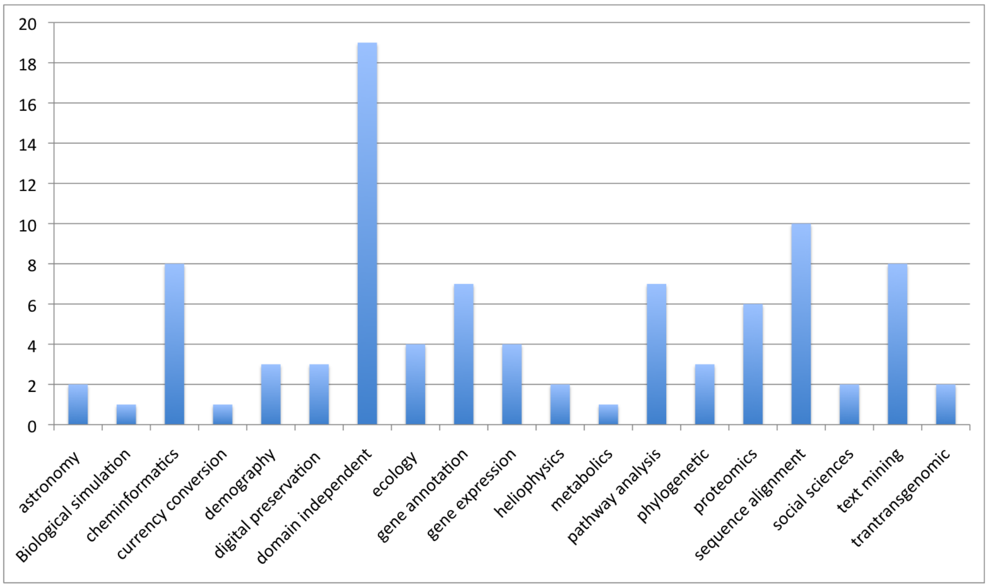
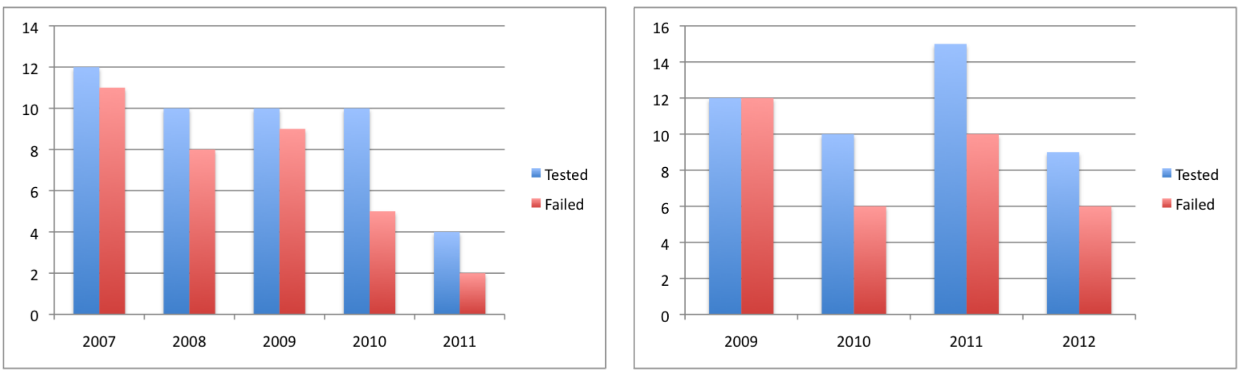


Figure 7: Distribution of the domain studied by our test workflows.

Although we focus on a particular family of workflows, i.e., Taverna workflows, we expect our approach and analysis to be applicable to many others and our analysis to be repeatable on a different corpus of workflows. To identify the causes of decay that the workflows we selected may suffer from, we attempted to execute them using the Taverna 2.3 workbench. We then manually examined their results, diagnosed broken links, etc. Our analysis showed that nearly 80% of the tested workflows failed to be either executed or produce the same results, and those from earlier years (2007-2009) had more than 80% failure rate (as shown in Figures 8). The causes of workflow decay can be classified into four categories, which we present in the rest of this section.



(a) Number of Taverna 1 workflows tested and failed.

(b) Number of Taverna 2 workflows tested and failed.

Figure 8: Number of Taverna workflows tested and failed.

8.1 Volatile third-party resources

Most of the workflows that we analysed make use of third-party resources such as web services and databases. The provision of such resources may be interrupted or changed, causing failure of the workflow to execute. In certain cases, the workflow cannot be run, even when the third party resources that it relies on are available, e.g., when such resources require authentication. Another cause that may lead to workflow decay, is changes to third party resources. For example, if the web service provider decides to change the implementation of the web service, then the workflow execution may not deliver the same results, or worse, it may not be possible to execute. Table 1 summarises these causes of decay with concrete examples.

