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PhD Thesis

Mining Abstractions in Scientific Workflows

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EL PRESIDENTE VOCAL 1 VOCAL 2

VOCAL 3 EL SECRETARIO

A mis padres

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Finally, after five years, I can finally say that I see light at the end of the tunnel. Maybe the other side is still a bit cloudy at the moment, but the important thing is to have arrived here. And, honestly, I think I wouldn't have made it to this point without all the people who have been by my side during these years.

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Abstract

Scientific workflows have been adopted in the last decade to represent the computational methods used in *in silico* scientific experiments and their associated research products. Scientific workflows have demonstrated to be useful for sharing and reproducing scientific experiments, allowing scientists to visualize, debug and save time when re-executing previous work. However, scientific workflows may be difficult to understand and reuse. The large amount of available workflows in repositories, together with their heterogeneity and lack of documentation and usage examples may become an obstacle for a scientist aiming to reuse the work from other scientists. Furthermore, given that it is often possible to implement a method using different algorithms or techniques, seemingly disparate workflows may be related at a higher level of abstraction, based on their common functionality. In this thesis we address the issue of reusability and abstraction by exploring how workflows relate to one another in a workflow repository, mining abstractions that may be helpful for workflow reuse. In order to do so, we propose a simple model for representing and relating workflows and their executions, we analyze the typical common abstractions that can be found in workflow repositories, we explore the current practices of users regarding workflow reuse and we describe a method for discovering useful abstractions for workflows based on existing graph mining techniques. Our results expose the common abstractions and practices of users in terms of workflow reuse, and show how our proposed abstractions have potential to become useful for users designing new workflows.

Resumen

Los flujos de trabajo científicos han sido adoptados durante la última década para representar los métodos computacionales utilizados en experimentos *in silico*, así como para dar soporte a sus publicaciones asociadas. Dichos flujos de trabajo han demostrado ser útiles para compartir y reproducir experimentos científicos, permitiendo a investigadores visualizar, depurar y ahorrar tiempo a la hora de re-ejecutar un trabajo realizado con anterioridad. Sin embargo, los flujos de trabajo científicos pueden ser en ocasiones difíciles de entender y reutilizar. Esto es debido a impedimentos como el gran número de flujos de trabajo existentes en repositorios, su heterogeneidad o la falta generalizada de documentación y ejemplos de uso. Además, dado que normalmente es posible implementar un mismo método utilizando algoritmos o técnicas distintas, flujos de trabajo aparentemente distintos pueden estar relacionados a un determinado nivel de abstracción, basándose, por ejemplo, en su funcionalidad común. Esta tesis se centra en la reutilización de flujos de trabajo y su abstracción mediante la exploración de relaciones entre los flujos de trabajo de un repositorio y la extracción de abstracciones que podrían ayudar a la hora de reutilizar otros flujos de trabajo existentes. Para ello, se propone un modelo simple de representación de flujos de trabajo y sus ejecuciones, se analizan las abstracciones típicas que se pueden encontrar en los repositorios de flujos de trabajo, se exploran las prácticas habituales de los usuarios a la hora de reutilizar flujos de trabajo existentes y se describe un método para descubrir abstracciones útiles para usuarios, basadas en técnicas existentes de teoría de grafos. Los resultados obtenidos exponen las abstracciones y prácticas comunes de usuarios en términos de reutilización de flujos de trabajo, y muestran cómo las abstracciones que se extraen automáticamente tienen potencial para ser reutilizadas por usuarios que buscan diseñar nuevos flujos de trabajo.

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Chapter 1

Introduction

In the last decade, the research output produced by the scientific community has almost doubled, from 1.3 million articles in 2003 to 2.4 million in 2013 (Ware and Mabe, 2015). The productivity of scientists is heavily influenced by their number of publications in high impact journals and conferences. Scientists are pressured to publish (Fanelli, 2010), but they are not always required to grant access to the digital outputs associated with their scientific publications. As a consequence, there is a general lack of transparency when communicating the computational methods used to obtain publication results.

In order to improve transparency, several initiatives for open science are underway. The European Comission includes funding for open publication of research results obtained in project grants[1]. The National Science Foundation requires a data management plan to ensure access and preserve the outputs of a project grant[2]. Publishers have promoted the notion of data and software journals[3] to store and preserve datasets as publications. Data repositories like FigShare[4] or Dryad[5] provide the means to share and cite any piece of a scientific investigation. Similarly, code repositories like GitHub[6] and Zenodo[7] allow sharing and documenting software for the community.

Although these initiatives are valuable efforts to address the access to the resources of an experiment, they do not focus on improving the communication of the meth-

[1] http://ec.europa.eu/research/science-society/open_access
[2] http://www.nsf.gov/pubs/policydocs/pappguide/nsf11001/gpg_2.jsp#dmp
[3] http://www.journals.elsevier.com/data-in-brief/
[4] http://figshare.com/
[5] http://datadryad.org/
[6] http://github.com/
[7] https://zenodo.org/

ods used in a scientific publication. Scientific articles usually describe computational methods informally, often requiring a significant effort from others to reproduce and to reuse. The reproducibility process can be very costly, even when the software and datasets used in the publication are available online (Garijo et al., 2013b). Retractions of publications have occurred in several disciplines (Marcus and Oransky, 2014; Rockoff, 2015). Some initiatives have started tracking and documenting the retracted papers of scientific journals[8], in order to alert the community about problematic papers. The repercussions of these bad practices can be seen beyond scientific circles. The public shows neutral to low trust for science on topics like pesticides, depression drugs or flu pandemics (American, 2010). Even publishers themselves have demanded researchers to submit detailed descriptions of the materials and methods used in a publication (Editorial, 2006).

Scientific workflows were proposed in the last decade in order to represent the computational methods used in scientific publications (Taylor et al., 2006). Scientific workflows define the set of computational tasks and dependencies needed to carry out *in silico* experiments (therefore improving their reproducibility), and have been increasingly adopted in domains like astronomy (Ruiz et al., 2014), brain image analysis (Dinov et al., 2009) and bioinformatics (Wolstencroft et al., 2013) among others. Besides execution and reproducibility, there are several benefits of using scientific workflows (Goderis, 2008) (Garijo et al., 2014b):

- Time savings: Individual users save a lot of time by copying and pasting whole previous working pipelines in new experiments. Other users save time as well when they reuse a workflow created by someone else, since they do not have to re-implement every single step.

- Teaching: Workflows can be used as an effective way to teach students about the sequence of steps and methods involved for processing an input. Breakpoints are often placed throughout the workflow to serve as checkpoints and make sure that execution was performed correctly.

- Visualization: With workflows, it is easier to understand how the overall method is structured, as well as the algorithms used in each step.

[8] `http://retractionwatch.com/`

- Design for modularity: Workflows provide a high-level view of the major steps involved in an analysis, and exposing those major steps drives the design of the code in a modular fashion.

- Design for standardization: Using a common workflow system allows researchers to see how others process certain kinds of data, what software packages they use, and what formats are more common among a group of collaborators. This leads to workflows that effectively capture emerging standards in the ways that data is formatted and processed, based on common practices adopted by a community of users.

- Debugging and inspectability: A workflow execution might fail due to incorrect setup, problems in the underlying code, missing files, incompatible file types, or server-related issues. Researchers use the workflow system's environment to debug errors in workflows.

Scientific workflows are relevant products of research, and "*key enablers for reproducibility of experiments involving large-scope computations*" (Gil et al., 2007). However, reusing a workflow or any of its parts may become a daunting task. Scientific workflows can become large and complex heterogeneous structures, and the lack of documentation and examples often increases the difficulty in understanding their main goals (Belhajjame et al., 2012b). In addition, there are large amounts of workflows in existing workflow repositories. A repository may contain hundreds or thousands of different workflows (Roure et al., 2009), and determining which ones are relevant to the problem at hand might become a hurdle for a researcher. In this regard, the creation of abstractions that group different workflows by certain criteria (e.g., common general functionality, shared workflow steps, etc.) is needed to improve workflow understandability.

In this work we address the issue of reusability and abstraction in scientific workflows. We propose to do so by exploring common relationships among groups of workflows in a workflow repository, mining abstractions that are useful for reuse.

1.1 Contributions

The work presented in this thesis makes the following contributions:

- **Workflow representation and publication**: We propose a model to represent scientific workflows in the different stages of their life cycle, as well as a methodology designed to publish scientific workflows and their resources in an open architecture in the Web.

- **A catalog of common workflow abstractions**: We define a catalog of workflow motifs, which aim to capture the most common steps in scientific workflows based on their functionality.

- **Automatic detection of commonly used workflow fragments**. We present an approach to automatically mine commonly used workflow fragments that are helpful for workflow reuse. Our approach exploits domain knowledge for generalizing workflows, which leads to the discovery of common abstract workflow fragments. We also define metrics for assessing the usefulness of our results.

- **Support for workflow annotation**. In addition to our workflow representation model, we define two models for semi-automatically annotating scientific workflows. The first model is a serialization of our catalog of workflow abstractions, along with the means to annotate workflow steps and groups of steps. The second model describes how workflow fragments are represented and linked to those workflows where they appear.

1.2 Thesis Structure

The thesis is structured as follows:

Chapter 2 introduces the state of the art, along with the main concepts that we will be handling throughout the thesis.

Based on the gaps identified in the state of the art, *Chapter 3* describes the work objectives and research hypotheses of this work.

Chapter 4 describes the model and methodology proposed to represent and publish scientific workflows in their different stages of their life cycle.

Chapter 5 presents the catalog of common domain independent workflow abstractions, as well as two analyses of workflow reuse (one from an automatic perspective and another one from a user community perspective) that help understand the current practices of workflow users.

Chapter 6 explains the method to mine commonly used workflow fragments in repositories of workflows, including how to filter and link the results. This approach is evaluated in *Chapter 7*, where the results are explained in detail.

Finally, *Chapter 8* describes conclusions and future lines of work.

1.3 Publications

The following publications have been accepted (in chronological order) during the research work presented in this thesis:

1. **Daniel Garijo** and Yolanda Gil. A new Approach for Publishing workflows: Abstractions, Standards, and Linked Data. Proceedings of the 6th Workshop on Workflows in support of large-scale science, pages 47-56, Seattle, USA. 2011.

2. **Daniel Garijo**, Pinar Alper, Khalid Belhajjame, Oscar Corcho, Yolanda Gil, and Carole Goble. Common Motifs in Scientific Workflows: An Empirical Analysis. 8th IEEE International Conference on eScience 2012, pages 1-8 Chicago, USA. 2012.

3. **Daniel Garijo** and Yolanda Gil. Augmenting PROV with Plans in P-Plan: Scientific processes as Linked Data. Second International Workshop on Linked Science: Tackling Big Data (LISC), held in conjunction with the International Semantic Web Conference (ISWC), Boston, USA, 2012.

4. **Daniel Garijo**, Oscar Corcho, and Yolanda Gil. Detecting Common Scientific Workflow Fragments Using Templates and Execution Provenance. Seventh International Conference on Knowledge Capture (K-CAP), pages 33-40, Banff, Alberta, Canada. 2013.

5. Khalid Belhajjame, Jun Zhao, **Daniel Garijo**, Aleix Garrido, Stian Soiland-Reyes, Pinar Alper and Oscar Corcho. A Workflow PROV-Corpus Based on Taverna and Wings. Proceedings of the Joint EDBT/ICDT 2013 Workshops, pages 331-332. Genova, Italy 2013.

6. **Daniel Garijo**, Pinar Alper, Khalid Belhajjame, Oscar Corcho, Yolanda Gil, Carole Goble. Common Motifs in Scientific Workflows: An Empirical Analysis (Extension of the 2012 conference paper for a journal). Future Generation Computer Systems, volume 36, pages 338-351. 2014.

7. **Daniel Garijo**, Oscar Corcho, Yolanda Gil, Boris A. Gutman, Ivo D. Dinov, Paul Thompson, and Arthur W. Toga. Fragflow: Automated Fragment Detection in Scientific Workflows. 10th IEEE International Conference on eScience 2014, pages 281-289, Guaruja, Brasil. 2014.

8. **Daniel Garijo**, Oscar Corcho, Yolanda Gil, Meredith N. Braskie, Derrek Hibar, Xue Hua, Neda Jahanshad, Paul Thompson, and Arthur W. Toga. Workflow Reuse in Practice: A Study of Neuroimaging Pipeline Users. 10th IEEE International Conference on eScience 2014, pages 90-99. Guaruja, Brasil. 2014.

9. **Daniel Garijo** and Yolanda Gil. Towards Workflow Ecosystems Through Standard Representations. 9th Workshop on Workflows in Support of Large-Scale Science (WORKS 14), pages 94-104. New Orleans, USA. 2014.

1.4 External Contributions

The main work presented in this thesis is an original contribution by the author of the manuscript. However, there are chapters which have been developed in collaboration with other researchers. This section summarizes their names and contributions to this thesis.

1. In **Chapter 5.1** Pinar Alper and Khalid Belhajjame contributed by manually inspecting many of the Taverna and VisTrails workflows. Together with Carole Goble, they were also key to the discussions and development of the workflow motif catalog, the associated ontology and the resulting publications.

2. In **Section 5.3**, Neda Jahanshad, Xue Hua, Meredith N.Braskie, Derrek Hibar and Yolanda Gil contributed to the discussions used to create the online survey.

3. In **Section 7.3**, Samuel Hobel, Ivo D. Dinov and Boris A. Gutman participated in evaluating the usefulness of the fragments produced by our approach. In addition,

some of the workflows of Boris A. Gutman have been used in the explanations of this thesis.

4. Zhizhong Liu helped to retrieve the multi-user corpus of workflows of the LONI Pipeline (WC3). This corpus was used in **Chapters 5** and 7.

Chapter 2

Related Work

A **scientific workflow** is defined as a template specifying the tasks needed to carry out a computational scientific experiment (Taylor et al., 2006). Each task, also known as a **workflow step**, uses none or more **inputs** and produces one or more **outputs**. The dataflow among the tasks, which we refer to as **workflow step dependencies** is captured by recording the relationship between each output and input of any step of the workflow. A **workflow input** is an input that has not been produced by any other workflow step. Similarly, a **workflow output** is an output that is not used by any other workflow step. An **intermediate result** is an output of a workflow step that has been used as an input by another workflow step in the workflow.

Scientific workflows have been used successfully in a wide range of domains, ranging from life sciences to geology or astronomy. Figure 2.1 shows an example of two scientific workflows from two different workflow systems. In both samples, we can see the most typical elements of a scientific workflow: their inputs (*textFile1*, *textfile2*, *threshold1* and *threshold2* for the workflow on the left and *projected_landmarks*, *average curve landmarks* and *skulpted* for the workflow on the right), intermediate results (only shown on the workflow of the left) and outputs (*LikelihoodFile* on the left and the upside triangle at the bottom of the *MINC obj 2 mesh* step on the right). Inputs of a scientific workflow may have been produced by other scientific workflows. Thus, an end-to-end experiment can be seen as a puzzle composed of different scientific workflows performing different aspects of it.

The main objective of this thesis is to mine repositories of workflows to find common abstractions that are helpful for workflow reuse. There are several areas of ongoing

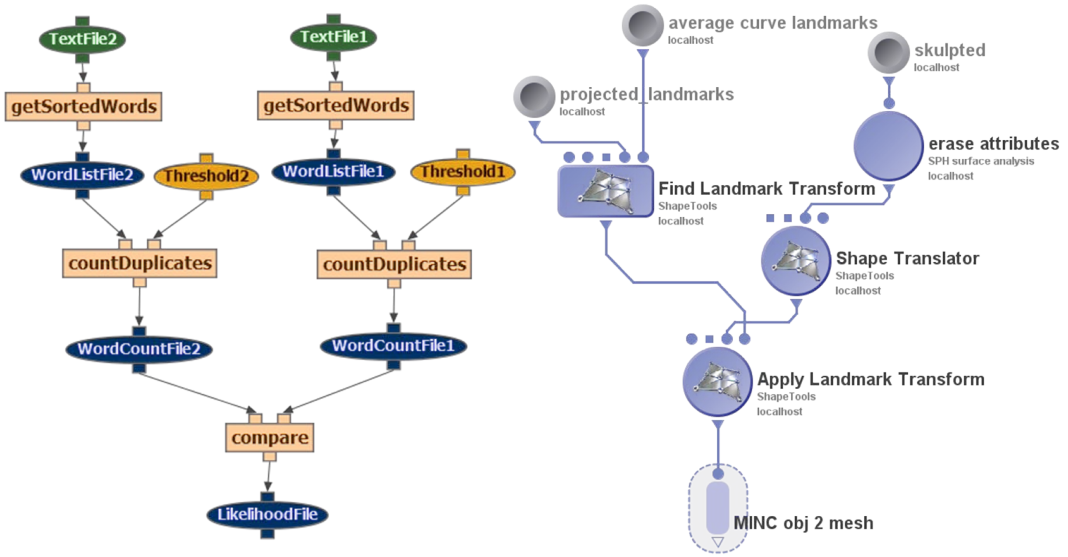


Figure 2.1: Two sample workflows from two different workflow systems. The one on the left is from the text analytics domain, while the one on the right is for neuro-image analysis.

related work.

The first one is **workflow representation**, key for understanding the functionality of the workflow steps at the different stages of the workflow life cycle.

The second area is **workflow abstraction**, which refers to the ability to generalize different workflows (or workflow steps) by their common functionality. Workflow abstraction is important for simplifying workflows and for finding relationships between them, which in the end make them easier to reuse and understand.

Finally, the third area is **workflow reuse**, as we aim to allow scientists to complete their experiments by using existent workflows (or parts of them) made by other researchers.

All three areas are closely related to each other. Having a clear representation of the workflow functionality and its relationships with other workflows at several levels of abstraction may help users decide whether a given workflow (or any of its sub-parts) can be adapted from a previous experiment for reuse or not.

In this chapter we analyze the current state of the art and limitations in workflow representation, abstraction and reuse; introducing the concepts that will be used throughout the rest of the thesis.

2.1 Scientific Workflow Representation

Scientific workflows have been often compared to business workflows[1], which are used to represent business processes in the corporate world (Cerezo et al., 2013). As stated in (Cerezo et al., 2013), *"nothing prevents a user from using a business workflow framework to model and perform a scientific experiment or a scientific workflow framework to capture and automate a business process"* and, in fact, there are examples of approaches for business workflows being adapted for scientific workflows (Mayer et al., 2012) (Slominski, 2007).

However, there are some important differences between scientific workflows and business workflows (Cerezo et al., 2013)(Tan et al., 2009)(Barga and Gannon, 2007). On the one hand, business workflows are generally robust, secure, reliable and control-driven (i.e., they often include control constructs like conditional branches and loops). Business workflows are designed to perform services rather than exploring whether an experiment can be successful or not. They also include policy and privacy concerns for their usage, as this is typical in the corporate world. On the other hand, scientific workflows represent *in silico* experiments that tend to be data driven, more dynamic and evolving, with an aim for shareability and reusability of the exposed scientific methods and with a flexible design for being extended by other researchers.

In our work we focus on scientific workflows. There have been several proposals for their representation, and all of them use a graph-based approach. We introduce the most relevant approaches in this section. Examples of workflow systems adopting each representation are further described in (Deelman et al., 2009).

Petri Nets (Reisig and Rozenberg, 1998) represent workflow steps as actions, which connect states of the workflow through directed arcs. Each state represents the status of the workflow after the execution of an action. The workflow always starts with an initial neutral state and reaches its final state only after the execution is completed. Figure 2.2 shows an example of a workflow represented as a Petri Net. The workflow retrieves a list of terms from a file (*Read*), adds annotations in parallel consulting two different data sources (*Annot1* and *Annot2*) and plots the results (*Plot*). Two additional steps (*Split* and *Merge*) distribute the data and merge it later in order to create the annotations in parallel.

[1] `http://www.wfmc.org/what-is-bpm`

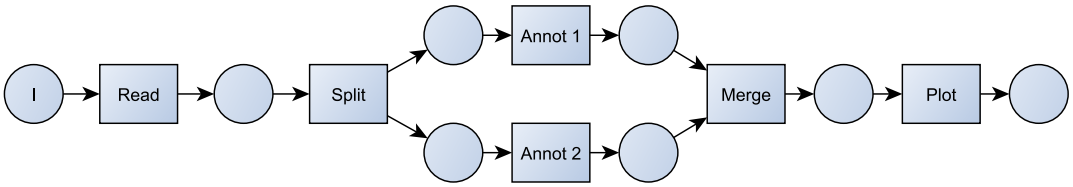


Figure 2.2: Example of a workflow represented as a Petri Net. The initial state is represented with an "I". Circles represent states of the workflow, and boxes represent the actions executed between states. The arrows represent data dependencies.

The Unified Modelling Language (UML) aims "*to provide system architects, software engineers, and software developers with tools for analysis, design, and implementation of software-based systems as well as for modeling business and similar processes*" (Bock et al., 2015). UML is one of the most popular languages for designing a system in software engineering, as it provides the means to create structure, integration and behavior diagrams. These include activity diagrams, which can be used to represent scientific workflows. Figure 2.3 shows an example illustrating the workflow depicted in Figure 2.2 (with a Petri Net) in UML.

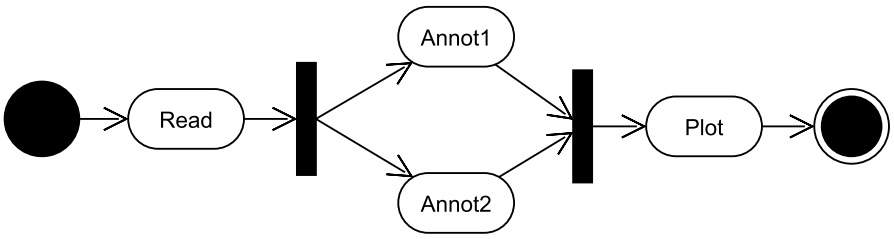


Figure 2.3: Example of a workflow represented in UML. The initial state is represented with a single black circle, while the final state has two circles. Workflow steps are represented as ellipses, and their data dependencies with arcs. Vertical bars represent fork and join nodes.

The Business Process Model and Notation (BPMN) (Aggarwal et al., 2011) provides a standard notation for implementing, managing and monitoring business processes. BPMN is widely used in business workflows, and it was designed to visualize business process execution languages such as the Business Process Execution Language (BPEL) (Jordan et al., 2007). Figure 2.4 shows how the workflow described in Figure 2.2 would

be represented in BPMN.

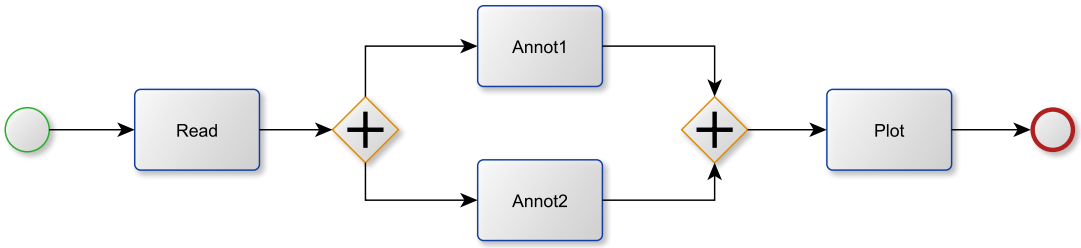


Figure 2.4: Example of a workflow represented in BPMN. The initial event is represented with a single circle, while the final event is depicted with a circle with a wider line. Workflow steps (tasks) are represented with rounded boxes. The flow is represented by arrows. Diamond boxes represent gateways, which indicate when two activities are performed in parallel.

However, the most typical representation for scientific workflows are graph-based models. In them, the nodes of the graph represent workflow steps and the edges capture their dataflow dependencies (e.g, (Gil et al., 2011) (Wolstencroft et al., 2013) (Goecks et al., 2010) (Fahringer et al., 2007) (Berthold et al., 2008) (Callahan et al., 2006) (Ludäscher et al., 2006)). Figure 2.1, shows two workflow examples from two different systems. It is worth mentioning that despite sharing the model, some systems represent differently the inputs, outputs and intermediate results. In this case, ellipses are used in the workflow of the left to refer to inputs, outputs and intermediate results, while small circles and a triangle represent inputs and outputs for the workflow on the right.

Graph-based models are usually based on the definitions proposed in (Bondy and Murty, 1976). Definition 1 summarizes the main concepts, which we use as basis for the rest of the thesis.

Definition 1 *A* ***graph*** $G = (V, E)$ *is defined as a non empty set of vertices (nodes)* $V = (v_1, ..., v_n)$ *which are interconnected by an empty or non empty set of edges (links)* $E = (e_1, ..., e_m)$ *with* $E \subseteq V \times V$ *and* V *disjoint from* E $(V \cap E = \emptyset)$*. Graphs are* ***directed*** *when an edge* $e = (u, v) \in E$ *means that the edge goes from* u *to* v *(having* $(u, v) \in V$*),* u *being the tail of the edge while* v *being its head. A* ***walk*** W *is a sequence of consecutive vertices* $(v_1, ..., v_n) \in V$ *such that for each pair of vertices* (v_i, v_{i+1}) *with* $i \in (1, ..., n-1)$ *there exists an edge* $e \in E$ *that connects them. If* $\forall\ (v_i, v_j) \in W\ v_i \neq v_j$ *with* $i \neq j$*,* W *is denoted as a* ***path****. Two vertices of a graph* G *are connected if there is a path between them. Connection is an equivalence relation on the vertex set* V*. Hence,*

a graph G (V,E) can be divided into sets of connected vertices, called ***components****. When G (V,E) has only one component, the graph is* ***connected****. Otherwise the graph is* ***disconnected****. A* ***cycle*** *C is a walk with* $(v_1, ..., v_n)$*, where* $v_1 = v_n$ *and where the edges* $(e_1, ..., e_k) \in C$ *are distinct. A graph without cycles is* ***acyclic****. Finally, a graph* $G = (V, E, L_V, L_E, \varphi_V, \varphi_E)$ *is* ***labeled*** *if* L_V *and* L_E *are sets of labels for the vertices and edges respectively; and* φ_V *and* φ_E *are functions that define how each vertex or edge is mapped to a label:* $V \rightarrow L_V$ *and* $E \rightarrow L_E$ *respectively. An illustrative example of each type of graph can be seen in Figure 2.5, according to its definition.*

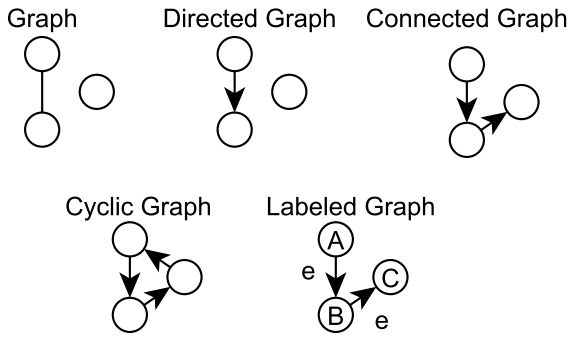


Figure 2.5: Different types of graph, as introduced in Definition 1.

Scientific workflows are typically data intensive, and they are often represented as directed acyclic graphs (DAGs). However, there are systems which allow for control flow constructs and use, when necessary, directed cyclic graphs (DCGs) like Kepler (Ludäscher et al., 2006), VisTrails (Callahan et al., 2006) or Moteur (Glatard et al., 2007). In the next section we introduce the main workflow management systems used in this work.

2.1.1 Scientific Workflow Management Systems

In order to design, monitor, execute and debug scientific workflows the community has created workflow management systems in different domains. Some examples are Wings (Gil et al., 2011), Taverna (Wolstencroft et al., 2013), GenePattern (Reich et al., 2006), the LONI Pipeline (Dinov et al., 2009), Galaxy (Goecks et al., 2010), VisTrails (Deelman et al., 2004), ASKALON (Fahringer et al., 2007), Knime (Berthold et al., 2008), Kepler (Ludäscher et al., 2006), Pegasus (Deelman et al., 2005) or Moteur (Glatard et al., 2007). These and other systems have already been described and compared in

detail in related work (Goderis, 2008) (Cerezo, 2013) (Deelman et al., 2009) (Yu and Buyya, 2005). Here we introduce the workflow systems that have been used for the experiments of this thesis. The rationale behind using each of these workflow systems is explained on Chapter 5.

2.1.1.1 Taverna

Workflow system that can operate in different execution environments and provides several possibilities of deployment (Wolstencroft et al., 2013). Taverna is available as a workbench[2], which embodies a desktop design user interface and an execution engine. Taverna also allows standalone deployments of its engine[3] in order to serve multiple clients. In its default configuration Taverna does not prescribe that the datasets and tools are integrated into an execution environment. In this sense it adopts an open-world approach, where workflows integrate (typically) remote third party resources and compose them into data-intensive pipelines. In addition, it also allows the development of plug-ins for the access and usage of dedicated computing infrastructures (e.g. grids) or local tools and executables. Its use has been extended in bioinformatics and in other domains including astronomy, chemistry, text mining and image analysis.

2.1.1.2 Wings

Workflow system that uses semantic representations to describe the constraints of the data and computational steps in the workflow (Gil et al., 2011). Wings can reason about these constraints, propagating them through the workflow structure and using them to validate workflows. It has been used in different domains, ranging from life sciences to text analytics and geosciences. Wings provides web based access and can run workflows locally, or submit[4] them to the Pegasus/Condor (Deelman et al., 2005) or Apache OODT (Mattmann et al., 2006) execution environments that can handle large-scale distributed data and computations, optimization and data movement.

[2]Taverna Workbench `http://www.taverna.org.uk/download/workbench/`
[3]Taverna Server `http://www.taverna.org.uk/download/server/`
[4]`http://www.wings-workflows.org`

2.1.1.3 Galaxy

Web-based platform for data intensive biomedical research (Giardine et al., 2005) (Blankenberg et al., 2007). One of the main features of Galaxy is its cloud back-end, which provides support for its extensive catalogue of tools. These tools allow performing different types of analysis of data from widely used existing datasets in the biomedical domain. Galaxy uses its own engine for managing the workflow execution, compatible with batch systems or Sun Grid Engine (SGE)[5]. Galaxy workflows can be run online[6] or by setting up a local instance[7].

2.1.1.4 VisTrails

System that tracks the change-based provenance in workflow specifications in order to facilitate reuse (Callahan et al., 2006). It has been used in different domains of life sciences like medical informatics and biomedicine, but also in other domains like image processing, climatology and physics. VisTrails uses its own engine to manage the execution and allows for the combination of specialized libraries, grid and web services. Its workflows can be run online[8] or locally[9].

2.1.1.5 The LONI Pipeline

Workflow system developed by the Laboratory of Neuro Imaging (LONI)[10] mainly for neuro-imaging applications (Dinov et al., 2011) (Dinov et al., 2009). It provides an efficient distributed computing solution to address common challenges in neuro-imaging research, enabling investigators to share, integrate, collaborate and expand resources including data, computing platforms, and analytic algorithms. The LONI Pipeline is mostly used for complex neuro-imaging analysis, which often requires knowledge about the input/output requirements of algorithms, data format conversions, optimal parameter settings, and a unique running environment since imaging studies tend to produce large amounts of data.

[5] http://star.mit.edu/cluster/docs/0.93.3/guides/sge.html
[6] https://main.g2.bx.psu.edu/root
[7] http://wiki.galaxyproject.org/Admin/Get%20Galaxy
[8] http://www.crowdlabs.org/vistrails/
[9] http://www.vistrails.org/index.php/Downloads
[10] http://loni.usc.edu/

2.1.2 Scientific Workflow Life Cycle

There are four main stages in the life cycle of a workflow (van der Aalst et al., 2003b): workflow design, workflow configuration, workflow enactment and workflow diagnosis. Rather than focusing on the phases themselves, here we describe the main workflow structures that are interchanged within a workflow management system during the workflow life cycle. We distinguish three major types of workflow structures:

1. **Workflow Template (WT)**: A generic reusable workflow specification that indicates the types of steps in the workflow and their dataflow dependencies. Workflow templates have also been referred to as "Workflow Orchestration" (Deelman et al., 2009). A workflow generation tool can take types of steps specified in the workflow template (e.g., "Sort") and specialize them to implemented algorithms and codes (e.g., "Quicksort in Python") to create a workflow instance.

2. **Workflow Instance (WI)**: A workflow that specifies the application algorithms to be executed and the data to be used (Deelman et al., 2009). Workflow instances are created from workflow templates when datasets are identified and are sometimes called abstract workflows because they do not specify execution resources (Cerezo et al., 2013). Since a type of step can have different implementations, the same workflow template could be used to generate very different workflow instances. A workflow instance can be submitted to a workflow mapping and execution system, which will identify and assign available resources at run-time, submit it for execution, oversee its execution, and return a workflow execution trace. Because different resources may be available at different times or in different execution environments, the same workflow instance may result in very different workflow execution traces.

3. **Workflow Execution Trace (WET)**: Also known as provenance trace, a workflow execution trace contains the details of what happened during the execution of a workflow, including what resources it was executed on, execution time for each step, links to the intermediate results, and possibly other execution details such as steps for data movements. When workflow steps fail to execute, a workflow execution contains annotations of what failed and in this way its dataflow structure may be different from the dataflow in a workflow instance.

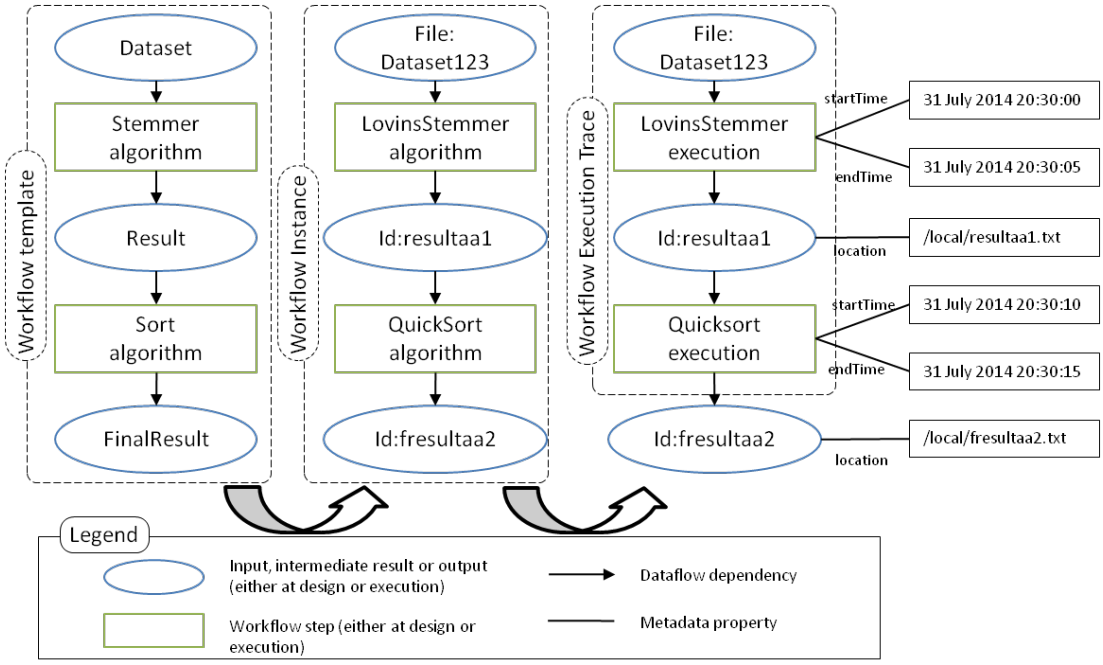


Figure 2.6: A workflow template (left), a workflow instance (center), and a successful workflow execution (right).

Figure 2.6 illustrates the difference between workflow templates, instances and executions with an example. The left of the figure shows a template with two steps (*Stem* and *Sort*), an input (*Dataset*) and an output (*FinalResult*). A workflow instance built from this template is shown in the middle of the figure, specifying *Dataset123* as the input and specific executable codes for each of the steps (the *LovinsStemmer* algorithm and *Quicksort* algorithm respectively). The workflow instance also has placeholders for the expected results (*Id:resultaa1*, and *fresutlaa2*). When this workflow instance is executed, the workflow execution engine produces the execution trace shown on the right (each step has its start and end time, and each intermediate result identifier (e.g., *Id:resultaa1*) has associated the path of the file it represents).

Figure 2.7 shows a failed execution of the same template and instance shown in Figure 2.6. The execution failed when executing the Quicksort component, which led to a trace with no final output and with different dataflow from the workflow instance.

Another crucial aspect to consider when representing workflows in their different stages is their granularity. Templates may be simplified or abstracted for helping in workflow design (Cerezo, 2013). Workflow execution traces and workflow instances may

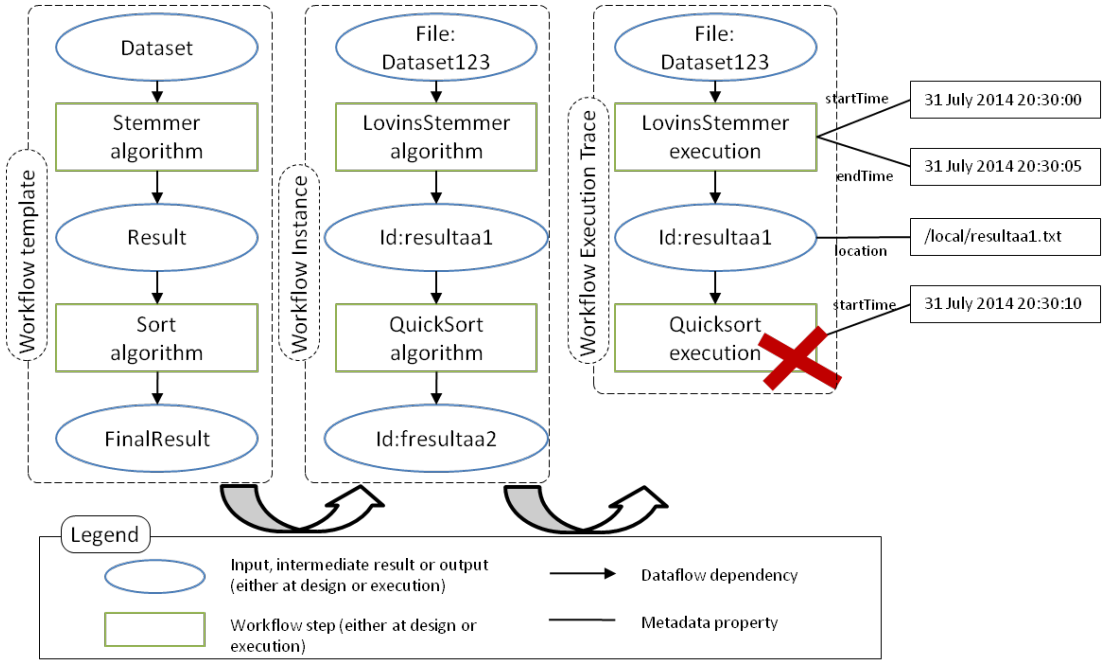


Figure 2.7: A workflow template (left), a workflow instance (center), and a failed workflow execution (right).

have very little in common after a workflow execution engine processes and optimizes the workflow instance for its execution (Deelman et al., 2004). Workflow traces can be summarized for providing an explanation of a failure. All these representations coexist, and are views of a workflow at the different phases of its life cycle.

2.1.3 Scientific Workflow Models

Most scientific workflow models aim at representing specifications of workflows (i.e., workflow instances and templates) and the results obtained after an execution. This section aims to illustrate some of the existing approaches with examples, focusing on those models that link workflow templates, instances and execution traces together with their metadata.

2.1.3.1 Workflow Template and Instance Specification Models

Workflow systems often declare their own model for specifying workflow instances or templates. These models are usually different from one system to another, as they depend on the particular system's supported features or domain specific requirements

(e.g., control-oriented constructs, enabling easy access to external web services, etc.). For example, Taverna has Scufl (Oinn et al., 2004), Pegasus uses DAX[11], Kepler uses MOML (Lee and Neuendorffer, 2000), Askalon uses AGWL (Fahringer et al., 2005), etc. Some additional examples can be seen in (Deelman et al., 2009).

There have been efforts towards creating a common workflow language. In the business workflow domain, Web Services BPEL (WS-BPEL) (Jordan et al., 2007) (Barga and Gannon, 2007) was designed for specifying business processes using web services. In the scientific workflow domain, the Data-Intensive Systems Process Engineering Language (DISPEL) was created to "*describe abstract workflows for distributed data-intensive applications*" (Atkinson et al., 2013). Another significant effort to develop a common workflow language was lead by the SHIWA project (Krefting et al., 2011), which developed the IWIR language (Plankensteiner et al., 2011) for representing workflows in a system-independent manner. Workflows represented in IWIR can be partitioned so that each partition is executed in a different workflow execution engine.

2.1.3.2 Workflow Execution Trace Models

These are the models designed to represent the provenance trace of a workflow. According to the recent W3C standard, provenance can be defined as *"a record that describes the people, institutions, entities, and activities involved in producing, influencing, or delivering a piece of data or a thing"* (Moreau et al., 2013).

The notion of provenance has been widely discussed in related work for a variety of domains, ranging from digital humanities[12] to e-science (Simmhan et al., 2005). In fact, several models have been proposed throughout the years to manage and represent generic provenance (Moreau, 2010). In an attempt to propose a common provenance standard, the workflow community started the Provenance Challenges[13], which focused on discussing different approaches for representing the same provenance problem and testing their interoperability. After the Third Provenance Challenge[14], the Open Provenance Model (OPM) (Moreau et al., 2011) consolidated itself as a *de facto* provenance standard and was adopted by a reasonable part of the community[15]. The

[11] `http://pegasus.isi.edu/wms/docs/schemas/dax-3.4/dax-3.4.html`
[12] `http://www.getty.edu/research/tools/provenance/`
[13] `http://twiki.ipaw.info/bin/view/Challenge`
[14] `http://twiki.ipaw.info/bin/view/Challenge/ThirdProvenanceChallenge`
[15] `http://openprovenance.org/`

interest in having a standard for provenance interchange vocabulary led to the creation of the W3C Provenance Incubator Group[16], which gathered the provenance requirements proposed by the scientific community in different domains (Groth et al., 2012) and set the first steps towards the creation of a standard (Gil et al., 2010). It was followed by the Provenance Working Group[17], whose effort finally materialized in the family of PROV specifications[18], a set of W3C recommendations on how to model and interchange provenance on the Web (Groth and Moreau, 2013).

Some workflow systems have started capturing their workflow executions by extending OPM and PROV models (most of them during the development of this thesis). Swift was perhaps one of the first workflow systems to export to OPM (Gadelha Jr. et al., 2011). The Taverna team followed with an experimental workflow export to OPM[19], but more recently they have moved to the Research Object model (Belhajjame et al., 2012a) to represent workflow descriptions and provenance according to PROV. Wings exports workflow executions following both OPM (Garijo and Gil, 2011) and PROV[20]. Some other approaches have used VisTrails to capture provenance traces according to PROV, using a more generic model (Missier et al., 2013). Systems like Pegasus or Kepler have been integrated with provenance management stores like PASOA (Miles et al., 2007) or Prov Manager (Marinho et al., 2012) to generically store provenance traces according to OPM and PROV respectively. To this date, there is no standard extension of OPM or PROV for representing scientific workflow execution traces.

Finally, other workflow systems like Galaxy, GenePattern or the LONI Pipeline create logs of workflow execution following their own conventions.

2.1.3.3 Linking workflow templates, instances and executions

The models shown in the previous sections tackle the representation of workflow templates, instances and executions separately. However, they depend on each other. For example, let us consider a scientist who wants to create a scientific workflow for the experiment he has been working on. The first step would be to complete a sketch of the workflow, which would be used to complete a workflow template. The workflow

[16] http://www.w3.org/2005/Incubator/prov/wiki/W3C_Provenance_Incubator_Group_Wiki
[17] http://www.w3.org/2011/prov/wiki/Main_Page
[18] https://dvcs.w3.org/hg/prov/raw-file/tip/namespace/landing-page.html
[19] http://dev.mygrid.org.uk/wiki/display/tav250/Provenance+export+to+OPM+and+Janus
[20] http://www.opmw.org/ontology/

template can then be implemented with specific algorithms using the input datasets selected for the experiment, creating one or several workflow instances. Then, a workflow instance may be executed one or several times, producing workflow execution traces that may be successful or not.

The relationships among workflow templates, instances and executions are often represented by different models with ontologies[21]. An ontology is defined as a *"formal specification of a shared conceptualization"*, where *conceptualization* refers to *"an abstract model of some phenomenon in the world by having identified the relevant concepts of that phenomenon"*, *formal* means that *"it should be machine-readable"* and *shared* means that *"the ontology captures consensual knowledge"* (Studer et al., 1998). Ontologies are usually implemented in RDFS (McBride et al., 2014) and OWL (McGuinness and van Harmelen, 2004), which are represented using the Resource Description Framework data model (RDF) (Klyne et al., 2004). RDF is a W3C recommendation that specifies the relationships between resources using a labeled graph with RDF statements. Each RDF statement consists on a triple with a subject node and an object node, connected by a predicate. Figure 2.8 shows an example, in which a file (*File1*, subject) is described with its creator (*Bob*, object) with the "*createdBy*" predicate.

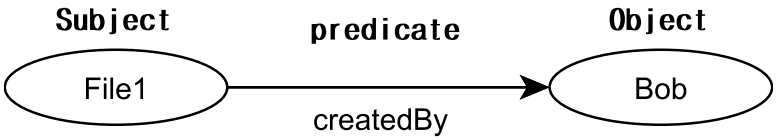


Figure 2.8: RDF example: a file is described with its creator.

Since graphs are a common representation for scientific workflows, several models have adopted RDF to represent their main concepts (Belhajjame et al., 2015; Cerezo, 2013; Missier et al., 2013). In addition, RDF provides a machine readable representation of the workflow, making it easier to process. During the development of this thesis, some models have been proposed to describe the links between scientific workflow templates, instances or executions:

The Research Object ontologies consist of a family of specifications for describing aggregations of resources related to a scientific experiment (Belhajjame et al.,

[21] Ontologies are commonly referred to as vocabularies when they are not complex. See `http://www.w3.org/standards/semanticweb/ontology`

2015). Scientific workflows play an important role, having two vocabularies for describing them. The workflow description vocabulary (wfdesc)[22] defines workflow instances and templates; and the workflow provenance vocabulary (wfprov)[23] defines workflow execution traces and how they link to the instances or templates. The vocabularies extend the PROV standard and support the definition of sub-workflows, but don't make a distinction between workflow instances and templates.

ProvONE is a recent PROV extension for capturing the "*most important information concerning scientific workflow computational processes*"[24]. ProvONE is based on D-PROV, another PROV extension that aims at representing the retrospective provenance (workflow execution traces) and prospective provenance (workflow instances) of scientific workflows (Missier et al., 2013). The model is similar to the Research Object ontologies, but tries to be more generic by representing dependencies among processes as links between ports or as channels.

Conceptual workflows have been designed to facilitate workflow abstraction and design (Cerezo, 2013). The model proposes a conceptual level (what we refer to as workflow template) which is then specified to an abstract level (workflow instance). A similar effort has been described in the Wings system, defining generic and concrete templates (Gil et al., 2009), but conceptual workflows are more generic by defining constructs to represent and link loops and conditional branches in workflow templates and instances. In both cases, the representation of workflow execution traces are out of the scope of the model.

P-Plan is designed to capture "*the plans that guided the execution of scientific processes*"[25] (Garijo and Gil, 2012). Hence, it is a simple high level model extending the PROV standard. P-Plan captures the main dataflow constructs and links them to the workflow execution. Since it is a general purpose vocabulary, P-Plan has been used for the description of laboratory protocols (Giraldo et al., 2014), description of the infrastructure of workflow steps (Santana-Pérez and Pérez-Hernández, 2015), scientific workflow invocation[26] or social science modeling (Markovic et al., 2014).

[22] `http://purl.org/wf4ever/wfdesc`
[23] `http://purl.org/wf4ever/wfprov`
[24] `http://purl.org/provone`
[25] `http://purl.org/net/p-plan`
[26] `http://purl.org/net/wf-invocation`

Other vocabularies aim to be more generic, in order to provide context for the whole experiment that led to the scientific workflow. These vocabularies do not necessarily attempt to describe any execution details, but rather a general purpose description that serves as documentation of the steps of the workflow. They include:

The **Investigation, Study, Assay (ISA) Model** differentiates between three concepts to describe biomedical research (Rocca et al., 2008). An *assay* represents the most specific part of an experiment, i.e., measurements performed on subjects. A *study* contains the experimental steps or sequence of steps and the *investigation* contains the overall goals and means used for an experiment. An investigation may have one or more studies, which themselves may consist of one or several assays. For each of these concepts, the model aims to capture metadata such as references, names, protocols or equipment.

The **Ontology for Biomedical Investigations (OBI)** defines a common framework for representing experimental descriptions and methods in biomedical research (Brinkman et al., 2010). OBI has been widely adopted and extended in the biomedical domain, and although its main focus relies on identifying the different types of inputs, outputs, roles and methods used by the community, it also defines basic relationships for specifying the inputs and outputs of a certain step or protocol.

The **EXPO Ontology** presents an ontology for scientific experiments. Although it is aimed at representing the scientific method (hypothesis, evaluation, interpretation of results, etc.), the ontology has also specific steps for modeling scientific tasks like those happening in a workflow along with their basic metadata (Soldatova and King, 2006).

Table 2.1 summarizes the scope and main features of the different approaches described above.

2.1.3.4 Scientific Workflow Metadata

The final aspect for representing scientific workflows is their metadata. Workflow metadata often captures basic attribution and other aspects that are typical of scientific workflows and their resources, such as the file size of the experiments, restrictions and descriptions of the workflow steps, license, start and end time of the workflow execution, whether an execution was successful or not, etc.

