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Nadia Cerezo, Johan Montagnat

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Scientific Workflows Reuse through Conceptual Workflows

Nadia Cerezo
CNRS, Univ. of Nice
I3S laboratory
cerezo@i3s.unice.fr

Johan Montagnat
CNRS, Univ. of Nice
I3S laboratory
johan@i3s.unice.fr

ABSTRACT

An increasing number of scientific experiments are “in-silico”: carried out at least partially using computers. Scientific Workflows have become a key tool to model and implement such experiments, but they tangle domain knowledge, technical know-how and non-functional concerns and are, as a result, difficult to understand, reuse or repurpose.

In order to ease Scientific Workflow Reuse, this paper defines a Conceptual Workflow model that is closer to the end-user’s domain and intentions. By placing our model higher on the abstraction scale, we can separate concerns and emphasize the in-silico experiment inside the workflow, thus improving readability and re-usability.

The conceptual representation can then be transformed into a regular Abstract Scientific Workflow, exploiting both domain and non-functional knowledge that are captured and harnessed through the use of Semantic Web technologies.

Categories and Subject Descriptors

D.2.13 [Software]: Reusable software

General Terms

Scientific Workflows, Reuse, Domain Engineering

1. INTRODUCTION

According to the Workflow Management Coalition¹, Terminology and Glossary 3.0, a *workflow* is the “*automation of a business process, in whole or part, during which documents, information or tasks are passed from one participant to another for action, according to a set of procedural rules*”. Originally geared towards the description of business processes, workflows have been increasingly used to describe scientific experiments, especially those performed on distributed computing infrastructures. *Scientific Workflows* are meant to perform *in-silico* (*i.e.* carried out en-

¹<http://www.wfmc.org/>

tirely or partially on computers) experiments, which usually imply large amounts of data. Workflow formalisms are appealing to scientists in that they provide means to formally describe complex experiments using an abstract (*i.e.* not too tightly coupled with an execution infrastructure) and versatile (*i.e.* accessible and adaptable) representation. Workflows ease the design and implementation of scientific experimental protocols.

“*Software Reuse is the use of existing software or software knowledge to construct new software.*” [6] Defined so broadly, *Software Reuse* has been an integral part of *Software Engineering* from the very beginning. The general tendency of programming languages and environments to provide developers with ever-coarser grained building blocks, at ever-higher levels of abstraction, is in itself *Software Reuse*. As a research area, *Software Reuse* lies at the crossroads of *Software Architecture* (to identify and handle reusable parts), *Domain Engineering* (to elevate the abstraction level) and *Separation of Concerns* (to integrate even cross-cutting concerns into reusable components).

Scientific Workflows Reuse, defined as a workflow system desideratum in [12] by “*Workflow systems should make it easy to design new workflows from existing workflows*”, is critical for two main reasons.

On the one hand, Scientific Workflows raise the need for flexibility a few notches above that of their Business counterparts [2]. Indeed, the scientific experiments they model result from neither precise specifications nor rigid protocols - no matter how rapidly evolving those may be - and are instead defined incrementally, through the exploration that is typical of scientific research. The very goal of Scientific Workflows, to represent in-silico experiments, entails frequent reuse and repurposing throughout their life-cycle.

On the other hand, scientific research thrives on collaboration between communities (*e.g.* teams, laboratories, countries). A lot of sharing is involved in those collaborations; of knowledge as well as of know-how. Since an increasing number of communities use Scientific Workflows not only to operate their (most often data-intensive) experiments, but also to record the associated protocols and techniques, the need to share Scientific Workflows is ever-growing and from it stems a greater need for reuse and repurposing, since they enable sharing when combined with discovery (*i.e.* finding suitable components).

Our goal is to provide tools for workflow designers to ease reuse, repurposing and ultimately sharing of Scientific Workflows. We believe that the main obstacle in most currently available frameworks is that their underlying models indis-

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criminally mix **core concerns** (the high-level concepts pertaining to the end-user’s scientific domain), **technical concerns** (functional in that they are needed to actually enact the workflow, but not directly relevant to the modeled in-silico experiment) and **non-functional concerns** (for instance *Quality of Service* considerations).