Table 1: Categorisation of decay caused by third-party resources

Causes	Refined causes	Examples
Third party resources are not available	Underlying datasets, particularly those locally hosted in-house datasets, are no longer available	Researcher hosting the data changed institution, server is no longer available
	Services are deprecated	(DNA Data Bank of Japan) DDBJ web services are not longer provided despite the fact that they are used in many myExperiment workflows
Third party resources are available but not accessible	Data is available but identified using different IDs than the one known to the user	Due to scalability reasons the input data is superseded by a new version making the workflow not executable or providing wrong results
	Data is available but permission, certificate, or network to access it is needed	Cannot get the input, which is a security token that can only be obtained by a registered user of ChemiSpider
	Services are available but need permission, certificate, or network to access and invoke them	The security policies of the execution framework are updated due to new hosting institution rules
Third party resources have changed	Services are still available by using the same identifiers but their functionality have changed	The web services are updated intentionally or unintentionally (e.g.malware) providing wrong results

8.2 Missing example data

It is not always obvious which data can be used as inputs to the workflow execution, and example inputs are often helpful. Example outputs can also be useful to gain an insight of the outcome anticipated from the workflow. However, our analysis revealed that they are not always made available. Provenance traces of previous runs are also useful as indications of where example data may be found.

8.3 Missing execution environment

The execution of a workflow may rely on a particular local execution environment, for example, a local R server[22] or a specific version of workflow execution software. Some of our test workflows exhibit this type

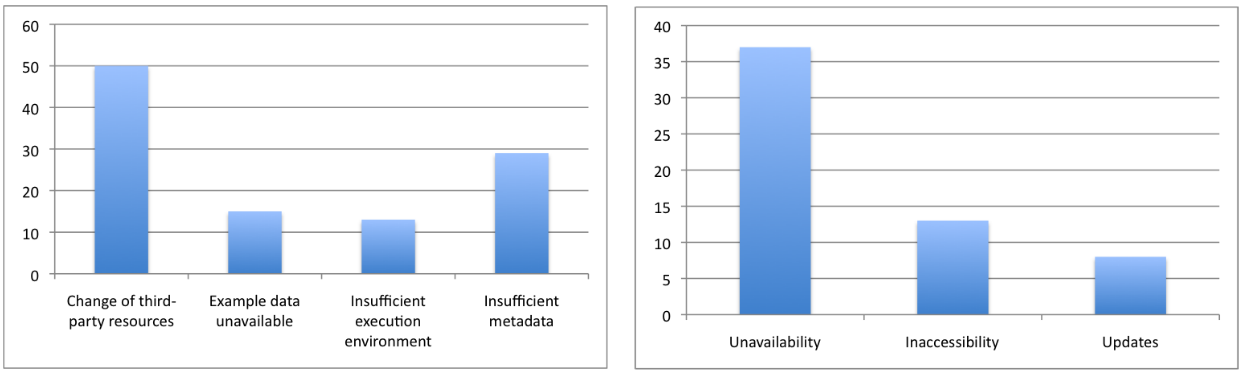
[22] http://www.r-project.org/

of decay. Taverna often provides sufficient information about missing libraries, and sometimes workflow descriptions provide a warning about the requirement for a specific library. This type of decay appears to be fixable by installing the missing software, albeit requiring some effort.

8.4 Insufficient descriptions about workflows

Sometimes a workflow workbench cannot provide sufficient information about what caused the failure of a workflow run. Additional descriptions in the workflow can play an important role in assisting re-users to understand the purpose of the workflow and its expected outcomes.

The results of the above analysis are summarised in Figure 9-a, which illustrates the number of workflows that suffer from each of the causes of decay presented above. It shows that 50% workflows suffer from decay due to third party resources.



(a) A summary of workflow decay causes

(b) Workflow decay due to third party resources

Figure 9: Results of workflow decay analysis.

To better understand the causes of decay due to third party resources. Figure 9-b illustrates the number of workflows that suffer from the causes presented in Table 1. It shows that the unavailability of third party resources is the leading cause of decay, followed by resources inaccessibility, and then resources changes.

The above results confirms our hypothesis that workflow decay is a serious problem. It also suggests that there is a need for additional information that can assist workflow designers detecting and repairing decayed workflows. We report in a separate deliverable [GC12a], on a minimal model and associated checklists, that were designed and developed with the objective to prevent and repair workflow decay.

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