Table 2.1: Summary of the different approaches for representing WT, WI, WET, their metadata and their connections. The asterisk (*) on the WT column indicates that the model makes no distinction when representing WT and WI.

Approach	Purpose	Control-based constructs	WT constructs	WI constructs	WET constructs	Metadata constructs
Research Object	Scientific workflows	No	Yes*	Yes	Yes	No
ProvONE	Scientific workflows	No	Yes*	Yes	Yes	No
Conceptual Workflows	Scientific workflows	Yes	Yes	Yes	No	No
P-Plan	Scientific processes	No	Yes*	Yes	Yes	No
ISA	Scientific experiments	No	Yes	No	No	Yes
OBI	Scientific experiments	No	Yes	No	No	Yes
EXPO	Scientific experiments	No	Yes	No	No	Yes

As we show on Table 2.1, very few models provide descriptive metadata for workflow templates, instances or executions. Specifically, as models become more generic, they contain less common metadata properties. When defining metadata, the models often reuse existing vocabularies, instead of defining new terms. Some of the most popular reused vocabularies for this purpose are the Dublin Core vocabulary [27], aimed at describing basic attribution and licensing; the SWAN-PAV ontology (Ciccarese et al., 2013), defined to describe detailed attribution, authoring, contributions and versioning of web resources; the FOAF vocabulary[28], which describes those agents that participated in the workflow; or the W3C PROV vocabulary for defining basic attribution and responsibility among the participating agents.

[27] `http://dublincore.org/documents/dcmi-terms/`
[28] `http://xmlns.com/foaf/spec/`

2.1.4 Scientific Workflow Publication

The ability to share workflows among scientists is critical for proper repurposing and reuse of existing workflows; as well as a means to providing attribution and feedback to other scientists for their work. In this section we review the current approaches for making a scientific workflow public.

2.1.4.1 Data Repositories

The simplest option for sharing scientific workflows is through data repositories and digital archives. In fact, general-purpose data repositories are gaining popularity for sharing the resources associated with a paper: input datasets, specific results, etc.

In this kind of repositories, workflows (and optionally, their associated resources) are compressed in a single file and stored or archived. The advantage of this approach is that the stored file becomes citable, as data repositories often provide a Digital Object Identifier (DOI)[29] for referring to them. The downside is that workflow bundles can be created in very heterogeneous ways, and without concrete guidelines, users may omit important information for proper workflow reusability. Some popular general data repositories are FigShare[30] and Dryad[31].

2.1.4.2 Workflow Repositories

In order to facilitate workflow reuse and to provide use examples, some workflow systems have created repositories for publishing workflow templates and instances. Galaxy has a catalog of public workflows[32] that can be downloaded and imported to one's workspace. VisTrails can push workflow specifications to CrowdLabs (Mates et al., 2011) in order to further document them. The LONI Pipeline also has a curated catalog of public workflows[33] and components. The most well known repository of workflows is probably myExperiment (Goderis et al., 2009), initially developed to store Taverna workflows, but currently containing more than 2000 workflows from systems like Kepler, the LONI Pipeline or RapidMiner[34].

[29] http://www.doi.org/
[30] http://figshare.com
[31] http://datadryad.org/
[32] https://usegalaxy.org/workflow/list_published
[33] http://pipeline.loni.usc.edu/explore/library-navigator/
[34] https://rapidminer.com/

Most public repositories store only workflow templates, although myExperiment has started moving towards capturing the context of experiments with Research Objects (called "packs"). Packs are collections of aggregated resources relevant to a particular experiment (e.g., executions, conclusions, hypothesis, diagrams, etc.).

The methodology for uploading a workflow into these repositories is usually through their workflow management systems or by manual submission through their publicly available APIs.

2.1.4.3 Science Gateways

Science gateways are applications, libraries of components, workflows and tools that are shared and integrated through a portal. Most workflow systems often choose this option for sharing workflows, as it can usually be combined with domain specific resources like models and software libraries. Examples of science gateways can be seen in (Filgueira et al., 2014) for the volcanology domain, in (Danovaro et al., 2014) for hydro-meteorology research or in the LONI Pipeline[35] for the neuro-image analysis domain.

The main difference between a science gateway and a workflow repository is that the former may provide the infrastructure to execute some of the shared components through community portals.

2.1.4.4 Virtual Machines and Web Services

Finally, another solution adopted by scientists is to encapsulate their workflows as part of virtual machines or web services that can be downloaded (or invoked) and then executed. For example, (Chirigati et al., 2013) tracks the provenance of experiments and then exposes the results and workflow specifications with a virtual machine. The advantage of this approach is that anyone can easily reproduce the results claimed by the scientist, since all the software dependencies are included as part of the virtual machine. However, there are two main disadvantages. The first one is that the workflow becomes a black box, hence very difficult to repurpose for other goals. The second one is that this approach cannot always be considered, specifically when the datasets used or produced by the experiment are large in size, or when the software uses non open

[35] `http://pipeline.loni.usc.edu/explore/library-navigator/`

source licenses, etc. Workflow reproducibility is a whole area of research, and is out of the scope of this thesis.

2.2 Workflow Abstraction

There are several approaches for creating abstractions from scientific workflows (i.e., creating generalizations of steps by some of their common features). As we have shown in the previous section, one possible way is based on the different stages of the workflow: workflow templates are more abstract than workflow instances, which themselves may be seen as representatives of a group of executions. Another possibility is based on the granularity at which each stage can be presented to the user. For example, a workflow execution trace may be simplified in part to facilitate understanding. In this section we describe the most common types of workflow abstractions based on their granularity, and give an overview on research developed to detect common workflow patterns.

2.2.1 Types of Abstractions in Scientific Workflows

Workflow templates and instances represent plans executed by a workflow engine. Hence, some of the abstractions defined for planning tasks can also be applied to scientific workflows. In this section we briefly define each of them with examples.

2.2.1.1 Skeletal planning

As stated in (Bergmann, 1992), a skeletal plan can be defined as a *"sequence of abstract and only partially specified steps which, when specialized to specific executable operations, will solve a given problem in a specific problem context"*. In this type of abstraction, the number of steps in the abstract plan is the same as in the concrete plan.

A particular case of this abstraction happens when only some of the steps of the plan are abstract, in which case we refer to it as *step abstraction*. In step abstraction, steps may be abstract classes of steps. These classes may be organized in a taxonomy designed by domain experts, for example if the steps share similar constraints on the conditions or effects. Figure 2.9 shows an example, where a generic workflow on the top is specialized as two different workflows on the bottom of the figure, based on the taxonomy of components depicted on the top right.

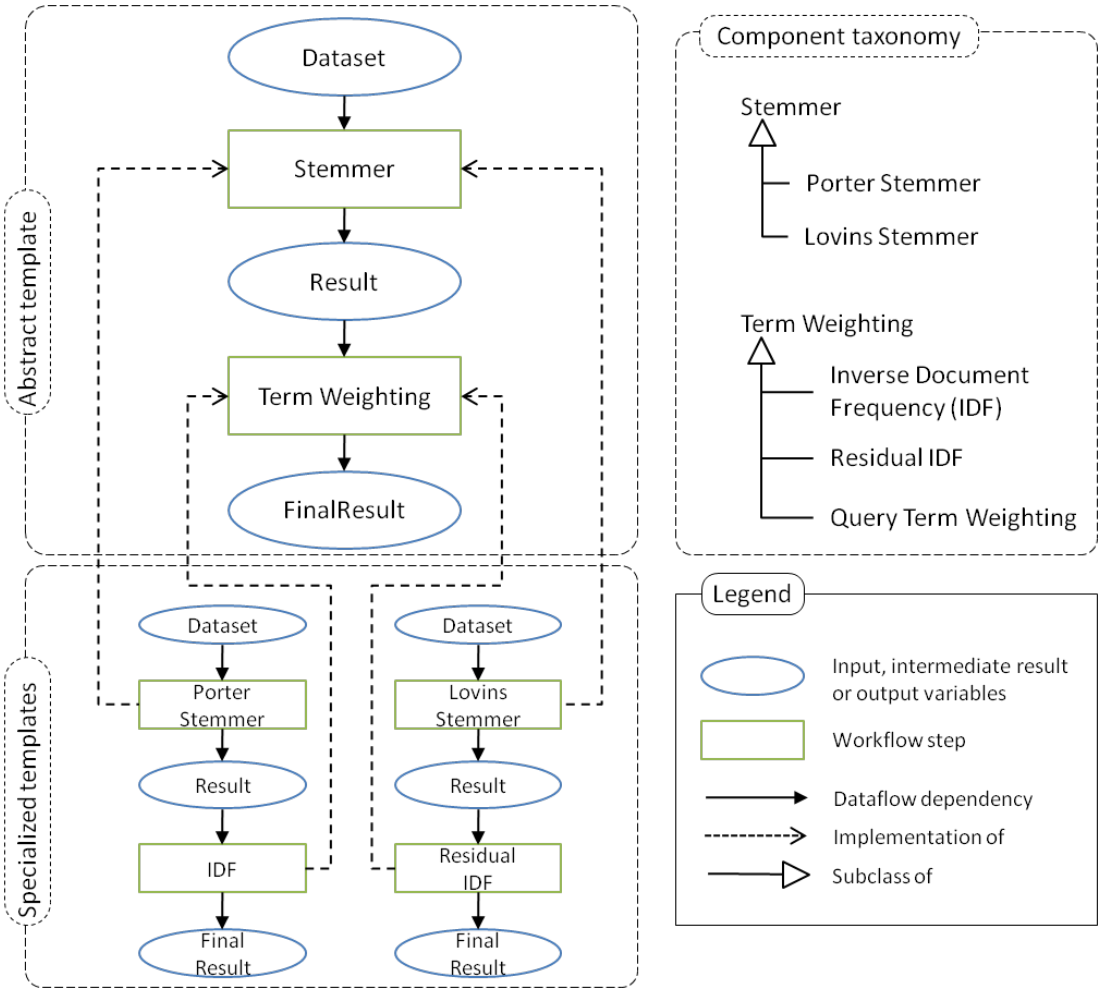


Figure 2.9: Skeletal planning abstraction based on a taxonomy. Two different templates (at the bottom) are two possible specializations of the template on the top, based on the taxonomy of components presented on the top right of the figure. Computational steps are represented with rectangles, while inputs, intermediate results and outputs are represented with ovals.

Some examples of this type of abstractions can be seen in scientific workflows. Wings uses abstract templates to specify its workflows (Gil et al., 2009). The notion of "abstract workflows" has also been discussed (Wood et al., 2012) for systems like SADI (Wilkinson et al., 2009). Other workflow systems like Galaxy and the LONI Pipeline define taxonomies of components for helping users build their workflows (implicitly using step abstraction).

2.2.1.2 Predicate abstraction

In this type of abstraction, entire predicates are dropped at any given abstraction level (Graf and Saidi, 1997). The intuition is that if a predicate requires less steps to be accomplished then it can be placed in a lower abstraction level so that adding actions to accomplish it will cause minimal disruption to the plan at higher levels. Ideally, the abstraction layers are designed to preserve downward monotonicity, which implies that any steps and orderings at higher layers of abstraction are unchanged as the plan is elaborated at lower abstraction levels. In workflows, this would be akin to dropping constraints or even inputs of steps at higher levels of abstraction. An example can be seen in Figure 2.10, where the workflow on the left is an abstraction of the workflow on the right, dropping the optional inputs *Dictionary* (used to train the stemmer component) and *Clusters* (which sets the number of clusters for the clustering algorithm).

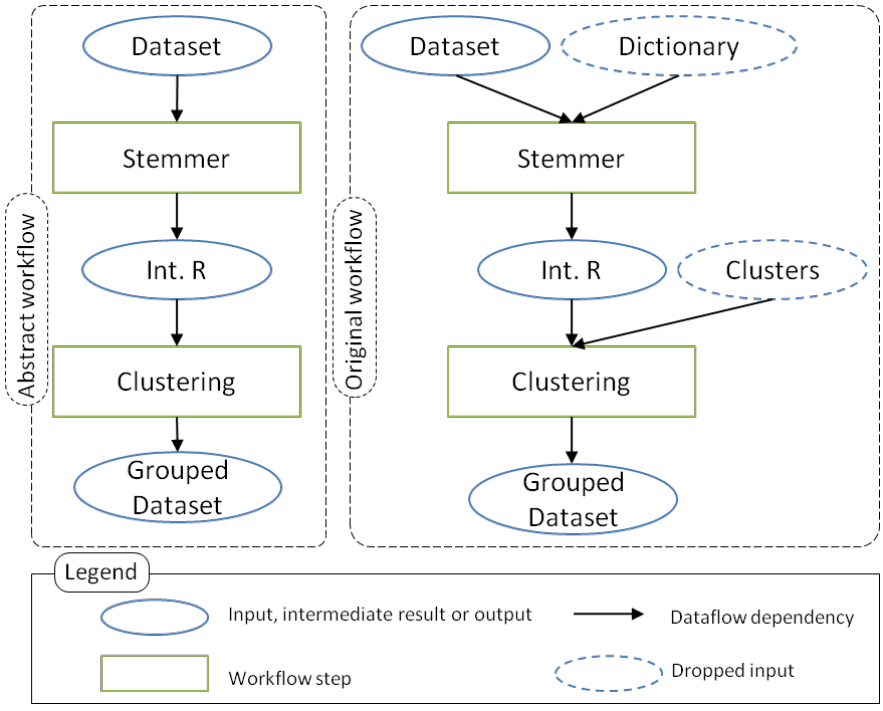


Figure 2.10: Predicate abstraction example: the workflow on the left is an abstraction of the workflow of the right. Two predicates (inputs *Dictionary* and *Clusters*) are omitted in creating the abstraction.

2.2.1.3 Macro abstraction

These are abstractions where several computation steps can be compressed together as one step in the abstract plan. The sub-steps do not disappear from the plan, they are hidden to the user in the abstract plan and can be shown inside the abstracted step. Figure 2.11 shows an example of a workflow in the LONI Pipeline, where two steps (*KL_MI_deform field* and *Interp Average pairs of 3*) are abstracted as a single step in the workflow on the left. Macro abstractions are a common feature in workflow systems, as they help simplify workflows for users.

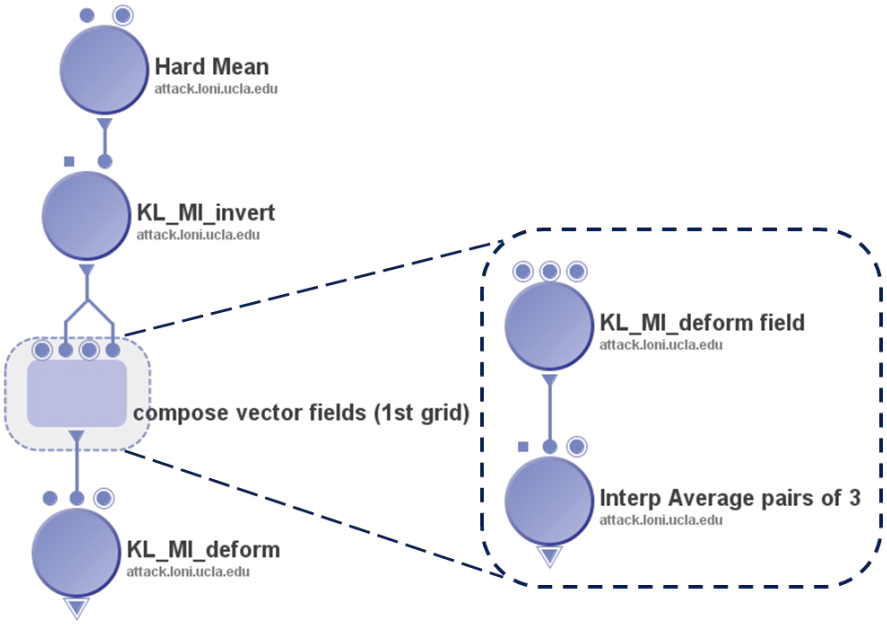


Figure 2.11: Macro abstraction example: two steps on the right are simplified as a single step on the workflow on the left.

Macro abstractions may be created by users as sub-workflows (e.g., as in systems like the LONI Pipeline and Taverna), or via algorithms that mine behavioral profiles of groups of steps of the workflow automatically (Smirnov et al., 2012).

2.2.1.4 Layered abstraction

This type of abstraction represents conceptual levels of detail that may have a very loose correspondence with one another. These abstractions can be seen as employing different

lenses to view the workflow depending on the perspective that users are interested in. This kind of abstraction is very useful to provide an explanation of a workflow for different purposes. For example, a scientist may be interested in seeing the main steps of the flow, while a developer wants to see exactly the preprocessing and post processing done in each step. An example can be seen in Figure 2.12, where a workflow instance (on the left) is enacted by a workflow execution engine creating a new workflow on the right. The enacted workflow is different from the workflow instance initially submitted, as it executes the first step in a distributed infrastructure. Therefore, the *FilterWords* step is separated in two parallel processes (*FilterWords1* and *FilterWords2*). A different workflow engine may have created a complete different instantiation from the workflow instance on the left.

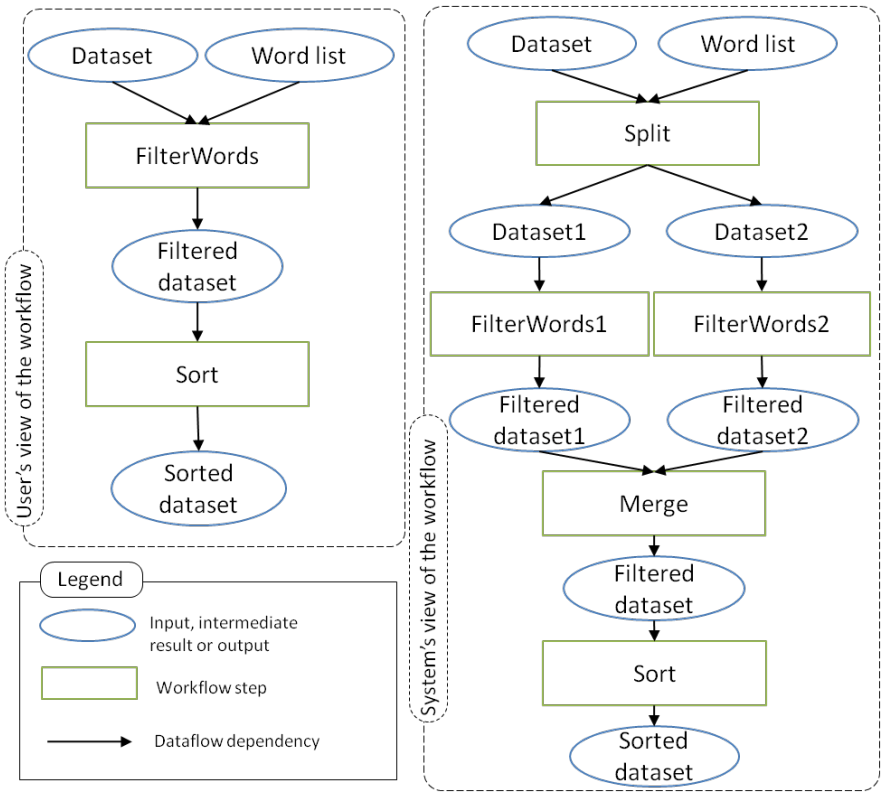


Figure 2.12: Layered abstraction example: the workflow of the left is an abstraction of the workflow of the right, which results when a workflow execution engine enacts it. Therefore the user's view of the workflow (left) is different form the system's view of the workflow (right).

Some approaches have explored this type of abstraction. In ZOOM*Userviews

(Biton et al., 2007), the authors proposed to exploit workflow execution traces to show different views to users according to their preferences. Conceptual workflows (Cerezo et al., 2013) define a mapping to convert workflows defined in a conceptual level into an intermediate representation that can be mapped itself to several target workflow systems. Workflow systems such as Pegasus (Deelman et al., 2004) or ASKALON (Wieczorek et al., 2005) often make use of this abstraction when mapping the workflow instance to their distributed infrastructure.

2.2.2 Workflow Patterns

In Software Development, a pattern is defined as "*the abstraction from a concrete form which keeps recurring in specific non-arbitrary contexts*" (Riehle and Züllighoven, 1996). This type of abstraction does not belong to any of the categories described in the previous section, but has been studied extensively in related work.

Repositories of workflow patterns have been developed based on different properties of workflows. The most popular approach is based on the *workflow structure and constructs* that are possible in different languages[36] (van der Aalst et al., 2003a). Other workflow patterns have been studied in terms of *workflow resources* (creation, distribution, allocation, etc.) (Russell et al., 2004b) and *workflow data* (e.g., visibility, interaction, transference, integration) (Russell et al., 2004a), including generic data intensive usage patterns (Corcho, 2013). Additional classifications are based on *the intrinsic properties of the workflows* (size, structure, branching factor, resource usage, etc.) (Ramakrishnan and Plale, 2010) (Ostermann et al., 2008) and their *environmental characteristics* (makespan, speedup, success rate, etc.) (Ostermann et al., 2008). The viability of some of these workflow patterns has even been studied and discussed for scientific workflows (Yildiz et al., 2009).

Workflow patterns represent common practices by the community, but do not always imply good practices for workflow design. For example, in (Cohen-Boulakia et al., 2014) authors outline anti-patterns in scientific workflows, which basically consist of redundancy and structural conflicts. Similarly, in (Velasco-Elizondo et al., 2013) the authors use architectural abstractions (i.e., workflow patterns) to deal with data mismatch issues between workflow steps (by suggesting the appropriate converters).

[36] `http://www.workflowpatterns.com/`

Generic workflow patterns based on the functionality of workflow steps have been explored superficially. In (Wassink et al., 2009), the authors perform an automated analysis of workflow scripts from life sciences, in order to obtain the frequency of different types of technical ways of instantiating workflow steps (e.g. service invocations, local scientist-developed scripting, local ready-madescripts, etc.). The authors also refine the category of local ready-made scripts with activity categories depending on their functionality (e.g., data access or data transformation). (Starlinger et al., 2012) extends the categories defined in (Wassink et al., 2009), identifying sub-categories at a workflow step level by analyzing 898 Taverna workflows in myExperiment.

Problem Solving Methods (PSMs) are other types of generic patterns that explore the functionality of the workflow steps in them. PSMs describe strategies to achieve the goal of a task in an implementation and domain-independent manner (Gómez-Pérez and Benjamins, 1999). PSMs are generic recipes, and some libraries have adapted them to model the common processes in scientific domains (Gómez-Pérez et al., 2010).

Other efforts aim at developing patterns based on workflow step functionality. Their goal is to categorize and group common functionality in a specific domain, and, in this regard, they may be used for generalizing workflows. For example, the Software Ontology (SWO)[37] models some of the typical operations in research regarding software functionality like data annotation, data visualization, image compression, etc. Other systems like Galaxy and the LONI Pipeline follow a similar approach. They have defined generic categories under which they group workflow libraries, such as "get data", "statistics", "structural analysis", etc.

2.3 Workflow Reuse

Scientific contributions are often built on previous existing work, and this also applies to scientists designing and creating scientific workflows. A proper workflow representation and abstraction enables better understanding of workflows created by other researchers, but it is difficult for scientists to explore whole datasets of workflows by themselves.

In order to facilitate this task, several approaches have been developed through the years for mining workflows for different purposes, ranging from workflow design to workflow discovery. In this section we first describe previous analyses on scientific

[37] `http://sourceforge.net/projects/theswo/`

workflow reuse, and then we summarize existing techniques that help users to reuse workflows.

2.3.1 Measuring Workflow Reuse

Scientific workflows can be considered as software artifacts that connect software components together (workflow steps). The barriers for software reuse have been analyzed in the literature (Boldyreff, 1989). Software engineering technologies have been compared and contrasted in terms of abstraction, selection, specialization and integration (Krueger, 1992), which, as we have shown in this the chapter, are common problems in scientific workflows as well. When focusing in the scientific domain, the incentives for software development in terms of reuse, collaboration and productivity (e.g., getting credit for software) have been discussed in (Howison and Herbsleb, 2011).

Regarding scientific workflows, some requirements for their reuse are defined in (Goderis, 2008). The main requirements consist on having a community open to workflow reuse, availability of reusable workflows (e.g., through a publishing and sharing infrastructure that manages interoperable workflows) and efficient workflow discovery.

The benefits of workflow reuse have been discussed in (Goderis et al., 2005), but (to our knowledge) there are not many studies on how users perceive workflow reuse. One of the few user surveys in the state of the art is (Goderis et al., 2005), which consisted of a questionnaire to 24 scientists from different institutions. According to the survey there are three main types of workflow reuse. These are "*for one's own purposes*", "*from a group of collaborators*" and "*from third parties*". The third type of workflow reuse was not reported by any of the participants in the survey. In (Sethi et al., 2012), the authors further defend the significance of reusing workflow fragments as well, by showing how certain parts of text analytics and image analysis workflows may be used for video activity recognition (and viceversa).

Automatic analyses of workflow repositories have also attempted to classify and quantify workflow reuse, with a special focus on the myExperiment repository and Taverna workflows. In (Tan et al., 2010), the authors use 280 Taverna workflows and 118 services of the BioCatalogue portal to find the connections among them (shared invocations and components). Furthermore, they apply social network analysis techniques to derive the centrality and betweenness of the nodes in the network. Unfortunately, the results show that "*services are currently reused in an ad hoc style instead of a*

federated manner". The work presented in (Wassink et al., 2009) also performs automatic analyses on Taverna workflows available in myExperiment, but with a corpus of 415 workflows. In this case, the authors divide the corpus into different categories of components (beanshells, scripts, etc.), and analyze their reuse. The work described in (Littauer et al., 2012) builds on (Wassink et al., 2009) to further analyze other characteristics of workflows (e.g., versioning, complexity, downloads) and proposes good practices for workflow reuse.

However, the most complete analysis of myExperiment is (Starlinger et al., 2012), which details how workflows, sub-workflows defined by users and steps (divided in different categories) are reused. The corpus consists of 898 workflows, and reuse is differentiated regarding the authors who contributed to the creation of a particular workflow. Reuse is common, and may happen in three main different manners: a workflow is reused as a new workflow (duplication), a sub-workflow is reused as a sub-workflow in another workflow, and workflows are reused as sub-workflows (or viceversa).

Although current approaches have analyzed reuse in a significant amount of workflows, the majority of the corpora have been designed in the same workflow system (Taverna) and leave out of the scope of their analysis groups of commonly occurring workflow steps that may not have been annotated as sub-workflows by users.

2.3.2 Workflow Mining for Reuse

There are several areas where mining approaches have been applied for different purposes, ranging from planning (Yang et al., 2005) (e.g., use previous plans to optimize a future execution) to database query pattern extraction (Lawrynowicz and Potoniec, 2014) (in order to obtain common queries that might help to optimize access to the dataset). In this section we introduce an overview of the efforts that are related to mining workflows, in particular to those that are data intensive (scientific workflows). These efforts are focused on three main goals: mining for the exploration of workflow repositories, mining for recommending or discovering existing workflows and mining to extract new workflows from existing ones.

2.3.2.1 Exploration of repositories

Repositories of workflows tend to be large, and it is difficult for users to analyze each entry individually. In order to address this issue, there are several efforts that try to

organize repositories for enabling better understanding. These efforts are based on machine learning techniques, namely clustering and topic modeling.

Clustering techniques are used to group sets of workflows together according to a given similarity metric. The main difference among the existing approaches is the similarity metric between workflows, the clustering technique being used and the number of clusters to which a workflow may belong. If we follow a chronological order, (Santos et al., 2008) started proposing two different metrics to define similarity among two given workflows: the maximum common sub-graph shared among them and the euclidean distance that separates both workflows when represented as vectors (considering the union of the names of the workflow steps in the workflow as the features of the vectors). In (Silva et al., 2011) the authors followed the previous approach by considering the structure of the workflow (e.g., connection between input ports and output ports) on its similarity measure. Both efforts use the K-means algorithm (MacQueen, 1967), commonly used for clustering in the information retrieval domain. Finally, in (Montani and Leonardi, 2012) the authors propose to use an edit distance in business workflows, taking also into account the temporal similarity of the workflow steps. In this case, the clustering technique is based on an unweighted pair group method with arithmetic means, which allows for hierarchical clustering.

Topic modeling techniques are common in text mining to determine the probability of a document belonging to a certain topic. A topic is not a single word, but a set of words which have a high probability of appearing together. (Stoyanovich et al., 2010) applies this paradigm to the workflow domain, using 2075 workflows from VisTrails and 861 from Taverna. The "words" in this case are the tags used to describe the workflow and the names of the workflow steps. As a result, a set of topics are derived, and workflows are organized around them.

A key difference between clustering techniques and topic modeling techniques is that clustering techniques are deterministic, while topic modeling techniques are probabilistic. This means that, when re-executed, a probabilistic technique may provide similar results but not necessarily the same ones obtained on a previous execution. The main disadvantage of both techniques is that a manual adjustment of the algorithm is needed in order to find the optimal number of topics or clusters depending on the similarity threshold set for the experiments.

2.3.2.2 Recommendation and discovery of existing workflows

The second goal for workflow mining focuses on suggesting workflows to users. This can be done in two different phases of the workflow life cycle (van der Aalst et al., 2003b): during workflow design, by suggesting the next workflow steps to the user, or during workflow diagnosis, when aiming to discover workflows similar to a particular one.

There are several approaches for next step suggestion while designing workflows, based on previous executions or templates. The most straightforward approach can be seen in (Oliveira et al., 2008), where the authors propose a probabilistic method by computing the relationships between components in pairs and suggesting the next most probable component. The approach proposed in (Koop, 2008) is more refined, by using paths in previous workflows to recommend the most likely next step. The suggestion may be either upstream or downstream the current fragment. Finally, (Leake and Kendall-Morwick, 2008) relies on case-based reasoning approaches to mine provenance traces in order to suggest users the next (single) step when editing new workflows. This technique uses a similarity metric, based on an edit distance combined with a structural comparison of the workflows.

Regarding workflow discovery, most approaches aim to deliver similar workflows to a given one. The similarity metric is once again critical, and there has been work that demonstrates that structural based approaches can outperform annotational ones (Starlinger et al., 2014a). In (Goderis, 2008), the authors perform several experiments comparing label-based approaches and sub-graph isomorphism techniques and perform benchmarks for workflow discovery on that basis (Goderis et al., 2009). In (Bergmann and Gil, 2014) the authors focus on structure according to a set of constraints set by the user (e.g., having a specific input or output type). In this regard, this approach is able to add specific requirements to the workflow the user is looking for. Finally, in (Starlinger et al., 2014b), the similarity metric is based on a direct comparison of the workflows by decomposing them into different layers, which provides fast results. It is worth mentioning that some of the similarity metrics used for clustering repositories may also be used for suggesting new workflows as well.

2.3.2.3 Deriving new workflows from existent corpora

The third goal for workflow mining aims to extract workflows from previous executions or templates. In prior work this has been explored in two different ways: by deriving an abstract workflow from a set of execution logs or by proposing new workflows from a repository of workflow templates (based on, for example, commonly used structures).

Log mining has been explored in both business and scientific workflows. In the business domain, (Herbst and Karagiannis, 1998) proposed to use hidden Markov models to find an approximation of a workflow from a set of execution traces. Other work aims at obtaining workflow patterns through process mining. In fact, the term process mining *"refers to methods for distilling a structured process description from a set of real executions"* (van der Aalst et al., 2003b). A detailed analysis of different approaches for process mining and research challenges can be read in (van der Aalst et al., 2003b). Some exemplar approaches can be found in (van der Aalst et al., 2005), where the resultant workflows are represented as Petri Nets, and (Rozinat and van der Aalst, 2006), which introduces a whole framework for process mining. In the scientific workflow domain (Gómez-Pérez and Corcho, 2008) mines provenance traces to map them against a problem solving method library. The goal of the work is similar to the aforementioned approaches in business workflows, but in this case the authors aim to generalize the provenance and to help understand the traces.

Case-based reasoning is often used to find substitute workflows for a given one. In (Müller and Bergmann, 2014) the authors discuss the adaptability of workflows and look for substitutes according to user needs. Another approach presents an algorithm that combines control flow and dataflow of workflow traces, reasoning to generalize and approximate a given workflow (Yaman et al., 2009). This is part of the POIROT project (Burstein et al., 2009) for creating an architecture for reasoning and learning components for workflows. Finally, (Smirnov et al., 2012) also generalizes workflows to group common sets of components based on existing behaviors in the business domain.

During the development of this thesis, graph mining techniques have started to be used to extract common patterns using the myExperiment repository. An overview of the problem by extracting patterns with different metrics has been proposed in (Kamgnia Wonkap, 2014). 258 Taverna workflows were analyzed in (Diamantini et al., 2012),

as a first approximation using inexact graph mining techniques. Recently, (García-Jiménez and Wilkinson, 2014a) has followed up by enriching 530 workflows with domain specific knowledge in the biomedical domain. However, the lack of a gold standard to measure precision and recall makes these approaches difficult to validate at the moment.

As happened with the approaches designed for exploring repositories, the main difference between case-based reasoning, graph mining and process mining is that while process mining is based on a network of probabilities, the other two approaches always produce patterns that are found in the input workflow corpus. Figure 2.13 illustrates the difference between the results of a process mining and a graph mining approach, using as input the three workflows depicted on top. The fragments produced by a graph mining technique can be seen on the right, while the network of probabilities extracted from the workflows can be seen on the left. Although both approaches mine patterns, they are used for different purposes.

2.4 Summary

In this chapter we have described the most relevant related work in the areas of workflow representation, abstraction and reuse. For each of the areas, we have also introduced the main concepts that will be used throughout the thesis along with the general limitations of each approach.

Most of the described approaches focus on either representation, abstraction or reuse, but none of them tackle the three areas as part of the same problem. Very few models consider linking abstractions and patterns to the templates or execution traces themselves; even in those approaches developed in parallel with this thesis. For example (Cerezo, 2013) links conceptual workflows to the workflow instances, but does not tackle the execution trace representation. Models like the Research Object and ProvONE address the template and execution representation and linking, but avoid dealing with abstractions of processes. To date, there are barely any approaches that use domain knowledge to extract abstract patterns that may help reusing and exploring workflows on a given repository. There is also a lack of a common simple model that can be used to represent the basic workflow functionality of all workflow systems for mining purposes, or that represents workflows based on their step functionality.

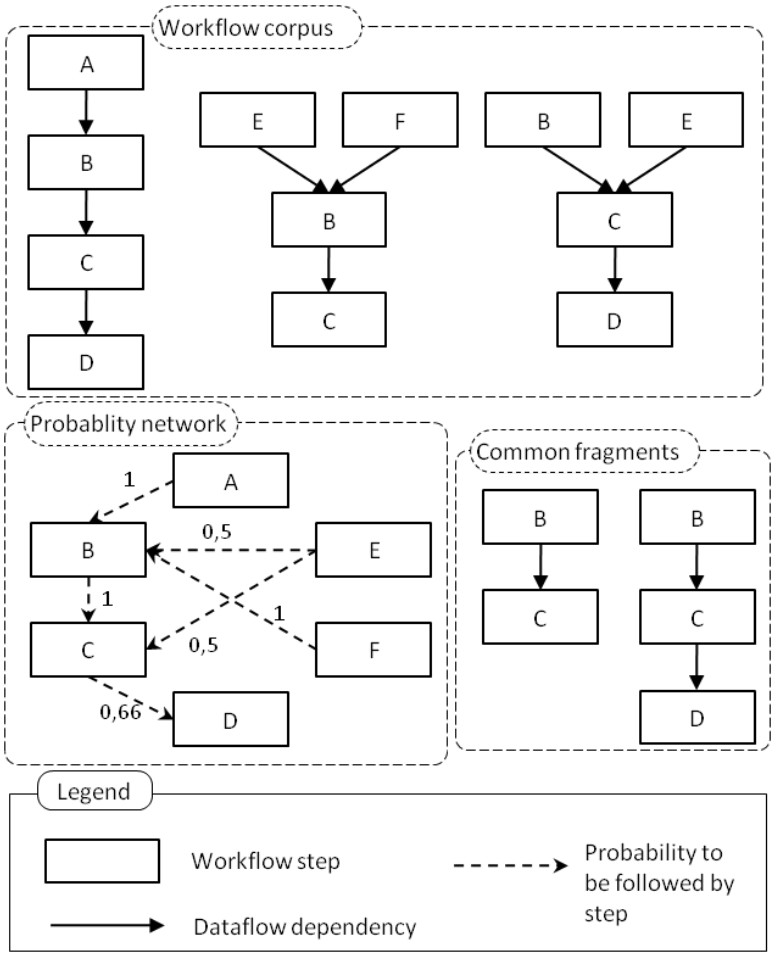


Figure 2.13: Difference in output: while process mining returns a network of probabilities, a graph mining approach focuses on the possible fragments found in the dataset. In the figure, the three workflows on the top lead to the probability network on the bottom left and to the two fragments on the bottom right. Inputs and outputs of each step have been omitted for simplicity.

Current mining approaches also present some limitations. Topic modeling, clustering and mining techniques may miss potential links between fragments of two dissimilar workflows. Graph mining or process mining techniques extract common workflow patterns, but they currently ignore whether these patterns are useful for reuse and how they can be used to link different workflow fragments together. Additionally, most of the approaches described for scientific workflows have been tested only in Taverna workflows. Further work is needed to analyze how users would interact in other types

of environment, e.g., smaller communities like a research lab, students of a university or a company.

In the next chapter we present our work objectives and hypothesis, relating them to some of the limitations that we have identified in the current state of the art.

Chapter 3

Research Objectives

The main goal of the research presented in this thesis is to facilitate workflow understanding and reuse by analyzing and abstracting an existent corpus of scientific workflows. This translates into three lines of work regarding scientific workflows. The first one is **workflow abstraction**, which refers to the ability of a system to generalize workflows (or workflow steps) by their common functionality. Workflow abstraction is key for simplifying workflows and for finding relations between them.

The second line, **workflow understanding**, relates to the ability of users to clearly determine the functionality of each of the steps (or group of steps) of the workflow. Workflow understanding benefits from workflow abstraction, as it helps simplifying the workflow at hand, and can be enhanced by including proper knowledge structure to documentation and examples on the target workflow. Workflow understanding is crucial to disseminate someone's work within the scientific community.

The third line is **workflow reuse**, closely related with the previous two. Having a clear understanding of the workflow functionality and its relationships with other workflows may help users decide whether a given workflow (or any of its sub-parts) can be adapted from a previous experiment or not.

This chapter introduces our main hypothesis (Section 3.1), its associated research challenges (Section 3.2) and defines our research methodology, research and technical goals (Section 3.3).

3.1 Research Hypotheses

We define our main hypothesis as follows:

Hypothesis 1 *Scientific workflow repositories can be automatically analyzed to extract commonly occurring patterns and abstractions that are useful for workflow developers aiming to reuse existing workflows.*

Our hypothesis can be divided into three different sub-parts, which overlap with the workflow understanding, reuse and abstraction aspects respectively. First, by *creating a catalogue of the most typical domain-independent scientific workflow patterns based on the functionality of workflow steps we can help users understand workflows better, independently of the workflow system where they were defined (**H1.1**).*

Second, *by detecting commonly occurring patterns and abstractions automatically we can find the implicit relationships between the workflows of a repository (**H1.2**).* Furthermore, for this purpose we hypothesize that the use of *graph mining techniques (**H1.2.1**) and the exploitation of domain specific metadata (**H1.2.2**) are good approaches for detecting and generalizing (or abstracting) common fragments automatically.*

Finally, by *highlighting those patterns that are potentially useful for users designing workflows we believe that we can help users reuse workflows (**H1.3**).*

A summary of the hypotheses and how they deal with workflow abstraction, understanding and reuse can be found in table 3.1

3.2 Open Research Challenges

Our hypotheses can be related to several research challenges. First, in order to determine a common format to deal with templates and provenance of workflows, we need to address the *workflow representation heterogeneity* in scientific workflows. Second, in order to find common reusable patterns, we must handle the *different levels of workflow abstraction* and *the difficulties for workflow reuse* of a given corpus. Finally, by detecting the common reusable patterns automatically we tackle the *lack of support for workflow annotation.* Each of these research challenges are further described below, and tackled throughout the thesis.

Table 3.1: Hypotheses and their respective addressed workflow research areas.

Hypothesis	Workflow Research Area
H1: Scientific workflow repositories can be automatically analyzed to extract commonly occurring patterns and abstractions that are useful for workflow developers aiming to reuse existing workflows	Abstraction, understanding, reuse
H1.1: It is possible to define a catalog of common domain independent patterns based on the common functionality of workflow steps	Abstraction, understanding
H1.2: It is possible to detect commonly occurring patterns and abstractions automatically	Abstraction, reuse
H1.3: Commonly occurring patterns are potentially useful for users designing workflows	Reuse

3.2.1 Workflow Representation Heterogeneity

As discussed in Chapter 2, a plethora of scientific workflow systems have been created to design, reuse, explore and execute scientific workflows for different scientific communities. Each community often has its own requirements for their experiments, which have led to the proliferation of heterogeneous formats for representing scientific workflows (e.g., for stream processing, distributed environments) specific built-in catalog support, cloud support, domain specific metadata capture, provenance exploration, etc. Despite some efforts to come up with a common workflow language, currently *there is no standard model for representing scientific workflows and their metadata (**RCRepresent1**).*

Furthermore, besides uploading resources individually to a public repository, *there are no general guidelines or methodologies for authors on how to expose a corpus of scientific workflows and their associated contents on the Web (**RCRepresent2**).*

3.2.2 Inadequate Level of Workflow Abstraction

Workflows may contain several scientifically-significant analysis steps, combined with other data preparation or result delivery steps (e.g., filtering, cleaning, etc.) that are auxiliary and not central to the science data analysis. In fact, studies have shown

that over half of the steps of workflows consist on data preparation steps that increase their complexity and obfuscate their main functionality (Garijo et al., 2012). Therefore in many cases *it is difficult to determine which are the main significant processing steps of the workflow (**RCAbstract1**)*, even when a textual description of the workflow functionality exists in a publication or other documentation. In this regard, patterns have been defined in other work to capture typical control flow properties on workflows (van der Aalst et al., 2003a). However, *there are no catalogs of the typical abstractions that can be found in scientific workflows based on their basic step functionality (**RCAbstract2**).*

3.2.3 Difficulties of Workflow Reuse

One of the key aspects of workflows is their potential shareability. Scientists often include workflows as sub-workflows (Starlinger et al., 2012) when the workflow system supports them. Several repositories of workflows like myExperiment, the LONI Pipeline, CrowdLabs or Galaxy store templates, metadata and sometimes even executions of past experiments. However, *it is difficult to determine the relation between different workflows regarding their functionality (**RCReuse1**)* and unless common reused workflow fragments are explicitly exposed by users as sub-workflows, *it is not easy to detect which workflows or workflow fragments are potentially useful for reuse (**RCReuse2**).*

3.2.4 Lack of Support for Workflow Annotation

Workflow authors have to describe manually the functionality of their workflows, their relationships to other workflows, their metadata and their inputs and outputs. *There are currently no approaches for facilitating these annotations in a semi-automatic way (**RCAnnot1**)*, even for the typical operations in workflows (e.g., formatting and merging inputs). Therefore, the textual annotations on workflows (besides basic metadata like creator, date and main purpose) are very few, and no standard is followed for describing workflow functionality and metadata.

A summary of the challenges tackled in this work and how they map to the hypotheses is presented in table 3.2.

Table 3.2: Open research challenges and their related hypotheses.

Research Challenge	Hypotheses
RCRepresent-1: There is no standard model for representing scientific workflows and their metadata	H1.1, H1.2
RCRepresent-2: There are no standard methodologies for publishing a corpus of scientific workflows and their associated resources in the Web	H1.1
RCAbstract-1: It is difficult to determine which steps perform the main significant processing steps in a scientific workflow	H1.1
RCAbstract-2: There are no catalogs of the typical abstractions that can be found in scientfic workflows based on their basic step functionality	H1.1
RCReuse-1: It is difficult to determine the relationship between different workflows regarding their functionality	H1.2
RCReuse-2: It is not easy to detect which workflows or workflow fragments are potentially useful for reuse	H1.3
RCAnnot-1: There are currently no approaches for assisting scientists with workflow annotation	H1.2

3.3 Research Methodology

The work presented in this thesis has been performed in an exploratory manner, following a layered approach motivated by the hypotheses. In each layer, the work has been validated experimentally, helping to refine the results obtained in previous layers.

Figure 3.1 shows a roadmap of the thesis work, where each layer represented on the left corresponds to a general problem. On the center and right of the figure we have specified our approach to tackle each of the layers and the evaluation followed to validate such approach. From top left to bottom right, the layers stand for the models we need for providing workflow descriptions reusing existing standards, validated through competency questions (Gruninger and Fox, 1994); the workflow abstraction effort for defining a catalog of typical abstractions in workflows (validated by comparing our proposal with workflow corpora from different systems); and the mechanisms developed to

automatically detect some of these abstractions on different workflow corpora (evaluated by defining concrete metrics and user feedback). We describe each of the layers next, indicating the technical objectives (i.e., objectives related to the development of software or analysis of existing solutions for a given challenge) and research objectives (i.e., those objectives aiming at finding new solutions for existing challenges) for each.

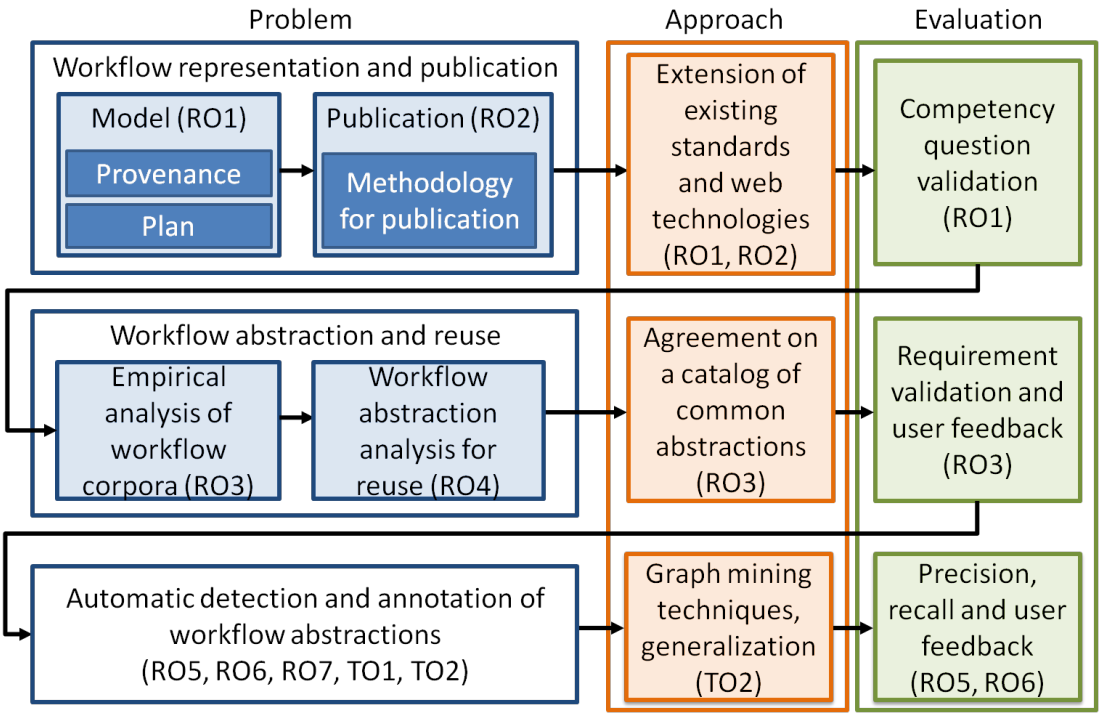


Figure 3.1: Roadmap of the thesis work, organized by the different problems, the approach followed to tackle each one and its proposed evaluation.

Workflow Representation and Publication: On a first layer, depicted as the top layer in Figure 3.1, we identify the requirements and develop the *models to represent workflow templates and their associated executions (**RO1**)*. The development is guided by the reuse of existing standards like the W3C Provenance Model, or commonly used vocabularies like the Open Provenance Model. The developed models are then used to *adapt an existing methodology for publishing content in the web to the scientific workflow domain (**RO2**)*. As a result, we produce a corpus of workflows which are accessible and easy to explore and exploit. The corpus also allows validating the requirements established for the models, helping to refine them accordingly.

Workflow Abstraction and Reuse: In our second layer we first perform a manual analysis on the published workflow corpus expanding it with the workflows available in other online repositories like myExperiment, CrowdLabs and Galaxy. The analyses aim at determining whether workflows in different domains and workflow systems share common functionality among their steps, producing as an outcome *a catalog of common workflow abstractions (**RO3**)*. The catalog is validated and refined with each new analyzed workflow, until no further abstractions can be obtained.

We then *analyze the current practices of users in workflows (and their fragments) in terms of workflow reuse, and we relate the results to the abstractions obtained in the catalog (**RO4**)*. This allows us to focus on the automatic detection of those abstractions that are relevant for workflow reuse.

Automatic Detection and Annotation of Workflow Abstractions: On our bottom layer we bridge the gap between a corpus of workflows and the catalog of abstractions defined in our second layer. We *apply graph mining techniques to detect potential abstractions automatically (**TO1**)*, *define filtering techniques for refining the obtained results (**RO5**)* and *propose metrics to validate our results against a corpus of annotated workflows (**RO6**)*. As a result, we *develop a system capable of finding common patterns automatically (**TO2**)*, and we validate it with further feedback from the users. Additionally, *we propose a model for describing workflow fragments and relate them to the workflows where they were found (**RO7**)*.

Table 3.3 summarizes the research objectives (ROs), technical objectives (TOs) and the research challenges from Table 3.2 that they tackle.