Rather than building yet another framework, our proposal is to define workflows at a higher level of abstraction, upstream from already plentiful Scientific Workflow models, then transform them into lower level workflows, readily executable by existing systems. In that, we fit the gap described in [7] as the need for distinct “*dimensions of abstraction [that] are experiment-critical versus non-experiment-critical representations, where the former refers to scientific issues and the latter is more concerned with operational matters.*” Our approach is one of *Generative Reuse*: new workflows are specified in a domain-specific language, then translated into executable code in a target language.

At the higher level we aim to formalize, we can overcome the aforementioned obstacle by:

- emphasizing domain concepts over technicalities,
- defining separately the *cross-cutting concerns* and the base process into which they are woven,
- providing a more flexible way to reuse components than the traditional encapsulation that is provided in most frameworks and
- leveraging *semantic annotations* to aid the design of new workflows from existing parts.

All the examples we give in the present paper, to illustrate the model we defined, come from the **Virtual Imaging Platform**² (VIP) project. The project’s goal is the integration of multiple modalities and organ models into a cohesive medical image simulation platform. The project aims to achieve (i) **interoperability** between various simulators that were never meant to interact, by using scientific workflows and semantic annotations, (ii) **data model federation** to handle all organ models in a standardized fashion, through the definition of the IntermediAte Model Format (IAMF) and (iii) **reliability and performance** on large-scale grid infrastructures needed to cope with the amount of data processed.

The platform is meant to be flexible and easy to extend with new simulators and organ models. To ensure maximum compatibility, the integration started with four medical imaging simulators, one for each of the four main medical imaging modalities: *SIMRI* [3] for *Magnetic Resonance Imaging (MRI)*; *FIELD-II* [10] for *UltraSonography (US)*; *Sindbad* [16] for *X-ray Computed Tomography (CT)*; and *Sorteo* [15] for *Positron Emission Tomography (PET)*.

The need for Scientific Workflow Reuse in the VIP project stems from its very objectives. Indeed, the goals of interoperability and data model federation themselves call for the design of new - and the identification of existing - common components. Furthermore, the need for flexibility (to ease the future introduction of new simulators) has already led to the identification of common ground between the simulators at the structural level.

The model we defined has three parts and the present article adopts the same structure: Section 2 further describes

²<http://www.creatis.insa-lyon.fr/vip/>

the abstraction level at which we work and defines the high-level elements of our model. Section 3 details the process of generating a workflow at a lower level of abstraction and defines the elements needed in our model to perform that transformation. Section 4 introduces the notion of Patterns and illustrates how it could enhance Scientific Workflow Reuse. Section 5 details how and to what extent we intend to automate the transformation process. We then present a few related projects in Section 6 and conclude with Section 7.

2. CONCEPTUAL LEVEL

A Scientific Workflow framework is essentially an interface between end-users (*i.e.* scientists) and computing infrastructures (most often distributed). In the field of Scientific Workflows, the distinction has long been made between **Concrete Workflows** that “*bind workflow tasks to specific resources*” and **Abstract Workflows** that do not [17]. The lack of stability on Grid infrastructures, where nodes and network failures are simply bound to happen every now and then, makes the manual definition of Concrete Workflows extremely impractical. As a result, most frameworks use Abstract Workflows for design as well as storage and generate the Concrete Workflows automatically at runtime.

Abstract Workflows pertain to the abstraction level of the framework, thus called the **abstract level**, whereas Concrete Workflows belong lower on the abstraction scale, on the infrastructure layer, thus called the **concrete level**. Yet, even though, as their name suggests, Abstract Workflows are more abstract than Concrete Workflows, they are meant to be readily executable and, as such, cannot avoid the clutter of technical concerns and workarounds that are necessary for the execution.