Table 3.3: Research and technical objectives and their related challenges.

Research Objective	**Research Challenge**
RO1: Define semantic models that represent workflow templates and executions, linking them together and capturing their basic metadata. The models should be based on existing standards	RCRepresent-1
RO2: Define or adapt a methodology for publishing workflows and their resources on the Web	RCRepresent-2
RO3: Define a catalog of common domain independent abstractions in scientific workflows	RCAbstract-1, RCAbstract-2
RO4: analyze the current practices of users in workflows in terms of workflow reuse, and we relate the results to the catalog	RCAbstract-1 RCAbstract-2
RO5: Define methods to filter non relevant fragment candidates	RCReuse-1, RCReuse-2
RO6: Define metrics for assessing the usability of a workflow fragment	RCReuse-1, RCReuse-2
RO7: Define a model for describing workflow fragments and relating them to the workflows where they were found	RCAnnot-1
TO1: Characterize the different types of existing graph mining algorithms, their features, their limitations and available implementations	RCReuse-2
TO2: Develop a framework for applying existing graph mining approaches on workflows, along with the means to refine and filter the results provided by the different algorithms	RCReuse-1, RCReuse-2, RCAnnot-1

Chapter 4

Scientific Workflow Representation and Publication

This chapter presents the Open Provenance Model for Workflows[1] (OPMW), our model to describe scientific workflows by capturing all their dataflow and dependencies, together with our approach for their publication. In doing so, we reuse existing standards and methodologies, which aim to make our results reusable and interoperable with other alternative approaches.

4.1 Scientific Workflow Model

We represent scientific workflows as labeled directed acyclic graphs (LDAGs). The nodes of the graph represent the steps, inputs, outputs and intermediate results and the edges represent the usage and generation dependencies among them. This choice of model is motivated by the amount of scientific workflow systems using this or very similar notation (as described on Chapter 2, some examples are Wings, the LONI Pipeline, Taverna, Galaxy, VisTrails, etc.). In addition, a graph based model enables the possibility of extending Semantic Web standards and reusing existing technologies to model and expose workflow information. In order to create a simple model, we focus on capturing data intensive workflow representations from a bottom up perspective, i.e., the most simple common constructs shared among all workflow systems. Therefore,

[1] `http://www.opmw.org/ontology/`

control constructs like loops and optional branches have been left out of the scope of the model.

Our model requirements, which have guided our development process, can be organized under three main categories:

- **Workflow template representation requirements**, which tackle the modeling of the workflow plan and its metadata. This includes the workflow template and workflow instance stages, introduced in Section 2.1.2.
- **Workflow provenance representation requirements**, which refer to the modeling of the execution of the workflow, its inputs, intermediate and final results. Provenance is crucial to determine the chain of events that led to a result of a scientific workflow, and which were the sources that influenced it.
- **Workflow attribution representation requirements**, which capture who created and collaborated in the creation of the workflow, its execution and documentation. Attribution is key for acknowledging the authors appropriately because it allows them to get credit for the work they have done. For example, the scientist responsible for designing the workflow (or a fragment of the workflow) may be different from the scientist who is responsible for its execution of a certain experiment.

The rest of the section describes how we have extended or reused existing vocabularies and standards to create OPMW and address each of the requirement categories described above. An Ontology Requirement Specification Document (ORSD) (Suárez-Figueroa, 2010) has been created for each of our proposed vocabularies, containing the competency questions (Gruninger and Fox, 1994) and the terms used to address them. The ORSD can be seen in the Annex A.

4.1.1 Representing the Provenance of Workflow Executions: The Open Provenance Model and W3C PROV

We use the W3C PROV standard and OPM (mentioned in Section 2.1.3.2) as foundational vocabularies and extend them to represent workflow executions as provenance records. In this section we briefly describe the core concepts of OPM and PROV that are relevant to our work, along with their main similarities.

4.1.1.1 The Open Provenance Model

OPM models the resources for which we want to obtain the provenance (e.g., an input of a workflow, an intermediate result, an output, etc.) as `artifacts`, which represent immutable pieces of state. The steps that use and produce artifacts are known as `processes` (action or series of actions performed on artifacts), and the entities that control those processes are `agents`. The relationships between artifacts, processes and agents are modeled in a provenance graph with five main causal edges: `used` (a process used some artifact), `wasControlledBy` (an agent controlled some process), `wasGeneratedBy` (a process generated an artifact), `wasDerivedFrom` (an artifact was derived from another artifact) and `wasTriggeredBy` (a process was triggered by another process). OPM also introduces the concept of `roles` to assign the type of activity that artifacts, processes or agents played when interacting with one another, and the notion of `accounts` and `provenance graphs`. An account represents a particular view on the provenance of an artifact based on what was executed. A provenance graph groups sets of related OPM assertions. OPM does not specify any concept for the modeling of plans, so it can only be used to describe workflow executions and it cannot be used to describe workflow instances or workflow templates.

OPM is available as two different ontologies that are built on top of each other. One is the OPM Vocabulary (OPMV)[2], a lightweight vocabulary implementation of the OPM model that only has a subset of the concepts in OPM but facilitates modeling and query formulation. Figure 4.1 (extracted from the online specification[3]) shows an overview of the main OPMV concepts, i.e., agents, processes and artifacts and their joint relationships. The other ontology is the OPM Ontology (OPMO)[4], which covers the full functionality of the OPM model, and can be used to represent OPM concepts that are not in OPMV, such as `account` or `role`. OPMO also includes the possibility of adding metadata to the relationships themselves (e.g., time of usage of an artifact in an activity) through a n-ary relationship pattern (Noy et al., 2006).

[2] `http://purl.org/net/opmv/ns`
[3] `http://open-biomed.sourceforge.net/opmv/img/opmv_main_classes_properties_3.png`
[4] `http://openprovenance.org/model/opmo`

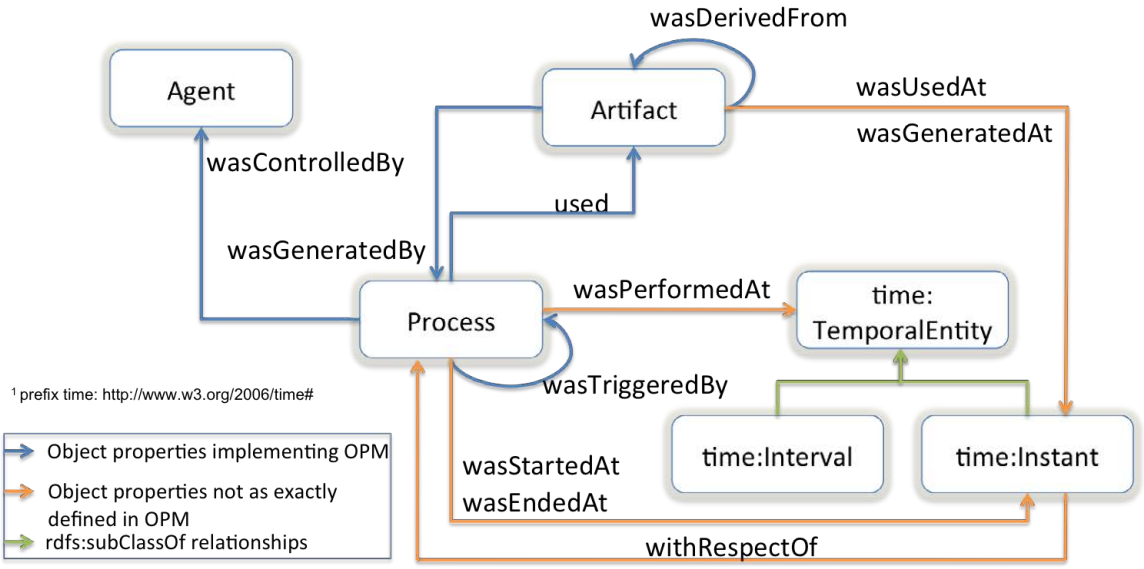


Figure 4.1: OPMV overview, extracted from its specification.

4.1.1.2 The W3C PROV Standard

The PROV model is heavily influenced by OPM. PROV models the resources as `entities` (which can be mutable or immutable), the steps using and generating entities as `activities`, and the individuals responsible for those activities as `agents`. As shown in Figure 4.2 (extracted from the online specification[5]), the relationships are also modeled in a provenance graph with seven main types of edges: `used` (an activity used some entity), `wasAssociatedWith` (an agent participated in some activity), `wasGeneratedBy` (an activity generated an entity), `wasDerivedFrom` (an entity was derived from another entity), `wasAttributedTo` (an entity was attributed to an agent), `actedOnBehalfOf` (an agent acted on behalf of another agent) and `wasInformedBy` (an activity used the entity produced by another activity).

PROV also keeps the notion of `roles` to describe how entities, activities and agents behaved in a particular event (usage, generation, etc.); and provides the means to qualify each of those roles using an n-ary pattern. Unlike OPM, PROV allows stating the `plan` associated with a certain activity, although the plan definition itself is out of the scope of the model (since it is not something that necessarily happened, for example, if a step of a plan failed).

[5] `http://www.w3.org/TR/prov-o/#starting-points-figure`

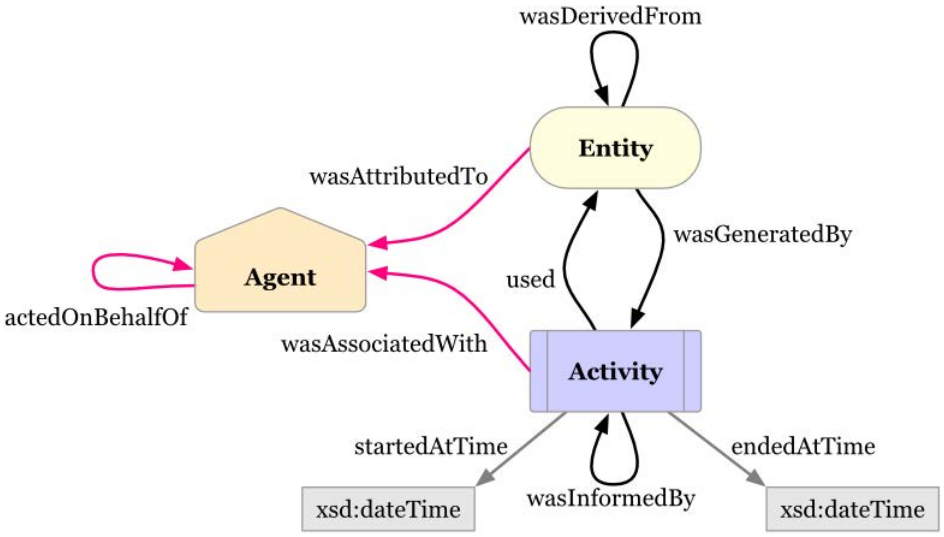


Figure 4.2: PROV overview, extracted from its specification.

PROV statements can be grouped in sets called `bundles`, which are entities themselves (thus allowing for their provenance to be described). The PROV standard is available as an ontology (PROV-O) (Lebo et al., 2013).

4.1.1.3 Comparison Between OPM and PROV

There is a very clear correspondence between OPM and PROV, and this facilitates the reuse of workflows represented in one language by tools that consume the other.

Figure 4.3 illustrates the commonalities between OPM and PROV that are relevant to our work. Entities and artifacts are depicted as ovals, activities and processes as boxes and agents as pentagons following the W3C notation[6]. Both models represent resources being used and generated by processes or activities which are controlled by an agent responsible for its execution. Entities (or artifacts, respectively) can be derived from other entities. Also, in OPM processes might be triggered by other processes, while in PROV activities might receive an input created by another activity (being informed by the other activity). We exploit these commonalities to integrate traces that comply with each of the models.

[6] `http://www.w3.org/2011/prov/wiki/Diagrams`

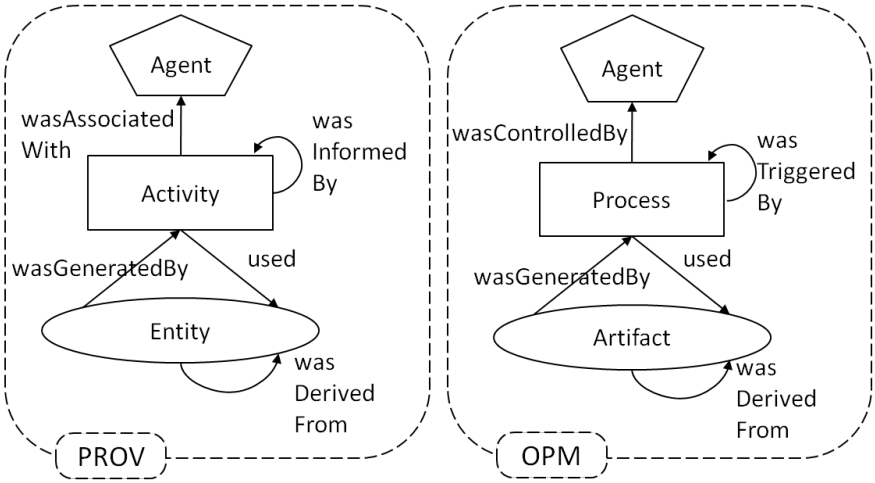


Figure 4.3: The commonalities between PROV (left) and OPM (right) facilitate mappings across both representations.

4.1.2 Representing Workflow Templates and Instances: P-Plan

We cannot use a provenance language like OPM or PROV to represent workflow templates and workflow instances: a provenance model describes things that have already happened, while templates and workflow instances are plans that will be executed at some point in time. Therefore we need a language that can represent process models or plans that when executed lead to a provenance trace that can be expressed in OPM or PROV.

P-Plan[7] (Garijo and Gil, 2012) is an extension of PROV for representing scientific processes (e.g. laboratory protocols (Giraldo et al., 2014), workflow infrastructure (Santana-Pérez and Pérez-Hernández, 2015), social computation (Markovic et al., 2014), etc.), and we use it to represent scientific workflows. Figure 4.4 shows an overview of the P-Plan vocabulary. In order to distinguish between the classes and properties of PROV and P-Plan, we have added prefixes to them ("`prov:`" and "`p-plan:`" respectively). A `plan` in P-Plan is a subclass of `plan` in PROV. The plan `steps` represent the planned execution activities. Plan steps may be bound to a specific executable step (`correspondsToStep` relationship) or refer to a class of steps, providing an abstraction layer over the execution. As a result, a plan step could be carried out in different ways in different executions of the same plan. A step may not have a corre-

[7] `http://purl.org/net/p-plan#`

sponding activity in the execution trace, (for example if there is an execution failure). A plan `variable` represents the inputs of a step and can have properties (i.e., type, restrictions, metadata, etc.). Plan steps may be preceded by plan steps (`isPrecededBy` relationship), and have variables as input (`hasInputVar` relationship). Variables are output of the plan steps (`isOutputVarOf` relationship) and may be bound to the inputs or outputs of executable steps (`correspondsToVariable` relationship). Both steps and variables are associated with a plan with the `isStepOfPlan` and `isVariableOfPlan` relationships respectively. The relation of the plan with agents involved in its execution is not specified in P-Plan, since it can be modeled with PROV. All the statements involved in the execution of the plan are grouped as part of a plan `bundle` (subclass of a `bundle` in PROV), which is `derivedFrom` the plan.

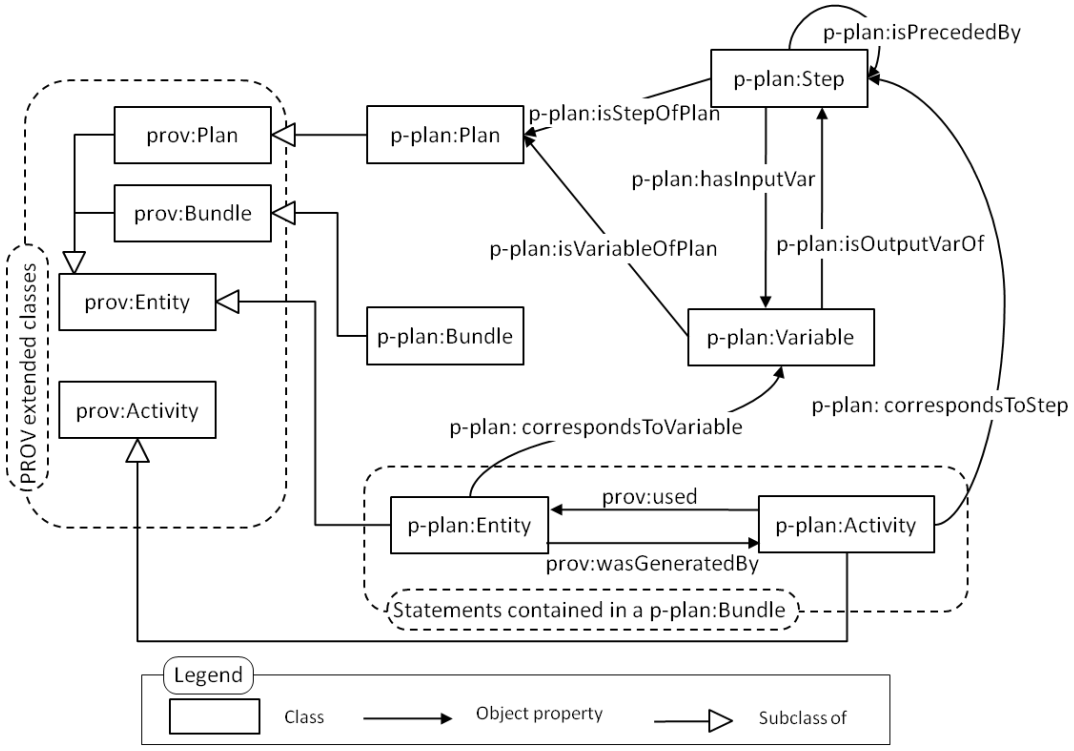


Figure 4.4: Overview of P-Plan as an extension of PROV.

Finally, plans may be included as part of other plans, e.g., when a set of steps are used several times through different plans. In order to capture this behavior, P-Plan defines the relationships `isSubPlanOfPlan`, which allows linking a plan to another, and the relationship `isDecomposedAsPlan`, which specifies how a step of a plan is expanded

itself as another plan. When this happens, the step representing the sub-plan becomes a `multiStep`. An example is shown in Figure 4.5, where a plan with two steps is used as part of another plan.

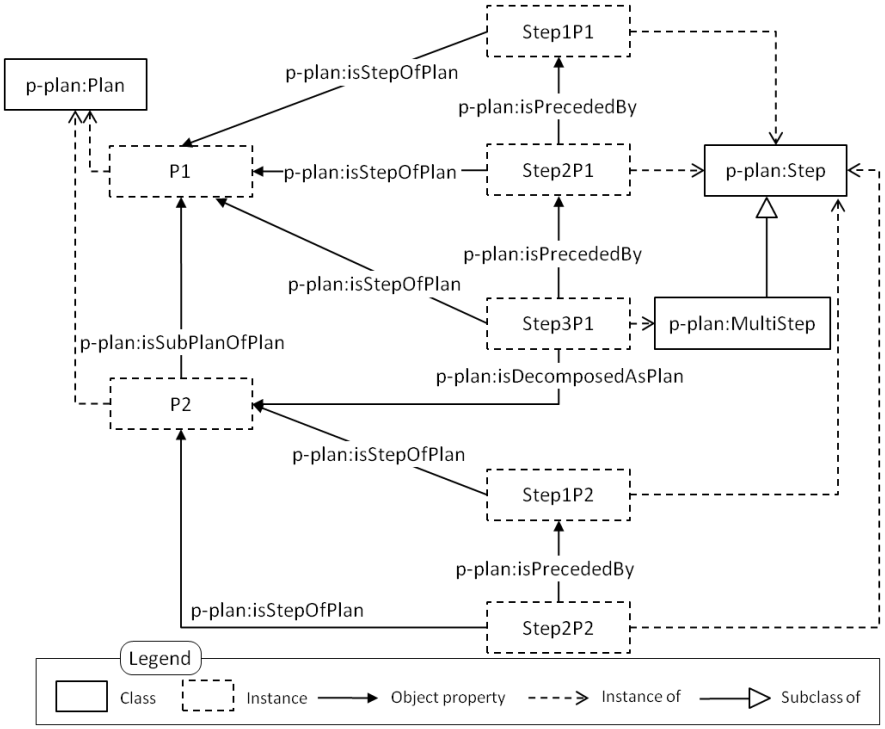


Figure 4.5: Sub-plan representation in P-Plan: A plan (P2) with two steps is contained as the third step of another plan (P1) with 3 steps.

4.1.3 OPMW

Workflow templates, instances, and executions can be represented with the OPMW model[8] (Garijo and Gil, 2011). OPMW extends P-Plan for addressing the template representation requirements, and PROV and OPM for the provenance representation requirements. OPMW supports the representations of workflows at a fine granularity with a lot of details pertaining to workflows that are not covered in those more generic models. OPMW also allows the representation of links between a workflow template, a workflow instance created from it, and a workflow execution that resulted from an instance. Finally, OPMW also supports the representation of roles and attribution

[8] `http://www.opmw.org/ontology/`

metadata about a workflow. Figure 4.6 shows the relationships between the different vocabularies and how OPMW extends PROV, OPM and P-Plan. Further details on linking between workflow templates, instances and executions, role modeling and workflow attribution in OPMW are described below.

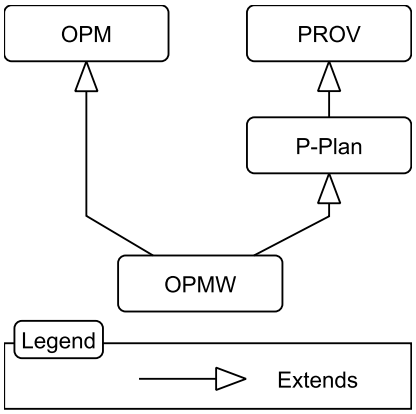


Figure 4.6: OPMW and its relationship to the OPM, PROV, and P-Plan vocabularies.

4.1.3.1 Linking templates, instances and executions in OPMW

In OPMW, a `workflow template` is a subclass of a P-Plan's `plan` (since it is a particular type of plan), a `workflow template process` is a subclass of P-Plan's `step` and a `workflow template artifact` extends the P-Plan's `variable` (since both of them refer to a particular domain). On the execution side, each `workflow execution process` (subclass of PROV's `activity` and OPM's `process`) is bound to a `workflow template process` via the `correspondsToTemplateProcess` relationship (subproperty of P-Plan's `correspondsToStep`). Similarly, each `workflow execution artifact` (subclass of PROV's `entity` and OPM's `artifact` respectively) is linked to its abstract `workflow template artifact` with the `correspondsToTemplateArtifact` relationship (subproperty of P-Plan's `correspondsToVariable`). Finally, the `workflow execution account` containing all the provenance statements of the execution is linked to the `workflow template` that contains all the assertions of the template with the `correspondsToTemplate` relationship.

Figure 4.7 shows an example of the OPMW vocabulary extending OPM, PROV and P-Plan. Each vocabulary concept and relationship is represented with a prefix to help understand its source (OPMW, P-Plan, PROV, OPMV or OPMO). In the

figure, a workflow template with one sorting step, an input and an output (on the top right of the figure, represented using P-Plan) is linked to its provenance trace on the bottom right of the figure (depicted with PROV and OPM). Each activity and artifact is linked to its respective step and variable. Additional metadata of the variables (e.g., constraints), steps (e.g., conditions for execution) activities (e.g., used code), artifacts (e.g., size, encoding), account (e.g., status) and template (e.g., associated dataflow graph) is modeled with OPMW, but has been omitted from the figure for simplicity.

As the figure illustrates, there is a clear correspondence between workflow templates (on the top) and workflow execution traces (on the bottom). The workflow instance is implicitly represented, as it can be derived from both the workflow template and the workflow execution trace: the workflow instance would have the same structure as the workflow template, using the workflow inputs and the references to the specific algorithms of the workflow execution trace.

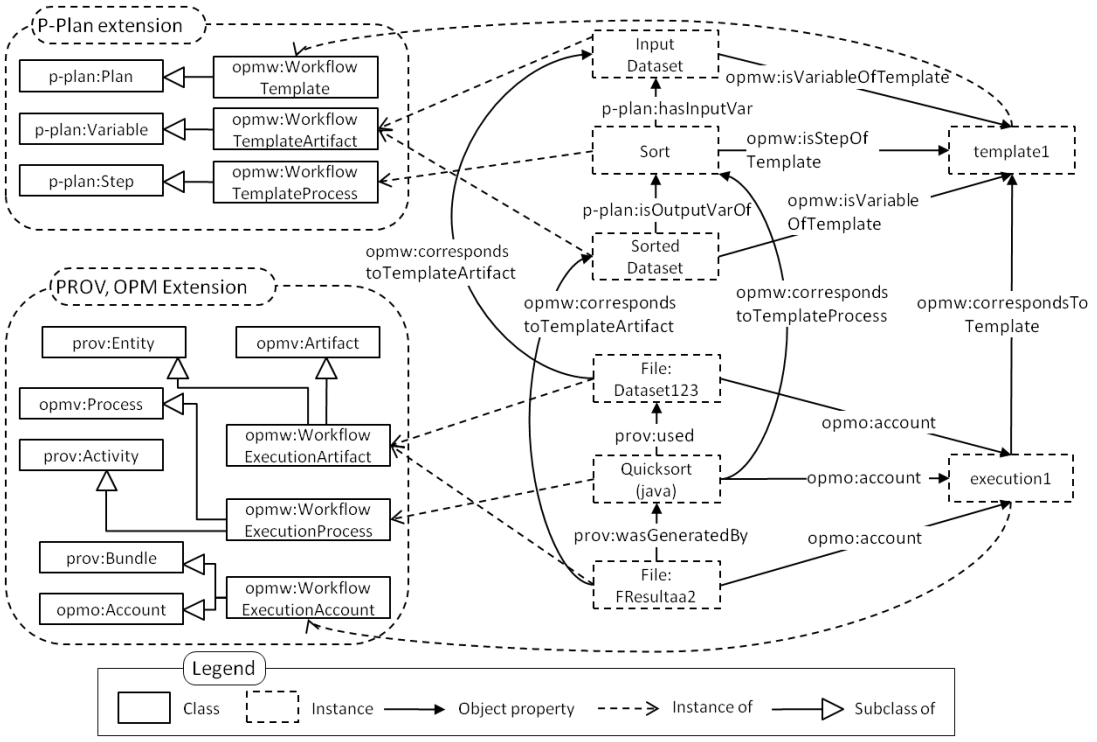


Figure 4.7: Example of OPMW as an extension of PROV, OPM and P-Plan. A workflow execution (bottom right) is linked to its workflow template (top right). Other details like attribution metadata have been omitted to simplify the figure.

4.1.3.2 Role Capture in OPMW

Workflow steps consume inputs and produce outputs with different roles, which may be crucial to understand how the execution process was carried out. For example, consider the execution of a component for removing duplicate genes that is depicted in Figure 4.8. The component had two datasets of genes as inputs and two datasets of genes as outputs. One of the inputs had the role *knownGenes*, the other had the role *foundGenes*. One of the outputs had the role of *discoveredGenes* and the other output was *discardedGenes*. All the inputs and outputs were datasets of genes, and their role labels are the identifiers that describe how each data was related to the process carried out. Thus, the *knownGenes* role qualifies the usage relationship in which the input *datasetA* and the process *removeDuplicates* were involved.

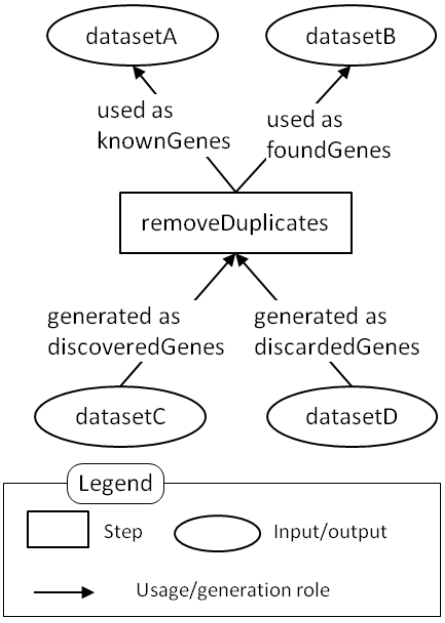


Figure 4.8: Example of roles: an executed workflow step used two datasets of genes (*Dataset A*, *Dataset B*) and produced two datasets of genes (*Dataset C*, *Dataset D*). Each dataset played a different role in the process.

In OPM and PROV this qualification of relationships is captured through an n-ary relationship pattern (Suárez-Figueroa et al., 2007), linking an instance of a role to the usage or generation edges. However, this option adds complexity to the model, as it forces us to introduce an indirection through intermediary resources in order to qualify

the relationship. An example can be seen in Figure 4.9, where we qualify in PROV (on the left) and OPM (on the right) the usage relationship between *removeDuplicates* and *datasetA* to introduce the role.

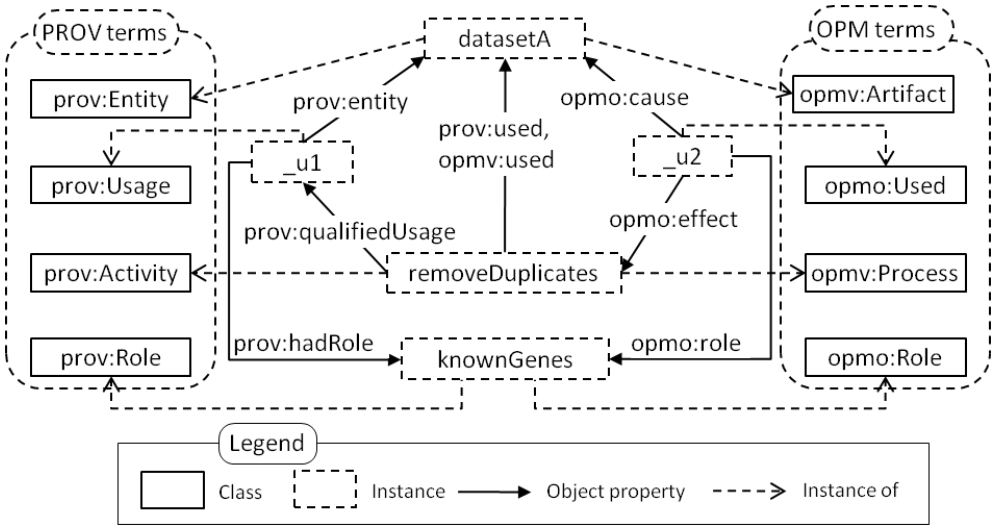


Figure 4.9: Qualifying a usage relationship in PROV (on the left of the figure) and OPM (on the right). Both models use an n-ary pattern (*Usage* and *Used*) to link *datasetA* with the *removeDuplicates* step and the *knownGenes* role.

Instead, we extend the usage or generation properties of both vocabularies with the role. The extension is not part of OPMW itself but part of the domain specific vocabulary used to describe the workflow steps. Figure 4.10 shows an overview of this approach, illustrating the example of Figure 4.8. The prefix "`ex`" has been used to identify the relationships extending OPM and PROV to identify the role (e.g., `ex:usedAs_knownGenes`). As shown in the figure, all the role subproperties are used to link the respective datasets with the process in a simpler manner than in Figure 4.10. Additional information of the property can be added as metadata description of the property (e.g., label, description, etc.).

4.1.3.3 Workflow Attribution in OPMW

Attribution is crucial for scientists who design, create and publish workflows, and OPMW can be used to represent such metadata in workflow templates, instances, and executions. For this, OPMW reuses terms from the Dublin Core (DC) Metadata

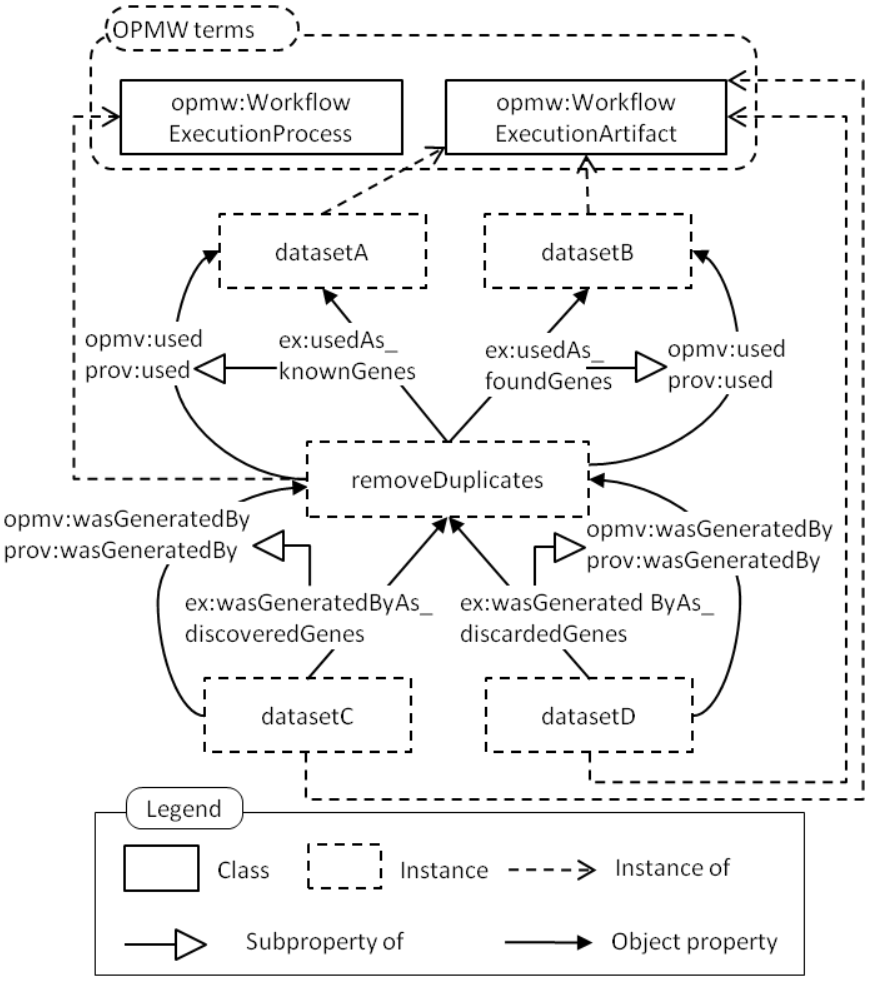


Figure 4.10: Role capture in OPMW: the roles of the inputs and outputs used and generated by the activity *removeDuplicates* extend the OPM and PROV usage and generation properties.

Vocabulary[9], namely author, contributor, rights and license. OPMW also defines additional terms for referring to the start and end of the whole execution of the workflow, the size of the produced files, the status of the final execution, the tool used to design the workflow, the tool used to execute the workflow, etc. Figure 4.11 shows an example, where a template created by an agent (*Phil*) and later modified by another agent (*Daniel*) using a workflow editor (*Wings*) has been successfully executed using two workflow execution systems (*Pegasus* and *Condor*).

[9] `http://dublincore.org/documents/dcmi-terms/`

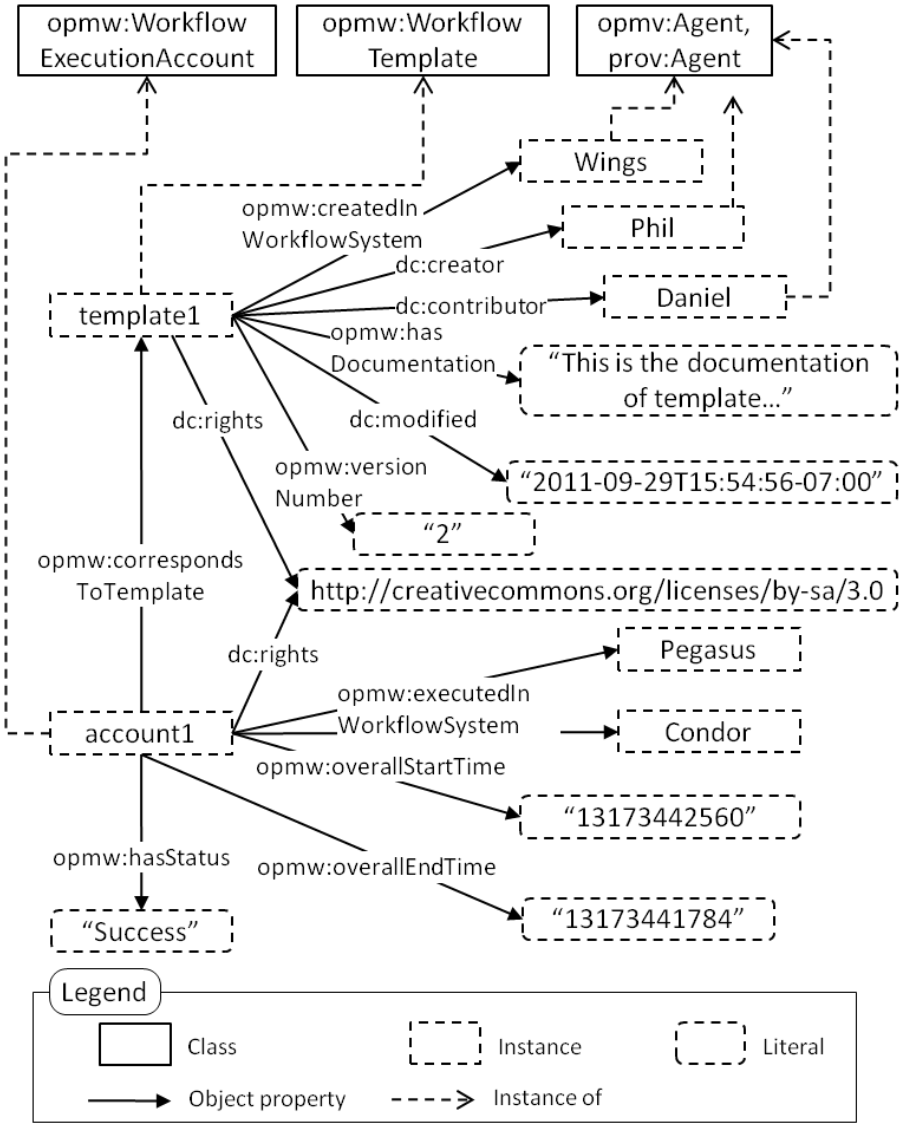


Figure 4.11: Example showing attribution metadata capture in OPMW.

4.2 Scientific Workflow Publication

As we have shown in the related work section, scientists make their workflows public using repositories like myExperiment, Galaxy or the LONI Pipeline. This normally follows a manual process, which relies on the users to describe the workflow and provide additional metadata. Furthermore, this only makes accessible the workflow itself, and to explore each workflow step it is necessary to download it locally. In this sec-

tion we describe our approach for publishing workflows and their executions as linked web resources, along with its benefits and showing a functional example in the Wings workflow system (Gil et al., 2011).

4.2.1 Workflows as Linked Data Resources

Publishing the templates and execution traces of scientific workflows is a crucial step for reuse, reproducibility and understanding. In order to be able to reference all the resources of a workflow template and its associated workflow executions properly, we use Universal Resource Identifiers (URIs) (Berners-Lee et al., 2005) following the Linked Data principles[10] (Bizer et al., 2009). URIs provide the mechanism to refer to the different resources of a workflow unambiguously, while the principles consist of a set of rules or expectations which indicate how the URIs should behave when someone (human or machine) accesses them.

The Linked Data principles state (Bizer et al., 2009): 1) that we should "*use URIs as names for things*", 2) that we should "*use HTTP URIs so that people can look up those names*" (making those URIs resolvable and available in any browser), 3) that we should "*provide useful information when someone looks up a URI*" (by showing the resources that are related to the URI) and 4) that we should "*include links to other URIs*", so that whoever is exploring the data can discover other resources. When a URI complies with the four principles, it becomes a *Linked Data URI*.

Using Linked Data URIs enables several important advantages to the publication of scientific workflows:

- **Linking to third party web resources**, which could be used for the input of scientific workflows. For instance, referring to proteins in the Protein Data Bank by using their published URI;
- **Get linked from other applications** by pointing to the URIs that we publish, which include both the workflows and the data generated by them;
- **Produce interoperable results** within different systems without having to define particular catalog structures and access interfaces.

[10] `http://www.w3.org/DesignIssues/LinkedData.html`

However, publishing Linked Data is not straightforward. There are several decisions and naming conventions to take into consideration when making the URIs accessible. In the following section we present a Linked Data publication methodology adapted to scientific workflows.

4.2.2 A Methodology for Publishing Scientific Workflows as Linked Data

Although there are publications that introduce and explain the Linked Data generation and publication process (Heath and Bizer, 2011), there are no methodologies that indicate the steps to follow in the scientific workflow domain. Therefore, we have adapted an existing methodology used in the publication of governmental data (Villazón-Terrazas et al., 2012, 2011) and other domains like energy consumption (Radulovic et al., 2015) to achieve our purpose.

The methodology consists on five main steps that are described as follows:

- **Specification**, which consists on an effort to identify the set of data sources to use, decide on their URI design and agree on a license for the resulting dataset.
- **Modelling**, where the users decide which vocabularies should be used to expose the data.
- **Generation**, which summarizes the process of transforming the data from their heterogeneous formats to RDF with the help of existing tools; cleaning the data and linking it with other existent sources.
- **Publication**, where the resulting dataset and its metadata is made available by using a triplestore (i.e., a database for the storage and retrieval of RDF (Villazón-Terrazas et al., 2011)).
- **Exploitation**, which consists on the usage of the published data through browsers for enabling their consumption manually or automatically.

Many of the steps of the methodology can be easily adapted to scientific workflows. For the *specification step*, the set of data sources to use is reduced to deciding the workflow management systems we want to integrate. From each workflow management

system it is necessary to identify how they specify workflow templates, workflow instances and execution traces, as those are the files that will have to be transformed and linked to each other when publishing the data.

The URI design is almost the same as in the original methodology. The base URI should be a URL under a domain of our control, the URIs for the ontology terms should have the word "ontology" on their schema and the URIs for the assertions or instances should have the word "resource" followed by the class name of the instance. In the scientific workflow domain we may want to distinguish different releases of the execution traces. Therefore we have included an optional parameter indicating the dataset name under which the data is made public:

Base URI = http://mydomain.org

Ontology URI = http://mydomain.org/ontology

Assertion URI = http://mydomain.org/[dataset/]resource/ClassName/instanceName

Regarding the appropriate license, publishers should first discuss the privacy issues and requirements of the data about to be released. In some domains privacy is a concern (e.g., for some workflows processing genomic data), in those cases an open license would not be appropriate. However, there are many areas of science where privacy is not an issue and that would benefit tremendously from an open license for sharing both data and workflows as Linked Data. Since the goal of publishing a scientific workflow is to make it available for others to reuse and repurpose, we recommend to use an open license. Several catalogs of licenses are already available on the Web[11] [12] [13], and can be used for selecting the most appropriate one.

For the *modeling step*, we propose to use and adapt the OPMW vocabulary introduced in Section 4.1.3, although other more recent PROV based vocabularies like the Research Object ontologies (Belhajjame et al., 2015) or ProvONE[14] could be used as well.

The *generation step* may be considered the most complex step in the whole process, as it depends on the features of the workflow system. Normally the templates, instances and execution traces can be exported from the workflow system and have to be mapped

[11] `http://datahub.io/es/dataset/rdflicense`
[12] `http://creativecommons.org/`
[13] `http://opendatacommons.org/licenses/`
[14] `http://purl.org/provone`

to the representation model chosen in the modeling step. Although several tools are proposed in the methodology to help in the conversion (Villazón-Terrazas et al., 2011), it is often necessary to develop a script that performs the transformation. The script should create the appropriate URIs to refer to the resources, instead of relying on the local IDs proposed by the workflow system. A very important aspect of this step is that templates, instances and traces have to be linked to each other according the representation model in order to be able to exploit these relationships later. In our methodology we exclude linking workflow inputs to other datasets of the Linked Open Data cloud, as we focus on making public the workflow contents for their reusability.

Finally, the *publication step* and *exploitation step* are followed as in the original methodology by using the set of tools proposed in (Villazón-Terrazas et al., 2011). We illustrate the whole methodology with an example in the next section.

4.2.3 Linked Data Workflows: An Example

In order to describe how each of the steps can be applied in practice, we have applied our methodology successfully to the Wings workflow system (Gil et al., 2011).

For the specification step, we chose to export and link workflow templates and execution traces out of the logs produced by the system. All the URIs generated by our system are "Cool URIs"[15], following the W3C recommendations. This means that they are produced under a domain under our control, they are unique, and they are not going to change. Each URI identifies a different resource that can be individually accessed and dereferenced with content negotiation (i.e., the same URI can handle requests for users (returning HTML) and machines (returning RDF)). By following our methodology, we decided to apply the following URI naming scheme:

Base URI = http://www.opmw.org/

Ontology URI = http://www.opmw.org/ontology/

Assertion URI = http://www.opmw.org/export/resource/ClassName/instanceName

As for the license, we chose the Creative Commons Attribution-ShareAlike 3.0[16], which allows anyone to reuse the published data if proper attribution is provided.

The modeling step is performed with the OPMW vocabulary. Then, in the generation step, Wings execution traces and instances are converted automatically to OPMW

[15] `http://www.w3.org/TR/cooluris/`

[16] `http://creativecommons.org/licenses/by-sa/3.0/`

with a transformation script[17]. Camel case notation is used for composing the identifiers of classes and instances, and a MD5 encoding (Rivest, 1992) is used to generate a unique identifier for each resource when necessary (e.g., a used file, an execution step, etc.).

For the publication step, the RDF files are loaded into a triple store and made public through a public endpoint (i.e., an access point for both human users and machines). We have selected Openlink Virtuoso[18] as our triple store because of its robustness, support from the community and mechanisms to create a public access. An additional file store is needed to store the files referred to in the links available in the triple store (inputs, intermediate results and outputs of the workflows). The file store is available in our local servers (http://www.opmw.org).

Now the endpoint can be exploited through generic visualizing tools like the linked data browser Pubby[19] or the workflow explorer WExp[20] (which we developed to explore the available data easily), but it can also be accessed programmatically from other applications. The access point for a workflow is simply a URI (of a workflow template or an execution), and all the components and datasets in the workflow can be accessed from it.

For example, a template called "Aquaflow_edm" would have the URI "`http://www-.opmw.org/export/resource/WorkflowTemplate/AQUAFLOW_EDM`" (template names are unique in Wings) and type `WorkflowTemplate`, (i.e. http://www.opmw.org/ontology/-WorkflowTemplate). As shown in Figure 4.12, by simply resolving the URI in a browser, a user would see an HTML page[21] with the descriptions involving that URI, i.e., the provenance of the template (contributor, license, primary source, documentation, etc.), the steps and variables that belong to the template, the executions associated with the template and the rest of its metadata. If we edit the request headers to ask for a machine-readable representation, we would receive the same information in the appropriate syntax (e.g., Turtle[22] or RDF/XML[23], depending on the request). This approach

[17] `https://github.com/dgarijo/WingsProvenanceExport`
[18] `http://virtuoso.openlinksw.com/`
[19] `http://wifo5-03.informatik.uni-mannheim.de/pubby/`
[20] `http://purl.org/net/wexp`
[21] `http://www.opmw.org/export/page/resource/WorkflowTemplate/AQUAFLOW_EDM`
[22] `http://www.w3.org/TR/turtle/`
[23] `http://www.w3.org/TR/rdf-syntax-grammar/`

can be used to access any resource (by resolving its URI) from any template or execution stored in the repository. If a user or program aims to perform a more complex query (e.g., returning all the stored templates with at least two executions), they may issue it to the public SPARQL endpoint[24], which will check and return the results in the desired format. Some query examples and pointers to resources can be browsed online[25].

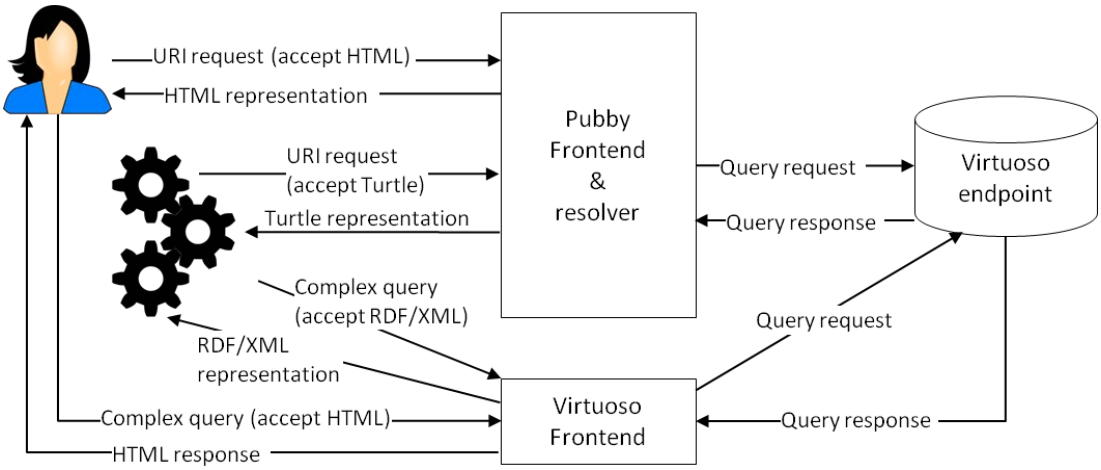


Figure 4.12: Different approaches for accessing workflow resources: a user may request to resolve a URI of a workflow by browsing a web page (HTML representation). Instead, a machine would request a machine readable format like RDF/XML or Turtle. For both machines and human users, more complex queries about resources may be issued through the public endpoint.

4.3 Summary

In Section 4.1.3 we have described OPMW, the model we developed to represent scientific workflow templates, instances and execution traces along with a methodology to make them public as linked data resources. OPMW is aligned to existing standards like PROV and reuses well-known models like OPM. In addition, we tested and validated OPMW by successfully answering our competency questions and by including the model as part of the WEST workflow ecosystem (Garijo et al., 2014d), where a set

[24] `http://opmw.org/sparql`
[25] `http://opmw.org/node/6`

of heterogeneous tools for workflow design, analysis and execution use it as an intermediate representation. Thus, OPMW is interoperable with applications consuming both PROV and OPM models and addresses the first research objective of this thesis (RO1, *definition of a model based on standards that represents and links workflow templates, execution and their associated resources*).

OPMW was designed to represent the most simple workflow constructs that are common to most scientific workflow systems (i.e., the relation between workflow templates, instance and executions, usage and generation of inputs, intermediate results and outputs and their key metadata), leaving more complex constructs like conditional branches or loops out of scope of the model. The rationale behind this decision is that a simpler representation may enable a better understanding (and hence, adoption) among the community, facilitating retrieving key metadata of each input and workflow step of the workflow and helping to understand the dataflow. In this regard, OPMW was designed to expose workflow information on the Web in a simple manner. As described in Section 2.1.3, there are more complex models for workflow interchange between different workflow systems (e.g., BPEL, SHIWA) to which OPMW can be mapped for exploiting this information.

Table 4.1 shows a comparison between OPMW and other recent approaches for representing scientific workflows and their relationships. On the one hand, the most similar approaches are the Research Object (Belhajjame et al., 2015) and ProvONE[26] models, which aim to provide a simple representation of workflows. In essence, the difference among the models is small, and part of the reason for the overlap is that they have been developed in parallel. Some of the differences are that the RO and ProvONE models have support for explicitly modeling sub-workflows and use data links to specify the connections between components of workflows. Instead, OPMW connects input data and output data to the workflow steps directly, in order to simplify the overall representation. Additionally, OPMW has explicit relationships for capturing workflow metadata. Since all these vocabularies extend the PROV standard, their representations are compatible at a higher level of abstraction.

On the other hand, the Conceptual Workflow model (Cerezo, 2013) is a top-down approach, with a different scope than OPMW. Rather than providing a simple representation between workflow templates and execution traces, the Conceptual Workflow

[26] `http://purl.org/provone`

Table 4.1: Comparison between OPMW and other scientific workflow vocabularies for representing workflow templates, instances and execution traces. The asterisk (*) on the WT column indicates that the model makes no distinction when representing WT and WI.

Approach	Domain	Control-based constructs	WT constructs	WI constructs	WET constructs	Metadata constructs
Research Object	Scientific workflows	No	Yes*	Yes	Yes	No
ProvONE	Scientific workflows	No	Yes*	Yes	Yes	No
Conceptual Workflows	Scientific workflows	Yes	Yes	Yes	No	No
OPMW	**Scientific workflows**	**No**	**Yes***	**Yes**	**Yes**	**Yes**

model studies how an abstract process can be transformed into a specific workflow. The scope is therefore in modeling and representing the relationship between abstract workflow templates and instances, which may follow a layered abstraction.

In section 4.2.2 we described a methodology that addresses the second research objective of this thesis (RO2, *definition of a methodology for publishing workflows and their resources on the Web*). The methodology facilitates the publication of whole sets of workflows and their associated resources automatically, simplifying this task for the user. Following our methodology, we created a repository of online accessible workflows and traces which will be used in the next stages of our work. To our knowledge, this is the first repository of fully resolvable linked scientific workflows and executions[27].

[27] accessible at `http://www.opmw.org/sparql`

Chapter 5

Workflow Abstraction and Reuse

As stated in Chapter 3, one of our hypotheses aims to determine whether patterns and abstractions can be obtained from a repository of workflows (H1.1). In particular, our goal is to find those abstractions that capture generic features of groups of workflows (or workflow fragments) independently from their contexts. For example, one way of achieving abstraction is by publishing workflow templates and linking them to their provenance executions traces. The templates act as a high level abstraction of a set of executions, grouping them as entities with the same original plan. Other types of abstractions may be obtained with the different types of workflow abstractions introduced in Chapter 2.2, such as macro abstraction, skeletal planning or layered abstraction.

However, even after defining these abstractions, workflows may be difficult to understand due to their their complex nature. A workflow may contain several scientifically-significant analysis steps, combined with auxiliary data preparation or result delivery activities, and in different implementation styles. This difficulty in understanding stands in the way of reusing workflows by potential adopters. In this chapter we aim to address this issue by performing several analyses, from both abstraction and reuse perspectives.

In Section 5.1, we characterize the domain independent conceptual abstractions for workflow steps that can be found in scientific workflows upon manual inspection. We refer to these abstractions as *workflow motifs*, and we have defined them after analyzing workflows manually from several workflow systems. Motifs are provided through (i) a characterization of the kinds of data-operation activities that are carried out within workflows, which we refer to as *data-operation motifs*, and (ii) a characterization of

the different manners in which those activity motifs are realized/implemented within workflows, which we refer to as *workflow-oriented motifs*.

In Sections 5.2 and 5.3 we explore how users reuse workflows and workflow fragments, analyzing whether those motifs related to workflow reuse are relevant for users or not. The analyses were performed from different perspectives. One analysis consists of an automatic processing of workflows, while the other one surveys users on the usefulness of reusing workflows and workflow fragments.

5.1 Workflow Motifs

In order to *define a catalog of common domain independent abstractions in scientific workflows* (objective RO3 of this thesis) we performed a manual analysis of the current practices in scientific workflow development. The objectives of the analysis were the following:

1. To reverse-engineer the set of current practices in workflow development through an empirical analysis.

2. To identify workflow abstractions that would facilitate understandability and therefore effective reuse.

In this section we present the results of the empirical analysis, performed manually over 260 workflow descriptions from four different workflow management systems. Based on this analysis, we propose a catalog of common workflow motifs.

5.1.1 Experimental Setup

We used workflows from Taverna (Wolstencroft et al., 2013), Wings (Gil et al., 2011), Galaxy (Goecks et al., 2010) and VisTrails (Scheidegger et al., 2008). The choice of these systems was due to the availability of workflow corpora through repositories (as introduced in Section 2.1.4.2, myExperiment (Roure et al., 2009) for Taverna, CrowdLabs (Mates et al., 2011) for VisTrails and the public endpoint we created in Section 4.2.2 (Garijo and Gil, 2011) for Wings) and portals (for Galaxy[1]), but also because of their core similarities:

[1] `https://main.g2.bx.psu.edu/`

- They provide similar workflow modeling constructs. The selected workflow systems are data flow oriented, which is consistent with our models, and they operate on large and heterogeneous data.

- All of them are open-source scientific workflow systems, initially focused on performing in-silico experimentation in the life sciences (Taverna, Galaxy, VisTrails) and geosciences (Wings) domains. Taverna, Wings and VisTrails now also have workflows across other different domains like astronomy, machine learning, meteorology, etc.

- All of these systems can interact with third party tools and services, and they include a catalog of components for performing different operations with data.

Despite being similar, we can still find some differences among the selected systems. In particular, VisTrails has explicit mechanisms for the basic control constructs (e.g., conditionals and looping), while Taverna, Wings and Galaxy are observers of the pure data flow paradigm (although there are implicit ways of implementing such control structures).

The variety of environments in which these systems operate highlights some other differences as well. While Taverna allows users to specify workflows that make use of third party services (i.e., an open environment), Wings requires that the resources and the analysis operations are made part of its environment prior to being used in experiments (i.e. a controlled environment). However, the differences between these systems are not a significant differentiating factor, as Taverna allows more control to be added to the environment through the addition of plug-ins, and Wings can establish connection to third party services via custom components. VisTrails and Galaxy may be positioned at an intermediate point, since they provide access to external web-services but also build on a comprehensive library of components.

A summary of the commonalities and differences among the workflow systems included in the analysis can be seen in Table 5.1.

5.1.2 Workflow Corpus Description

For our analysis, we have chosen 260 heterogeneous workflows in a variety of domains. We analyzed a set of public Wings workflows (89 out of 132 workflows), part of the

Table 5.1: Summary of the main differences in the features of each workflow system: explicit support for control constructs (i.e., conditional, loops), whether the user interface is web-based or not, whether the environment is open or controlled, and the execution engine used.

Workflow System	**Control Constructs**	**GUI**	**Environment type**	**Engine**
Taverna	No	Desktop/Web	Open/Controlled	Taverna
Wings	No	Web	Controlled	Pegasus, Apache OODT
Galaxy	No	Web	Open/Controlled	Galaxy
VisTrails	Yes	Desktop/Web	Open/Controlled	VisTrails

Taverna set (125 out of 874 Taverna2 workflows in myExperiment), a set of Galaxy workflows (26 out 145 of workflows) and part of the VisTrails set (20 out of 274 workflows).

- For Wings, we analyzed all workflows from drug discovery, text mining, domain independent, genomics and social network analysis domains.
- For Taverna we analyzed workflows that were available in myExperiment (Roure et al., 2009). We determined the groups/domains of workflows by browsing the myExperiment group tags[2] and identifying those domains which contained workflows that were publicly accessible at the time of the analysis. For the Taverna dataset we analyzed cheminformatics, genomics, astronomy, biodiversity, geoinformatics and text mining domains. The distribution of workflows to domains is not even, as it is also the case in myExperiment. Taverna is the workflow system with the largest public collection of workflows, in order to obtain a manageable subset of workflows for manual analysis, we made random selections from each identified domain.
- For Galaxy we chose all the documented workflows available in the public workflow repository[3] (i.e., those workflows with annotations explaining the functionality of their components). Since Galaxy is specialized in the biomedical domain,

[2] `http://www.myexperiment.org/groups`
[3] `https://main.g2.bx.psu.edu/workflow/list_published`

most of the workflows are from the genomics domain, although three of them do text analysis operations in files.

- For VisTrails we chose a set of documented workflows available in CrowdLabs and tutorials, which include domains in medical informatics and genomics. It is worth mentioning that some workflows are domain independent (machine learning workflows, visualization and rendering of datasets, annotation of texts, etc.), so they have been included under a new category.

When selecting workflows for this analysis we made sure to include workflows that were developed with the intention of backing actual data-intensive scientific investigations. We didn't include any example or testing workflows, which are used for demonstrating the capabilities of different workflow systems. A summary of the number of workflows analyzed from each domain can be seen in Table 5.2, while Table 5.3 provides additional information on the size of workflows analyzed in terms of the range and average number of analysis tasks.

Table 5.2: Number of workflows analyzed from Taverna (T), Wings (W), Galaxy (G) and VisTrails (V).

Domain	**No of workflows**	**Source**			
		T	W	G	V
Drug Discovery	7	0	7	0	0
Astronomy	51	51	0	0	0
Biodiversity	12	12	0	0	0
Cheminformatics	7	7	0	0	0
Genomics	90	38	28	23	1
Geo-Informatics	6	6	0	0	0
Text Analysis	45	11	31	3	0
Social Network Analysis	5	0	5	0	0
Medical Informatics	7	0	0	0	7
Domain Independent	30	0	18	0	12
TOTAL	260	125	89	26	20

Table 5.3: Maximum, minimum and average size in terms of the number of steps within workflows per domain.

Domain	Max. Size	Min. Size	Avg. Size
Drug Discovery	18	1	7
Astronomy	33	1	7
Biodiversity	12	1	4
Cheminformatics	20	1	9
Genomics	53	1	6
Geo-Informatics	14	3	8
Text Analysis	15	1	5
Social Network Analysis	7	3	6
Medical Informatics	29	8	4
Domain Independent	20	1	6

5.1.3 Methodology for Workflow Analysis

Our analysis was performed based on the workflow template, documentation, metadata and traces available for each of the workflows within the corpus studied. Each workflow was inspected using the associated workbench/design environment. Documentation on workflows is provided within workflow descriptions and in repositories in which the workflows are published. We performed a *bottom-up manual* analysis that aimed to surface two orthogonal dimensions regarding workflow steps in workflows: 1) outline what kind of data-operation activity is being undertaken by a workflow step and 2) how that activity was implemented. For example, a visualization step (data oriented activity) can be implemented in different ways: via a stateful multi-step invocation, through a single stateless invocation (depending on the environmental constraints and nature of the services), or via a sub-workflow.

The only automated part of the data collection was associated with the workflow size statistics for Taverna workflows. The myExperiment repository provides a REST API[4] that allows retrieving information on Taverna workflows. Using this facility we were able to automate the collection of partial statistics regarding the number of workflow steps and the number of input/output parameters of Taverna workflows.

[4] `http://wiki.myexperiment.org/index.php/Developer:API`

Rather than hypothesizing possible motifs up front, we built up a set of motifs as we progressed with the analysis. For each workflow we recorded the number of occurrences of each motif according to the documentation, and metadata descriptions provided by the original authors (independently of the workflow system it belonged to). In order to minimize misinterpretation and human error, the motif occurrences identified for each workflow were cross-validated by at least another colleague. Whenever there was a conflict in the annotation, the metadata and documentation associated with the workflow was reviewed again, discussing the possible interpretations until agreement was reached.

5.1.4 A Motif Catalogue for Abstracting Scientific Workflows

We divided motifs into two categories: data-operation motifs (i.e., the motifs related to the main functionality undertaken by the steps of the workflow), and workflow-oriented motifs (i.e., how the data-operation motifs are undertaken in the workflow). An overview of the motif catalog is provided in Table 5.4. In this section we describe each type of motif in detail.

5.1.4.1 Data-Operation Motifs

Data Preparation

Data, once it is retrieved, may need several transformations before being able to be used in a workflow step. The most common activities that we have detected in our analysis are described below.

Combine: Data merging or joining steps are commonly found across workflows. The *combine* motif refers to the step or group of steps in the workflow aggregating information from different inputs. An example can be seen in Figure 5.1, where the results of two branches are merged for presenting a single output result.

Filter: The datasets brought into a pipeline may not be subject to analysis in their entirety. Data could further be distilled, sampled or could be subject to extraction of various subsets.

Table 5.4: Overview of our catalog of workflow motifs.

- Data-Operation Motifs
  - Data Preparation
    - Combine
    - Filter
    - Format Transformation
    - Input Augmentation
    - Output Extraction
    - Group
    - Sort
    - Split
  - Data Analysis
  - Data Cleaning
  - Data Movement
  - Data Retrieval
  - Data Visualization
- Workflow-Oriented Motifs
  - Inter-Workflow Motifs
    - Atomic Workflows
    - Composite Workflows
    - Workflow Overloading
  - Intra-Workflow Motifs
    - Internal Macros
    - Human Interactions
    - Stateful (Asynchronous) Invocations

Format Transformation: Heterogeneity of formats in data representation is a known issue in many scientific disciplines. Workflows that bring together multiple access or analysis activities usually contain steps for format transformations, sometimes called "Shims" (Hull et al., 2004), that typically preserve the contents of data while converting its representation format.

Input Augmentation: Data access and analysis steps that are handled by external services or tools typically require well formed query strings or structured requests as input parameters. Certain tasks in workflows are dedicated to the generation of these queries through an aggregation of multiple parameters. An example of this is provided in the workflow of Figure 5.2: For each service invocation (e.g. *getJobState*) there are steps (e.g. *getJobState_Input*) that are responsible for creating the correctly formatted inputs for the service.

Output Extraction: Outputs of data access or analysis steps could be subject to data extraction to allow the conversion of data from the service format to the workflow internal data carrying structures. This motif is similar to the *format transformation* and *filter* motifs, and is associated with steps that perform the inverse operation of *input augmentation*. An example is given in Figure 5.2, where output extraction steps (e.g. *getJobState_output*) are responsible for parsing the XML message resulting from the service (*getJobState*) to return a singleton value containing solely the job state.

Group: Some steps of the workflow reorganize the input into different groups or classify the inputs on a given collection of data items. For example, grouping a table by a certain category or executing a SQL GROUP-BY clause on an input dataset. *Group* is different from *combine*, as the former may reorganize the information in an input without the need to aggregate it from several sources.

Sort: In certain cases datasets containing multiple data items/records are to be sorted (with respect to a parameter) prior to further processing. The *sort* motif refers to those steps. Figure 5.1 shows an example where the inputs resulting from the data analysis (*comparisonResults*) are sorted (*ComparisonResultsV2* component) before being merged in a subsequent step.

Split: Our analysis has shown that many steps in the workflows separate an input (or group of inputs) into different outputs. For example, the splitting of a dataset into different subsets to be processed in parallel in a workflow.

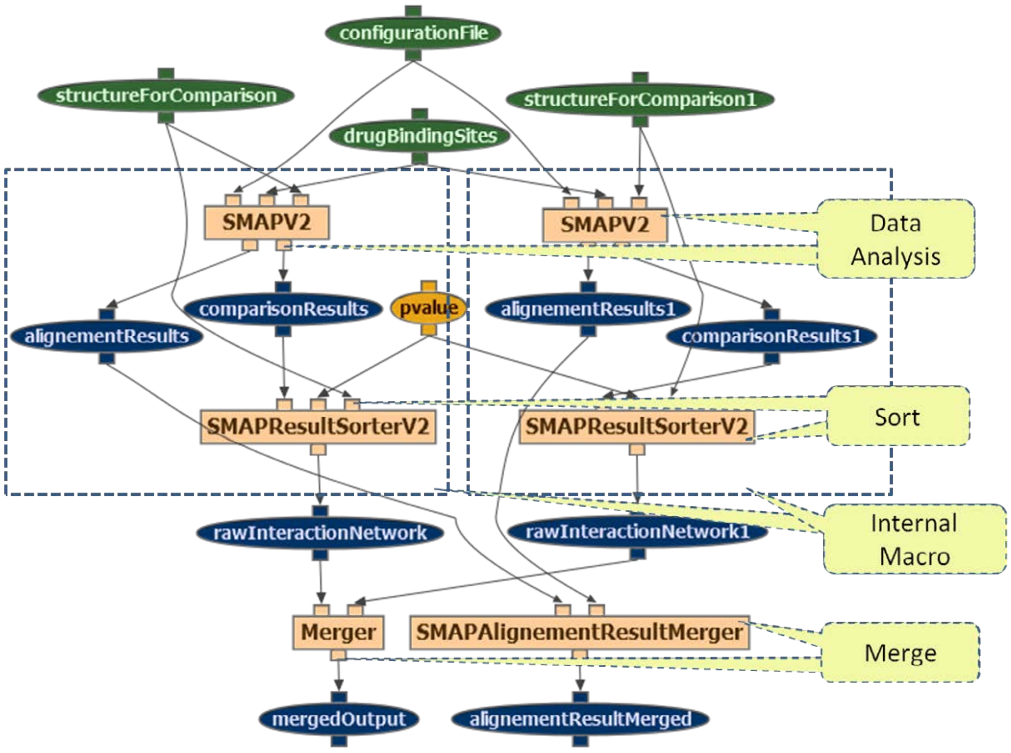


Figure 5.1: Sample motifs in a Wings workflow fragment for drug discovery. A comparison analysis is performed on two different input datasets (SMAPV2). The results are then sorted (SMAPResultSorter) and finally merged (Merger, SMAPAlignementResultMerger).

Data Analysis

This motif refers to a broad category of tasks in diverse domains, and it is relevant because it often represents the main functionality of the workflow. An important number of workflows are designed with the purpose of analyzing or evaluating different features of input data, ranging from simple comparisons between the datasets to complex protein analysis to see whether two molecules can be docked successfully or not. An example is given in the workflow of Figure 5.2 with a processing step named *warp2D*, and the steps named *SMAPV2* in Figure 5.1 with a ligand binding sites comparison of the inputs. These steps carry out the main functionality of the workflow, but they are surrounded by other data preparation and filtering steps.

Data Cleaning/Curation

We have observed the steps for cleaning and curating data as a separate category from data preparation and filtering. Typically these steps are undertaken by sophisticated tooling/services, or by specialized users. A cleaning/curation step essentially preserves and enriches the content of data (e.g., by a user's annotation of a result with additional information, detecting and removing inconsistencies in the data, etc.).

Data Movement

Certain analysis activities that are performed via external tools or services require the submission of data to a location accessible by the service/tool (i.e., a web or a local directory respectively). In such cases the workflow contains dedicated step(s) for the upload/transfer of data to these locations. The same applies to the outputs, in which case a data download step is used to chain the data to the next steps of the workflow. The data deposition of the workflow results to a specific server would also be included in this category. In Figure 5.2, the *DataUpload* step ships data to the server on which the analysis will be done.

Data Retrieval

Workflows exploit heterogeneous data sources, remote databases, repositories or other web resources exposed via SOAP or REST services. Scientific data stored in these repositories are retrieved through query and retrieval steps inside workflows. Certain tasks within the workflow are responsible for retrieving data from such external sources into the workflow environment. We also observed that certain data integration workflows contain multiple linked retrieval steps, being essentially parametrized data integration chains. *Data retrieval* is different from *data movement*, as it refers to those steps of the workflow selecting particular data to be consumed by the workflow (through a query, REST API, etc.) instead of performing a bulk upload of the workflow resources.

Data Visualization

Being able to show the results is as important as producing them in some workflows. Scientists use visualizations to show the conclusions of their experiments and to take important decisions in the pipeline itself. Therefore, certain steps in workflows are

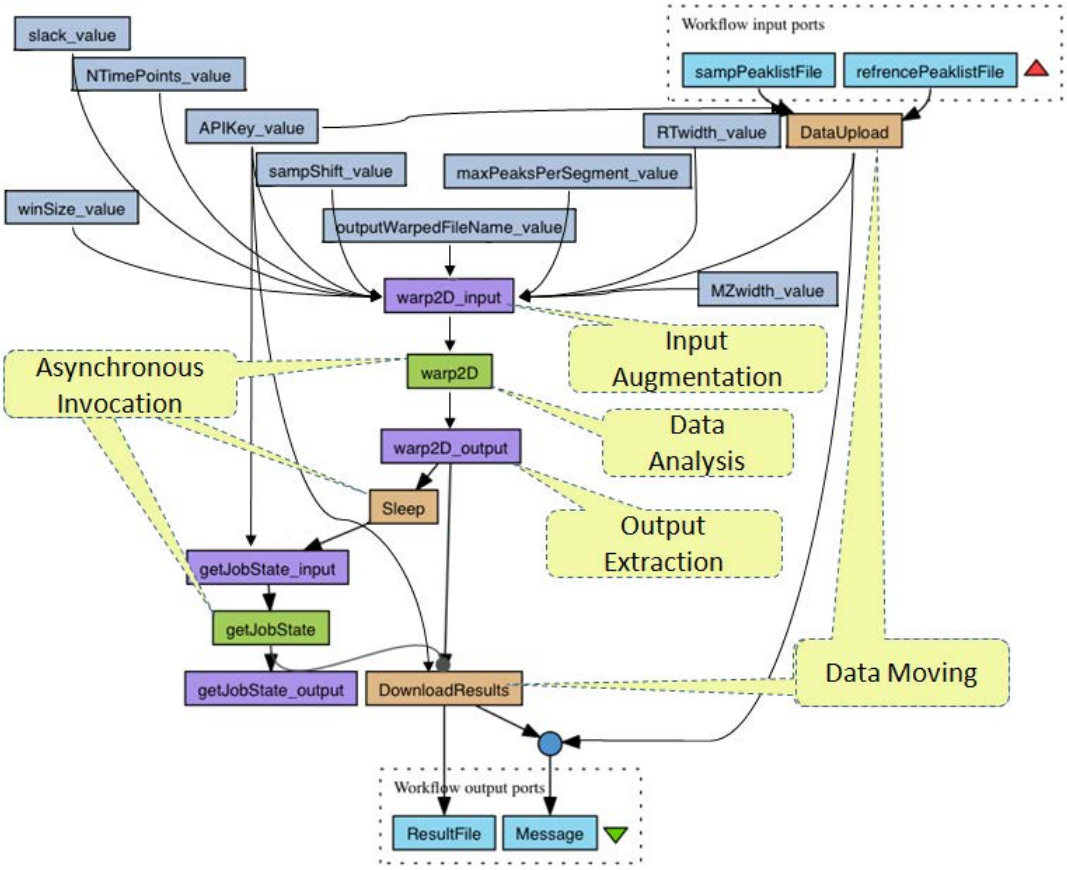


Figure 5.2: Sample motifs in a Taverna workflow for functional genomics. The workflow transfers data files containing proteomics data to a remote server and augments several parameters for the invocation request. Then the workflow waits for job completion and inquires about the state of the submitted job. Once the inquiry call is returned the results are downloaded from the remote server.

dedicated to generation of plots, graphs, tables and XMLs or CSV file outputs from input data. This category is essentially for result delivery of the experiment results.

5.1.4.2 Workflow-Oriented Motifs

We divide this category into two different groups, depending on whether motifs are observed *among* workflows, by analyzing the relations of the workflow with other workflows (*inter workflow motifs*); or *within* workflows, by exploring the workflow itself (*intra workflow motifs*).

Inter Workflow Motifs

Atomic Workflows: A significant number of workflows perform an atomic unit of functionality, which does not require to be decomposed into smaller workflow fragments. Typically, these workflows are designed to be included in other workflows as sub-workflows, part of a larger experiment. *Atomic workflows* are the main mechanism of modularizing functionality within scientific workflows.

Composite Workflows: This motif refers to those workflows including one or more workflows as a sub-workflow. The usage of sub-workflows appears as a common practice for reusing modular functionality from multiple workflows. It is important to note that there are two ways in which this motif may appear in a collection of workflows: highlighted explicitly by the creator of the workflow (i.e., the user deliberately included other workflows as part of the one being designed) or detected implicitly by the analysis (i.e., a given workflow was created without any sub-workflows, but there are other existing workflows on the collection that are equivalent to fragments of the current workflow). The latter is common in systems were the creation of sub-workflows is not included among the features of the workflow system.

Workflow Overloading: Our analysis has shown that authors tend to deliver multiple workflows with the same functionality, but operating over different input parameter types. An example is performing an analysis over a *string* input parameter versus performing it over the contents of a specified file, generalizing a workflow to work with collections of files instead of single inputs, etc. Overloading is a response to the heterogeneity of environments, directly related to workflow re-use (as most of the functionality of the steps in the overloaded workflow remains the same).

Intra workflow motifs

Internal Macros: This category refers to those groups of steps in the workflow that correspond to repetitive patterns of combining tasks. An example can be seen in Figure 5.1, where there are two branches of the workflow performing the same operations in the same order (SMAPV2 plus SMAPResultSorterV2 steps).

Human Interactions: We have observed that some scientific workflows systems increasingly make use of human interactions to undertake certain activities within workflows. These steps are often necessary to achieve some functionality of the workflow that cannot be (fully) automated, and requires human computation to complete. Typical examples of such activities are manual data curation and cleaning steps (e.g., annotating a CSV file), manual filtering activities (e.g., selecting a specific data sub-set to continue the experiment), etc.

Stateful/Asynchronous Invocations: Certain activities such as analyses or visualizations could be performed through interaction with stateful (web) services execution (i.e., that allow for creation of jobs over remote grid environments). Such activities require invocation of multiple operations at a service endpoint using a shared state identifier (e.g. Job ID). An example is given in the workflow of Figure 5.2, where the service invocation *warp2D* causes the creation of a stateful warping job. The call then returns a job ID, which is used to inquire about the job status (*getJobStatus*), and to retrieve the results (*DownloadResults*).

The workflow motif catalog is available as an ontology for annotating workflows[5]. Usage examples can be seen in the ontology documentation[6].

5.1.5 Workflow Analysis Results

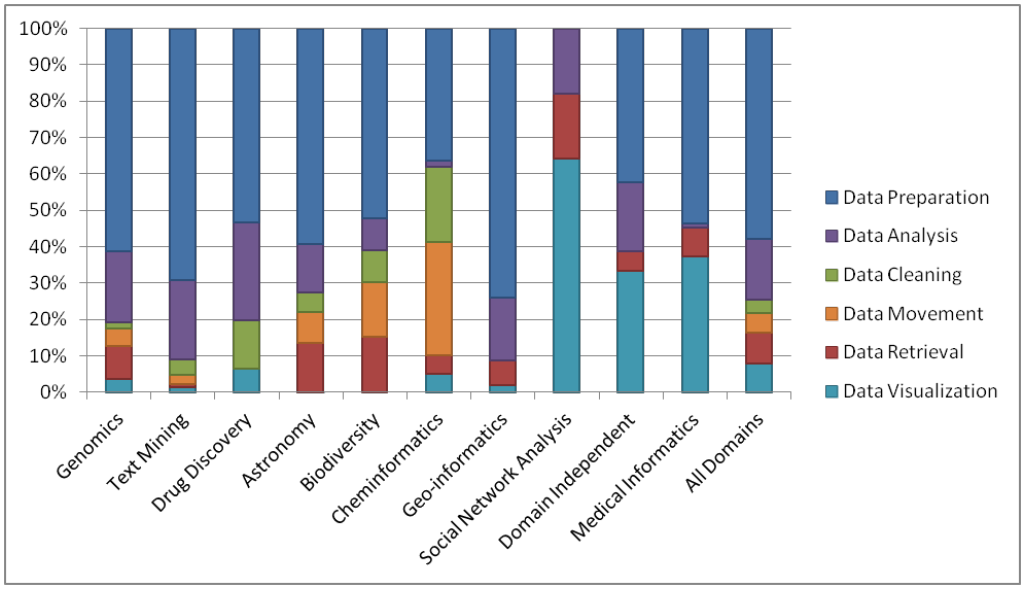
In this section we report on the frequencies of the data-operation and workflow-oriented motifs within the workflows selected for our analysis. We also discuss how they are correlated with the workflow domains. The data resulting from this analysis is available online[7]. A detailed explanation of the frequencies for each domain and for each workflow system can be seen in (Garijo et al., 2014a).

Figure 5.3(a) illustrates the distribution of data-operation motifs across the domains. The analysis of this figure shows the predominance of the data preparation motif, which constitutes more than 50% of the data-operation motifs in the majority of domains. This is an interesting result as it implies that data preparation steps are more

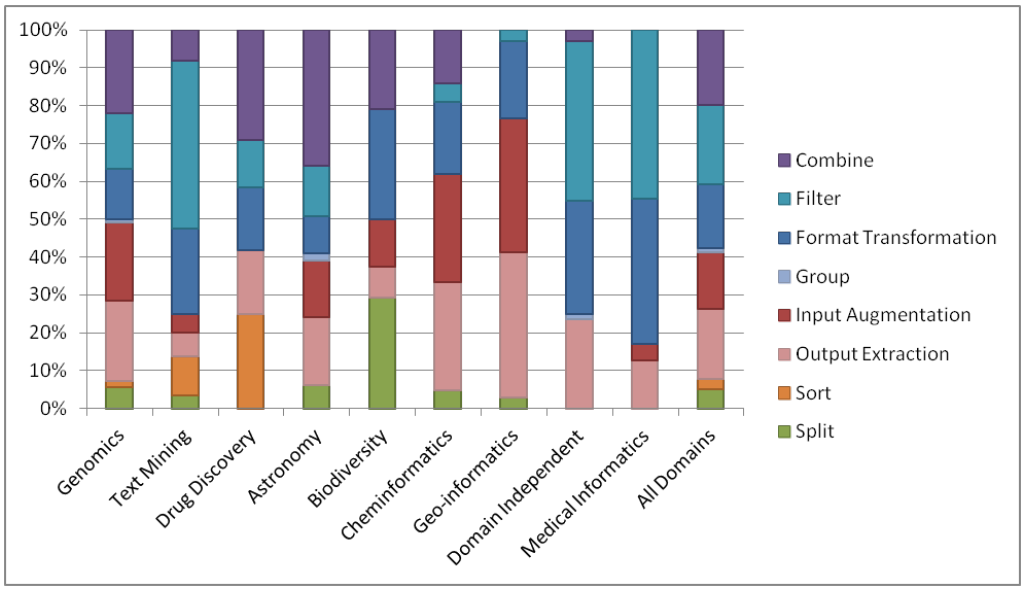
[5] `http://purl.org/net/wf-motifs`

[6] `http://vocab.linkeddata.es/motifs/version/14062013/`

[7] Results available at `http://dx.doi.org/10.6084/m9.figshare.1598104`, `http://purl.org/net/ro-motifPaper#inputs`



(a) Distribution of data-operation motifs per domain.



(b) Distribution of data preparation motifs per domain. The social network analysis domain is not included, as it does not have any data preparation motifs.

Figure 5.3: Distribution of the data-operation and data preparation motifs by domain.

common than any other activity, specifically those that perform the main (scientifically-significant) functionality of the workflow. The abundance of these steps is one major obstacle for understandability, since they burden the documentation function and cre-

ate difficulties for the workflow re-user scientists. The social network analysis domain is an exception, as it consults, analyzes and visualizes queries and statistics over concrete data sources without performing any data preparation steps. Figure 5.3(a) also demonstrates that within domains such as genomics, astronomy, medical informatics or biodiversity, where curated common scientific databases exist, workflows are used as data retrieval clients against these databases.

Drilling down to data preparation, Figure 5.3(b) shows the dominance of filter, input augmentation and output extraction motifs for most domains. Input augmentation and output extraction are activities which can be seen as adapters that help plugging data analysis capabilities into workflows. Their number is higher in workflows relying on third party services, i.e., most Taverna domains (biodiversity, cheminformatics, geoinformatics); while filtering is higher in Wings, Galaxy and VisTrails workflows. Figure 5.3(b) also demonstrates how the existence of a widely used common data structure for a domain, in this case the VOTable in astronomy[8], reduces the need for domain-specific data transformations in workflows.

Some of the differences between the systems are reflected in the motifs results. As displayed in the comparative Figure 5.4 for the life sciences domain (a general domain shown in Table 5.5 including the genomics, drug discovery, biodiversity, chemical informatics and medical informatics domains), in Wings, Galaxy and VisTrails input augmentation and output extraction steps are much less required (around 30%, 20% and 20% respectively versus almost 50% in Taverna) as the inputs are either controlled (Galaxy, VisTrails) or strongly typed (Wings) and the data analysis steps are pre-designed to operate over specific types of data. In Figure 5.5(a) we observe that Wings workflows do not contain any data retrieval or movement steps, as data is pre-integrated into the workflow environment (data shipping activities are carried out behind the scenes by the Wings execution environment) whereas in Taverna the workflow carries dedicated steps for querying databases and shipping data to necessary locations for analysis. Galaxy and VisTrails also include components to retrieve content from external datasets into the environment (2% and 10% respectively), although we didn't find steps for moving the data of intermediate steps to external services among the set of workflows analyzed. In the case of Galaxy this happens because most data

[8] `http://www.ivoa.net/Documents/VOTable/`

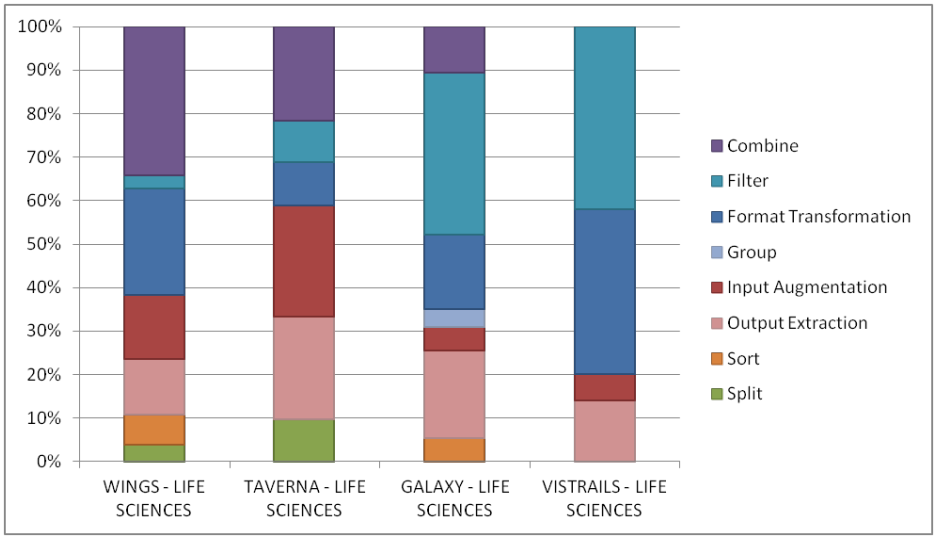


Figure 5.4: Distribution of the data preparation motifs in the life sciences workflows.

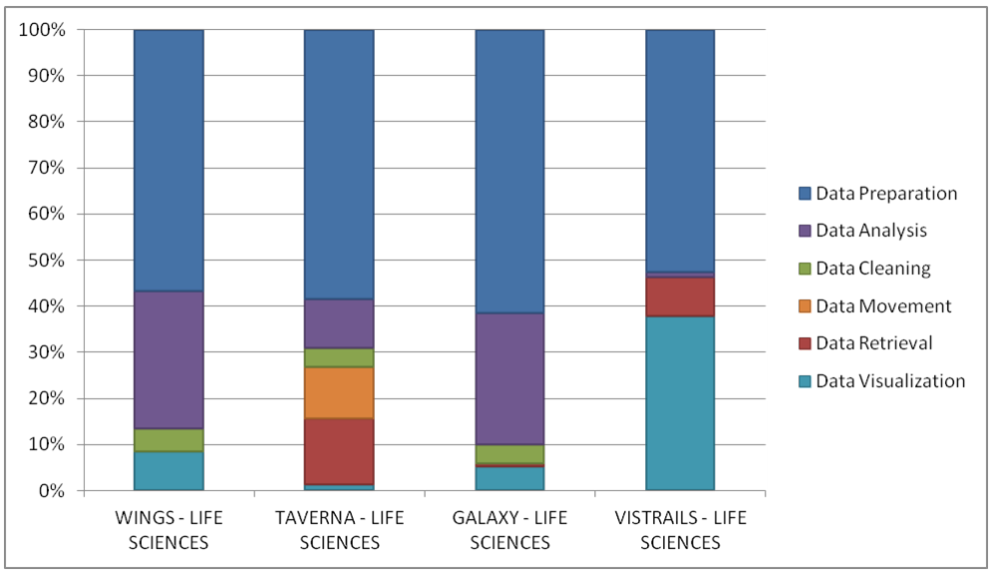
Table 5.5: Distribution of the workflows from Taverna (T), Wings (W), Galaxy (G) and VisTrails (V) in the life sciences domain.

Domain	No. of workflows	Source
Drug Discovery	7	W
Biodiversity	12	T
Cheminformatics	7	T
Genomics	90	T (38), W(28), G (23), V (1)
Medical Informatics	7	V
Total	123	

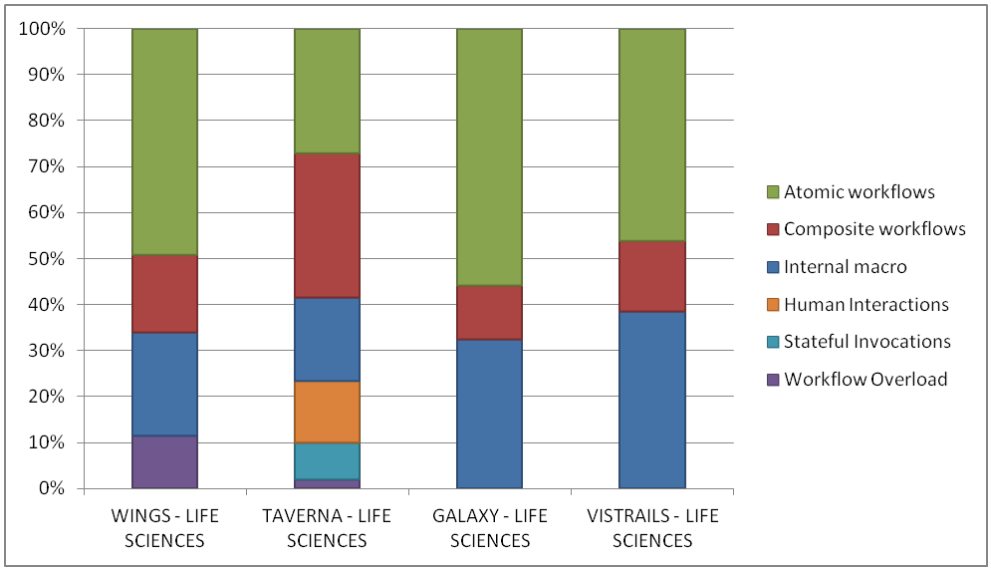
retrieval and moving steps are performed transparently to the workflow execution (individual components are used to retrieve the data to the user domain, and that data is then used as input of the workflow); while in VisTrails the main analysis steps of the analyzed workflow set were performed using custom components.

Another interesting finding is the amount of visualization steps found in the life sciences domain (Figure 5.5(a)). One feature of VisTrails and Galaxy are the tools included for the visualization of workflow results. In VisTrails workflows almost 40% of the motifs found are visualization steps, but this percentage is very reduced in Galaxy (less than 5%). This is due to a separate visualization tool in Galaxy[9] which

[9] `https://main.g2.bx.psu.edu/visualization/trackster`



(a) Distribution of the data-operation motifs in the life sciences workflows.



(b) Distribution of the workflow-oriented motifs in the life sciences workflows.

Figure 5.5: Distribution of motifs in the life sciences workflows.

reduces the need for visualization steps in the workflows. As shown in Figure 5.5(a), the visualization steps in Taverna and Wings are considerably smaller (around 2% and 10% respectively).

The impact of the difference in the execution environments of the analyzed workflow systems is also observed on the workflow-oriented motifs, as can be seen in Figure 5.5(b). Stateful invocations motifs are not present in Wings, Galaxy and VisTrails workflows, as all steps are handled by a dedicated workflow scheduling framework/pipeline system and the details are hidden from the workflow developers. In Taverna's default configuration, there are no execution environments or scheduling frameworks prescribed to the users. Therefore the workflow developers are 1) either responsible for catering for various different invocation requirements of external resources, which may include stateful invocations requiring execution of multiple consecutive steps in order to undertake a single function 2) they can develop specific plug-ins that wrap-up stateful interactions and boiler plate steps.

Regarding workflow-oriented motifs, Figure 5.6 shows that human interaction steps are increasingly used in scientific workflows, especially in the biodiversity and cheminformatics domains. Human interaction steps in Taverna workflows are handled either through external tools (e.g., Google Refine[10]), facilitated via a human-interaction plug-in, or through local scripts (e.g., selection of configuration values from multi-choice lists). However, we observed that several boiler-plate *set-up* steps are required for the deployment and configuration of external tooling to support the human tasks. These boiler plate steps result in very large and complex workflows. Wings and VisTrails workflows do not contain human interaction steps. Galaxy is an environment that is heavily based on user-driven configuration and invocation of analysis tools (some parameters and inputs of the workflows can even be changed after the execution of the workflow has started). However, based on our definition of human interactions, i.e. analytical data processing undertaken by a human, the Galaxy workflows that we have analyzed do not contain any human computation steps either.

The workflow overload motif also plays a relevant role, appearing in almost 10% of the analyzed workflows. Workflows containing this motif are considered advanced forms of sub-workflow development. By executing workflows in different settings, authors

[10] `https://code.google.com/p/google-refine/`

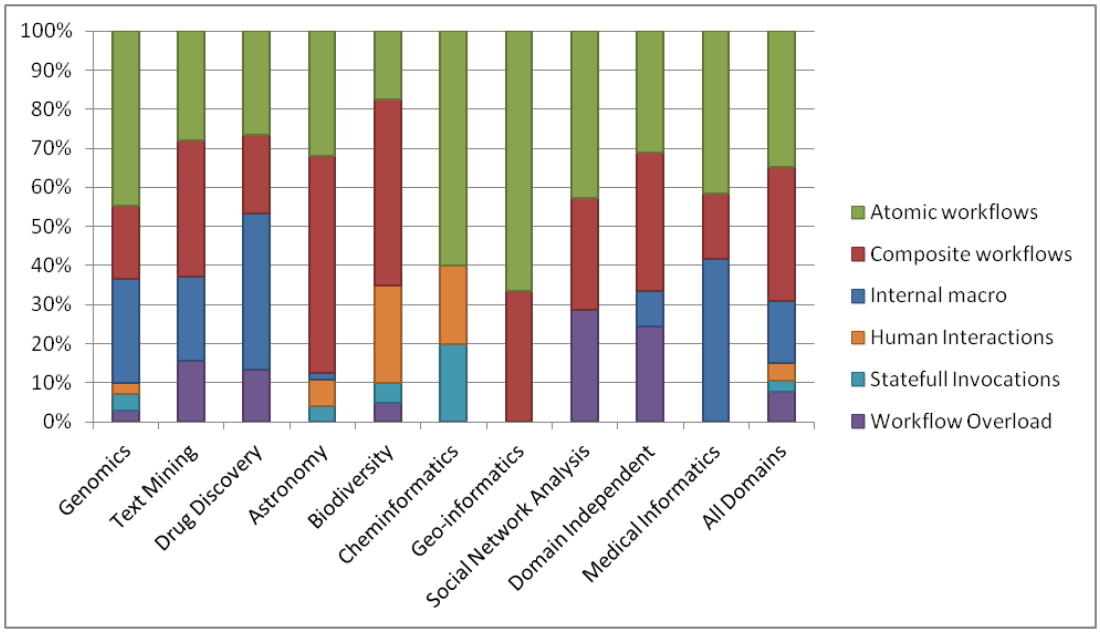


Figure 5.6: Distribution of workflow-oriented motifs grouped by domain.

provide overloaded versions of the same functionality in different workflows to increase the coverage on target uses.

Finally, Figure 5.6 shows a *large proportion of the composite workflows and internal macro motifs*, up to more than 60% in some domains. This confirms that the use of sub-workflows (or repetitions of sets of steps among a group of workflows) is an established best practice for modularizing functionality and reuse. Sub-workflows can also be used to encapsulate the preparation steps and multi-step service invocations within "components" (Davies, 2011), in order to reduce obfuscation. However, users usually have to identify these sub-workflows with common functionality by hand. Ideally, a workflow system would suggest ways to simplify a workflow based on other published workflows, instead of relying on users to do so. We will address this point in Chapter 6.

5.1.6 Summary

The main findings of our analysis can be summarized as follows:

- We identified 6 major types of data-operation motifs and 6 types of workflow-oriented motifs that are used across different domains. From the former group,

the most common motif is the data preparation, highlighting that an important effort in the creation of the workflow is dedicated to tool integration and data operation activities. Regarding workflow-oriented motifs, the amount of internal macro motifs and composite workflows indicate that reuse is a common practice among scientists publishing their workflows.

- Some differences in the motif distribution are caused due to the features of the workflow systems. The frequency by which the motifs appear depends on the differences among the workflow environments and differences in domains. For instance, data preparation motifs are correlated with the type of execution environment for which the workflow is designed. In a workflow system such as Taverna, many steps in the workflow can be dedicated to the moving and retrieval of heterogeneous datasets, and stateful resource access protocols. On the contrary, in a workflow system such as Wings, VisTrails and Galaxy we notice that some data preparation motifs, such as data moving, are minimal and in certain domains absent.

According to the analysis, common workflow fragments seem to be crucial for understanding how different workflows relate to each other and for creating different types of abstractions, which should have an impact on workflow reuse. Here we hypothesize that it is possible to detect commonly occurring workflow fragments automatically (H1.2), and that they can be useful for potential reusers (H1.3). Thus, in an effort to understand in depth the relation between workflows, workflow fragments and their reuse among the workflow corpora, the following sections perform two types of analysis. The first one, on Section 5.2, details an automatic analysis exploring over more than 850 unique workflows in order to confirm the findings found manually. The second analysis, in Section 5.3, aims to explore the user perspective on workflow fragment reuse and usefulness, highlighting the common practices of a community of users.

5.2 Analysis of Workflow and Workflow Fragment Reuse

Given the results obtained in the manual analysis presented in Section 5.1, we explore in this section how workflows are reused among a collection of workflows. Furthermore, we analyze how workflow fragments defined by users (as sub-workflows) are reused in

other workflows. In order to do so, we first introduce the corpus used in the analysis, and then we analyze how many of the workflow fragments (and workflows) defined by users actually appear in other workflows. The analysis is made from two perspectives: reuse in a corpus mainly designed by single users and reuse in a corpus with workflows from many users.

It is worth mentioning that the corpus used for this analysis is different from the one presented in the motif analysis presented in Section 5.1, and there are several reasons for this decision. The first one is to test whether the high number of composite workflows found in the previous workflow corpus is consistent with the reuse analysis on a corpus from a different workflow system. Similarly, the second reason is that most workflow reuse analyses presented in the state of the art (Chapter 2) are from the Taverna workflow system, and we wanted to confirm whether workflow reuse was also common in other workflow systems or not. The third reason is the amount of available workflows from the workflow system being explored, the LONI Pipeline (described in Chapter 2). Finally, the fourth reason is the lack of support for sub-workflow creation by some of the systems considered in the motif manual analysis, which would reduce considerably the corpus, as we want to assess the reuse of user-defined workflow fragments as well.

5.2.1 Experimental Setup

We performed our analysis on 6815 workflows created with the LONI Pipeline workflow system. From these workflows, 854 are unique, obtained after applying a simple filter to remove duplicates and single step workflows. Additionally, we have selected the LONI Pipeline because it has two features that are of interest for this work:

- **Grouping tools** that allow users to define a "*grouping*" of components in a workflow. A grouping is a user-defined sub-workflow, which can be copied/pasted in different workflows and annotated. Groupings are shown in workflows as single steps which can be explored (and expanded) when necessary, following a macro abstraction.

- **A public library of components** identified in a unique way with well defined functionality, which allows users to reuse popular components, although they can create their own.

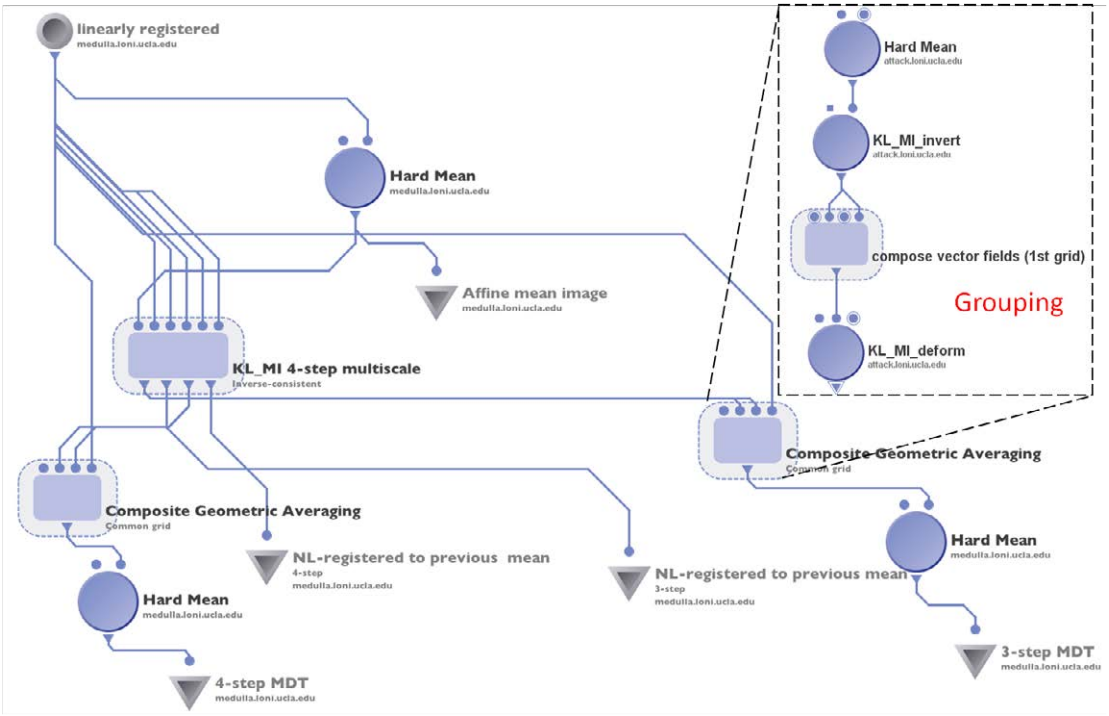


Figure 5.7: An example of a workflow in the LONI Pipeline, with workflow steps (components) shown as circles. Outputs are shown as triangles while the input (*linearly registered*) is a smaller circle. The connections among steps represent the dataflow. Users can select sub-workflows to create groupings of components (shown with dashed lines), which can be reused in the same workflow and in others (shown as rectangular components).

Figure 5.7 shows an example of a workflow with groupings defined by scientists using the LONI Pipeline. The figure shows a minimal deformation target (MDT) pipeline to serve as an unbiased average brain template for neuro-imaging studies. The grouping, which has been expanded in the figure (on top right) contains three steps and another grouping (*compose vector fields*).

5.2.1.1 Workflow Corpus

The workflows are distributed among four different corpora. Originally, we obtained two corpora from two different users, containing all the workflows created by them or in collaboration with other people. A third corpus contains the runs of 62 unique users submitted to the LONI Pipeline servers during January 2014. Finally, on a second iteration of our analysis, another user incorporated more workflows to the experiment.

The main features of each corpus are described below:

1. User Corpus 1 (WC1) A set of 790 workflows (441 workflows after filtering duplicated structures and single-step workflows) designed mostly by a single user. Some of the workflows are the result of collaborations with other users, which produced different versions of workflows originally produced by this user. The domain of the workflows is in general medical imaging (brain image understanding, 3D skull imaging, genetic modeling of the face, etc.), and some are still used by the LONI Pipeline community. Other workflows were designed for a specific purpose and are not reused anymore.

2. User Corpus 2 (WC2) A set of 113 well-documented workflows (94 after filtering) created, validated and curated by one user, sometimes in collaboration with others. Most of the workflows have been made public for others to reuse, and range from neuro-imaging to genomics. Some of the workflows were developed as early as 2007, and many of them are being used in different institutions.

3. Multi-user Corpus 3 (WC3) A set of 5859 workflows (269 after filtering), submitted to LONI pipeline for execution by 62 different users over the time lapse of a month (Jan 2014). The number of filtered workflows descends drastically from the input corpus as many of the executions are of the same workflow or are one-step workflows designed for testing.

4. User Corpus 4 (WC4) A set of 53 workflows (50 after filtering), designed mainly by a single user. The domains of the workflows are focused also on medical imaging (ranging from genomics to neuro-image analysis), and contain workflows that have been reused or are versions of other workflows of the corpora. Some of these workflows are large (more than 90 steps).

In all four corpora, workflows are likely to reuse components from the public library, that allows groupings to be reused across different workflows. Table 5.6 provides an overview of the size of each corpus before and after filtering.

Table 5.6: Corpus overview.

Corpus	Original size	Size after Filtering
WC1 (Single User)	790	441
WC2 (Single User	113	94
WC3 (Multi User)	5859	269
WC4 (Single User)	53	50

5.2.1.2 Analysis Methodology

The analysis was performed in an automated way for each corpus, once duplicate workflows and single-step workflows had been removed. In order to have a full notion on how workflows and groupings are reused, we performed two independent sub-analyses respectively.

In both analyses, each workflow or grouping was transformed to a labeled graph (according to P-Plan) and compared against another in terms of its steps. Since in the LONI Pipeline each component has a unique identifier, we use them to label the nodes of the graph (the label becomes the type of the workflow step). Therefore, two nodes are the same if they have the same label (i.e., the same type). Both analyses follow a similar approach. First, an initial pass over the dataset gathers the different workflows or groupings to compare. Then, a second iteration compares each graph (workflow or grouping) against all the workflows of the corpus, annotating those workflows where the graph is found. The method to do this comparison is by transforming each graph to a SPARQL query (i.e., the standard language for querying RDF data (Harris et al., 2013)) and issue it against the target workflow. Further details of this approach are described in Chapter 6, where we use it to find workflow fragments in workflows.

It is worth mentioning that with our approach we compare whether a workflow or a grouping is included in another workflow regardless of the grouping annotations made by users in the target workflow. That is, if a grouping consists on three steps A, B and C where C consumes the output of B and B consumes the output of A; and we find these steps in a workflow with the same dependencies among them, we consider that the grouping is found in that workflow (even if the steps A, B and C of the workflow have not been annotated as a grouping by a user). This is a key difference with other related work, where reuse is measured just in terms of the explicit workflows and sub-workflows

created by users.

Similarly to what happens with workflows, if a grouping is duplicated we will only consider it once, and single-step and empty groupings are not considered for reuse. Groupings are not further compared against groupings, just against workflows.

5.2.2 Workflow Reuse Analysis Results

Table 5.7 shows how workflows are reused in the corpora, while tables 5.8 and 5.9 refer to the distribution and reuse of the groupings.

As we already suspected, **a significant portion of the workflows are reused** (an average of 25.5% of the workflows are reused in the four corpora) considering those workflows that have been reused at least one time in the rest of the corpus. The more workflows the corpus has (as in the first and third corpora), the more workflows are reused. This makes sense, as the workflows of each corpora are designed for the same domain, and many have overlapping functionality.

Table 5.7: Reuse of workflows (wfs) for each corpus.

Corpus	Unique filtered workflows	Reused wfs. (f>=2)	Total times wfs. are used in corpus	Most occur of a wf.
WC1	441	175	1638	94
WC2	94	13	43	9
WC3	269	106	619	25
WC4	50	7	19	5

As shown in table 5.8, the total number of groupings is more than twice of the number of unique groupings, indicating that it is a common practice adopted by the users of the workflow system. Also, groupings are not found alone in workflow corpora. It is common to find more than four groupings in a workflow (when a workflow uses groupings).

Table 5.9 illustrates how **groupings are heavily reused, more than workflows are reused**. A range of 44% to 65% of the unique groupings are reused in other workflows for the four corpora, and the number of times they are used in a corpus is much higher than the total number of groupings defined by users. This suggests that some users include in their workflows steps that other users have defined as groupings.

The number of workflows with groupings is higher when a single user created the corpus (309 out of 441, 41 out of 94 and 17 out of 50 from corpus WC1, WC2 and WC4 versus 70 out of 269 of corpus WC3). In WC1, WC2 and WC4 the creators of the workflows are experienced users who know their previous workflows and are likely to reuse them, while the high number of users contributing to WC3 makes it difficult for all of them to be aware of the workflows from other colleagues.

Another interesting fact is the size of the groupings, being up to 92 in corpus WC4 and down to 0 in corpora WC2 and WC4. After exploring several workflows showing this practice, we have realized that the high number of steps for some groupings happens because users sometimes declare a whole workflow as a grouping. A possible explanation is that this would either facilitate copying and pasting the grouping into other templates, or help organizing the workflow for the creator: when workflows are too complex, users often separate their functionality in several smaller workflows. Then, each smaller workflow is declared a grouping and copied and linked in a bigger workflow.

Regarding the minimum size of groupings, we have discovered that sometimes workflow creators group unused inputs or outputs in workflows, leading to groupings of 0 steps. A possible explanation for groupings of size 1 is that the workflow creators annotate extra instructions when using a specific component in a workflow (in our analysis only groupings of size bigger than one are considered, shown in the unique multi-step grouping column of Table 5.8).

Table 5.8: Statistics and distribution of groupings in the corpora.

Corpus	Total qroup.	Unique multi-step qroup.	Wf with qroup.	Avg. group. per wf	Max nof steps in qroup.	Min n of steps in qroup.
WC1	1379	146	309	4	56	1
WC2	294	87	41	7	39	0
WC3	277	79	70	4	60	1
WC4	245	40	17	14	92	0

In summary, our automated analysis confirms what our manual analysis initially highlighted: *workflow reuse is a common practice*. However, it *is less frequent than grouping reuse*. Groupings not only identify commonly reused fragments of workflows, but also seem to be used to modularize and simplify them for a better understanding.

Table 5.9: Reuse of groupings (group) for each corpus.

Corpus	Unique filtered groupings	Reused group. (f>=2)	Total times group. are used in corpus	Most occurrences of a grouping
WC1	146	65	1842	176
WC2	87	40	227	29
WC3	79	47	246	24
WC4	40	26	103	7

Groupings are widely reused independently of the users that have contributed to the corpora, although their number is higher when single users contribute to the corpus. After seeing the results of the analysis, we believe that suggesting some of these commonly used groupings may be beneficial for users designing and visualizing workflows. Thus, in order to explore this possibility, we present in the following section a user survey on workflow reuse and discuss the results.

5.3 Workflow and Workflow Fragment Reuse: User Survey

Although some workflow reuse analysis and benefits have been introduced in Section 2.3, there are barely any studies that ellaborate on the reasons that users give for reusing workflows and workflow fragments. In this section we aim to understand such reasons by discussing the results of a survey on workflow reuse performed in labs that use the LONI Pipeline to create workflows. The LONI Pipeline community of users provides a great opportunity to study how workflow fragments are used in practice, whether they improve reuse or not, and the barriers that users find in reusing workflows and workflow fragments.

5.3.1 Experimental Setup

We selected the LONI Pipeline as our system of choice for this analysis for three main reasons. First, the automatic analysis described in Section 5.2 has shown that it is a workflow system with a high rate of reused workflows and groupings. Second, the LONI Pipeline defines the ability to define groupings, as introduced in Section 5.2, allowing users to define and reuse groups of steps that could be copied and pasted in

new workflows. Finally, the third reason is the interest of the community for exploring workflows and their fragments. Workflow mining tools like the Workflow Miner[11] have been developed for helping users browsing how different workflow components depend on each other in a catalog of workflows.

The fact that the LONI Pipeline includes tools to create, mine and view workflow groupings is an indication that users and/or developers have found a need for reusing workflow fragments. In our analysis, we set out to understand the current level of adoption, the perceived benefits, and the barriers regarding reuse of workflows and workflow fragments.

We created a survey and sent it to the mailing list of users of the LONI Pipeline. We included users who use the LONI Pipeline system installed at the University of Southern California (USC), but due to time limitations we did not include many other users that have downloaded the system and run it themselves in their own servers. The survey was conducted on-line, and the responses were anonymous. The complete survey can be found in Annex B, while the the responses are available online[12].

The survey included two kinds of questions. Some questions presented a choice of answers using a five-level Likert scale (Likert, 1932). For example, for the question "*Is reusing workflows from others useful?*" we offered five answers: very often, often, sometimes, occasionally, and never. Other questions offered a list of possible answers and allowed users to provide their own answers. For example, for the question "*Why is reusing previously created workflows useful?*" the list of possible answers included "*It saves time*", "*Workflows give a high-level diagram that helps remember what was done*", and "*Other*". If the latter was chosen, respondents could provide text with their own reasons. Respondents could do more than one selection.

It is worth mentioning that the survey tackles the issue of workflow reuse gradually. First, it issues questions regarding the reusability of software. Then it asks for the reusability of methods (i.e., workflows) and ends up prompting questions regarding the reusability of fragments of those workflows. This way we ensure that we cover all the possible aspects of workflow reuse.

[11] `http://pipeline.bmap.ucla.edu/products-services/workflow-miner/`
[12] `http://dx.doi.org/10.6084/m9.figshare.1572327`

5.3.2 User Survey Report

We received a total of 21 responses from the users in the lab, ranging from students to experienced users and programmers. In this section we discuss the results of the survey, highlighting in boldface our findings.

5.3.2.1 Writing and Sharing Code

We wanted to have some reference for comparing the responses about workflow sharing, so the survey included some questions about code sharing. Figure 5.8 shows responses regarding the importance of writing code and reusing code. **Writing code is considered very important** for this area of research. **Sharing code is not considered to be as important**. These answers imply that the responders are well aware of the importance and value of their software.

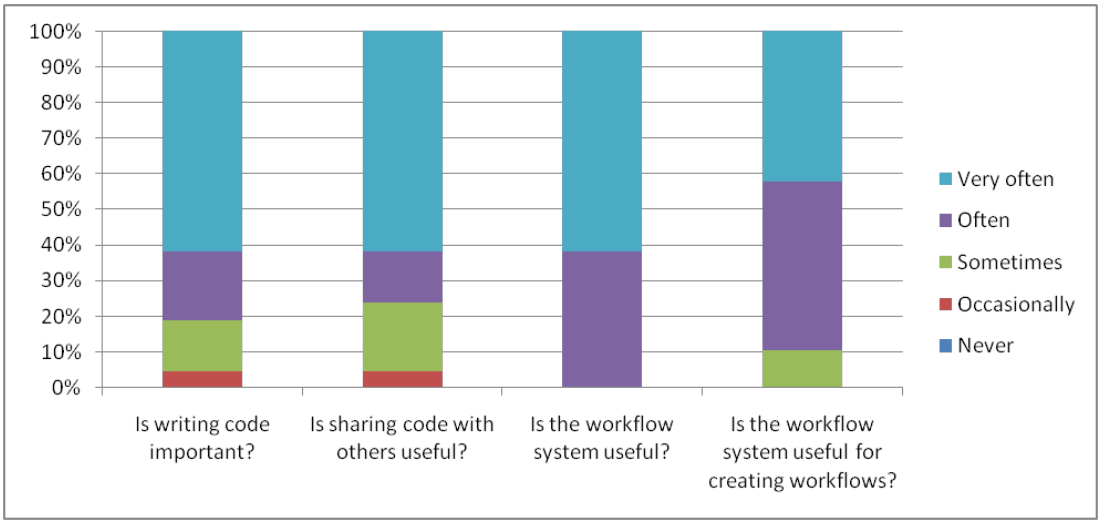


Figure 5.8: Distribution of the answers regarding the utility of writing and sharing code and the utility of the workflow system.

5.3.2.2 Adopting a Workflow System

Figure 5.8 also shows responses regarding the workflow system basic utility in creating workflows for their work. **The overwhelming majority of responders found the workflow system useful**. This perhaps reflects a self-selection bias of the user population that responded, but is nevertheless useful to put in perspective the survey

responses and the conclusions of this study. Figure 5.9 shows the most usual sizes of workflows according to the respondents. Workflows of fewer than 10 steps seem to be the most common. We asked for the reasons not to use the workflow system. We assumed that even users of the workflow system may not use it for all their analyses. We offered one choice and then free text answers. Two respondents selected the given choice of "*It takes time to learn to create workflows*". Free-form answers included "*Minor changes to underlying scripts or tuning of parameters may require more work than just editing scripts themselves*," and "*Sometimes it is easier to run a certain command in loops or batches or to edit the various input/output parameters (file names, paths, options, etc.) on the command line, rather than clicking through the workflow GUI*". Overall, all respondents seem to find utility in the workflow system.

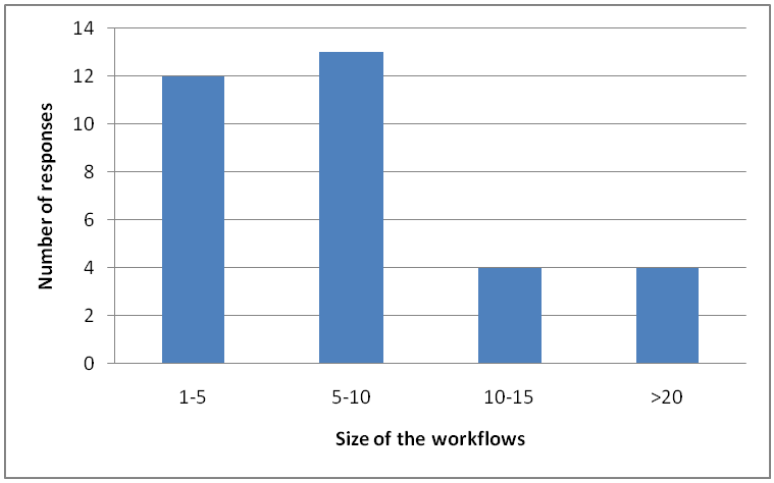


Figure 5.9: Preferred size of created workflows.

5.3.2.3 Using Workflows

Figure 5.10(a) shows the survey answers regarding the utility of creating and sharing workflows. Respondents responded overwhelmingly that **creating workflows is very useful, but, although useful, the reuse of workflows was seen as less useful**. Therefore, reuse is not the only reason why workflows are created. Reusing workflows from a user's prior work is considered as useful as reusing workflows from others.

When asked "*Why is creating workflows useful?*", respondents were given the choices shown in Table 5.10. The number of respondents that selected each choice is also shown

in that table. **The benefits of workflows that the majority of respondents agreed with include time savings, organizing and storing code, having a visualization of the overall analysis, and facilitating reproducibility**. Many respondents agreed to other benefits that included debugging complex code, and encouraging the adoption of standard ways to do things. Free-form responses included: "*Workflows are mainly used for population studies so that you can run many subjects in the same time, and it is easy to pass around to someone who doesn't know how to code*", "*The main reason is that it is easy to send a prepared pipeline to another researcher and they can usually figure out how to use it, regardless of their programming knowledge*", "*It's a really intuitive visualization of the underlying code. Sort of brings the code 'to life'!*" and "*Parallelizing without having to use the Sun Grid Engine script*".

Table 5.10: Survey results concerning why it is useful to create workflows.

Workflows save time	13
Easier to track and debug complex code	9
Convenient way to organize/store code	11
Help write more organized code	6
Help make code more modular/reusable	4
Help make methods more understandable	8
Visualization of overall analysis	11
Workflows facilitate reproducibility	10

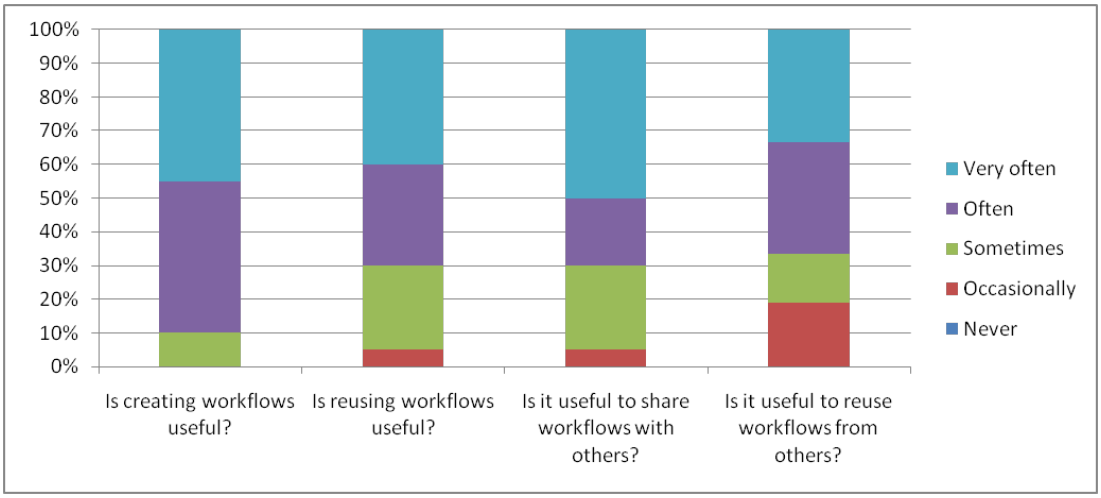
Table 5.11(a) shows responses for the question of why it is useful to reuse workflows in new analyses. Overwhelmingly, **users found that using workflows saves them time**. They also found the visualization of the workflow useful. Free form answers included: "*We often re-run the exact same or very similar analysis steps on our data (e.g., pre-processing, statistical tests), so often we only need to change the inputs and outputs (and maybe some parameters)*".

Table 5.11(b) shows responses for why it is useful to share workflows with others. The overwhelming majority of respondents said that **workflows are useful for both non-programmers and for teaching new students**. It also saves them time because they do not need to re-implement code. No free form answers were specified.

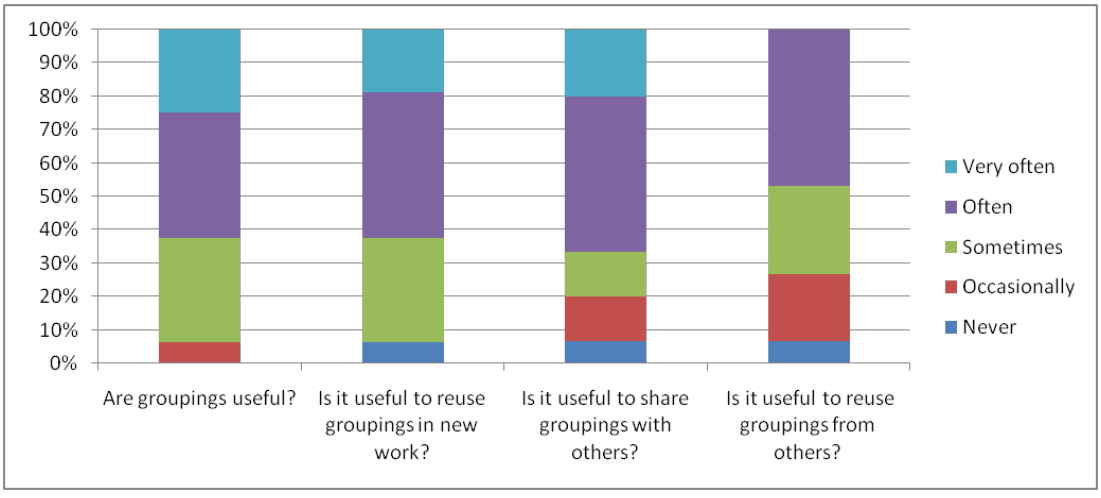
Table 5.11(c) shows answers for why are workflows not shared. Respondents did not offer very overwhelming reasons for not sharing workflows. Free form answers included

"*The best pipelines to share are the ones that have all the kinks worked out, so we can explain how to edit the input and output file names and then the person can just run it*".

Table 5.11(d) shows responses for why it is not useful to reuse workflows from others. Respondents did not offer very overwhelming reasons for not reusing workflows from others. Free form answers included "*Documentation can be easily fixed by adding comments or providing a verbal/written explanation along with the pipeline*".



(a) Distribution of the answers regarding the utility of sharing and reusing workflows.



(b) Distribution of the answers regarding the utility of sharing and reusing groupings.

Figure 5.10: Utility of workflows and groupings.

Table 5.11: Survey results with multiple choice answers concerning benefits of sharing workflows.

(a) Is reusing workflows in new analyses useful?

Saves time	19
Gives a diagram of what was done	13

(b) Why is it useful to share workflows with others?

Non-programmers can use them	20
New students can easily learn	19
No need for others to re-implement code	14
Adoption of standard ways to do things	9

(c) Why are workflows not shared?

Others would not want to use them	1
Others ask too many questions to the creators	2
Workflows from others are difficult to understand	3
It is difficult to understand how to prepare data for a workflow	3

(d) Why is it not useful to reuse workflows from others?

Workflows from others are difficult to understand	4
It is difficult to understand how to prepare data for a workflow	2
Workflows created by others are too specific	1
It is hard to take workflows created by others and make them work	2

5.3.2.4 Using Groupings

Figure 5.10(b) shows the answers regarding the utility of sharing and reusing groupings. As with workflows, **reuse is not the only reason why groupings are created**. Unlike workflows, **reusing groupings from one's own work is more useful than reusing groupings from others**.

Table 5.12 shows the results for the multiple-choice questions about groupings. Most respondents agreed that **groupings help simplify workflows**. **Groupings also make workflows more understandable by others**. Like workflows, groupings save time. Groupings also **make code more modular and more understandable, more so than workflows**. Groupings are seen as useful to non-programmers and students. Very few respondents gave any reasons for not sharing groupings and not

reusing groupings from others. A free-form answer for why groupings are not used was "*It is a pain to dissect when debugging to know where things failed*". For why are groupings not shared, one respondent selected that it is hard to explain what they do, and a free form answer was "*Others want a finished product, not pieces that they have to put together on their own*".

Table 5.12: Survey results with multiple choice answers concerning benefits of sharing groupings.

(a) Why is creating groupings useful?

Visualization of the analysis	10
To simplify workflows that are complex overall	12
To make workflows more understandable to others	12

(b) Is reusing groupings in new analyses useful?

Groupings save time	12
Help make code more modular/reusable	10
Help make methods more understandable	7

(c) Why is it useful to share groupings with others?

Non-programmers can use them	12
New students can easily learn	11
No need for others to re-implement code	9
Adoption of standard ways to do things	6

(d) Why are groupings not shared?

Others would not want to use them	0
Others ask too many questions of the creators	1
Workflows from others are difficult to understand	4
It is difficult to understand how to prepare data for a grouping	1

(e) Why is it not useful to reuse groupings from others?

Groupings from others are difficult to understand	2
It is difficult to understand how to prepare data for a grouping	3
Groupings created by others are too specific	1
It is hard to take groupings created by others and make them work	4

In summary, if we compare the responses in Figures 5.10(a) and 5.10(b) and Tables

5.11 and 5.12, **workflows are considered generally more useful than groupings. However, more respondents said that groupings help make their code more modular and understandable**.

5.4 Summary

In this chapter we defined the scope of the workflow abstractions tackled in our work, focusing on those related to workflow reuse. We defined a catalog of common workflow motifs, which are domain independent conceptual abstractions of workflow steps, by doing an empirical analysis on a corpus from four different workflows systems. This addresses the third research objective of this thesis (RO3, *define a catalog of domain independent abstractions in scientific workflows*) and contributes to the research challenges RCAbstract-1 (*difficulty of determining which are the significant steps of a workflow*), RCAbstract-2 (*absence of catalog of abstractions based on workflow step functionality*) and RCAnnot-1 (*facilitate workflow annotation*). The results of the analysis highlight that three motifs in particular are widely used among the corpora: atomic workflows, composite workflows and internal macros, which indicate that workflow reuse is a common practice among scientists of different domains.

We have attempted to confirm and understand further two aspects of workflows and workflow fragments: reuse and usefulness. Therefore we have performed analyses on another workflow system (the LONI Pipeline), different from the ones explored in the manual analysis, with an active community of users and a significant corpus of workflows.

We first performed an automated analysis of workflows to measure reuse, based on the sets of steps users have defined in the corpora (user groupings). We also performed a user survey on 21 users to find out their opinion with respect of workflow and sub-workflow sharing and reuse. The results speak for themselves: the workflow reuse rate is high (with a minimum of 12% and increasing up to 30% in cases where the size of the collection is more than 200 workflows), and the grouping reuse rate is even higher (44% to 65% of the groupings are reused). It is interesting that users consider workflows more useful than groupings from the point of view of reuse, although they recognize that groupings help modularizing and understanding their code better.

Given that users tend to reuse groupings and workflows, our hypothesis is that by mining commonly used fragments of workflows we can discover new groupings or even workflows that are useful for them when designing workflows. Hence, in the next chapter we describe our approach for detecting these common workflow fragments automatically.

Chapter 6

Workflow Fragment Mining

As we showed in the survey described in Section 5.3, common groupings are helpful mechanisms for simplifying workflows and helping users understanding them. However, currently the grouping definition is completely manual. Unless published online and documented, the only way to explore other people's groupings is to individually download their workflows and explore them locally. As shown in Chapter 3, we hypothesize that by mining an existing workflow corpus we will be able to extract common sub-workflows and suggest them as potential useful groupings to users. In this chapter we introduce our approach for detecting automatically common sub-workflows of a workflow corpus, which we refer to as common *workflow fragments*, defined as in Definition 2 below and using (Jiang et al., 2012) as reference.

Definition 2 *A **workflow fragment** $Wf = (N, A, L_N, L_A, \varphi_N, \varphi_A)$ of a workflow $W = (V, E, L_V, L_E, \varphi_V, \varphi_E)$ is a connected sub-workflow of W, i.e., $N \subseteq V$ with $L_N \subseteq L_V$ and $\forall v \in N \varphi_N(v) = \varphi_V(v)$ and $A \subseteq E$ with $L_A \subseteq L_E$ and $\forall a \in A \varphi_A(a) = \varphi_E(a)$. Given a workflow fragment wf, a corpus of workflows $C=(c_1, c_2, ..., c_n)$ and function $F: < wf, C > \rightarrow \mathbb{N}$ that calculates the number of times wf appears in C, a **common workflow fragment** is a workflow fragment which appears at least f times on the workflow corpus (with F(wf)=f and $f \geq 2$). There are two ways in which F could count the occurrences of a workflow fragment wf in a corpus. If F considers all the occurrences of wf in C, then we refer to F as **frequency**. If F counts only one occurrence of a workflow fragment per workflow, (i.e., $F =\mid c_i \mid / wf \subseteq c_i$) then we refer to F as **support**.*

An overview of our approach for workflow fragment mining is shown in Figure 6.1. This approach is implemented in **FragFlow** as an open source framework and it is

available online[1].

First, a data preparation step is necessary to filter and format the workflow corpora according to the models proposed in Chapter 4 (Section 6.1). Then we apply different graph mining techniques (further described on Section 6.2.1), and filter the results to produce a set of candidate common workflow fragments (Section 6.3). Finally, the fragments are visualized, linked to the workflows of the corpus where they appear and statistics with their frequency and size are calculated (Section 6.4 and 6.5).

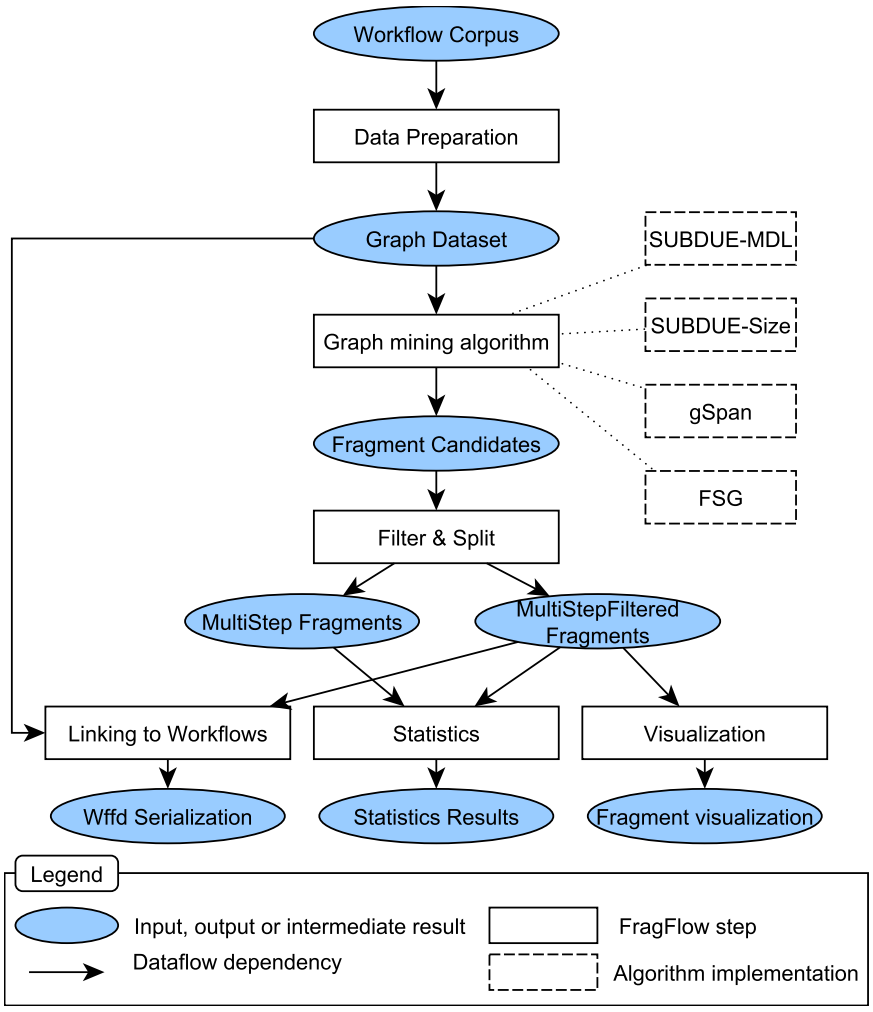


Figure 6.1: An overview of our approach for common workflow fragment mining. The rectangles represent major steps, while the ellipses are the inputs and results from each step. Arrows represent where an input is used or produced by a step.

[1] `https://github.com/dgarijo/FragFlow`, `http://dx.doi.org/10.5281/zenodo.11219`

6.1 Data Preparation

FragFlow takes as input a workflow corpus, which may integrate worfklows from one or more workflow systems represented with OPMW's labeled directed acyclic graphs (LDAGs, see Chapter 4). Other serializations are supported, but OPMW's facilitates the conversion of workflows to each of the formats needed by the tools introduced in the following sections.

In this step workflows are converted to a simplified LDAG format. For each LDAG, the labels of the vertices in the graph corresponds to the types of the step in the workflow, while the edges capture the dependencies between different steps (using the P-Plan vocabulary). Data dependencies are removed to simplify the graph and reduce the overhead of the graph mining techniques applied in further steps. An example can be seen in Figure 6.2, where the full workflow in the left is represented as the LDAG in the middle, which is itself represented with P-Plan as shown in the right. By removing the data dependencies, four nodes in the graph are eliminated. Workflows are processed at their lowest granularity, i.e., groupings and other user annotations are ignored.

Duplicated workflows are removed from the input corpus. This is necessary for reducing the noise of the sample and avoiding obtaining misleading common workflow fragments. For example, if the source of the corpus are the monthly executions submitted to a server, then it is likely to have workflows that were submitted several times for execution (hence, repeated). If duplicated workflows are not removed, the most common fragments would be the most frequently executed workflows, which would not indicate fragments that are reused a lot.

Single step workflows are also removed, as they are not meaningful workflow fragments. Single step workflows are often run for testing individual components, which are then plugged into a bigger workflow.

6.2 Common Workflow Fragment Extraction

The second step of FragFlow is the graph mining algorithm. Our approach for detecting common fragments in a corpus of workflows relies on the application of existing graph mining techniques. In this section we introduce an overview of the main different graph mining approaches related to the problem of sub-graph mining, along with their features and the candidate algorithms adopted in the thesis. For a detailed explanation of these

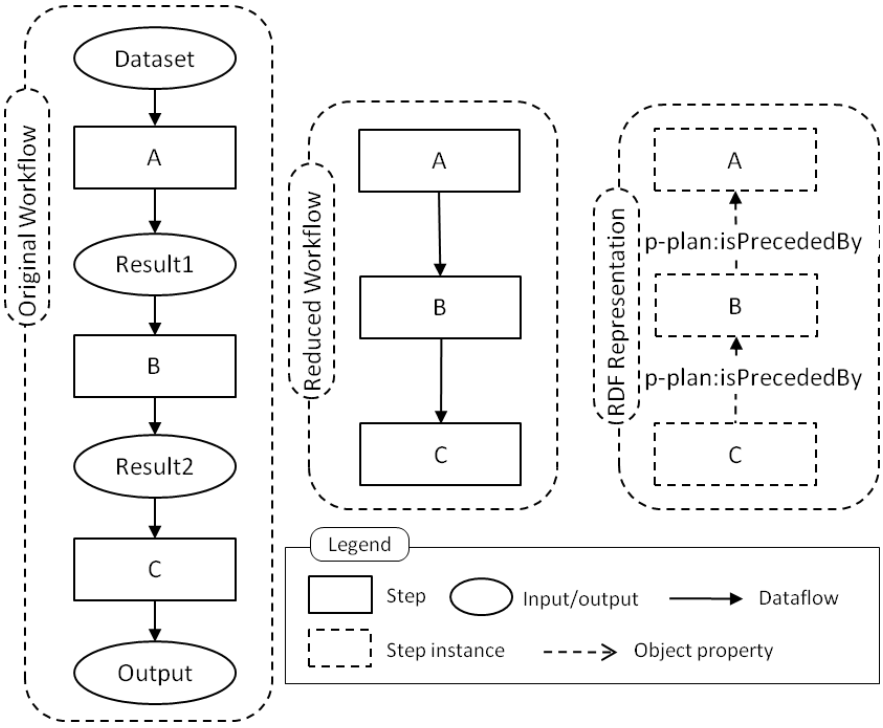


Figure 6.2: Simplifying workflows: by removing the data dependencies on the input graph of the left, we reduce the overhead for graph mining algorithms (middle and right).

and other similar techniques for graph and tree mining we refer the reader to (Jiang et al., 2012).

6.2.1 Frequent Sub-graph Mining

When representing workflows as graphs, finding the common workflow fragments of an input corpus is an adaptation of the Frequent Sub-graph Mining (FSM) problem, also referred to as Frequent Sub-graph Matching in the literature (Jiang et al., 2012). The objective of FSM is *"to extract all the frequent sub-graphs, in a given data set, whose occurrence counts are above a specified threshold"* (Jiang et al., 2012). The main difference with our case is that we are not interested in obtaining *all* the workflow fragments, just those that are *useful* for potential reuse. Hence, we first mine all the common workflow fragments and then we filter them with the techniques explained in section 6.3.

The core of FSM is sub-graph isomorphism detection, a problem with NP-Complete

complexity (Cook, 1971). In our case, we will base our work on the definitions introduced in (Jiang et al., 2012), briefly summarized in Definition 3.

Definition 3 *A graph* $G_1 = (V_1, E_1, L_{V_1}, L_{E_1}, \varphi_{V_1}, \varphi_{E_1})$ *is* ***isomorphic*** *to another graph* $G_1 = (V_2, E_2, L_{V_2}, L_{E_2}, \varphi_{V_2}, \varphi_{E_2})$ *if there is a* ***bijective function*** $f : V_1 \rightarrow V_2$ *which maps all the vertices of G1 to all the vertices of G2 and viceversa, i.e.,* ***(i)*** $\forall v \in V_1, \varphi_{V_1}(v) = \varphi_{V_2}(f(v))$ ***(ii)*** $\forall e = (u, v) \in E_1 \Leftrightarrow \forall (f(u), f(v)) = e' \in E_2$ *and* ***(iii)*** $\forall$ *(u,v)* $\in E_1$ $\varphi_{E_1}(u, v) = \varphi_{E_2}(f(u), f(v))$. *We say that* G_1 *is* ***sub-graph isomorphic*** *to* G_2 *if and only if there is a sub-graph* $g \in G_2$ *that is isomorphic to* G_1.

There are two main types of FSM approaches that are relevant to our work: inexact FSM techniques (which can find generic workflow fragments, although may not deliver all the existing frequent sub-graphs in the corpus) and exact FSM techniques (which discover all the possible frequent sub-graphs in the input corpus). These techniques are either frequency based or support based depending on the algorithm implementing them. We describe and discuss them further bellow.

6.2.1.1 Inexact FSM Techniques

These are techniques that use approximate measures to calculate the similarity between two graphs and detect the commonalities among them (Jiang et al., 2012). Figure 6.3 shows an example with three workflows (on top) in which an inexact mining technique is applied (in this case, an iterative graph clustering approach). The most common patterns detected by the technique can be seen in the lower part of the figure. *Fragment 1* has an exact match in the three workflows, but the second fragment found groups two very similar parts of the workflow together (a connection from a step A to *Fragment 1*).

In general, these techniques apply heuristics to detect the most common workflow fragments efficiently. However, the solution provided is not always complete. Therefore, these techniques may not identify all the possible common fragments in the corpus of graphs.

There are many existing inexact graph mining algorithms, which have been developed for different domains (detection of molecules in genomics and chemistry, grammar learning, etc.). Some common examples are SUBDUE (Cook and Holder, 1994; Holder et al., 2002), which uses a graph clustering approach by applying various metrics to

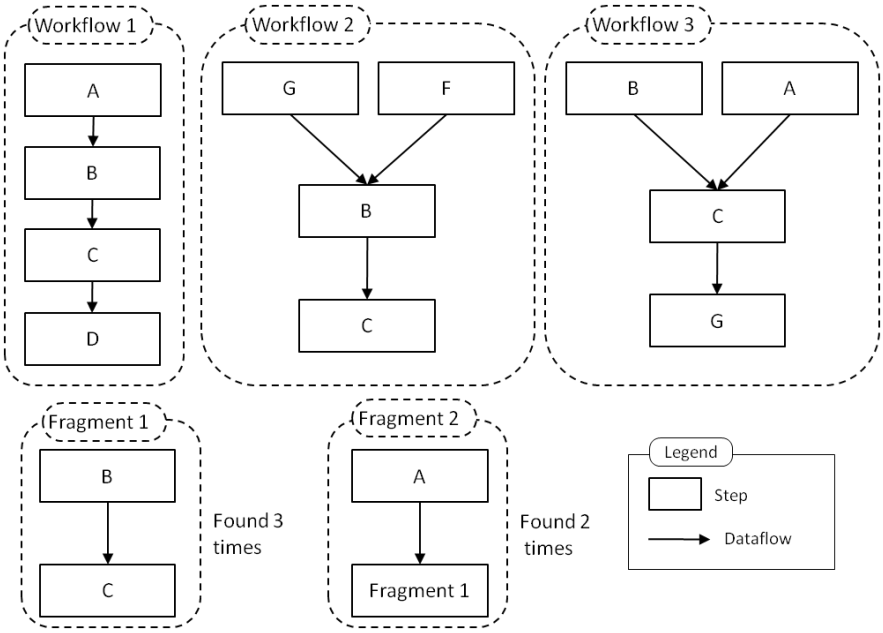


Figure 6.3: Example of an inexact graph mining technique applied to three different workflows (on top of the figure). The results can be seen in the lower part of the figure.

reduce the input graph on each iteration of the algorithm; GREW (Kuramochi and Karypis, 2004b), which uses a similar approach by contracting the edges of the input graph while rewriting it and adding special heuristics to find longer and denser fragments; or SIGMA (Mongiovi et al., 2010), which uses a set-covered based approach by associating a feature set with each edge of the candidate fragment. An extended list of other algorithms can be found in (Jiang et al., 2012).

6.2.1.2 Exact FSM Techniques

These are techniques that aim to deliver all the possible frequent sub-graphs included in a graph corpus. Since these techniques look for all possible solutions, the computational overhead may be excessive in some cases, specially when the size of the common sub-graphs grows. An example of results from this technique can be seen in Figure 6.4, where it is applied to three different workflows (we have ignored single step fragments for simplicity). In the results, we can see that the pattern A followed by B (A$\rightarrow B$), which is included in $A \rightarrow B \rightarrow C$ with the same number of occurrences, is returned as a solution as well.

Exact FSM techniques are more common than inexact FSM approaches. Exact FSM techniques can be based on breadth first search (BFS) or depth first search (DFS) of the graph. Well stablished examples of BFS are the Apriori Graph Mining algorithm (AGM) (Inokuchi et al., 2000), which uses and adjacency matrix to represent graphs in combination with an efficient level-wise search to discover common sub-graphs; or the FSG algorithm (Kuramochi and Karypis, 2001), which builds on the Apriori algorithm by adding a sparse graph representation to reduce storage and computation and incorporating optimizations for the generation of candidates. Common DFS examples are gSpan (Yan and Han, 2002), which uses a canonical representation for encoding each sub-graph and establishes a lexicographic order for efficiently applying the DFS strategy; or Gaston (Nijssen and Kok, 2004), which detects the common sub-graphs by detecting first common paths, transforming them to trees and evolving them into graphs. Additional exact graph mining techniques are described in (Jiang et al., 2012).

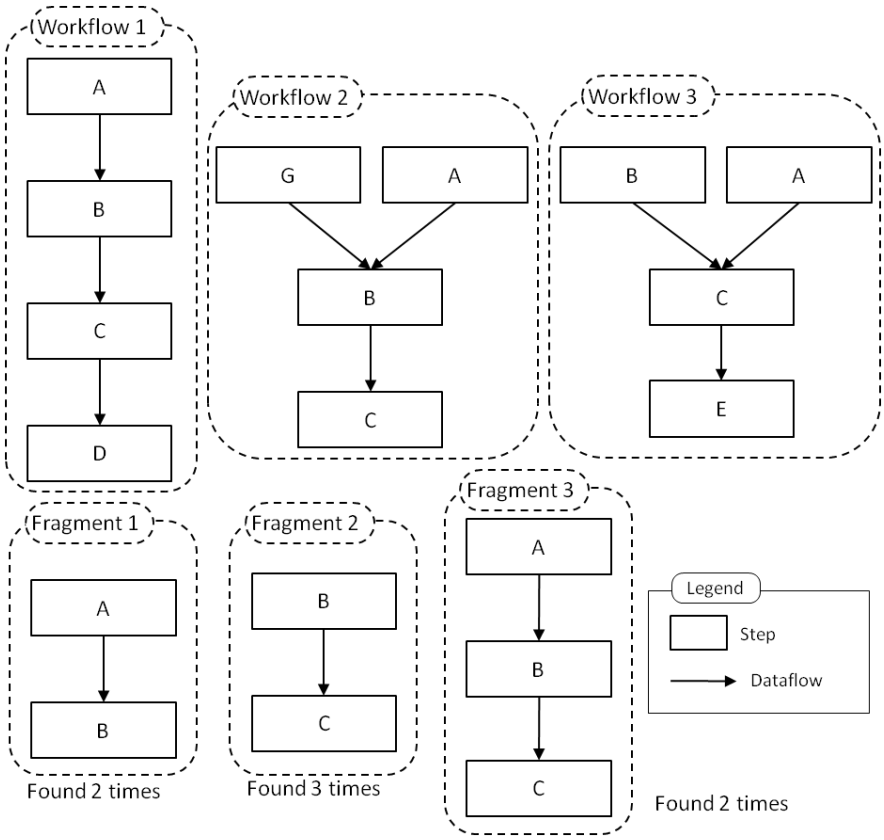


Figure 6.4: Example of an exact match graph mining technique applied to three different workflows (on top of the figure). The results can be seen in the lower part of the figure.

6.2.1.3 Exact FSM versus inexact FSM techniques

Both exact and inexact FSM techniques have advantages and disadvantages. On the one hand, inexact FSM techniques tend to find smaller but highly frequent patterns, including some interesting patterns not detected by exact graph mining techniques. However, they might not identify all potential useful workflow fragments since the results they provide are incomplete.

On the other hand, exact FSM techniques identify all possible fragments in the input corpus. However, when the frequent sub-graph size in the input dataset is high, exact FSM techniques might return too many fragment candidates, while consuming significant computational resources. Adjusting the parameters of the search (e.g., frequency of the desired workflow fragments) is important in order to obtain the best results.

6.2.1.4 Frequency-based versus support-based techniques

Another important aspect is how each technique considers the graphs of the input corpus. Some approaches are **frequency-based** (see Definition 2), i.e., they consider each candidate structure based on the number of times it appears, while others are **support-based** (see Definition 2), i.e., they only consider a candidate structure once per input graph. An example is depicted in Figure 6.5: if we consider our threshold for detecting fragments to be at least two occurrences, the two step fragment $A \rightarrow D$ would not be recognized by a support based approach, since it only occurs on *Workflow 3*. However, since it appears two times, a frequency based approach would consider the sequence of steps as a candidate fragment. Similarly, the fragment $A \rightarrow B$ would be considered to have occurred three times on a frequency based approach (two times on the first workflow and one on the second), while on a support based approach it would occur only two times. Both techniques produce valuable workflow fragments, and are worth considering for detecting common workflow fragments.

6.2.2 Frequent Sub-graph Mining in FragFlow

FragFlow integrates three different existing techniques for extracting common workflow fragments, one inexact graph mining approach with two different heuristics and two exact graph mining techniques. These techniques were selected for several reasons:

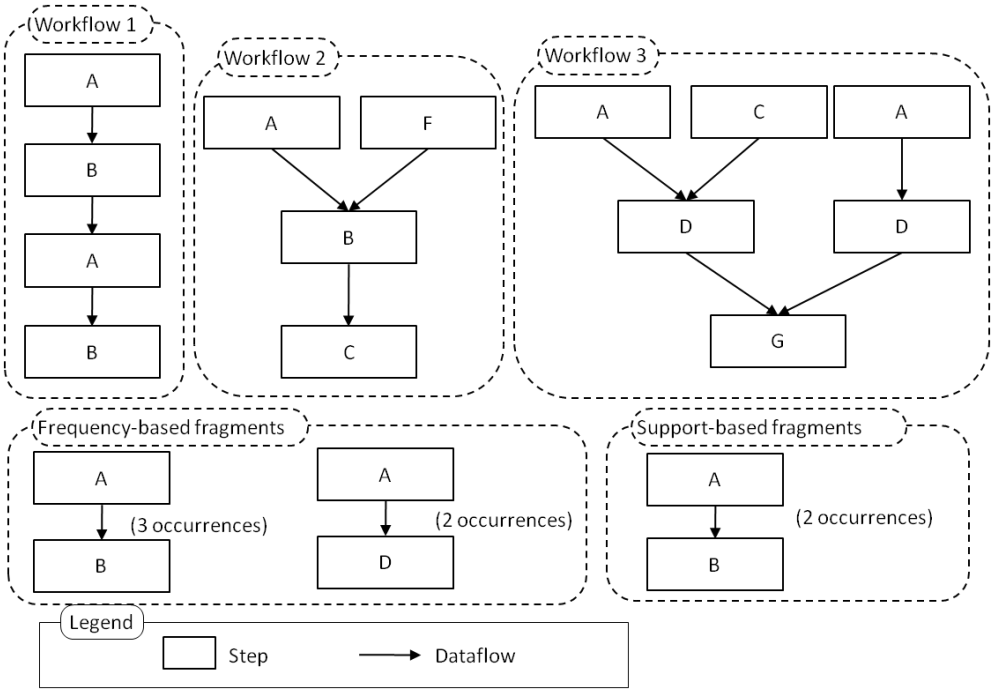


Figure 6.5: Example of a support-based approach versus a frequency-based approach. In a support-based approach, the occurrences of the fragment $A \rightarrow B$ are two (one occurrence in the first workflow and another one on the second workflow), while in a frequency-based approach the occurrences would be three (two times in the first workflow and one in the second).

- Technique features: the algorithm represents a type of technique that could provide different results than other integrated graph mining techniques (i.e., inexact graph mining techniques with different heuristics, exact mining techniques versus inexact mining techniques, etc.). In this work we have tried to use techniques that could retrieve different types of patterns. Table 6.1 includes the different techniques we have taken into account, based on the discussion presented in Section 6.2.1.

- Availability: the algorithm is open source and available for download, as the focus of the work is not to reimplement algorithms described in papers.

- Documentation: the algorithm is documented or has guidelines describing how to use it, providing examples, details of the input format, additional configuration parameters, etc. Some of the algorithms described in the state of the art are

domain-specific and not trivial to reuse without a proper documentation.

- Input/output representation: the input of the algorithm follows a standard or conforms to well used representation.

As shown in Table 6.1, FragFlow integrates two different heuristics of the SUBDUE algorithm (Cook and Holder, 1994) as an inexact graph mining technique, the gSpan algorithm (Yan and Han, 2002) as an exact match depth first search technique and the FSG algorithm (Kuramochi and Karypis, 2004a) as an exact match breadth first search technique. All the currently integrated inexact FSM techniques are frequency based, while exact FSM techniques are support based. The rest of this section provides details of each of the integrated approaches.

Table 6.1: Frequent sub-graph mining algorithms integrated in FragFlow.

Algorithm	**Mining type**	**Occurrences**	**Search Strategy**
SUBDUE	Inexact	Frequency	N/A
FSG	Exact	Support	BFS
gSpan	Exact	Support	DFS

6.2.2.1 SUBDUE

This algorithm was created to detect the most common and repetitive substructures within structural data (Cook and Holder, 1994). SUBDUE uses a hierarchical graph clustering approach by detecting on each iteration of the algorithm the most adequate candidate structure and compressing the input graph with it. Each candidate structure is selected by applying an heuristic, which determines the benefits of reducing the total graph with that candidate structure. SUBDUE uses two main heuristics, which we have used in our analyses:

1. Minimum description length (MDL): heuristic based on the minimum description length introduced by Risannen (Rissanen, 1978). At each iteration, the best candidate substructure is chosen by trying to minimize $I(S) + I(G \mid S)$, where S is the substructure, G is the input graph, I(S) is the number of bits necessary to encode the substructure and $I(G \mid S)$ is the number of bits necessary to encode G with respect to S (Cook and Holder, 1994). After the candidate has

been chosen, the algorithm compresses the graph and continues iterating until no further reduction can be applied.

2. Size: at each iteration, the best fragment is chosen according to how the overall size of graph collection is reduced. That is, this heuristic aims to minimize $size(S) + size(G \mid S)$, where S is the substructure, G is the input graph, $size(S)$ is the number of vertices plus the number of edges of the substructure and $size(G \mid S)$ is the number of vertices plus the number of edges of G with respect of S. Thus, the most repetitive and the bigger the candidate substructure is, the more possibilities it has to be selected.

SUBDUE has been updated through the years with different implementations to make it able to operate with incremental data (Coble et al., 2005) (Coble et al., 2006) or to allow it to recognize recursive structures (e.g., for concept learning) (Holder et al., 2002). Even though more recent efforts have outperformed it, SUBDUE is recognized in the literature as one of the most common algorithms for inexact sub-graph mining (Jiang et al., 2012). In this work, we have used the implementation available on the SUBDUE project website[2], slightly tuned to produce additional metadata with the results[3].

6.2.2.2 FSG

Algorithm that uses a breadth first strategy based on the level-by-level expansion adopted by the Apriori algorithm (Inokuchi et al., 2000).

FSG (Kuramochi and Karypis, 2004a) was designed to work efficiently on undirected labeled graphs and scale reasonably well to very large graph datasets. FSG tackles the problem of common sub-graph detection by applying the following approach: first, it gathers all the single-edged and double-edged graphs. Then the algorithm iterates generating candidate sub-graphs (whose size is one edge greater than the previous frequent ones) counting their frequencies and pruning any candidates that do not satisfy the minimum support constraint (i.e., established minimum number of occurrences). The algorithm stops when no further sub-graphs are generated in an iteration (Kuramochi and Karypis, 2004a).

[2] `http://ailab.wsu.edu/subdue/`

[3] `https://github.com/dgarijo/FragFlow/tree/master/SUBDUE_TOOL`

For efficiency, FSG uses a canonical representation of the graphs, i.e., a unique code to represent the graph without depending on the order of its vertices and edges. Unfortunately, this causes some of the fragments mined to be in an incorrect order when applied to directed graphs (or LDAGs, as it is our case). In order to solve this issue, we match the resulting fragments against those workflows were they were found and fix the directionality of the fragment. We use the FSG implementation included in the PAFI framework[4].

6.2.2.3 gSpan

One of the most popular exact FSM techniques (Jiang et al., 2012), and the first one designed using a DFS strategy. The gSpan algorithm (Yan and Han, 2002) uses a canonical labeling system (a DFS lexicographic order) where each graph is assigned a minimum DFS code. By doing this, gSpan turns the problem of finding common sub-graphs to finding their respective minimum DFS codes. Based on the code, a hierarchical graph is constructed and traversed, discovering all the most frequent sub-graphs. Finally, gSpan applies pre-pruning, post-pruning and partial count pruning to improve its performance (Yan and Han, 2002). In our work, we use the gSpan implementation available on the ParSeMiS framework[5].

6.3 Fragment Filtering and Splitting

The next step in FragFlow is filtering and splitting workflow fragments. The FSM algorithms introduced in the previous section may return many results, including fragments that overlap or that are included as part of other fragments. In order to present to users only those fragments considered to be useful, we filter and refine the initial results by introducing different classes of fragments, as described in Definition 4.

Definition 4 *Given a workflow fragment wf, we denote it as a* ***candidate workflow fragment*** *if it was produced by applying different FSM algorithms to a workflow corpus. The* ***order*** *of a workflow fragment is a function* $o : wf \rightarrow \mathbb{N}$ *which returns the number of vertices in the workflow fragment* ($o(wf) = |V(wf)|$). *Fragments where* $o(wf) > 1$ *are referred to as* ***multi-step workflow fragment****. Finally, if we have a set of workflow*

[4] `http://glaros.dtc.umn.edu/gkhome/pafi/overview/`

[5] `https://github.com/timtadh/parsemis`

fragments $Wf = (wf_1, wf_2, ..., wf_n)$*, we denote as* ***multi-step filtered fragments*** *(Mff) those multi-step workflow fragments that are not part of bigger workflow fragment with the same number of occurrences, i.e.,* $wf_i \in Mff\ (1 \leq i \leq n) \Leftrightarrow$ ***(a)*** $o(wf_i) > 1$*,* ***(b)*** $\forall wf_j \in Wf, (1 \leq j \leq n), j \neq i, wf_i \subseteq wf_j \Rightarrow F(wf_i) \neq F(wf_j)$ *(where F stands for the frequency or support as defined in Definition 2).*

Figure 6.6 shows an example, where five fragments are represented (*f0*, *f1*, *f2*, *f3* and *f4*). As all the fragments have been produced by applying FSM techniques, all of them are considered as candidate fragments. Candidates *f1* to *f4* have more than one step, and are thus considered multi-step fragments. From this group, two fragments are part of other fragments (*f1* is included in *f2* and *f3* in *f4*). However, the frequency of *f1* is equal to *f2*, while *f3* occurs more times than *f4*. Therefore, *f2*, *f3* and *f4* are considered multi-step filtered fragments, while *f1* is not.

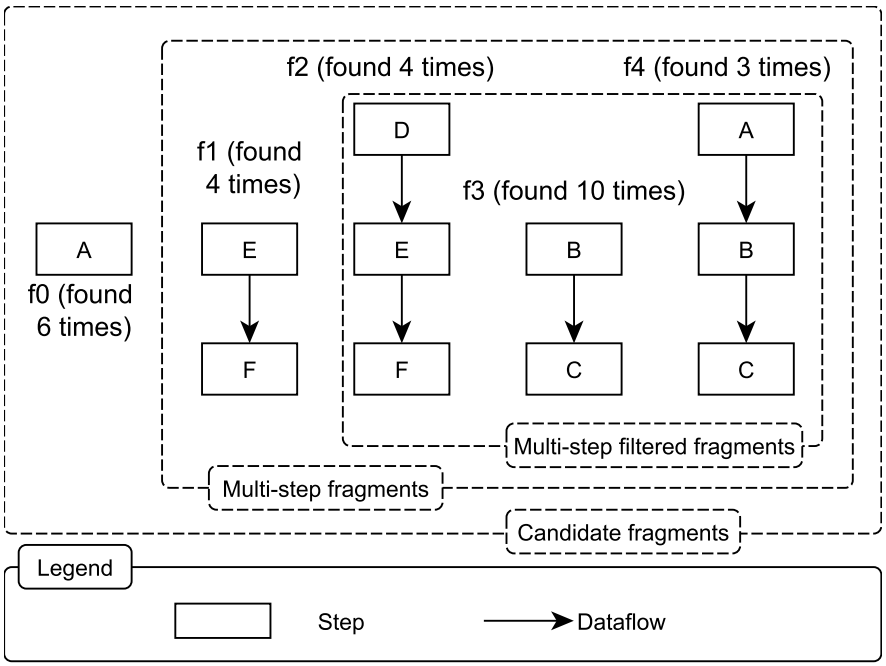


Figure 6.6: Types of fragments for filtering FSM results.

Our interest is to present to the user only the multi-step filtered fragments, that is, fragments that have several steps and occur more than a minimum number of times. Single step fragments are not relevant, as they are already the minimum pieces of functionality when creating a workflow. By filtering multi-step fragments we maximize

the size of the fragments presented to the user without removing those common smaller fragments that are included as part of bigger fragments.

After filtering, the candidate fragments are split according to their category (multi-step or multi-step filtered). This helps selecting the group of fragments to visualize, calculate statistics or link to the original corpus.

6.4 Fragment Linking

Once the workflow fragments have been filtered, the next step in FragFlow is to bind each fragment to its occurrences in the original workflow corpus, so as to make explicit the conexion between workflows and their common fragments. This section introduces first the model used to represent and bind fragments to results by extending the P-Plan ontology; and then it describes how the different fragments are bound to the workflows of the original corpus.

6.4.1 Workflow Fragment Representation

We created the Workflow Fragment Description Ontology (Wf-fd[6]) to represent workflow fragments and link them to their occurrences in a workflow dataset. Wf-fd was built by extending the P-Plan ontology, as workflow fragments are always part of a workflow template (a `plan` in P-Plan). Figure 6.7 shows an overview of the model, highlighting the extended terms and how the workflow fragment representation benefits from P-Plan. In order to differentiate between the classes and properties of both models, we use the "`p-plan`" and "`wffd`" prefixes respectively. In Wf-fd, a `WorkflowFragment` is a subclass of P-Plan's `plan`. A workflow fragment has steps (reusing the `step` concept in P-Plan) which represent the individual data manipulation steps of a particular fragment. The order among the steps is also captured with the P-Plan property `isPrecededBy` between fragment steps.

In Wf-fd there are two types of `workflow fragments`. On the one hand, a `detected result workflow fragment` is a workflow fragment found after applying FSM techniques or manual analyses on a workflow dataset. It identifies a unique fragment that can be found in a workflow dataset (e.g., a workflow fragment result provided by any of the graph mining techniques presented in Section 6.2.1). On the other hand,

[6] `http://purl.org/net/wf-fd`

a `tied workflow fragment` represents how a `detected result workflow fragment` was found in the workflow dataset, pointing to the particular steps of the workflows that correspond to the fragment.

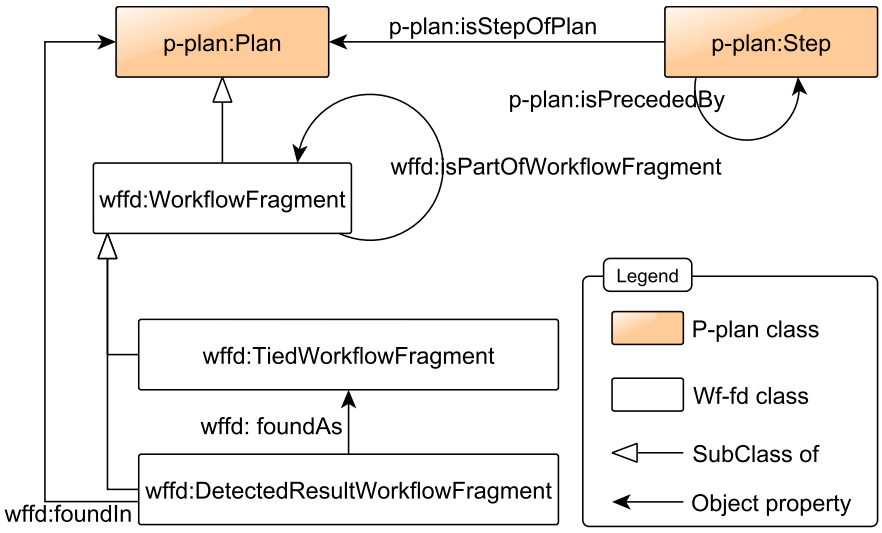


Figure 6.7: Wf-fd overview, extending the P-Plan ontology.

An example is represented in Figure 6.8, where two fragments (*resultF1* and *resultF2*) are found two times (linked through their respective tied result workflow fragments) in the workflows *Workflow 1* and *Workflow 2*. As the figure shows, resultF2 is composed of two steps with types <B> and <C>, while *resultF1* is composed by the step <A> followed by the fragment *resultF2*. This relationship is represented with the `wffd:isPartOfWorkflowFragment` relationship.

ResultF2 is represented with a P-Plan's `multiStep` (*step2F1*) in *resultF1*. The additional step (*step2F1*) is necessary as the fragment *resultF2* could be part of many other fragments, and including it directly as part of *resultF1* would lead to inconsistencies when representing the rest of the results. For example, if we want to represent the three fragments depicted in Figure 6.9 and we don't make use of a `multiStep` step, the modeling would result as shown in Figure 6.10(a), which is inconsistent (the precedence relationship in *R2* would not be properly represented) and adds complexity for retrieving fragments based on their `isPrecededBy` relationship. Instead, if we use the modeling proposed in Figure 6.10(b) (i.e., using the `mutliStep` to model fragment inclusion in other fragments), the fragments would be represented properly and their

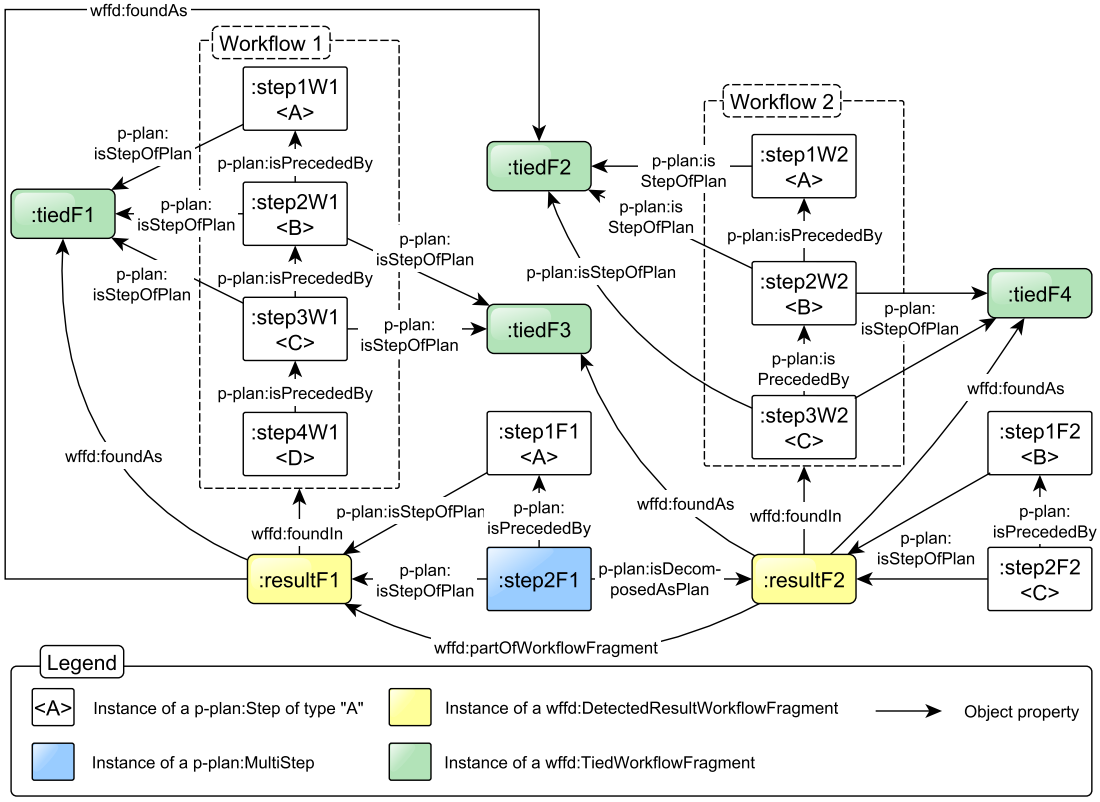


Figure 6.8: Wf-fd example. Two fragments (*resultF1* and *resultF2*) are found twice on the workflows *Workflow1* and *Workflow2*. Their respective tied workflow fragments indicate where in each of the workflows the fragments were found. Also, *resultF2* is part of *resultF1*, being recorded appropriately.

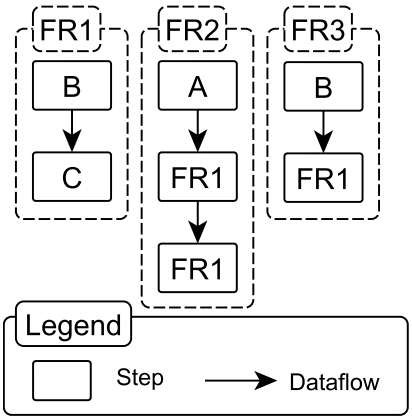


Figure 6.9: Three sample fragments. Arrows represent the dependencies among the steps.

retrieval could be done by using just the `isPrecededBy` relationship.

This representation also allows each fragment to point to the specific steps of the workflow where it was found (`foundAs`), as well as the workflow itself (`foundIn`). Thanks to the model and the reuse of P-Plan, we enable queries to retrieve additional metadata for each fragment and workflow step (e.g., number of times that a fragment has been detected in a workflow, how the fragment was found, etc.).

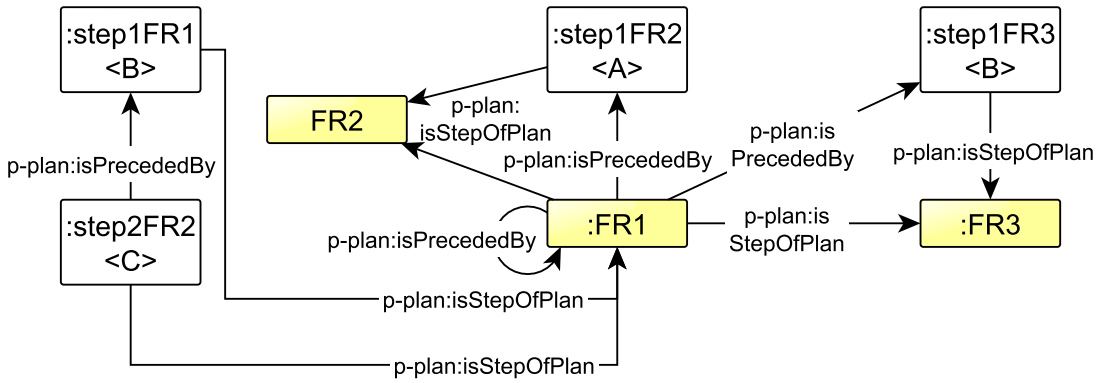
6.4.2 Finding Fragments in Workflows

Once the final set of fragments has been obtained and refined, we link them to the original workflow corpus, represented with the Wf-fd ontology. Since the FSM approaches do not always indicate where the fragments were found, we use a generic simple method to link the obtained results of both exact and inexact FSM techniques to the input workflow corpus: we create queries from each fragment.

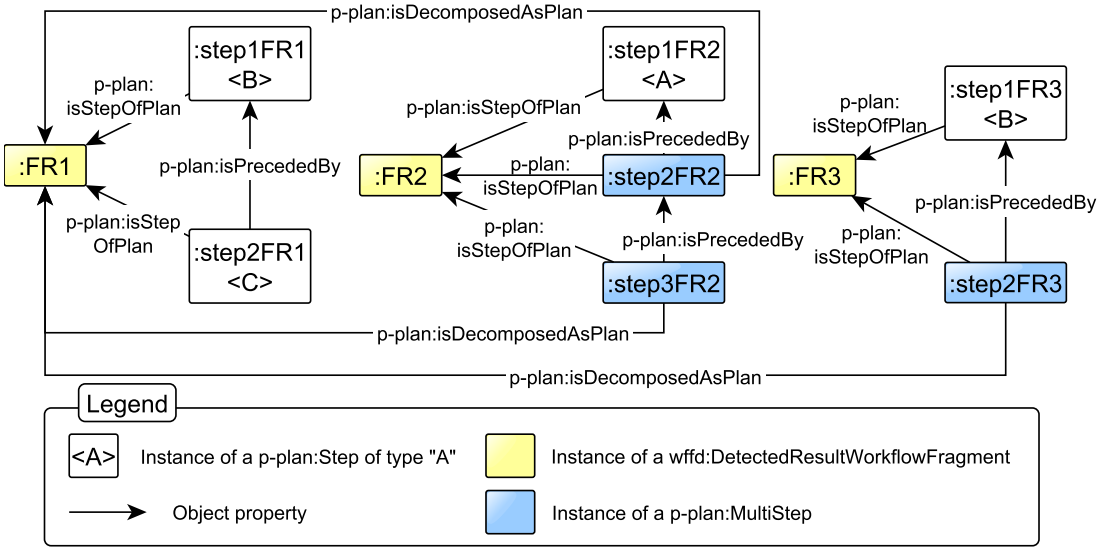
At this stage the input workflows are already represented in P-Plan from previous steps. Thus, workflow fragments detected by exact FSM techniques are trivial to transform to queries: each node is transformed to a `step` in P-Plan, and each dependency among two steps is represented with the `isPrecededBy` relationship. As an example, the fragment depicted in Figure 6.11(a), is transformed to the query below (expressed in SPARQL):

```
SELECT ?wf ?stepA ?stepB ?stepC WHERE{
  ?stepA a <A>.
  ?stepB a <B>.
  ?stepC a <C>.
  ?stepA p-plan:isStepOfPlan ?wf.
  ?stepB p-plan:isStepOfPlan ?wf.
  ?stepC p-plan:isStepOfPlan ?wf.
  ?stepC p-plan:isPrecededBy ?stepA.
  ?stepC p-plan:isPrecededBy ?stepB
}
```

Workflow fragments detected with inexact mining techniques are more complex to transform. For example, consider the fragment represented on the top of Figure 6.11(b) (*Fragment 1*), where step A is followed by *Fragment 2* (composed of two steps B and C). *Fragment 1* represents that step A is followed by *Fragment 2*, but it does not

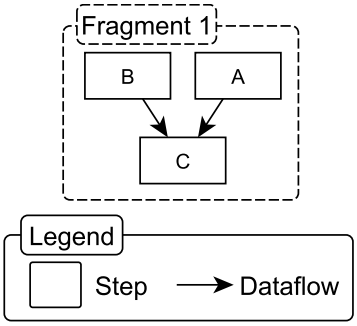


(a) Inconsistent model: Modeling the fragments of Figure 6.9 without using `p-plan:MultiStep`.

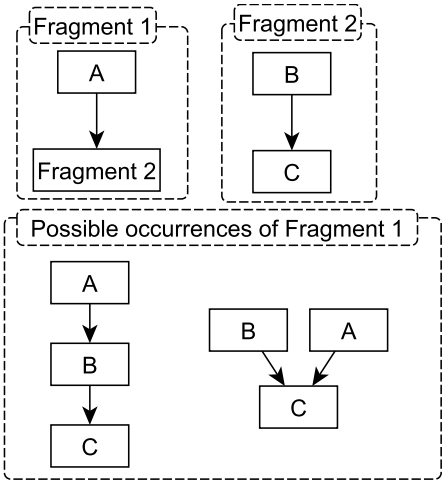


(b) Consistent model: Modeling the fragments of Figure 6.9 using `p-plan:MultiStep`.

Figure 6.10: Inconsistent and consistent modeling of the fragments depicted in Figure 6.9.



(a) A simple fragment example obtained by an exact FSM technique.



(b) Transforming inexact FSM fragments to queries. The fragment on top of the figure can be transformed in two different ways, shown in the middle of the figure.

Figure 6.11: Transforming fragments obtained with exact FSM techniques (left) and inexact FSM techniques (right).

specify if step B or C (due to the inexact mining approach). Therefore, we try both possibilities, translating the fragment to the two possible interpretations shown on the bottom of the figure. Both interpretations queries are issued within the same query as follows (represented in SPARQL):

```
SELECT ?wf ?stepA ?stepB ?stepC WHERE{
  ?stepA a <A>.
  ?stepB a <B>.
  ?stepC a <C>.
  ?stepA p-plan:isStepOfPlan ?wf.
  ?stepB p-plan:isStepOfPlan ?wf.
  ?stepC p-plan:isStepOfPlan ?wf.
  ?stepC p-plan:isPrecededBy ?stepB.
{
  ?stepB p-plan:isPrecededBy ?stepA.
}UNION{
  ?stepC p-plan:isPrecededBy ?stepA.
}}
```

The answers for each query (or union of queries in the case of inexact mining) are all the possible bindings within all workflows, showing how and where each fragment was found in each of the workflows of the original corpus.

6.5 Fragment Statistics and Visualization

Once the fragments have been filtered and bound to the workflow corpus, the next step in FragFlow is to produce statistics and visualizations of the fragments. For this purpose we created scripts for calculating the minimum frequency of the fragments and number of times they were found in the corpus, which is particularly useful for the evaluation of our approach (as we describe in Chapter 7). Additionally, we created a graph-based visualization for a collection of fragments, helping users understand the shape and dependencies of each fragment.

6.6 Summary

In this chapter we have introduced our approach for extracting workflow fragments by reusing different graph mining techniques. In doing so, we have proposed a way to clean the input workflow dataset to avoid incorrect results and we have characterized and selected existing graph mining techniques that broaden the types of fragments being found by our approach. This addresses the technical objective of this thesis TO1 (*characterize the different types of existing graph mining algorithms, their features, their limitations and available implementations*).

We have also introduced a set of novel techniques to filter irrelevant fragments and link the results to the parts of the input corpus where they occur, thus addressing the technical objective TO2 (*develop a framework for applying existing graph mining approaches on workflow templates and executions, along with the means to refine and filter the results provided by the different algorithms*).

It is worth mentioning that our effort has been driven towards usefulness rather than efficiency, as the second was not part of the scope of this thesis. For example, if the number of workflows of the input corpus is high, doing a SELECT query retrieving *how* a complex fragment was found on the corpus might be too time consuming. In those cases, our approach could be divided into smaller sub-problems (e.g., issuing queries

against single workflows instead of workflow dataset) or simplifying our approach (e.g., issuing ASK queries instead of SELECT queries). Improving the performance and efficiency of our approach is future work.

In the next section we will assess usefulness of our results by performing three evaluations on two different workflow systems.

Chapter 7

Evaluation

In this chapter we evaluate our hypotheses by describing the results of our approach for automatically detecting abstractions on scientific workflows. Given that H1.1 (i.e., *it is possible to define a catalog of common domain independent patterns based on the functionality of workflow steps*) has already been addressed in Section 5.1 by defining a catalog of common workflow motifs, in this chapter we focus on evaluating H1.2 (*it is possible to detect commonly occurring patterns and abstractions automatically*) and H1.3 (*commonly occurring patterns are potentially useful for users designing workflows*).

First, Section 7.1 defines the evaluation metrics associated with each hypothesis, and then Sections 7.2 and 7.3 describe the results obtained on each of the evaluations. Finally, section 7.4 summarizes our contributions with respect to each hypothesis.

7.1 Evaluation Metrics

There are different techniques to identify patterns in a workflow corpus, as we have described on Chapter 6. In order to evaluate our hypotheses H1.2 and H1.3, we need to assess the genericity and usefulness of our proposed frequent workflow fragments. However, to our knowledge *there are no standard metrics that define if a given workflow pattern is generic or useful.* Therefore we propose a metric for assessing frequent generic fragments and two for evaluating fragment usefulness, as described in Definition 5. These metrics will be adapted and used later for performing independent evaluations, as they have different requirements on the input corpus.

Definition 5 *A workflow fragment is* ***generic*** *if it appears in two or more workflows with different levels of abstraction. We consider a workflow fragment to be* ***useful*** *if it has been reused and annotated by one or several users designing workflows (either as a workflow or as a sub-workflow).*

7.1.1 Occurrence and Generalization Evaluation Metrics

Our proposed metric aims to confirm whether a workflow fragment is commonly occurring and generic. In order to do so, we compare our proposed fragments to those motifs from our catalog that are related to workflow reuse, i.e., *internal macros* and *composite workflows*. Internal macros detect the reused parts of a workflow among the workflow itself, and therefore a fragment matching an internal macro is commonly occurring. Composite workflows indicate that a target workflow is composed by other existing workflows. Hence, any fragment matching those sub-workflows is commonly occurring. Additionally, these motifs may apply a step abstraction to relate workflows with the same abstract functionality, and we can use them to assess the genericity of our proposed fragments. For measuring our results, we use precision (P_{motifs}) and recall (R_{motifs}), defined as:

$$P_{motifs} = \frac{|F \cap M|}{|F|}$$

$$R_{motifs} = \frac{|F \cap M|}{|M|}$$

Where **F** represents the resultant set of fragments and **M** stands for the set of motifs we are looking for (in this case, M would represent either the set of internal macros in the corpus or the sub-workflows included in any composite workflow in the corpus). Precision and recall values range from 0 (low) to 1 (high). In order to be able to apply this metric, *a workflow corpus with annotated motifs is necessary.*

7.1.2 Usefulness Evaluation Metrics

In this case, the first metric we propose aims at comparing whether the workflow fragments found by our approach match those fragments or workflows designed and reused by users (i.e., *user groupings*). We also measure our results in terms of precision and recall for this task. On the one hand, the precision measures how many of the common

fragments correspond to the reused groupings and workflows identified by users. On the other hand, the recall identifies the percentage of detected reused structures out of the total reused groupings and workflows. Since our focus is to detect useful workflow fragments, we prioritize precision over recall. The recall measure is relevant, but some of the reused groupings or workflows may have a low frequency and may avoid detecting higher frequency fragments, motivating our decision.

It is worth mentioning that workflows are considered in the metric as well. Some workflows are reused as part of other bigger workflows in the workflow corpus and our fragments may correspond to them. Precision (P_{group}) and recall (R_{group}) metrics are defined as:

$$P_{group}(overlap) = \frac{|F \cap (G \cup W)|}{|F|}$$

$$R_{group} = \frac{|F \cap (G \cup W)|}{|G \cup W|}$$

Where **F** represents the set of proposed fragments, **G** stands for the set of user-defined groupings and **W** corresponds to the set of reused workflows. The intersection between fragments and the union of all groupings and workflows is calculated by measuring which fragments overlap with a grouping or a workflow. The *overlap* term stands for the percentage of steps that are equal between our proposed fragments and groupings or workflows when calculating $|F \cap (G \cup W)|$, with P(100%) meaning that the fragments found are exactly the same as one of the the groupings or workflows defined by users. Figure 7.1 shows an example by comparing the overlap of two fragments against the same grouping. The fragment on the left (*Fragment1)* is equal to *Grouping1* (overlap 100%), while in *Fragment2* only two steps out of three are the same (with an overlap of 66%). This additional measure determines how similar our fragments are with respect to a user-defined grouping or workflow, and helps identifying whether our fragments are close to what they defined or not. As in the last metric, precision and recall values range from 0 (low) to 1 (high). A requirement for applying this technique is to *have a workflow corpus with user-defined groupings specified.* Note that the overlap is not introduced for the recall (R_{group}), as it could lead to inconsistent results: if the number of candidate fragments similar to the groupings and workflows designed by

users is higher than the number of groupings and workflows, then the recall would be superior to 1.

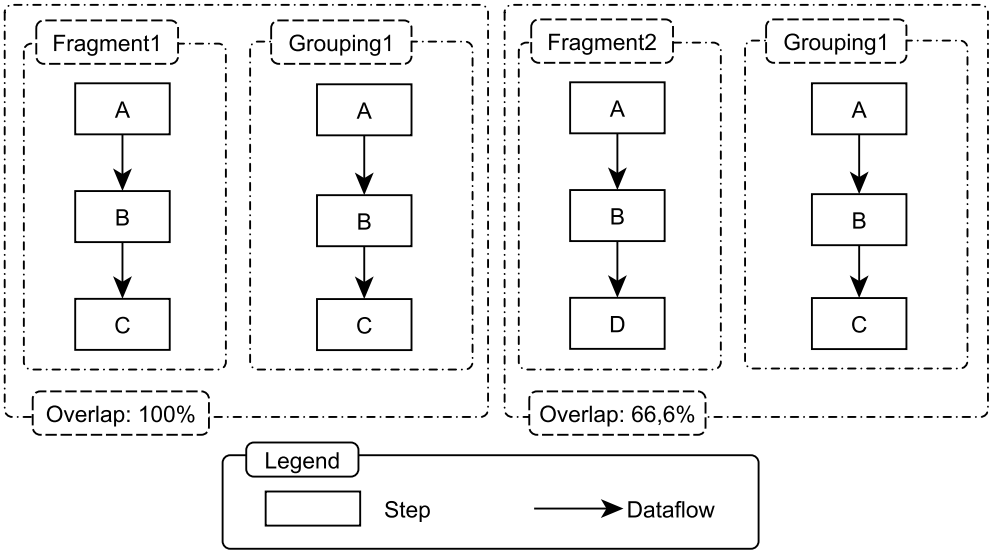


Figure 7.1: Overlap example: two fragments are compared against the same grouping. *Fragment1* is exactly the same as *Grouping1*, while only two out of three steps of *Fragment2* are equal to *Grouping1* (hence 66,6% overlap).

For the second metric, we rely on user feedback. Thus, we target the accuracy (Acc) of our results, defined as:

$$Acc = \frac{|FA|}{|F|}$$

Where $|FA|$ stands for the number of fragments the user found useful and $|F|$ represents the total number of fragments proposed to the user.

Table 7.1 shows a summary of our proposed metrics and their requirements for evaluation, which will be applied on the following sections on different user corpora.

Table 7.1: Proposed metrics with their requirements for evaluation.

Metric	**Requirement for evaluation**
P_{motif}, R_{motif}	Workflow corpus annotated with motifs
P_{group}, R_{group}	Workflow corpus annotated with user-defined groupings
Acc	Workflow corpora and respective user feedback.

7.2 Workflow Motif Detection and Workflow Generalization

In this section we describe the results of applying our first metric (P_{motifs} and R_{motifs}) to an input corpus of workflows in order to test our hypothesis H1.2 (*it is possible to detect commonly occurring patterns and abstractions automatically*). Therefore, generalization of workflows is applied (using a step abstraction with the workflow system's taxonomy of components) to determine whether abstract workflow patterns can be mined successfully. Section 7.2.1 describes the experimental setup of the evaluation, while sections 7.2.2 and 7.2.3 elaborate on the results obtained by applying inexact and exact graph mining techniques. The evaluation presented here is based on our previous results (Garijo et al., 2013a), which have been further refined.

7.2.1 Experimental Setup

We have selected a dataset that contains 22 workflow templates in the domain of text analytics (17 after removing one-step workflows), specified using the Wings workflow system (Gil et al., 2011). The templates are annotated according to the Open Provenance Model for Workflows (OPMW) and belong to the Wings corpus presented in Section 5.1. This specific domain and dataset have been selected for our experiment for two main reasons:

- They contain abstract and specific templates in the same domain, which provide some alternatives for generalization of workflows. This means that some specific templates may share commonly occurring steps with other templates of the corpus after applying a step abstraction (i.e., after a generalization of their steps).

- They have been manually analyzed, before and after generalizing the workflows (as described in (Garijo et al., 2012)), so as to identify all internal macros motifs and workflows part of a composite workflow motif. The annotations highlight maximal motifs, i.e., if an internal macro consists of 4 steps, it has been annotated only once, without including the three-step and two-step possible internal macros contained. An example can be seen in Figure 7.2, where a workflow for document classification has an internal macro with six steps (appearing two times, one on each branch of the workflow). The internal macro annotated would be the one

highlighted in the figure, and all the possible combinations of its sub-workflows ignored. Motif annotations are required by the reusability metrics tested in this section, and we use them in our evaluation to assess the workflow fragments found.

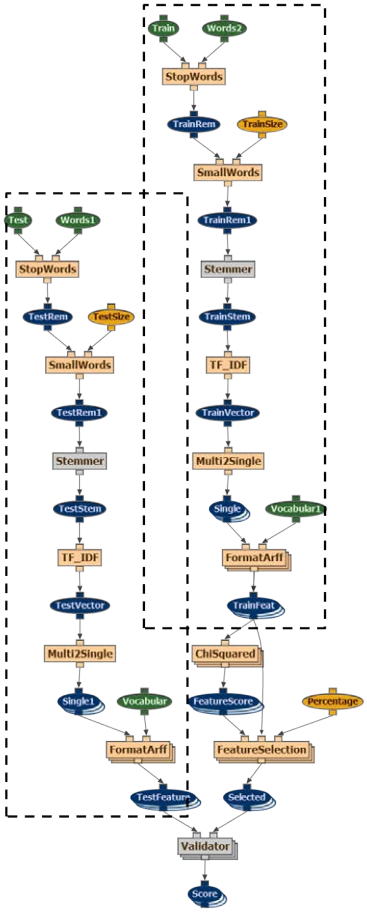


Figure 7.2: Example of an internal macro, annotated with a dashed line. The internal macro consists on the sequence of steps that are included in each branch, ignoring all the possible 2, 3, 4 and 5 sub-workflows included in it.

We apply inexact and exact FSM techniques for detecting the desired motifs, as described in Section 6.2.2. For detecting internal macros, we run the FSM algorithms on each template separately, while for detecting those workflows included in composite workflows we run the FSM techniques over the whole corpus. It is important to note that the techniques that are support-based will not be able to find any internal macros, as they only consider one occurrence of a fragment per input graph, and internal macros

Table 7.2: Summary of the manual analysis on the Wings corpus.

		No Generalization		Generalization	
Templates	Filtered Templates	Int. Macro	Wf in Comp. Workflow.	Int. Macro	Wf in Comp. Workflow.
22	17	3	2	5	7

aim to find the common parts of a single workflow.

Table 7.2 summarizes the detected motifs on the input corpus, before and after generalizing all the steps of the workflows (more details can be found in Annex C.1). The table shows how the size of the corpus and the number of motif annotations are not big, as the corpus had to be extended from the motif analysis to annotate all internal macros and workflows in composite workflows when generalizing the corpus. However, we consider the corpus significant enough for validating our hypothesis and analyzing our results in detail because the annotated motifs are based on commonly reused patterns. Furthermore, having a smaller corpus might highlight the limitations of the applied algorithms when some common patterns overlap.

The evaluation *will assess whether we can obtain a high recall on the proposed results, rather than a high precision*: we aim for an automatic detection of **all** the internal macros and workflows part of composite workflows on the input corpus. More precision in our results may avoid finding all the abstractions we are looking for.

7.2.2 Evaluation of the Application of Inexact FSM techniques

We apply the SUBDUE-MDL and SUBDUE-Size techniques described in Section 6.2.2 to the input corpus. The description of the results for each motif can be found below.

7.2.2.1 Internal Macro Results

Table 7.3 shows the precision and recall of the results obtained for the inexact FSM techniques on the input corpus (both returned the same results). The table shows the results according to the generalization (i.e., using the input corpus as is (no generalization) and after applying step abstraction (generalization)); and the type of fragment: candidate (raw result returned by the inexact FSM technique), multi-step (fragments with more than one step) and multi-step filtered (product of applying our filtering

techniques described on Section 6.3). All the fragments are obtained assuming the minimum frequency (i.e., a minimum of 2 occurrences on the analyzed structure). Due to the size of the corpus, we avoid comparing the results at different frequencies, as the results would not differ significantly.

Table 7.3: Inexact FSM techniques for the detection of internal macro motifs, using the templates without and with generalization of their steps.

	SUBDUE MDL/Size			
	No Generalization		Generalization	
Fragment type	$P_{i.macro}$	$R_{i.macro}$	$P_{i.macro}$	$R_{i.macro}$
Candidate	0,13	1,0	0,19	1,0
Multi-step	0,22	0,67	0,36	0,8
Multi-step filtered	**1,0**	**0,67**	**1,0**	**0,8**

As the results show, all the internal macros are detected with the candidate fragments for the non generalized and generalized corpus ($R_{i.macro} = 1{,}0$). However, one of the annotated internal macros is not detected when applying our filtering techniques (1 out of 3 in the non-generalized corpus and 1 out of 5 in the generalized corpus). Figure 7.3 shows the explanation of this result. On the left, the workflow where the internal macro has been annotated is depicted. On the right we can see its reduced form, showing just the dependencies among the different steps. It turns out that the internal macro consists of just a one step fragment (*Stemmer*), which is filtered by our approach (on the multi-step filtered fragments) since one-step fragments are just single-step components and are already available for a workflow designer as atomics pieces of functionality. Therefore, although the internal macro is not detected, the behavior of our results is the desired one. Note that in our motifs and fragments we don't consider overlapping structures, that is why the *Vocabular* component is not included as part of the internal macro.

Regarding the precision, the best results are obtained on the multi-step filtered fragments ($P_{i.macro} = 1{,}0$). In this case, this is due to the nature of the motif we are looking for. We explore every workflow by itself, so the number of fragments found tend to be reduced and included on each other.

Finally, a key finding of our results is that they show how our approach can handle both generalized workflows and non-generalized workflows. As shown in Table 7.2,

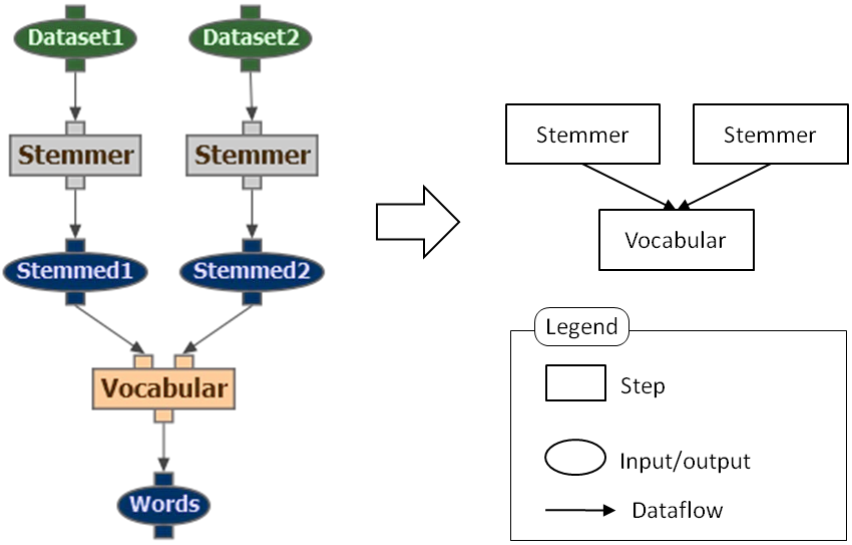


Figure 7.3: Workflow where the internal macro annotated could not be detected. When transforming the workflow to its reduced form, the internal macro is just a one-step fragment, which is ignored.

when applying generalization, two new internal macros are detected in the corpus. Both of them are found by our approach.

7.2.2.2 Composite Workflow Results

Tables 7.4 and 7.5 show the results obtained after applying both SUBDUE-MDL and SUBDUE-Size metrics on the corpus respectively.

Table 7.4: Inexact FSM techniques for the detection of workflows in composite workflow motifs, using the templates as they are and with generalization and the SUBDUE MDL evaluation. The asterisk represents the results when a target workflow is included as part of a bigger detected fragment.

	SUBDUE MDL			
	No Generalization		Generalization	
Fragment type	$P_{c.wf}$	$R_{c.wf}$	$P_{c.wf}$	$R_{c.wf}$
Candidate	0,14	0,50	0,67 (1,0)*	0,57 (0,86)*
Multi-step	0,14	0,50	0,67 (1,0)*	0,57 (0,86)*
Multi-step filtered	**0,14**	**0,50**	**0,67 (1.0)***	0,57 (0,86)*

Table 7.5: Inexact FSM techniques for the detection of composite workflow motifs, using the templates as they are and with generalization and the SUBDUE Size evaluation. The asterisk represents the results when a target workflow is included as part of a bigger detected fragment.

	SUBDUE Size			
	No Generalization		Generalization	
Fragment type	$P_{c.wf}$	$R_{c.wf}$	$P_{c.wf}$	$R_{c.wf}$
Candidate	0,03 (0,07)*	0,50 (1,0)*	0,15 (0,22)*	0,57 (0,86)*
Multi-step	0,11 (0,22)*	0,50 (1,0)*	0,57 (0,86)*	0,57 (0,86)*
Filtered multi-step	**0,125 (0,25)***	**0,50 (1,0)***	**0,57 (0,86)***	**0,57 (0,86)***

Some of the results on the table include a second measure in brackets with an asterisk. The measure indicates the precision or recall when the target workflow reused in a composite workflow has not been detected, but it is included as part of a bigger fragment which has been detected by the applied FSM technique. We decided to include this measure for two main reasons. The first one is because the workflows designed by users may not correspond entirely with how they are reused in other workflows. The second reason is due to the algorithm used by the graph mining techniques, tending to maximize the size of the patterns found when they overlap. An example can be seen in Figure 7.4, where three workflows are depicted. The one on the left (*Workflow 1*) is reused in the other two workflows. The workflow in the middle is also reused in the workflow on the right (*Workflow 3*). Since *Workflow 1* is included in a bigger reused workflow (*Workflow 2*), the graph mining technique may select the bigger fragment (*Workflow 2*) instead of *Workflow 1*, depending on its frequency in the rest of the corpus.

Due to this overlapping issue, our results for detecting workflows included in the composite workflow motifs are not as good as those obtained for internal macro motifs. The best results are obtained by the SUBDUE-Size technique, with one out of two detections (50%) for non generalized workflows (the other composite workflow is detected as part of a bigger fragment) and four out of seven (57%) detections in generalized workflows (which increases to six out of seven (86%) if we consider those fragments

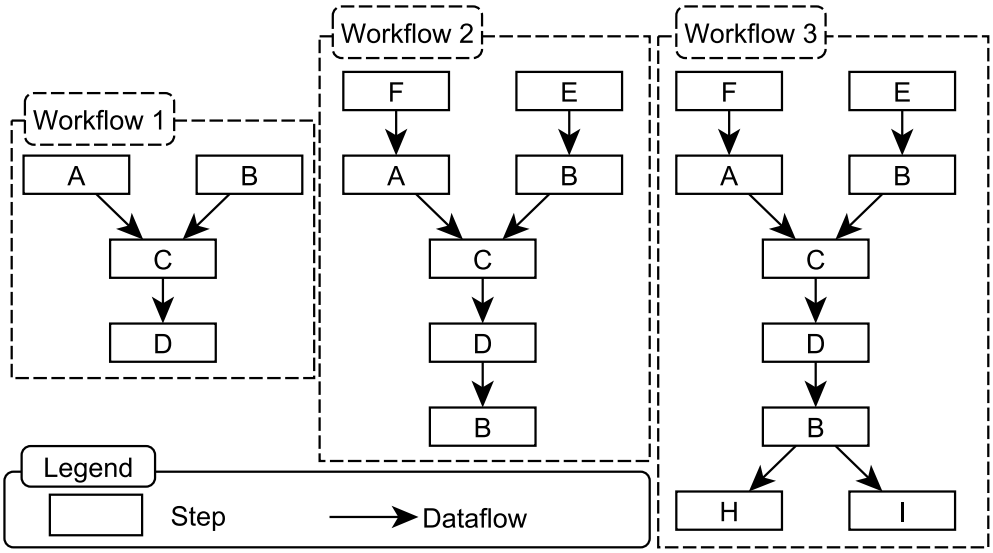


Figure 7.4: Fragment inclusion: The workflow on the left is included in the workflow in the middle which itself is included in the one on the right. If maximal patterns are chosen by the applied FSM technique, *Workflow 1* may not be detected as a common workflow fragment.

overlapping with the target workflow). The results demonstrate that, up to a reasonable percentage, inexact FSM fragments are a good technique for detecting which workflows are part of composite workflows, even if not all of them are detected.

It is worth mentioning that even taking into consideration those results included in bigger fragments, there are target workflows that are not detected by the algorithm. This can be explained by further analyzing the overlapping issue and the way SUBDUE operates. SUBDUE reduces each candidate fragment in the input dataset on each iteration. If a fragment overlaps with another and the algorithm chooses one to reduce, the other candidate might not be detected. Figure 7.5 shows an example where three workflows have two overlapping fragments. *Workflow 1* and *Workflow 2* share a three step fragment (highlighted with a dotted line). *Workflow 2* and *Workflow 3* share a two step fragment. Due to the overlap between the two fragments, if SUBDUE decides to reduce the bigger one, the smaller fragment will not be detected. Some of these issues disappear when applied to bigger corpora, as the smaller patterns tend to be more frequent and are detected even if there are overlapping issues.

Finally, precision is better for the SUBDUE-MDL technique, which produced fewer results than SUBDUE-Size. As was the case with the internal macros, by generalizing

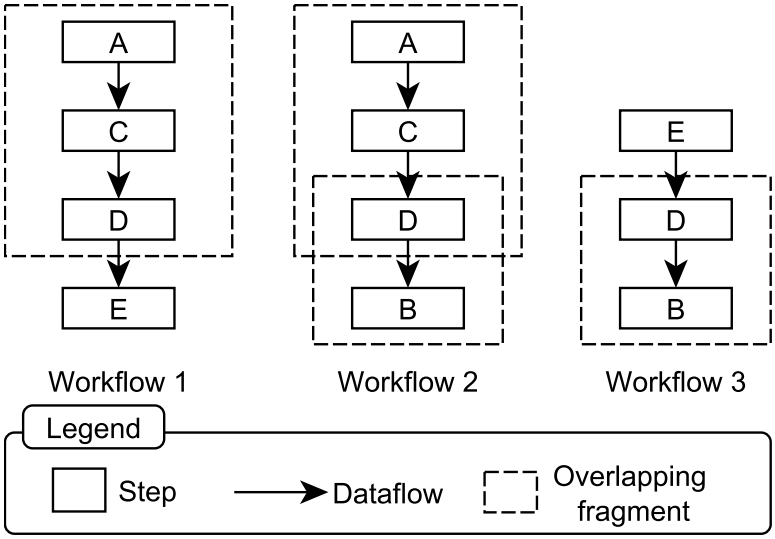


Figure 7.5: Fragment overlap in SUBDUE: three workflows overlap without being included in each other (their common parts have been highlighted with a dotted line). If the FSM technique selects the bigger fragment, the smaller one (step D followed by B) would not be detected.

the workflows we obtain more workflow fragments, which match more than half of the workflows detected manually.

7.2.3 Evaluation of the Application of Exact FSM Techniques

Table 7.6 summarizes the results of applying the gSpan technique to the input corpus (an additional evaluation with the FSG algorithm was not included, as all exact FSM techniques deliver very similar results). The results are obtained with minimum support two (similarly to what we stablised for the frequency of inexact FSM techniques), and filtering out one-step results (can be set as a parameter for the algorithm).

As expected, *all the workflows included in composite workflows are found among the provided results*, improving the outcome generated by the inexact FSM techniques. This happens because exact mining techniques return all the possible fragments in the input corpora. Thanks to our filtering techniques, we are able to decrease the number of candidate fragments (hence augmenting the precision) from 41 to 11 (4% to 18%) when no generalization is applied and from 70 to 15 (10% to 47%) when it is. Meanwhile, the recall is preserved at 100%, which indicates the validity of our proposed filtering techniques. Even after filtering the fragments, the precision is, in general, still worse

than inexact FSM methods due to the number of candidate fragments produced by the technique.

Table 7.6: Exact FSM techniques for the detection of workflows included in composite workflow motifs, using the templates with and without generalization.

	GSpan			
	No Generalization		Generalization	
Fragment type	$P_{c.wf}$	$R_{c.wf}$	$P_{c.wf}$	$R_{c.wf}$
Candidate	0,04	1,0	0,10	1,0
Multi-step	0,04	1,0	0,10	1,0
Multi-step filtered	**0,18**	**1,0**	**0,47**	**1,0**

7.2.4 Summary

In this section we have described our first evaluation, which aims at addressing whether it is possible to detect commonly occurring patterns and abstractions automatically (H1.2) on a small hand-annotated corpus. In order to do so, we have compared our proposed fragments to the commonly occurring motifs, i.e., internal macro motifs and those workflows included as part of a composite workflow motif. One of the advantages of using a small controlled corpus is that we are able to detect and analyze potential issues of the applied fragment mining techniques. We have explained our experimental setup and analyzed the results in detail. Overall, the results show that inexact FSM techniques are a good approach to detect internal macros, while exact FSM techniques obtain perfect recall for detecting those workflows that are part of the composite workflow motifs (since exact FSM techniques detect all commonly occurring fragments, this is an expected result). Additionally, both approaches are able to deal successfully with a scenario in which the workflows are declared at different levels of abstraction.

In the following section we describe our second evaluation, aimed at determining whether our proposed fragments are useful for reuse based on what users have previously defined (H1.3). A detailed discussion of the results with respect to the hypotheses can be seen on Section 7.4.

7.3 Workflow Fragment Assessment

As we have seen in our previous evaluation, our proposed workflow fragments are a feasible means to find the workflows participating in composite workflow and internal macro motifs annotated by users on a workflow corpus. However, the results in general have low precision (under 50%). This indicates that the fragments returned by our approach suggest additional typical structures in the workflow corpus that could be potentially useful for workflow reuse. Hence, in this section we aim to determine whether our proposed fragments are actually useful or not, thus addressing our hypothesis H1.3 (*common reusable patterns are potentially useful for users*).

The Section is organized as follows. We first introduce the common experimental setup in Section 7.3.1, common to both of the following evaluations. Section 7.3.2 checks whether our proposed fragments are similar to the reused structures manually identified by users (user groupings and workflows) in a workflow system. Then, in Section 7.3.3, we discuss the outcome of a survey that domain experts filled to determine the usefulness of a set of proposed workflow fragments. The evaluation presented here is based on our previous findings (Garijo et al., 2014c), which have been expanded and refined.

7.3.1 Experimental Setup

Our evaluation has been performed using four workflow corpora from the LONI Pipeline system. The corpora are WC1, WC2, WC3 and WC4, previously introduced in Section 5.3. We have chosen these corpora for two main reasons:

- *High reusability*: The workflows belong to the same domain, have been created by single and multiple users, and are reused as a whole or included as part of other workflows (as shown in Section 5.3).
- *User groupings*: Users have the means to annotate their sub-workflows as groupings. These can be taken as a reference to compare our candidate fragments and are a requirement for applying the metrics proposed for this type of analysis ($P_{group}(overlap)$ and $R_{group}(overlap)$).

We first performed a comparison between our proposed fragments and the workflows and groupings in the corpora defined by users. We used the $P_{group}(overlap)$ and R_{group}

metrics. Different values of the frequency of the common fragments and the overlap with our solution were considered in order to analyze the quality of the candidate fragments. The evaluation prioritizes a *high precision in the proposed candidate fragments rather than a high recall*: we aim at obtaining common workflow fragments that are useful for the workflow designers, instead of aiming at finding all the possible fragments actually reused by users. Table 7.7 provides a summary of the workflows and groupings that have been reused by users. These numbers will be used to evaluate our approach.

Table 7.7: Unique workflows, groupings and their reuse. These numbers will be later used to calculate the precision and recall of the proposed fragments.

	Unique multi-step workflows		Unique multi-step groupings	
Corpus	Created	Reused	Created	Reused
WC1	441	175	146	71
WC2	94	13	87	40
WC3	269	106	79	47
WC4	50	7	40	26

Candidate fragments that did not overlap with user-defined groupings or workflows were collected and used as a part of a user survey. The survey aimed at testing whether these fragments were still a useful suggestion to the users. Hence, we used the usefulness metric (Acc) defined in Section 7.1.2. A high accuracy determines that our suggested fragments were potentially useful for that user.

In this case generalization is not applied, as no domain-specific taxonomy modeling the components of the workflows in the corpora was provided.

7.3.2 FragFlow Fragments versus User Defined Groupings

We applied inexact techniques (SUBDUE-MDL, SUBDUE-Size) and exact FSM techniques (gSpan) to measure the precision and recall of our approach. The results of the evaluation are described below.

7.3.2.1 Evaluation of the Application of Inexact FSM techniques

Figures 7.6, 7.7, 7.8 and 7.9 show the number of fragments found and their precision ($P_{group}(overlap)$) for every corpus. Each figure shows two evaluations, corresponding

to the MDL and Size heuristics of the SUBDUE algorithm. Both of these techniques are frequency-based approaches, that is, the frequency represents the number of times (occurrences) a fragment is found in the corpus (counting several times if the fragment appears several times in one workflow). The fragment frequencies are normalized according to the size of the dataset, in order to show how different frequencies affect the precision and the found FragFlow fragments. The "min" metric stands for the minimum frequency for a fragment to be detected, i.e., it appears at least two times in the corpus. Given that the number of multi-step fragment and multi-step filtered fragments is similar in both evaluations, we only show the latter (Mff) in the precision graphs.

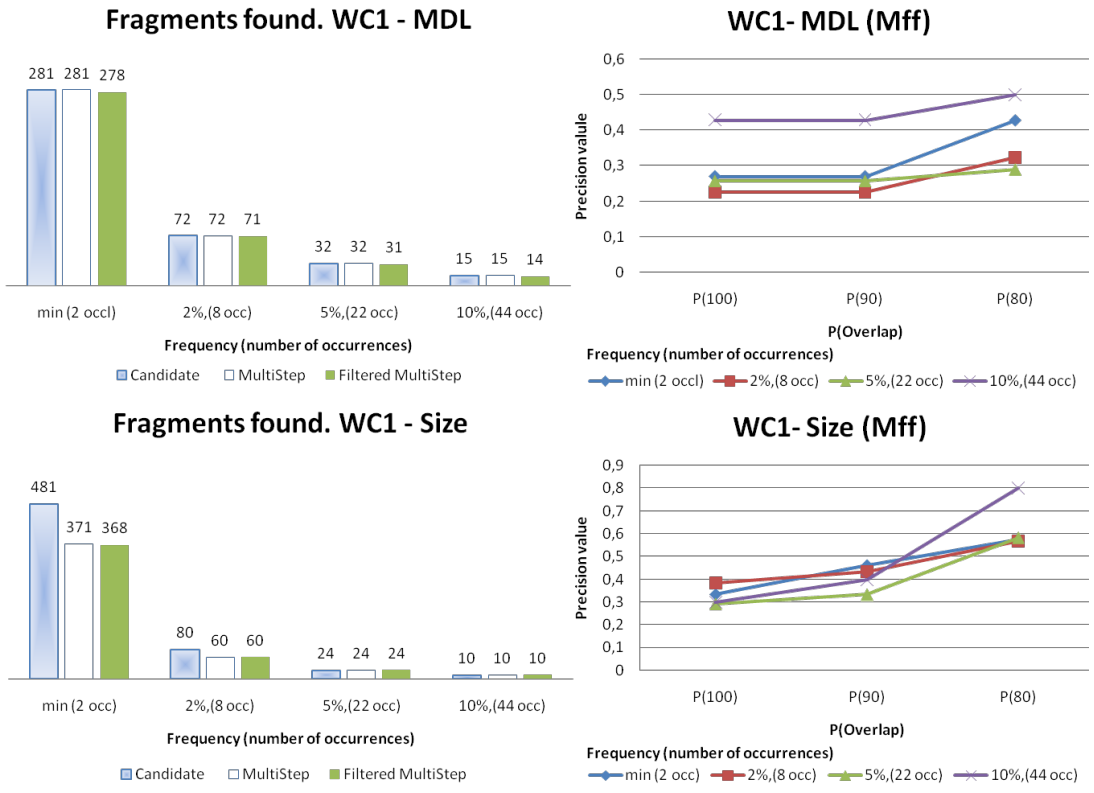


Figure 7.6: Number of fragments found and precision results for WC1 with the MDL and Size evaluations. For the precision, only multi-step filtered fragments are shown.

Finally, the precision metric shows different values for the *overlap*, indicating the *overlap* percentage between the proposed fragments and the groupings and workflows designed by the users. The rationale for having an overlap different to 100% is to

consider fragments that are very similar to the chosen workflows or groupings created by the users. The minimum overlap value, 80% , was chosen empirically, as the main differences with the proposed fragments tend to be too many if this value is decreased. Additional information on the fragments found can be found in Annex C.2.

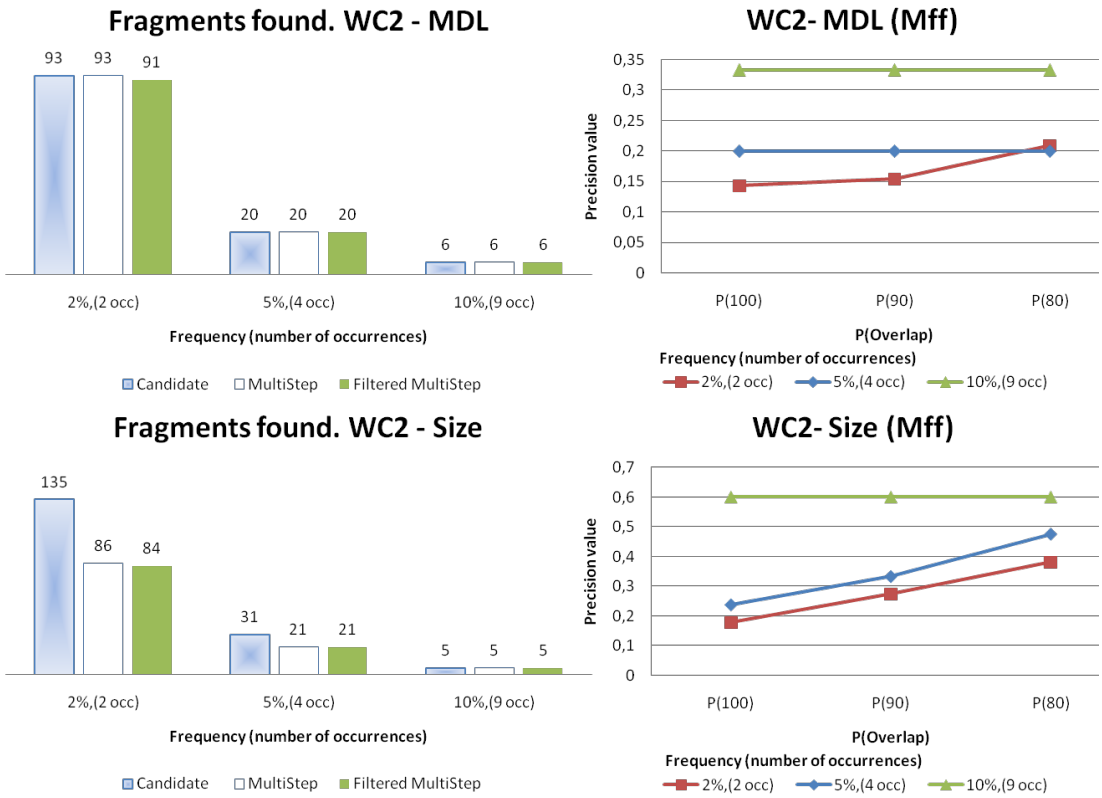


Figure 7.7: Number of fragments found and precision results for WC2 with the MDL and Size evaluations. For the precision, only multi-step filtered fragments are shown.

The results show that many workflow fragments are found to be commonly reused for all four corpora. However, there are more common workflow fragments with high frequency in the single-user corpora (WC1, WC2 and WC4) than in the multi-user corpus (WC3). This result can be explained by looking at the high number of users contributing to WC3 (over 60, as described in Section 5.2) and the nature of the corpus, which is a collection of executions submitted by those users during a month. Given that all users were unlikely to be part of the same team, they would not have the means of knowing the workflows submitted by other users to the repository, thus decreasing their reuse. Instead, the other three corpora had one main contributor who was aware

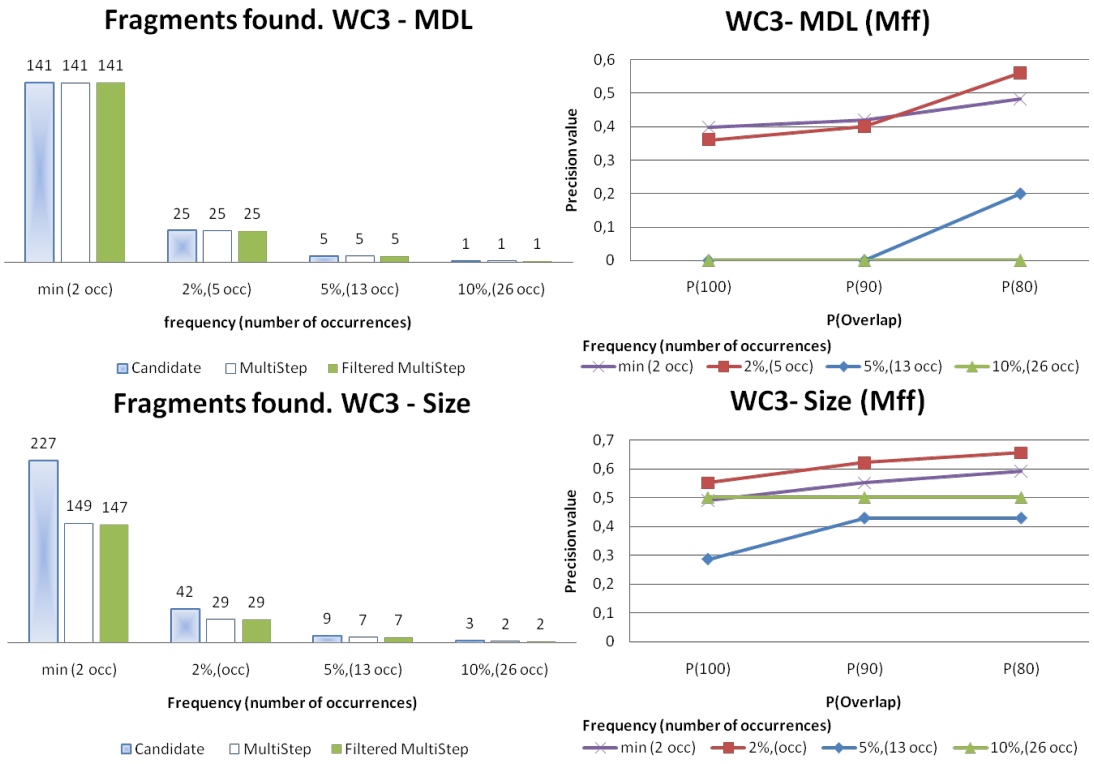


Figure 7.8: Number of fragments found and precision results for WC3 with the MDL and Size evaluations. For the precision, only multi-step filtered fragments are shown.

of the previous work in the respective corpus, facilitating their reuse.

In general, a good number of the workflow fragments found with inexact FSM techniques match those workflows or groupings designed by users. The maximum precision with 100% overlap ranges from 35% (WC2, WC4) to 60% (WC3), increasing to 60% to 80% when considering an overlap of 80% of the workflow steps.

An individual analysis of each corpus can explain the differences in the corpora results:

- In WC1 we see a high reuse and number of workflows, which leads to producing a high number of precise fragments. This finding is confirmed when analyzing the overlap, as a high number of fragments (up to 80%) is similar to the groupings or workflows designed by the user.

- WC2 consists on a set of curated workflows made public for the LONI Pipeline community to reuse. Although they share some common parts, workflow reuse

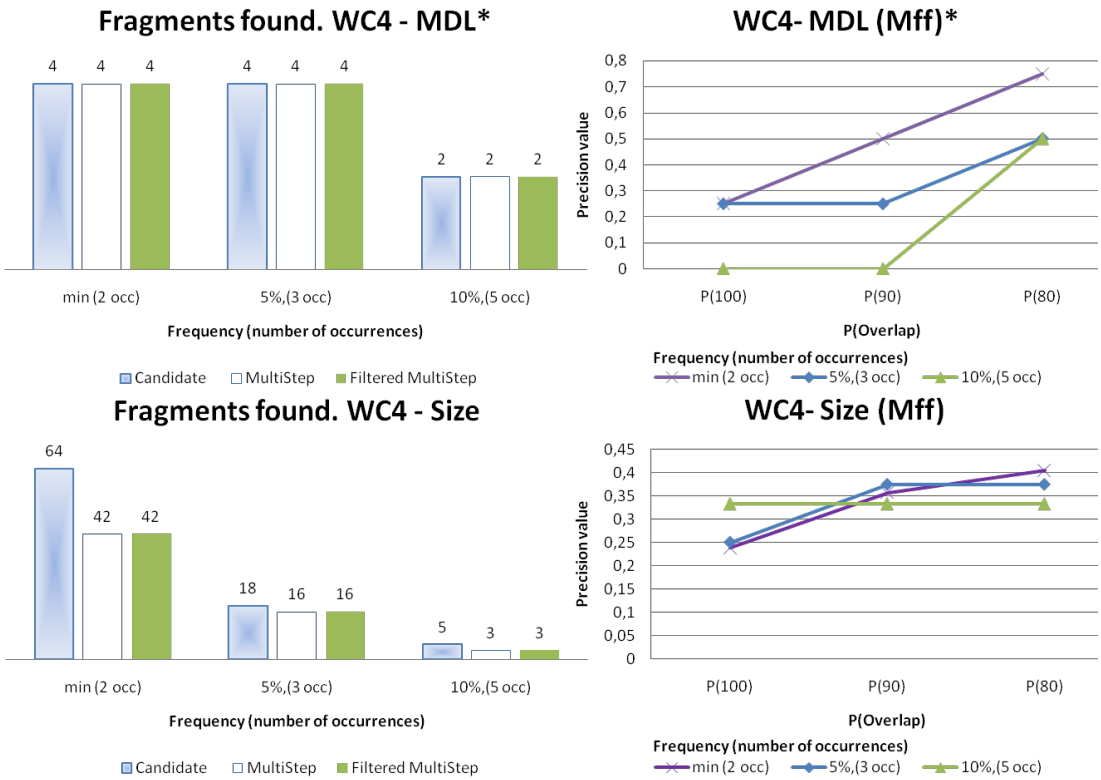


Figure 7.9: Number of fragments found and precision results for WC4 with the MDL and Size evaluations. For the precision, only multi-step filtered fragments are shown. The asterisk indicates an execution failure for WC4.

is not that high in the corpus. Hence the number of fragments found at high frequency is lower (not higher than 6), and the precision is higher (60%).

- WC3 does not produce a high number of frequent patterns (less than seven multi-step filtered fragments are found with f>5%), due to the lower reusability issue discussed above. However, when looking at a lower frequency (f>2%) more than half of our fragments are equal to the users' choice. This means that although different users may not be aware of what other users have designed, they still reuse similar substructures in their workflows at the grouping level.

- WC4 is a small corpus of heavyweight workflows, some of which reuse parts of more than 90 steps from other workflows. Due to the nature of the corpus, the MDL evaluation produced only four common workflow fragments before failing,

although the Size evaluation was obtained successfully. In this case the precision of our results is worse than in the previous corpora (reaching no more than 40% for the Size evaluation). This is caused by two main reasons: the design decisions made by the user to create the groupings in a workflow, and the way the evaluation metric works. If a user defines a grouping within a workflow that appears several times on the workflow corpus, the associated fragment found could merge it with some other workflow steps. Figure 7.10 shows an example, where a workflow contains two user-defined groupings on the left (*Grouping 1* and *Grouping 2*). Assuming that the workflow is reused elsewhere in the corpus, our proposed fragment (on the right of the figure) would include the union of both groupings, instead of two separated fragments.

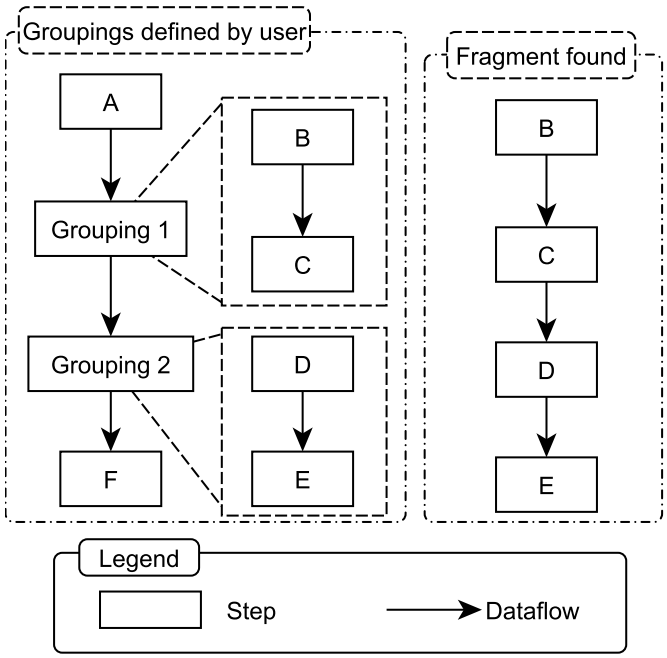


Figure 7.10: Groupings defined by user versus a fragment found. If a user defines connected sub-groupings that co-occur with the same frequency, then the fragment found will merge them.

Regarding the type of evaluation, SUBDUE-Size returns the most precise results both in $P_{group}(100)$ and $P_{group}(80)$ (excluding the MDL evaluation of WC4, which produced errors) according to the evaluation metrics we defined. When looking at the frequency, if a significant number of fragments is returned (i.e., the number of

fragments is superior or equal to 5) then the more frequent those fragments are higher the precision is for the technique. This indicates that in corpora with high reusability such as WC1, users tend to annotate common steps of workflows for their reuse.

As shown in Table 7.8, in all four corpora the recall is very low (21% for the best case, and usually under 10%). This is an expected result, as for calculating the recall metric all the user-designed workflows and groupings are taken into account, whether reused or not. Additional noise is introduced by several user practices that we have detected in the corpora. For example, different users tend to design similar workflows and groupings differently (by adding or removing just a few steps), thus increasing their total number. Other users tend to group certain steps of the workflow for simplifying the view of their current experiment, some others group sets of steps, inputs or outputs that are not relevant for their experiment, etc.

The results also show that by increasing the frequency of the found fragments the recall decreases. This is natural, as the high frequent fragments are fewer than those found at lower frequencies.

7.3.2.2 Evaluation of the Application of Exact FSM techniques

Table 7.9 shows the number of fragments found on the four corpora by the gSpan exact FSM technique. Results are sorted by support, which represents the percentage of workflows in the corpora where a FragFlow fragment was found at least once. The support is normalized to the corpora size, showing in parenthesis the number of templates corresponding to that percentage.

As we described in Section 6.2.1.2, exact FSM techniques aim to find all the possible workflow fragments in the corpora. Thus, Table 7.9 only contains multi-step filtered fragments (mff), due to the large amount of candidate and multi-step fragments returned by the technique. In fact, those rows where an asterisk is shown (in WC1, WC2 and WC4) indicate that the results could only be obtained after fixing the maximum size of a fragment for the gSpan technique. Otherwise the algorithm produces memory errors due to the combinatory explosion produced by the amount of fragments that have to be taken into account for mining results. This is highlighted on WC4, where the size of the reused structures tends to be very large. On the contrary, in corpora where the size of the reused of the patterns is lower, like WC3, all the multi-step filtered

Table 7.8: Recall result summary: for each corpus (WC1 to WC4) and inexact FSM technique, the table displays the lowest and highest recall obtained, along with the frequency at which it was obtained.

Corpus	Inexact FSM	Lowest Recall (freq)	Highest Recall (freq)
WC1	MDL	0,010221465 (10%)	0,127768313 (min)
	Size	0,005110733 (10%)	0,209540034 (min)
WC2	MDL	0,011049724 (10%)	0,071823204 (2%)
	Size	0,016574586 (10%)	0,082872928 (2%)
WC3	MDL	0 (5%)	0,16091954 (min)
	Size	0,002873563 (10%)	0,206896552 (min)
WC4	MDL	0 (10%)	0,011111111 (5%)
	Size	0,011111111 (10%)	0,111111111 (min)

fragments can be mined successfully. Annex C.3 shows additional details on the results obtained.

Figure 7.11 shows the precision results for the four corpora. Except for WC4 (for which we cannot consider the gSpan to work properly due to the results obtained), the precision of the exact FSM technique is around 40%, increasing from 47% to 71% when considering an overlap of 80% between the proposed fragments and the workflows or groupings taken into consideration. In general, most of the observations made for the inexact FSM techniques apply for exact FSM. The best precision is obtained in WC1 due to the amount of available workflows and their reusability. WC2 and WC3 do not have many high frequent patterns (with support over 15%), showing their best precision when selecting support between 2% and 5%. Finally, WC4 shows limited results due to its nature, as it contains a small set of workflows which reuse large fragments of others.

Table 7.9: Number of multi-step filtered fragments found by corpus at different support percentages. The number of workflows that the support corresponds to is indicated in brackets. Due to memory problems, some executions (indicated with an asterisk) at lower frequencies had to be limited to a maximum size of fragment (around 10-15).

Corpus	Support % (no. of templ)	Multi-step filtered fragments
WC1	2% (8)	637*
	5% (22)	1996
	10% (44)	110
	15%(66)	33
WC2	2% (2)	127*
	5% (4)	48
	10% (9)	14
	15% (14)	2
WC3	2% (5)	108
	5% (13)	29
	10% (22)	9
	15% (40)	0
WC4	2% (1)	NA
	5% (3)	out of memory
	10% (5)	10*
	15% (7)	3

* Execution limited to fragment size

However, there are some differences between exact and inexact FSM techniques. The first one is the number of multi-step filtered fragments found, being higher for exact FSM. This is expected, as it follows the behavior established for exact FSM techniques, which is to find all possible fragments, even those that are included in bigger ones. The disparity in the number of fragments is also relevant for a second difference: as shown in bold in Table 7.10, inexact FSM techniques provide equal or better precision for all the corpora, including overlap. Even if more fragments are found to be equal to templates or groupings, the higher number decreases the precision metric.

Another key aspect is that, unlike inexact FSM results, the more frequent a fragment is does not necessarily imply a better precision (this only happens in WC1, where

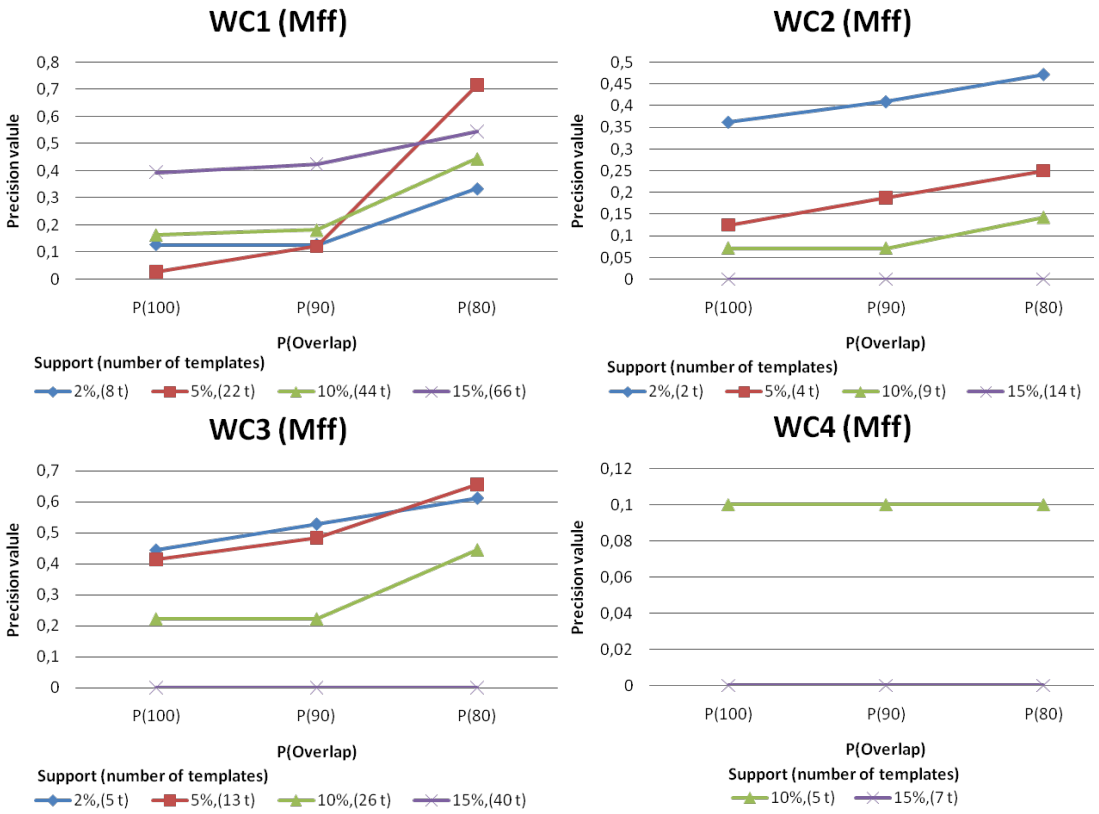


Figure 7.11: Exact FSM results for corpus WC1 to WC4 using the gSpan algorithm.

Table 7.10: Inexact FSM technique results versus exact FSM techniques in terms of precision, considering exact comparison and overlap.

Corpus	Highest P(100) (inexact FSM)	Highest P(100) (exact FSM)	Highest P(80) (inexact FSM)	Highest P(80) (exact FSM)
WC1	**0,42**	0,39	**0,8**	0,71
WC2	**0,6**	0,36	**0,6**	0,47
WC3	**0,55**	0,44	**0,65**	0,65
WC4	**0,33**	0,1	**0,4**	0,1

workflow reuse and grouping reuse is very frequent). The precision value is influenced by the amount of fragments found in exact FSM techniques and the design criteria followed by users (like preferred size or organization of workflow steps). Therefore, although some users tend to group common workflow steps of their workflows for reusability in the four corpora, it cannot be considered the only reason for doing so. High frequency

fragments that do not correspond to any workflows or groupings could be suggested to users, as we will discuss in the next section.

Finally, Table 7.11 shows a summary with the recall of the obtained results, which resembles the one obtained with inexact FSM techniques. If all the candidates proposed by gSpan were considered, the recall would be higher, as all possible fragments would be mined. However that would decrease the precision of our results dramatically. Similarly, if only the reused workflows and groupings are compared, the recall is likely to increase.

Table 7.11: Recall results summary obtained for the gSpan algorithm on each corpus. The support percentage at which each result was obtained is highlighted in brackets.

Corpus	**Lowest Recall (support %)**	**Highest Recall (support %)**
WC1	0,022146508 (15%)	0,137989779 (2%)
WC2	0 (15%)	0,254143646 (2%)
WC3	0 (15%)	0,137931034 (2%)
WC4	0 (15%)	0,011 (10%)

7.3.3 User Evaluation

After comparing our results with the user defined workflows and groupings, we performed a survey with the collaboration of three domain experts responsible for the single-user corpora used in the previous evaluation (WC1, WC2 and WC4). The purpose of the survey was to measure whether the FragFlow fragments that were different from the user designed workflows or groupings would still be useful for each of the domain experts or not.

In order to avoid overloading the domain experts with fragments, each of them was presented with 10 to 18 fragments randomly selected at different frequencies and support. The number of fragments presented varied according to the number of fragments found, and each domain expert answered on the usefulness of the fragments with regard to their own corpus.

Similar to what we did in the fragment versus grouping evaluation (Section 7.3.2), we relaxed the accuracy metric by asking domain experts if they would have modified some parts of the proposed fragment before adopting it. Thus, candidate FragFlow fragments could be *used as proposed* if the user would use the proposed fragment as it was, *used with minor changes* if the user would change less than one third of the fragment; *used with major changes*, if the user would change more than one third of the fragment, or *not used* if the user did not think the proposed fragment would be useful. In this section we describe and discuss the results of the survey. Additional details on the survey can be seen in Annex C.4, while the responses and additional resources are available online[1].

7.3.3.1 User Evaluation Results

The responses to our survey are summarized in Table 7.12, with good results on average. The first user would reuse more than half of the proposed fragments (66% accuracy), using 11% of candidate fragments as proposed, changing slightly 16% of them and doing major changes to 38% of them. When asked about the reasons to not use the other third of the proposed FragFlow fragments, the user answered that they were too simple (two or three steps).

User 2 would reuse all of the proposed fragments (100% accuracy), almost half of them (43%) as FragFlow detected them, half of them by changing more than one third of the components, and 6% with minor changes. When asked about the complexity of the fragments, user 2 argued that sometimes additional sub-groupings would be necessary, since they help clarifying and organizing the workflow.

Finally, user 3 would also reuse all of the proposed fragments, 40% of them without any change, 30% with minor changes and 30% with major changes. When asked about the complexity of the proposed fragments, this user also said that some of the fragments had too many steps (30%), but that some others were too simple (20%).

7.3.4 Summary

In this section we introduced our second main evaluation, which aims at addressing whether our automatically detected common workflow fragments are commonly occurring (H1.2) or useful (H1.3). We divided this activity into two main sub-evaluations.

[1] `http://dx.doi.org/10.6084/m9.figshare.1577564`

Table 7.12: User evaluation of FragFlow fragments.

User	Use as Proposed	Use with minor changes	Use with major changes	Not use
User 1 (WC1)	11%	16,6%	38%	33,3%
User 2 (WC2)	44%	6%	50%	0%
User 3 (WC4)	40%	30%	30%	0%

The first one performed an automatic assessment of our proposed fragments by comparing them to the workflows and groupings designed by users of four different workflow corpora. The second sub-evaluation consisted of a domain expert survey for assessing the usefulness of our fragments.

For each evaluation, we described our experimental setup, discussed and compared thoroughly the results obtained by different FSM techniques on the workflow corpora. In contrast with the evaluation presented in Section 7.2, in this section we dealt with a big workflow corpora, which allowed us to highlight any limitations that the FSM techniques might suffer when dealing with a high volume of workflows (e.g., poor performance for WC4). It also allowed us to analyze how the design decisions followed by different users on the workflow corpora affect our results.

It is worth mentioning that, despite our efforts, we have not found a unique configuration for obtaining the most precise workflow fragments. Inexact FSM techniques are slightly more precise than exact FSM techniques, and frequency plays a role only when there is high reuse in the workflow corpus. Also, inexact FSM techniques are interesting because they tend to cluster workflows in fewer fragments, which facilitates their presentation to the user.

7.4 Evaluation Conclusions

Throughout this chapter, we have introduced the metrics, rationale, experimental settings and results of our evaluations. In this section we discuss whether these results validate the main hypothesis of the thesis (H1), described in Chapter 3: *"Scientific workflow repositories can be automatically analyzed to extract commonly occurring patterns and abstractions that are useful for developers aiming to reuse existing workflows"*. The hypothesis has been divided into three different sub-parts, *"it is possible to define a*

catalog of common domain independent patterns based on the functionality of workflow steps" (H1.1), *"it is possible to detect commonly occurring patterns and abstractions automatically"* (H1.2) and *"commonly occurring patterns are potentially useful for users designing workflows"* (H1.3). Since H1.1 has already been addressed by the catalog proposed in Section 5.1, in this section we discuss the relationship between our results, H1.2 and H1.3.

7.4.1 Commonly Used Workflow Patterns and Abstractions

H1.2 states that it is possible to detect *commonly occurring patterns and abstractions automatically* by making use of *graph mining techniques* (H1.2.1) and the *exploitation of domain specific metadata* (H1.2.2). Our evaluations have shown that workflow fragments can be mined successfully from a workflow corpus using inexact and exact graph mining techniques. However, the key remaining question to answer is: are these fragments commonly occurring and generic?

We have addressed this question in our first evaluation, by comparing our proposed fragments with two groups of motifs related to workflow reuse: internal macros (which identify the common sets of tasks within a single workflow) and composite workflows (which detect whether a workflow is a composition of other existing workflows). These motifs help identifying *commonly occurring* workflows and workflow fragments; and our evaluation has shown that inexact mining techniques can find most of the internal macros and workflows participating in composite workflows, while exact graph mining techniques find all the target structures related to both motifs. Therefore, *graph mining techniques are adequate for finding commonly occurring patterns automatically* (addressing successfully H1.2.1).

Internal macros and composite workflows can be also used to assess the generality of our fragments, as the corpus used in the evaluation had them annotated. Therefore, in order to evaluate H1.2.2, we performed the same type of evaluation generalizing the workflow corpus. Our results show that generic workflow fragments can also be mined successfully (we obtained a high recall), even improving the results produced by the inexact graph mining techniques. Therefore, we can confirm that our approach *is able to detect commonly occurring patterns and abstractions in a scientific workflow corpus*, thus confirming H1.2.2 and H1.2.

However, our evaluation also showed that, apart from the target motifs, other commonly occurring workflow fragments were included among the results found by our approach (our precision in some cases was low). Therefore, the objective of our second and third evaluations consisted of measuring whether these other common workflow fragments are useful for workflow design or not.

7.4.2 Workflow Fragment Usefulness

Our hypothesis H1.3 states that *commonly occurring patterns are potentially useful for users designing workflows*. In order to evaluate our hypothesis, we first introduced a definition for usefulness (considering a fragment *useful* if it had been reused and annotated as a workflow or a grouping by one or several users when designing workflows) and designed two different evaluations.

The first evaluation compared our proposed fragments against several corpora of user-annotated workflows and groupings. The results show that, on average, almost half of the proposed fragments matched exactly those groupings (or workflows) reused by users in their workflows. This number increases to more than half of our proposed fragments (around 60%) if we also take into account those fragments that are similar to a user-defined grouping or workflow. Therefore, according to our results *we have enough evidence to confirm hypothesis H1.3*, as up to 60% of the commonly occurring patterns that we detect automatically have demonstrated to be useful for users designing workflows.

Our second evaluation aimed at determining if the other 40% of our suggested fragments were useful as well. Therefore, we performed a user survey with three domain experts, asking them about the usefulness of the fragments found on their respective corpora. On average, the accuracy of our results turned out to be very high. Most of the proposed fragments were considered useful by users (nearly 90%), even if they would change around half of the fragments according to their personal preferences (e.g., size, complexity, frequency, etc.). These preferences can be set up as parameters to filter fragments, thus increasing the performance of our approach.

There is clearly not enough evidence to state that ***the majority*** *of our proposed commonly occurring workflow fragments* ***are useful***, as half of our candidate fragments were found to be useful and only three domain experts participated in the survey. However, the analysis presented in this chapter supports this hypothesis. A more

complete analysis could not be completed due to the difficulty of finding volunteer users with a significant corpus of workflows.

Chapter 8

Conclusions and Future Work

The main goal of this thesis was to facilitate scientific workflow understanding and reuse by automatically mining commonly used workflow fragments of a workflow corpus. To this end, we developed workflow provenance and template representation models that extend existing standards, we created a catalog of workflow abstractions based on workflow step functionality, we developed and implemented workflow fragment mining techniques and we defined metrics and used them to measure the usefulness of workflow fragments.

Based on the evaluation of our results, we extract two main conclusions. The first conclusion is that *commonly occurring workflow fragments can be mined automatically from a corpus of workflows using graph mining techniques.* Furthermore, *commonly occurring workflow fragments are generally useful for users designing workflows.* However, an important finding is that *not all commonly used workflow fragments are useful*, as this depends partly on user preferences and context.

The second conclusion is that *workflow abstraction plays an important role in understanding how different workflows relate to each other.* Therefore, it is possible to find additional occurring workflow fragments using step abstractions.

The rest of the section discusses our assumptions and restrictions, contributions, impact, current limitations and future lines of work. All the inputs, outputs and intermediate results of the thesis are available online as Research Objects (Belhajjame et al., 2015) that define the datasets, structure and metadata of our experiments[1].

[1] `http://purl.org/net/mining-abstractions-in-scientific-wfs`

8.1 Assumptions and Restrictions

Throughout the thesis, we have taken a series of assumptions and restrictions for our work. Our first assumption for applying the methods described here is that *workflow repositories should be available for exploiting workflow definitions of their steps and dependencies* (A1) or *their provenance traces* (A2).

Also, in order to apply successfully our fragment mining techniques, we convert the workflow corpus to *directed labeled acyclic graphs* (R1). We restrict to this type of representation because it is the most common in data intensive scientific workflows. Other types of workflows (e.g., business workflows) may benefit from this work, but have been excluded from the scope of the thesis.

Furthermore, we assume that *all the steps of a workflow can be assigned a label with their type* (A3). The type of the workflow step helps identify its functionality, and it is normally chosen from a library of components by the workflow designer. *If two steps perform the same function in a workflow, they are assumed to have the same type* (A4). Thus, *two workflows are assumed to have equivalent functionalities if their dependency graphs are isomorphic and their nodes share the same types* (A5).

Finally, our last assumption is that, when designing workflows, *researchers aim to reuse workflows and workflow fragments in their work, if they find them useful* (A6).

Tables 8.1 and 8.2 summarize our assumptions and restrictions according to their description.

8.2 Contributions

In this section we summarize our contributions regarding the research challenges defined on Chapter 3.

8.2.1 Workflow Representation Heterogeneity

Our main contributions to this research challenge are the OPMW model (addressing partly RCRepresent-1, *there is no standard model for representing scientific workflows and their metadata*), and a methodology for publishing scientific workflows as Linked Data (addressing RCRepresent-2, *there are no methodologies for publishing a corpus of scientific workflows and their associated resources as Linked Data*).

Table 8.1: Assumptions considered in this thesis.

Assumption	Description
A1	Available workflow repositories exist for exploiting definitions of workflow steps and dependencies
A2	Available workflow repositories exist for exploiting workflow provenance traces
A3	All the steps of a workflow can be assigned a label with their type
A4	If two steps perform the same function in a workflow, they are assumed to have the same type
A5	Two workflows are assumed to have equivalent functionality if their dependency graphs are isomorphic and their nodes share the same type
A6	Researchers aim to reuse workflows and workflow fragments in their work, if they find them useful

Table 8.2: Restrictions considered in this thesis.

Restriction	Description
R1	Workflows are represented as directed acyclic graphs

8.2.1.1 The OPMW Model

In Chapter 4 we described our rationale and requirements for designing the OPMW model, the first contribution of this thesis. OPMW is a lightweight vocabulary created to represent workflow templates, workflow instances and workflow executions along with their relationships and metadata. The requirements were gathered by looking at the main workflow operations available in data intensive workflow management systems, and selecting the minimum common group among all of them. In this regard, the main scope of the model is to be able to exploit workflow data belonging to several heterogeneous workflow systems.

Another key requirement of the model was to be aligned with existing vocabularies and standards. By extending both OPM and PROV, OPMW ensures backwards compatibility with applications using OPM, as well as with those using the W3C PROV standard. Additionally, by extending P-Plan, OPMW can be combined with other vocabularies, as it happened in (Santana-Pérez and Pérez-Hernández, 2015) for specifying

workflow execution infrastructure.

The OPMW vocabulary has evolved since its creation, and has been tested as part of the WEST ecosystem (Garijo et al., 2014d), where a set of workflow tools for design, analysis and execution use it as a simple intermediate representation during the whole workflow life cycle. We have used this implementation to further evaluate the effectiveness of the OPMW model.

8.2.1.2 A methodology for publishing scientific workflows as Linked Data

Our second contribution consists of a methodology to make the different resources associated with workflow templates, workflow instances and workflow executions openly accessible as web resources. Our proposal is to publish all the workflow related resources following the Linked Data paradigm. This allows easy accessibility and reuse for both humans and machines aiming to consume the workflow related information.

Our proposed methodology adapts a generic approach successfully applied for the publication of data in other domains like energy consumption, meteorology or geography. As described in Section 4.2.2, the methodology consists of five main steps (specification, modelling, generation, publication and exploitation), which have been adapted for the publication of scientific workflows. An example of each step is provided in Section 4.2.3.

8.2.2 Addressing the Inadequate Level of Workflow Abstraction

Generalizing workflows by hand is a daunting task, and may require domain specific knowledge from expert users. In this respect, we have made two main contributions in this thesis: a catalog of common workflow motifs based on workflow step functionality, addressing partly RCAbstract-1 (*it is difficult to determine which steps perform the main significant processing steps in a scientific workflow*), and RCAbstract-2 (*there are no catalogs of the typical abstractions that can be found in scientific workflows based on their basic step functionality*); together with an approach to use domain specific knowledge in order to find additional workflow fragments in a workflow corpus (based on step abstraction).

8.2.2.1 A catalog of common workflow motifs

In Section 5.1 we described the result of a manual analysis over 260 scientific workflows from four different workflow systems. As a result, we obtained a catalog of common domain independent conceptual abstractions, which we refer to as *common workflow motifs*.

The motif catalog consists of 6 major types of data-operation motifs (related to the main functionality undertaken by the steps of the workflow) and 6 types of workflow-oriented motifs (which indicate how the data-operation motifs are implemented in the workflow). The most common motif is data preparation, highlighting that an important effort in the creation of workflows is dedicated to data integration, filtering and reformatting activities. Regarding workflow-oriented motifs, the amount of internal macro motifs and composite workflows indicate that reuse is a common practice among scientists publishing their workflows.

Workflow motifs categorize workflow steps by their functionality. Hence, they provide the means to create an adequate level for workflow abstractions.

8.2.2.2 Workflow generalization

Chapter 5 describes how a step abstraction may help connecting workflows that seemed to be unrelated. In principle, this can be achieved by using domain experts to create taxonomies of components with the same functionality. As we have demonstrated in Chapter 7, this approach can be used to find additional generic motifs that help creating relationships among different scientific workflows.

8.2.3 Difficulty of Workflow Reuse

We presented several contributions related to this open research challenge. First, we analyzed how users reuse workflows in different corpora, addressing RCReuse-1 (*it is difficult to determine the relation between different workflows in a corpus*).

Second, we have designed and evaluated an approach to find commonly occurring workflow fragments automatically, along with the metrics to assess whether a workflow fragment is useful or not in terms of reuse. This addresses RCReuse-2 (*It is not easy to detect which workflows or workflow fragments are potentially useful for reuse*), as our approach generates fragments that are potentially useful for reuse.

Finally, we defined a method for exploring how different workflow fragments can be linked to their original workflows, enabling linking distinct workflows thet share common functionality (and also addressing RCReuse-1).

8.2.3.1 Workflow reuse analysis

In order to dig into the level of workflow reuse exposed in Section 5.1, Sections 5.2 and 5.3 describe two analyses from two different perspectives. One consists of an automatic analysis of four workflow corpora, counting the number of unique workflows and groupings (i.e., user hand made sub-workflows) and how many of them are finally reused. An interesting conclusion of this analysis is that, despite the current difficulty for workflow reuse, a high number of workflows appear in other workflows, specially when the repository belongs to a single contributor. Groupings are also heavily used, even more than workflows.

The second analysis describes a user survey on code, workflow and grouping reuse. The rationale for the analysis was to understand the user perspective on reuse, in order to confirm the findings from previous analyses. According to the results, workflows are generally considered more useful than groupings (although groupings are considered useful as well). Groupings are not created solely for reuse purposes, but also to organize workflows and make them easier to modularize and simplify.

These analyses are a strong contribution, since they are unique on measuring sub-workflow reuse in a workflow corpus.

8.2.3.2 Automatic workflow fragment detection

Another contribution to address the difficulty of workflow reuse is our approach to the automated detection of workflow fragments using graph mining techniques. This approach, described in Chapter 6, is able to detect successfully commonly occurring workflow fragments using graph mining techniques and filtering the fragments to simplify the results. As shown in the evaluation in Section 7.3, more than half of the resulting fragments are equal or very similar to what users identified as useful in their own designs. Furthermore, those fragments that were not similar to what users indicated in their workflows, were still considered useful by three different domain experts on their respective corpora. This indicates that our approach is able to find fragments

that are useful for workflow reuse, although further analysis is needed to confirm that the majority of our proposed fragments are useful for that purpose.

8.2.3.3 Workflow fragment assessment metrics

Another contribution regarding the difficulty for workflow reuse are the metrics we have defined for assessing whether a workflow fragment is useful or not. These metrics are described in Section 7.1, and are based on precision and recall. The first metric relies on the ability to find fragments as motifs that are either commonly occurring or generic like internal macros and composite workflows. The second metric assesses whether our fragments are similar to the structures defined by users when they design workflows.

8.2.3.4 Workflow fragment linking

In addition to obtaining the resulting set of commonly occurring workflow fragments, we have described in Section 6.4 a generic method to link a fragment to the workflow or workflows where the fragment appears. This is a contribution towards easing workflow reuse and discoverability, as the workflows of a repository are related to each other by their commonly occurring workflow fragments.

8.2.4 Lack of Support for Workflow Annotation

We have described in the thesis two contributions *for facilitating annotation of workflows and workflow fragments in a semi-automated way* (RCAnnot1), in the form of two different vocabularies. The first one is a vocabulary for common workflow motifs and the second one is a vocabulary for workflow fragment description and linking.

8.2.4.1 Workflow motif vocabulary (wf-motifs)

Wf-motifs[2] is a vocabulary encoding the catalog of common workflow motifs presented in Section 5.1. This vocabulary is a contribution towards workflow annotation for two reasons. First, it provides a machine readable description of the catalog of motifs, stating how different motifs are related or depend on each other. Second, it defines explicit relationships to annotate workflows and workflow steps with any of the motifs described on the catalog.

[2] `http://purl.org/net/wf-motifs`

8.2.4.2 Workflow fragment description vocabulary (wf-fd)

The Wf-fd vocabulary[3] is the means we use to expose the links found between fragments and the original workflows where they were found. In this regard, the vocabulary itself is a contribution because we use it to automatically annotate workflows with their associated workflow fragments.

8.3 Impact

The contributions of this thesis have already started to be used in recent work by other researchers. The OPMW model has been used for exposing automatically annotated bio-informatic workflows (García-Jiménez and Wilkinson, 2014b) and for documenting the results of scientific research[4]. Our catalog of motifs has been adopted and extended by analyzing workflows in distributed environments (Olabarriaga et al., 2013) and summarizing workflows (Alper et al., 2013).

Other contributions may impact different workflow research areas, as we describe below:

- **Workflow exploration**: By knowing how each fragment is found on a workflow, it is possible to derive a network where the nodes represent the different workflows and the edges are the common fragments (dependencies) found among them. Thus, the higher the number of common fragments the stronger the connection would be between two workflows. This kind of network would help users to see how different workflows are connected with each other in a repository, facilitating the exploration between workflows with the same parts of functionality.

- **Workflow abstraction**: Approaches like (Cerezo, 2013) use fragment knowledge bases to create abstractions. These approaches can benefit from our commonly occurring workflow fragments.

- **Workflow discovery**: Commonly occurring workflow fragments, when supported in many workflows, may become valuable workflow candidates themselves. Repository maintainers may offer these potentially reusable fragments to users to include in their workflows.

[3] `http://purl.org/net/wf-fd`

[4] `http://linked-research.270a.info/linked-research.html`

- **Workflow visualization**: As stated in the user survey of Section 5.3, one of the reasons why groupings are created is for summarization and organization purposes. Hence, commonly occurring workflow fragments can be used to simplify the complexity of a workflow by collapsing their nodes under a single one. If a workflow has overlapping fragments it would be possible to create different views according to user preferences, simplifying the overall complexity shown to the final user.

- **Workflow compression**: Similarly, if several workflows share the same fragment, it would be possible to store the common relevant workflow fragments instead of every expanded workflow, for efficiency. This would be particularly useful when dealing with similar or identical provenance traces.

- **Suggestions for workflow design**: Commonly occurring fragments may be used to suggest how a user may complete a workflow under development. By comparing the current workflow with the commonly occurring fragments, it would be possible to recommend the next step or sets of steps of the workflow.

- **Workflow ranking**: Once the catalog of fragments is linked to a workflow corpus, it would be possible to order the workflows by different criteria and create rankings. Possible examples of rankings are the degree of reusability of the workflow (i.e., how much of the workflow can be found in other workflows), workflows with most reused fragments, etc.

8.4 Limitations

In this section we discuss the main limitations associated with the contributions and methods described in this thesis.

8.4.1 Workflow Representation and Publication

OPMW aims to represent scientific workflow templates, instances and executions and their relationships as labeled directed acyclic graphs (as stated on restriction R1). More complex workflow structures, such as sub-workflows, loops and conditionals (the last two being more typical of business workflows) have been deliberately left out of the model for simplicity. In this regard, OPMW captures the minimum set of workflow

operations common to most workflow systems. In order to represent more complex structures, additional extensions of the model would be necessary.

Regarding the publication of workflows, one possible issue is privacy. In some domains privacy is a concern (e.g., if the workflow processes sensitive clinical data), and in those cases the open publication of all the workflow resources as Linked Data would not be appropriate. However, there are many areas of science where privacy is not an issue and that would benefit tremendously from a more open architecture for sharing both data and workflows. Besides, it is possible to publish workflows as Linked Data for local consumption, by restricting the access to the Linked Data server.

8.4.2 Common Workflow Motifs

Our catalogue of common workflow motifs is the result of an extensive analysis on workflows from different domains and different platforms. We believe that the sample collected is statistically significant for the life-sciences domain, as for most of the systems we have chosen the majority of the workflows available.

However, there may be other motifs in other domains and types of workflows (e.g., business workflows) or in workflows prepared to be executed in other settings like distributed systems (as happened in (Olabarriaga et al., 2013)). Since the catalog is exposed as an online vocabulary, we have provided the means to extend it whenever additional analyses are made.

In addition, one of the objectives of this work tackled the automatic detection of abstractions from a repository of workflows. In this regard, we have only addressed the detection of those motifs related to workflow reuse. The rest of the motif catalog has been left out of scope, and it would present a challenging line of future work.

8.4.3 Workflow Fragment Mining

As discussed in Chapter 6, there are two possible limitations introduced by graph mining techniques: the *size of the result* (i.e., number of mined workflow fragments) and the *time* needed to compute the results.

Regarding the size of the result, we have developed filtering techniques that prune the response and return only those fragments that are relevant to our purposes. However, our results have shown that there are cases where the size of the commonly

occurring fragments leads the exact graph mining techniques to produce memory errors (e.g., when many versions of a big workflow are included as part of the corpus). This limitation can be handled by augmenting the amount of memory allocated to the application, increasing the minimum frequency or support for a fragment to be found in the workflow corpus, limiting the maximum size of the fragment to be found or by using an inexact graph mining technique (which simplifies greatly the number of responses, even when all the possible fragments are not returned).

Regarding the time, sub-graph isomorphism is known to be a NP-Complete problem (Cook, 1971). Different techniques optimize their algorithms in order to reduce the execution time as much as possible, being able to handle a large amount of graphs in a reasonable time. Although we state time as a limitation of graph mining techniques, we do not consider it critical in our analyses. Workflow fragment mining can be performed as an automated back-end task on a repository, executed once in a fixed period of time (e.g., week or month). Time can also be reduced greatly by modifying the parameters of the mining algorithms, such as maximum size of the fragment to look for in the dataset or the minimum support or frequency of the fragments to find (the bigger the support, the fewer the candidates and therefore the faster we obtain the results), etc. However, adding these kinds of limitations may have an impact on the quality of the results.

8.4.4 Workflow Generalization

In our work, we use taxonomies and domain knowledge to generalize workflows and find abstract fragments in a workflow corpus, if they exist. These abstractions depend on how domain experts model the domain, and thus different workflows may be simplified differently according to how each user models their domains. The main limitation in this regard is that the domain knowledge must come from an expert or a community of experts in the form of a taxonomy or an ontology, in order for us to be able to generalize workflows. The creation of a taxonomy from a repository of workflows is out of the scope of this work.

8.5 Future Work

Our work may be expanded in several ways. In this section we discuss possible future lines of work related to our research challenges.

8.5.1 Towards Workflow Ecosystem Interoperability

Workflow heterogeneity has been an issue in the workflow community for years, and some interchange languages for workflow specification interoperability have been specified by part of the community (e.g., IWIR). However, the workflow life cycle (including workflow instances and workflow executions) is still represented differently for each workflow tool.

We believe that a way to consolidate an intermediate representation between different workflow design and execution tools is through a workflow ecosystem (Garijo et al., 2014d). A workflow ecosystem brings together heterogeneous tools that consume and produce workflow templates, instances and executions at different moments of the workflow life cycle. Different tools may also consume workflows at different granularity (e.g., a workflow depiction tool would aim to consume an abstract provenance trace, while a workflow execution tool would require the full dependency graph among the workflow steps and where to find the scripts to run each of them). This forces tools to cooperate in order to communicate with a consistent representation. In this thesis we have proposed and tested a model that tries to minimize the common workflow operations in order to successfully communicate different applications in a workflow ecosystem. However, this is only a first step, and a community of adopters and producers is necessary to push forward a robust and consolidated standard model.

8.5.2 Automating Detection of Workflow Abstractions

In this thesis we have discussed two ways of creating abstractions from workflows: workflow generalization (which is generated automatically by using a taxonomy provided by domain experts) and a catalog of workflow motifs (some of which we find automatically by using graph mining techniques). Even though we have contributed towards the automatic detection of workflow abstractions, our work may be expanded, as we further describe below.

Workflow Generalization: One of the limitations we have devised for workflow generalization is the need for a domain expert to create the taxonomy used to generalize the workflow steps. The ability to derive a domain specific taxonomy automatically would improve the process, in case no domain experts can be consulted. The extraction of the taxonomy may be performed by exploring workflows and by mining domain specific knowledge bases with description of the workflow steps.

Workflow Motifs: In Section 5.1 we described a catalog of common workflow motifs in scientific workflows. As discussed in the limitations section, a future line of work would be to expand this catalog with other types of workflows (e.g., business workflows) or execution environments (e.g., high performance workflows or distributed workflows).

We have left the detection of any motif unrelated to workflow reuse out of the scope of this thesis. A challenging line of work would be, given a workflow as an input, to be able to recognize and annotate all its motifs automatically. This would help understand the workflow better, as in many cases there is not enough documentation to determine what a particular step of a workflow does unless we execute it.

After extracting and refining the motif catalog we have analyzed some of the features of the motifs. Below we highlight some of the features which might help for their automated classification, specially those under the "data preparation" category:

- **Input and output number:** by determining whether the number of inputs is bigger than the number of outputs we can (usually) discard certain types of motifs. For example, a merging component normally has several inputs of the same type and produces a lesser amount of outputs of the same type.

- **Input and output size:** when combined with the number of inputs, their size can be combined as a metric to speculate about the type of operation going on the component. For example, if a dataset file is used as input of a step and the result is a similar reduced dataset, the input may have been filtered.

- **Input and output type:** This feature can be combined with the previous two to speculate about the type of motif being applied. For example, if the type of the input is the same as the type of the output, we might be applying different data transformations (filter, clean, merge, group) to the same file.

- **Name similarity:** It is common for the authors to name their components after the function they perform. For example, if a component merges a dataset, it is likely to be named "MergeDataset" (or similar). By measuring the distance of the workflow step name from a controlled vocabulary (merge, filter, concatenate, curate, add, etc.) we could speculate about its function.

These features may be combined into feature vectors and then used to train classifiers with them. Additionally, algorithms to differentiate between inputs and outputs could be run, in order to determine the type of transformations happening in each workflow step. Adding these kind of annotations to a workflow corpus automatically would also allow categorizing workflow steps in order to derive their taxonomy.

8.5.3 Improving Workflow Reuse

There are several ways in which our candidate workflow fragments may be improved to be more useful. First, it would be necessary to study the different features of a workflow fragment in order to allow users to customize their results. As we have seen in our evaluations, different users prefer fragments of different sizes and frequencies. Other metadata like the number of different workflows in which they appear (support) or the technique used to obtain them (inexact or exact FSM) may be relevant for filtering a set of useful fragments for a particular user.

Second, it should be possible to rank a set of fragments once they have been automatically characterized and annotated. Rankings make a set of fragments easily comparable in order to recommend similar workflows to a particular given one (based on their fragment similarity). It would be an interesting line of work to determine if a recommendation based on similar workflow fragments provides similar or better results than other approaches existent in the state of the art.

Third, a set of workflow fragments may be used for suggestions in workflow design, in combination with process mining approaches. Process mining approaches have been demonstrated to obtain good results to predict the next step of the workflow. When using process mining techniques with common workflow fragments (which have been repeatedly used among the dataset), we suspect that better results may be obtained with less processing, as the common workflow fragments filter out those structures that are unlikely to be used.

Finally, another area of improvement is the efficiency with which the workflow fragments are obtained. The size of the commonly occurring fragments may cause the fragment detection process to be slow. We have deliberately left out the issue of efficiency from this thesis, as our main objective was to assess whether graph mining techniques would be appropriate for obtaining a set of useful workflow fragments for designing workflows or not. Therefore, we have tested representative graph mining algorithms of inexact and exact FSM techniques. In Annex D we discuss additional algorithms with potential to either discover other types of workflow fragments (as inexact FSM), or return the results more efficiently.

ANNEX A

Competency questions for OPMW

Here we introduce the competency questions created for the development of OPMW, described in Section 4.1.3. The competency questions can be seen in table A.1, A.2, A.3, A.4 and A.5 below.

Table A.1: Competency questions for OPMW (1).

Competency Question	Terms created/reused to address it
What are the input data variables of a workflow step?	DataVariable, uses, WorkflowTemplateProcess
What are the output data variables generated by a workflow step?	DataVariable, isGeneratedBy, WorkflowTemplateProcess
What are the parameters used for a workflow step (name, type)?	ParameterVariable, uses
What are the files associated to a workflow execution?	WorkflowExecutionArtifact, opmo:account, WorkflowExecutionAccount
What are the intermediate results produced in a workflow execution?	WorkflowExecutionArtifact, opmo:account, WorkflowExecutionAccount

Table A.2: Competency questions for OPMW (2).

Competency Question	Terms created/reused to address it
Which processes where run in a workflow execution?	WorkflowExecutionProcess, opmo:account, WorkflowExecutionAccount
What are the parameters and variables of a workflow?	DataVariable, isVariableOfTemplate, WorkflowTemplate
Where was a particular workflow executed?	WorkflowExecutionAccount, executedInWorkflowSystem
Which codes were used to run a workflow step?	WorkflowExecutionProcess, hasExecutableComponent
This execution step, to which template step does it correspond to?	WorkflowExecutionProcess, correspondsToTemplateProcess, WorkflowTemplateProcess
This execution file (intermediate result, input or result) to which part of the workflow template does it correspond?	WorkflowExecutionArtifact, correspondsToTemplateArtifact, WorkflowTemplateArtifact
To which workflow template does this execution correspond?	WorkflowExecutionAccount, correspondsToTemplate, WorkflowTemplate
Which step produces this data variable in the workflow template?	DataVariable, uses, WorkflowTemplateProcess
Which steps use this data variable in the workflow template?	DataVariable, isGeneratedBy, WorkflowTemplateProcess
This parameter, to which template does it correspond to?	ParameterVariable, isParameterOfTemplate, WorkflowTemplate

Table A.3: Competency questions for OPMW (3).

Competency Question	Terms created/reused to address it
This variable, to which template does it correspond to?	DataVariable, isVariableOfTemplate, WorkflowTemplate
This intermediate result, to which execution does it correspond to?	WorkflowExecutionArtifact, opmo:account, WorkflowExecutionAccount
This result, to which execution does it correspond to?	WorkflowExecutionArtifact, opmo:account, WorkflowExecutionAccount
Who is the responsible for the execution of the workflow (or steps of the workflow)?	WorkflowExecutionProcess, opmv:wasControlledBy, prov:wasAssociatedWith, opmv:Agent
Which steps use a particular dataset in an execution?	WorkflowExecutionProcess, opmv:used, prov:used, WorkflowExecutionArtifact
Which step has generated this output?	WorkflowExecutionArtifact, opmv:wasGeneratedBy, prov:wasGeneratedBy, WorkflowExecutionProcess
Where was this workflow created?	WorkflowTemplate, createdInWorkflowSystem
Does this workflow have a documentation?	WorkflotTemplate, hasDocumentation
Are there any collections on the workflow?	WorkflowTemplateArtifact, hasDimensionality

Table A.4: Competency questions for OPMW (4).

Competency Question	Terms created/reused to address it
How long did an execution last?	WorkflowExecutionAccount, hasOverallStartTime, hasOverallEndTime
Was the execution finished successfully?	WorkflowExecutionAccount, hasStatus
What is the start time and end time of this execution process?	WorkflowExecutionProcess, prov:startedAtTime, prov:endedAtTime
Can I see a diagram of the execution?	WorkflowExecutionAccount, hasExecutionDiagram
Can I see a diagram of the workflow?	WorkflowTemplate, hasTemplateDiagram
What is the original template designed by the workflow system?	WorkflowTemplate, hasNativeSystemTemplate
What is the execution log?	WorkflowExecutionAccount, hasOriginalLogFile
Is a template component abstract? (i.e., it has multiple possible implementations)	WorkflowTemplateProcess, isConcrete
What is the name of this file?	WorkflowExecutionArtifact, hasFileName
What is the size of this file?	WorkflowExecutionArtifact, hasSize
What is the URL with the location of this file?	WorkflowExecutionArtifact, hasLocation
What is the version number of this workflow?	WorkflowTemplate, versionNumber
What was the value of this parameter?	WorkflowExecutionArtifact, hasValue

Table A.5: Competency questions for OPMW (5).

Competency Question	**Terms created/reused to address it**
Is there a license associated to this workflow or to any of its outcomes?	WorkflowTemplate, WorkflowExecutionArtifact, WorkflowExecutionProcess, dc:rights, dc:license
Who created this workflow?	WorkflowTemplate, dc:creator, prov:wasAttributedTo
Who contributed to this workflow?	WorkflowTemplate, dc:contributor, prov:wasAttributedTo

ANNEX B

Reuse Questionnaire

Tables B.1, B.2 and B.3 illustrate the set of questions included in the user survey described on Section 5.3.

Table B.1: List of the questions included in the user survey (1).

Number	Survey Question
Q1	Is,writing code important for being able to do research in a neuro-imaging lab?
Q2	If it is, is sharing code with other researchers useful?
Q3	Is the LONI pipeline workflow system useful?
Q4	Is the LONI pipeline useful for creating workflows (pipelines)?
Q5	If not, why? - It takes time to learn how to create workflows - Other:
Q6	Is creating workflows (pipelines) useful?
Q7	Why is creating workflows (pipelines) useful? Select all that apply: - It saves time to reuse components from my previous workflows - Workflows make it easier to track and debug complex code -Workflows are a convenient way to organize and store my code -Workflows make me think of organizing my code better -Workflows make me think of making my code modular and more reusable -Workflows are a convenient way to make my methods more understandable -Workflows are a useful visualization of an overall analysis -Workflows facilitate reproducibility - Other
Q8	Is reusing previously created workflows (pipelines) in new analyses useful?

Table B.2: List of the questions included in the user survey (2).

Number	Survey Question
Q9	Why is reusing previously created workflows (pipelines) useful? Select all that apply - It saves time to reuse components from my previous workflows - Workflows give a high-level diagram that helps remember what was done - Other:
Q10	Is it useful to share workflows (pipelines) with other researchers?
Q11	Why is it useful to share workflows (pipelines) with other researchers? Select all that apply - Non-programmers can use the workflows to run code easily - New students and new people in the lab can easily use workflows - It saves them time because they do not have to re-implement the code - It makes everyone think of standards by adopting the ways others do things - Other:
Q12	If not, why are workflows (pipelines) not shared? Select all that apply - Others would not want to use them - Others ask too many questions to the creators of the workflows - Workflows created by others are difficult to understand - It is difficult to understand how to prepare the data for a workflow - Other:
Q13	What is the most usual size of workflows (pipelines)? Select all that apply - 1-5 components - 5-10 components - 10-20 components - >20 components
Q14	Is it useful to reuse workflows (pipelines) from other researchers?
Q15	If not, why? Select all that apply - Workflows created by others are difficult to understand - It is difficult to understand how to prepare the data for a workflow - Workflows created by others are often too specific - It is hard to make them work - Other:
Q16	Is the groupings functionality of the workflow system useful?
Q17	If not, why?
Q18	What are,the benefits of using groupings? Select all that apply. - To have nice visualizations of an analysis - To simplify workflows that are complex overall - To make workflows more understandable to others - Other:
Q19	Is it useful to reuse previous groupings in new work?

Table B.3: List of the questions included in the user survey (3).

Q20	Why is reusing previously created groupings useful? Select all that apply. - It saves time to reuse groupings instead of whole workflows - Groupings are a convenient way to make my code modular - Groupings are a convenient way to make my methods more understandable - Other:
Q21	Is it useful to share your own previous groupings with other researchers?
Q22	Why is it useful to share your own previous groupings with other researchers? Select all that apply. - Non-programmers can use groupings more easily than whole workflows - New students and new people in the lab can easily use groupings - It saves them time because they do not have to re-implement the code - It makes everyone think of standards by adopting the ways others do things - Other:
Q23	If not, why are groupings not shared? Select all that apply - Others ask too many questions to the creators of the workflows - Others would not want to use them - It is difficult to explain what they do - It is difficult to explain how to prepare the data - Other:
Q24	Are groupings from other researchers reused?
Q25	If not, why are they not reused? - It is difficult to understand what they do - It is difficult to understand how to prepare the data - They are too specific - It is hard to make them work - Other:
Q26	Are workflows (pipelines) linked to publications?
Q27	How is this done? Select all that apply - Keeping personal notes about what workflows were used in a paper - Posting links publicly in a project or personal Web site - Other:
Q28	When workflows are not linked to publications, why is that? Select all that apply - People do not know how to do it -People do not find it useful - Other:
Q29	Would you like to add any other comments on the topics of the questions above?

ANNEX C

Evaluation Details

This annex provides additional details of the results described in Chapter 7.

C.1 Motifs found in the Wings Corpus

Table C.1 provides details on how the internal macro motifs are found in the Wings corpus used in Section 7.2. Regarding composite workflows, we analyze whether a particular workflow is part of another workflow (i.e., is part of a composite workflow) or not. More details on any of the templates can be browsed online[1].

C.2 Details on the evaluation of the Application of Inexact FSM techniques

Table C.2 introduces the details used to create the figures depicted on Section 7.2.2 of the evaluation.

C.3 Details on the evaluation of the Application of Exact FSM techniques

Table C.3 introduces the details used to create the figures depicted on Section 7.3.2.2 of the evaluation.

[1] `http://purl.org/net/wexp`

Table C.1: Motifs found in the Wings corpus. Templates with one step are omitted.

Template name	**N of Steps**	**Part of comp. workflows?**	**Part of comp. workflows? (generalizing)**	**N of internal macros**	**N of internal macros (generalizing)**
1 Classify	1	-	-	-	-
2 CorrelationScore	1	-	-	-	-
3 DocumentClassificationMutli	15	no	no	1 (5 steps)	2 (2 steps and 5 steps)
4 DocumentClassificationSingle	13	no	no	1 (6 steps)	1 (6 steps)
5 DocumentClustering	6	no	no	0	0
6 FeatureGeneration	4	no	yes	0	0
7 FeatureSelection	7	no	no	0	0
8 GenerateVocabular	3	no	no	1 (1 step)	1 (1 step)
9 Model	3	no	no	0	0
10 ModelThenClassify	2	no	no	0	0
11 MultiLabel	3	no	yes	0	0
12 PlotCorrelationScore	3	no	no	0	0
13 PlotTopics	1	-	-	-	-
14 PrepareDataset	2	no	no	0	0
15 ReduceDataset	1	-	-	-	-
16 Similar	2	no	yes	0	0
17 SimilarWords	6	no	yes	0	0
18 SimilarWordsTopics	6	no	yes	0	0
19 Stemming	3	yes	yes	0	0
20 TermWeighting	1	-	-	-	-
21 Topic Modeling	6	no	no	0	1 (2 step)
22 Validate	2	yes	yes	0	0

C.4 Usefulness Questionnaire

The questionnaire issued to the three different users and used in Section 7.3.3 followed the template described in table C.4:

Table C.2: Details on precision and recall of inexact FSM techniques on corpora WC1-WC4, used in the LONI Pipeline evaluation. The frequency indicates the minimum number of occurrences for a fragment to appear in the corpus. The precision and recall are shown only for multi-step filtered fragments (Mff) for simplicity.

Corpus	Inexact FSM	Freq (num occurr. (occ))	Candidate	Multi-Step	Mff	P100 (Mff)	P90 (Mff)	P80(Mff)
WC1	MDL	min (2 occ)	281	281	278	0,269784173	0,269784173	0,428057554
		2%,(8 occ)	72	72	71	0,225352113	0,225352113	0,323943662
		5%,(22 occ)	32	32	31	0,258064516	0,258064516	0,290322581
		10%,(44 occ)	15	15	14	0,428571429	0,428571429	0,5
	Size	min (2 occ)	481	371	368	0,33423913	0,461956522	0,573369565
		2%,(8 occ)	80	60	60	0,383333333	0,433333333	0,566666667
		5%,(22 occ)	24	24	24	0,291666667	0,333333333	0,583333333
		10%,(44 occ)	10	10	10	0,3	0,4	0,8
WC2	MDL	min (2 occ)	93	93	91	0,142857143	0,153846154	0,208791209
		2%,(2 occ)	93	93	91	0,142857143	0,153846154	0,208791209
		5%,(4 occ)	20	20	20	0,2	0,2	0,2
		10%,(9 occ)	6	6	6	0,333333333	0,333333333	0,333333333
	Size	min (2 occ)	135	86	84	0,178571429	0,273809524	0,380952381
		2%,(2 occ)	135	86	84	0,178571429	0,273809524	0,380952381
		5%,(4 occ)	31	21	21	0,238095238	0,333333333	0,476190476
		10%,(9 occ)	5	5	5	0,6	0,6	0,6
WC3	MDL	min (2 occ)	141	141	141	0,397163121	0,418439716	0,482269504
		2%,(5 occ)	25	25	25	0,36	0,4	0,56
		5%,(13 occ)	5	5	5	0	0	0,2
		10%,(26 occ)	1	1	1	0	0	0
	Size	min (2 occ)	227	149	147	0,489795918	0,551020408	0,591836735
		2%,(5 occ)	42	29	29	0,551724138	0,620689655	0,655172414
		5%,(13 occ)	9	7	7	0,285714286	0,428571429	0,428571429
		10%,(26 occ)	3	2	2	0,5	0,5	0,5
WC4	MDL (failed exec)	min (2 occ)	4	4	4	0,25	0,5	0,75
		2%,(1 occ)	NA	NA	NA	NA	NA	NA
		5%,(3 occ)	4	4	4	0,25	0,25	0,5
		10%,(5 occ)	2	2	2	0	0	0,5
	Size	min (2 occ)	64	42	42	0,238095238	0,357142857	0,404761905
		2%,(1 occ)	NA	NA	NA	NA	NA	NA
		5%,(3 occ)	18	16	16	0,25	0,375	0,375
		10%,(5 occ)	5	3	3	0,333333333	0,333333333	0,333333333

Table C.3: Details on precision and recall of exact FSM techniques on corpora WC1-WC4, used in the LONI Pipeline evaluation. The support indicates the minimum number of templates in which to appear in the corpus. The precision and recall are shown only for multi-step filtered fragments (Mff) for simplicity. The asterisk (*) means that the execution was limited by setting a maximum fragment size, in order to avoid out of memory errors.

Corpus	Support (%), (templ (t))	Multi-Step	Mff	P100 (Mff)	R100 (Mff)	P90(Mff)	P80(Mff)
WC1	2%,(8 t)	out of memory	637*	0,127158556	0,137989779	0,127158556	0,334332834
	5%,(22 t)	out of memory	1996	0,02755511	0,093696763	0,121743487	0,717935872
	10%,(44 t)	54714	110	0,163636364	0,030664395	0,181818182	0,445454545
	15%,(66 t)	5819	33	0,393939394	0,022146508	0,424242424	0,545454545
WC2	2%,(2 t)	out of memory	127*	0,362204724	0,254143646	0,409448819	0,472440945
	5%,(4 t)	out of memory	48	0,125	0,033149171	0,1875	0,25
	10%,(9 t)	368877	14	0,071428571	0,005524862	0,071428571	0,142857143
	15%,(14 t)	25	2	0	0	0	0
WC3	2%,(5 t)	out of memory	108	0,444444444	0,137931034	0,527777778	0,611111111
	5%,(13 t)	2850	29	0,413793103	0,034482759	0,482758621	0,655172414
	10%,(26 t)	37	9	0,222222222	0,005747126	0,222222222	0,444444444
	15%,(40 t)	0	0	0	0	0	0
WC4	2%(1 t)	NA	NA	NA	NA	NA	NA
	5%, (3 t)	out of memory	out of memory	NA	NA	NA	NA
	10%,(5 t)	out of memory	10*	0,1	0,011111111	0,1	0,1
	15%,(7 t)	268840	3	0	0	0	0

Table C.4: User questionnaire for assessing the usefulness of the proposed fragments.

Question	**Possible responses**
Q1: Would you consider the proposed fragment a valuable grouping?	I would not select it as a grouping (0) I would use it as a grouping with major changes (i.e., adding/removing more than 30% of the steps) (1) I would use it as a grouping with minor changes (i.e., adding/removing lessthan 30% of the steps) (2).
Q2: What do you think about the complexity of the fragment?	The fragment is too simple (0) The fragment is,ne as it is (1) The fragment has too many steps (2)

ANNEX D

Additional FSM Algorithms for Mining Useful Fragments

As described in Chapter 6, there are many existing algorithms for FSM (Jiang et al., 2012). However, finding the associated implementations for each of the algorithms is not always trivial. In this annex we discuss three algorithms with available implementations that may improve some aspects of the current results obtained by our approach. Other algorithms with available implementations exist[1,2], but according to their descriptions they may not return results significantly different to what we have already obtained with the ones implemented in our approach (as most of them are exact FSM techniques).

- Sigma (Mongiovi et al., 2010) is an inexact FSM algorithm that performs over a dataset of graphs. Being inexact, Sigma may return commonly occurring fragments that are similar, discovering new levels of abstraction among the workflow corpus. Additionally, according to the authors, it outperforms other state of the art inexact FSM algorithms, which makes it a potential candidate for us to consider when finding fragments in workflows.

- GRAMI (Saeedy and Kalnis, 2011) is another inexact FSM algorithms for efficiently mining large single graphs. GRAMI uses an edit distance to group together similar commonly occurring fragments, instead of using an exact mining approach.

[1] `http://hms.liacs.nl/graphs.html`
[2] `http://www.borgelt.net/fpm.html`

However, GRAMI has been designed for single large graphs, and it would be required to explore whether it would be appropriate for finding patterns in multiple graphs, as it is our case.

- MIRAGE (Bhuiyan and Hasan, 2013) implements an exact FSM algorithm using a MapReduce approach. In this regard, the results would not differ from other exact FSM algorithms already implemented in FragFlow, but by parallelizing their approach with MapReduce, the total amount of time needed to process the input corpus would be significantly reduced.

Glossary

AGM

The Apriori Graph Mining algorithm (AGM) is an exact FSM technique that uses an adjacency matrix to represent graphs in combination with an efficient levelwise search to discover common sub-graphs (Inokuchi et al., 2000). 117

AGWL

ASKALON's language for specifying scientific workflows (Fahringer et al., 2005). 20

ASKALON

Workflow management system developed by the University of Innsbruck (Austria) (Fahringer et al., 2007). 14

BFS

Breadth first search (BFS) is a technique for exploring a graph by visiting first all the neighbours of a node. 117

BPMN

The Business Process model and Notation (BPMN) provides a standard notation for implementing, managing and monitoring business processes (Aggarwal et al., 2011). 12

Business workflow

Templates designed to model, automate and execute a flow of business activities in the corporate world[3]. 11

[3] `http://www.wfmc.org/what-is-bpm`

Candidate workflow fragment

A workflow fragment identified by any of the FSM approaches integrated in FragFlow. 122

Case-based reasoning

Group of techniques that aim to solve a given problem based on past experience with similar cases. 38

Clustering

Set of techniques that aim to group together individuals sharing a particular set of common features. 37

Common workflow fragment

Given a workflow corpus, a workflow fragment is common if it appears at least f times in the corpus, with f bigger than 2. The number "f" can be calculated in two different ways. If each occurrence is counted once per workflow then "f" represents the **support** for the workflow fragment. If all the occurrences of the fragment are counted (even if it appears several times on the same workflow) "f" represents the **frequency** of the workflow fragment. 111

Competency question

A requirement to be fulfilled by an ontology (i.e., the data modeled by an ontology must be able to answer the question). 52

Conceptual workflows

Workflow model that aims to facilitate workflow abstraction and design by separating workflows in conceptual and abstract levels (Cerezo, 2013). 23

CrowdLabs

Workflow repository for VisTrails' workflows, created by the University of New York (USA)(Mates et al., 2011). 26

D-PROV

Provenance model for representing workflow execution templates, instances and executions (Missier et al., 2013). It extends the PROV standard. 23

DAX

Syntax used by the Pegasus workflow system for specifying scientific workflows[4]. 20

DFS

Depth first search (DFS) is a technique for exploring a graph by visiting each branch associated to a node of the graph before backtracking to the next neighbor. 117

Directed acyclic graph

A non empty set of nodes and edges that connect those nodes. All the edges have a direction, i.e., they go from a source node (tail) to a target node (head). This type of graph has no cycles, i.e., from a node it is not possible to reach the same node by following its edges. 14

Directed cyclic graph

A non empty set of nodes and edges that connect those nodes. All the edges have a direction, i.e., they go from a source node (tail) to a target node (head). This type of graph contains cycles, i.e., from a node it may be possible to reach the same node by following its edges. 14

DISPEL

Data-Intensive Systems Process Engineering Language, defined to "*describe abstract workflows for distributed data-intensive applications*" (Atkinson et al., 2013). 20

DOI

A Digital Object Identifier (DOI)[5], is a standard way for accessing resources on electronic networks. It has been commonly used to refer to electronic documents, like journal articles. 26

[4] `http://pegasus.isi.edu/wms/docs/schemas/dax-3.4/dax-3.4.html`
[5] `http://www.doi.org/`

Dryad

Data repository for the international scientific and medical literature. Maintained by the North Carolina State University (USA)[6]. 26

Dublin Core

Popular vocabulary for defining a set of common metadata terms (e.g., attribution, licensing, etc)[7]. 25

EXPO

Ontology designed to represent the methodological aspects of a scientific experiment, including the scientific tasks required to carry it out (Soldatova and King, 2006). 24

FigShare

Popular data repository for archiving resources in digital sciences[8]. 26

FOAF

Popular vocabulary for describing agents on the Web and their interactions[9]. 25

FragFlow

The approach proposed in this thesis for mining frequent workflow fragments. 111

FSG

Exact FSM technique that builds on the Apriori algorithm by adding a sparse graph representation to reduce storage and computation, while incorporating optimizations for the generation of candidate fragments (Inokuchi et al., 2000). 117

FSM

The Frequent Sub-graph Mining (FSM) problem aims to *"to extract all the frequent sub-graphs, in a given data set, whose occurrence counts are above a specified*

[6] `http://datadryad.org/`
[7] `http://dublincore.org/documents/dcmi-terms/`
[8] `http://figshare.com`
[9] `http://xmlns.com/foaf/spec/`

threshold"(Jiang et al., 2012). FSM techniques can be exact (if they retrieve all the frequent sub-graphs of an input corpus) or inexact (if they group together similar sub-graphs to create common abstractions. 114

Galaxy

Workflow management system developed by the Johns Hopkins University for intensive biomedical research (Goecks et al., 2010). 14

GenePattern

Workflow management system specialized in the genomics domain and developed by the Broad Institute of MIT and harvard (USA) (Reich et al., 2006). 14

Graph

A non empty set of nodes which are interconnected by a set of edges. 11

Graph mining

Term used to refer to the application of graph-based techniques to extract commonalities among the nodes and edges of a dataset expressed as a LDAG. 39

GREW

Inexact FSM technique based on the contraction of the edges of the input graph while rewriting it, adding special heuristics to find longer and denser fragments (Kuramochi and Karypis, 2004b). 116

Grouping

User-defined sub-workflow, which can be copied and pasted in different workflows and annotated as a unit of single functionality. 94

GSpan

Exact FSM technique that uses a canonical labeling system (a DFS lexicographic order) where each graph is assigned a minimum DFS code (Yan and Han, 2002). 122

ISA

The Investigation, Study, Assay Model (ISA) (Rocca et al., 2008) aims at describing the main steps and metadata involved in a scientific experiment. 24

IWIR

The Interoperable Workflow Intermediate Representation (IWIR) is a syntax for defining workflows in a system-independent manner (Plankensteiner et al., 2011). 20

Kepler

Workflow management system designed as a collaborative effort between the University of Davis (USA), the University of Santa Barbara (USA) and the University of San Diego (USA) (Ludäscher et al., 2006). 14

Knime

Workflow management system developed by the University of Konstantz (Germany) (Berthold et al., 2008). 14

Labeled directed acyclic graph

A directed acyclic graph that uses labels to represent the different types of nodes and edges. See also directed acyclic graph. 51

Layered abstraction

Type of abstraction where conceptual levels of detail may have a very loose correspondence with one another. 31

Linked Data principles

Set of guidelines that indicate how to publish a resource and its metadata on the Web[10] (Heath and Bizer, 2011). 65

Macro abstraction

Abstractions where several computation steps can be compressed together as one step. 31

[10] `http://www.w3.org/DesignIssues/LinkedData.html`

MOML

Kepler's language for specifying scientific workflows (Lee and Neuendorffer, 2000). 20

Moteur

Workflow management system designed at the I3S Laboratory (France) (Glatard et al., 2007). 14

Multi-step filtered fragment

Multi-step workflow fragments which are not part of bigger workflow fragments with the same number of occurrences as them. For more details, see Definition 4. 123

Multi-step workflow fragment

A workflow fragment with more than one step. 122

OBI

The Ontology for Biomedical Investigations (OBI) defines a common framework for representing experimental descriptions and methods in biomedical research (Brinkman et al., 2010). 24

Ontologies

An ontology is defined as a "formal specification of a shared conceptualization", where *conceptualization* refers to *"an abstract model of some phenomenon in the world by having identified the relevant concepts of that phenomenon"*, *formal* means that *"it should be machine-readable"* and *shared* means that *"the ontology captures consensual knowledge"* (Studer et al., 1998). 22

OPM

The Open Provenance Model (OPM) is a generic model for describing the provenance of a given resource (Moreau et al., 2011). 20

OPMO

The Open Provenance Model Ontology (OPMO)[11] is an ontology that extends on OPMV to represent the full functionality of OPM. 53

OPMV

The Open provenance Model Vocabulary (OPMV)[12] is a lightweight implementation of the OPM model that only has a subset of the concepts in OPM but facilitates modeling and query formulation. 53

OPMW

The Open Provenance Model for Workflows (OPMW) is the model proposed in this thesis to describe scientific workflows by capturing all their dataflow, dependencies and provenance. 51

ORSD

The Ontology Requirement Specification Document (ORSD) (Suárez-Figueroa, 2010) describes the competency questions that an ontology must be able to answer when modeling a particular domain. 52

OWL

The Web Ontology Language (OWL) is designed to *"explicitly represent the meaning of terms in vocabularies and the relationships between those terms"*. OWL *"has more facilities for expressing meaning and semantics than XML, RDF, and RDFS, and thus OWL goes beyond these languages in its ability to represent machine interpretable content on the Web"* (McGuinness and van Harmelen, 2004). 22

P-Plan

PROV extension designed to "*capture the plans that guided the execution of scientific processes*" (Garijo and Gil, 2012). 23

[11] `http://openprovenance.org/model/opmo`
[12] `http://purl.org/net/opmv/ns`

PASOA

Provenance Aware Management System (PASOA), integrated with some workflow management systems to manage their execution traces (Miles et al., 2007). 21

Pegasus

Workflow management system developed at the Information Sciences Institute of the University of Southern California (USA) (Deelman et al., 2005). 14

Petri Net

A model for representing states and local actions in the world of information processing (Reisig and Rozenberg, 1998). When adapted to scientific workflows, the actions correspond to workflow steps, which connect states of the workflow through directed arcs. 11

POIROT

Architecture for integrating reasoning and learning components for workflows (Burstein et al., 2009). 39

Predicate abstraction

Type of abstraction where entire predicates (e.g., constraints, inputs of steps, etc.) are dropped at any given abstraction level (Graf and Saidi, 1997). 30

Problem Solving Methods

Resources that describe strategies to achieve the goal of a task in an implementation and domain-independent manner (Gómez-Pérez and Benjamins, 1999). 34

PROV

W3C standard for specifying provenance on the Web (Groth and Moreau, 2013). 21

Provenance

"*A record that describes the people, institutions, entities, and activities involved in producing, influencing, or delivering a piece of data or a thing*" (Moreau et al., 2013). 20

Prov Manager

Provenance management system designed to store the executions of workflows according to PROV (Marinho et al., 2012). 21

ProvONE

Provenance model extending the PROV standard to represent workflow execution templates, instances and executions[13]. 23

Pubby

Tool used as a front-end for browsing Linked Data of SPARQL endpoints[14]. 69

RapidMiner

Workflow management system aimed at creating workflows for predictive analysis[15]. 26

RDF

The Resource Description Framework (RDF) is a W3C standard that specifies the relationships between resources using a labeled graph with RDF statements. Each RDF statement consists on a source node and an object node, connected by the property that is linking them (Klyne et al., 2004). 22

RDFS

The RDF Schema (RDFS) is an extension of the RDF vocabulary to provide a data-modeling vocabulary for RDF (McBride et al., 2014). 22

Research Object

Family of specifications for representing the aggregation of resources that are part of a research work. In addition, the RO model contains vocabularies for specifying workflow templates and executions (Belhajjame et al., 2012a). 21

[13] `http://http://www.purl.org/provone`
[14] `http://wifo5-03.informatik.uni-mannheim.de/pubby/`
[15] `https://rapidminer.com/`

SADI

The Semantic Automated Discovery and Integration (SADI) (Wilkinson et al., 2009) is a framework for discovering and integrating distributed and analytical resources[16]. 29

Scientific workflow

Template defining the "*set of tasks needed to manage a computational science process*" (Deelman et al., 2009). 2

Scufl

Taverna's language for specifying scientific workflows (Oinn et al., 2004). 20

SIGMA

Inexact FSM technique which uses a set-covered based approach by associating a feature set with each edge of the candidate fragment (Mongiovi et al., 2010). 116

Skeletal plan

"*Sequence of abstract and only partially specified steps which, when specialized to specific executable operations, will solve a given problem in a specific problem context*" (Bergmann, 1992). 28

Software Ontology

Ontology designed to represent the typical operations in software development[17]. 34

SPARQL

W3C standard for querying RDF data (Harris et al., 2013). 97

Sub-graph isomorphism

Problem aimed at determining whether a given graph is part of another graph or not. 38

[16] `http://sadiframework.org/content/about-sadi/`
[17] `http://sourceforge.net/projects/theswo/`

SUBDUE

Inexact FSM technique based on a iterative clustering approach, by applying two heuristics to reduce the input graph on each iteration (Cook and Holder, 1994). The two heuristics used by SUBDUE are the Minimum Description Length (MDL) (Rissanen, 1978) and the current size of the graph. 115

SWAN-PAV

Vocabulary defined to describe detailed attribution, authoring, contributions and versioning of web resources (Ciccarese et al., 2013). 25

Taverna

Workflow management system developed at the University of Manchester (UK) (Wolstencroft et al., 2013). 14

The LONI Pipeline

Workflow management system designed for neuro-image analysis by the University of California Los Angeles (USA) and the University of Southern California (USA) (Dinov et al., 2009). 14

Topic modeling

Set of techniques that aim at generating the common topics of a set of documents. A topic is not necessarily a single word, it may be a common subset of words among the documents. 37

UML

The Unified Modelling Language (UML) is a common language for describing system architectures and behavior in software engineering (Bock et al., 2015). In the workflow domain, it can be used to represent the data dependencies among the steps of a workflow. 12

URI

A Universal Resource Identifier (URI) is "*is a compact sequence of characters that identifies an abstract or physical resource*" (Berners-Lee et al., 2005). 65

VisTrails

Workflow management system developed at the University of Utah (USA) and the University of New York (USA) (Callahan et al., 2006). 14

WExp

The Workflow Explorer (WExp)[18] is a simple browser for workflows and their metadata. 69

Wf-fd

The Workflow Fragment Description Ontology (Wf-fd) is our proposed extension of the P-Plan ontology to model the relationship between workflow fragments and the workflows where they were found. 124

Wings

Workflow management system developed at the Information Sciences Institute of the University of Southern California (USA) (Gil et al., 2011). 14

Workflow abstraction

The ability to generalize workflows (or workflow steps) by their common functionality. Workflow abstraction is key for simplifying workflows and for finding relations between them. 10

Workflow execution trace

Provenance trace that contains the details of the execution of a workflow: used inputs, intermediate results, final outputs, etc. 17

Workflow fragment

Given a workflow W, a workflow fragment is a connected sub-workflow of W. 111

Workflow instance

A workflow that specifies the application algorithms to be executed and the concrete data to be used. Workflow instances do not specify execution resources. 17

[18] `http://purl.org/net/wexp`

Workflow management system

Systems made to design, monitor, execute and debug scientific workflows. 14

Workflow motif

Domain independent conceptual abstraction for workflow steps that can be found in scientific workflows. 73

Workflow pattern

"*The abstraction from a concrete form which keeps recurring in specific non-arbitrary contexts*" (Riehle and Züllighoven, 1996). 33

Workflow representation

The models created to serialize a workflow on the different phases of its life cycle. 10

Workflow reuse

The ability to adapt an existing workflow (or any of its sub-parts) for composing a new workflow. 10

Workflow template

Generic reusable workflow specification that indicates the types of steps in the workflow and their dataflow dependencies. 17

Workflow understanding

The ability of users to clearly determine the functionality of each of the steps (or group of steps) of the workflow. 43

WS-BPEL

Web Services Business Process Execution Language (WS-BPEL), a standard language for defining web service composition pipelines (Jordan et al., 2007). 20

ZOOM*Userviews

System designed to represent the different views of the same workflow according to their relevance (Biton et al., 2007). 32

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