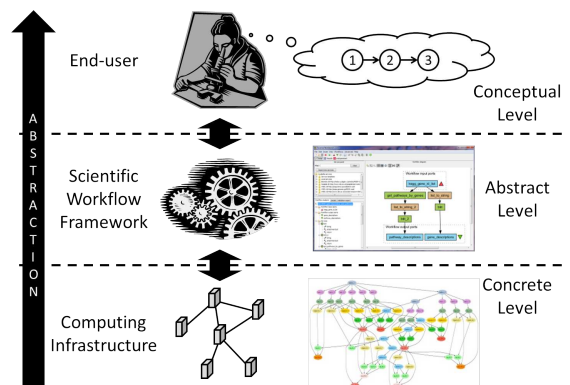


Figure 1: Scientific Workflow Abstraction Levels

To ease reuse and repurposing, we work at a higher level than that of Abstract Workflows on the abstraction scale: the so-called **conceptual level**, as shown on Figure 1. This level enables the modeling of in-silico experiments closer to the end-users’ domains.

The Scientific Workflow model we defined at that level is what we call **Conceptual Workflow**. Conceptual Workflows aim at capturing the user intentions when he or she designs a scientific experiment, independently from concerns such as reliability, performance, security and so on. They focus on the scientific process itself, distinguishing it from non-functional and technical aspects. Hence Conceptual Workflows are easier to manipulate, understand and reuse.

2.1 Model

A **Conceptual Workflow** represents all or part of an in-silico experiment. At that high-level, they consist in domain functions performed over input objects to obtain desired products.

Most of the existing scientific workflow models are directed graphs whose vertices represent data or processing nodes and whose edges represent data or control flow. We believe that representation to be straightforward enough for users who are not accustomed to process modeling and thus adopt it as a basis for our own model.

A **Conceptual Workflow** is a *Directed Graph*:

- whose *vertices* are **Conceptual Inputs** (representing input objects), **Conceptual Outputs** (representing desired products) or **Conceptual Workflows** themselves (representing domain functions)
- and whose *edges* are **Conceptual Links** (representing the data and control flow).

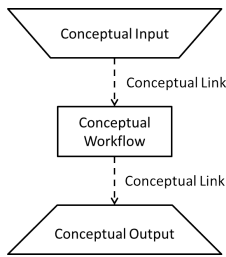


Figure 2: Graphical Convention - High-level elements

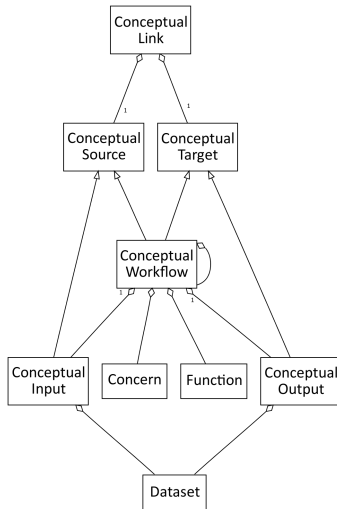


Figure 3: Meta-model - High-level elements

All those elements are shown on Figure 2 and their relationships are described in UML³ on Figure 3 (default cardinality is * (many)).

³Unified Modeling Language, current specification available at <http://www.omg.org/spec/UML/Current>

Conceptual Workflows are nested so as to provide encapsulation: parts of the workflow that are deemed too detailed or that are reused can be kept inside a sub-workflow and thus hidden in a black box from the viewpoint of the parent workflow. That mechanism is provided by most Scientific Workflow frameworks.

Each **Conceptual Workflow** can be associated to any number of:

- **Functions**: domain concepts such as **Align Image** or **Generate Photons**
- and **Concerns**: functions outside the scope of the domain, pertaining to a lower, more technical, level of abstraction such as **Append Prefix** or **Convert to String** or to cross-cutting non-functional areas of expertise (e.g. Quality of Service) such as **Compress data** or **Retry 3 times**.

Conceptual Inputs represent the starting materials of the in-silico experiment, whereas **Conceptual Outputs** represent its results. Both can be associated to any number of **Datasets**: domain concepts such as **Brain Model** or **Synthetic Sonogram**.

Conceptual Links represent interactions between 3 possible pairs of source/target elements:

- Conceptual Input \rightarrow Conceptual Workflow,
- Conceptual Workflow \rightarrow Conceptual Workflow or
- Conceptual Workflow \rightarrow Conceptual Output.

Because a **Conceptual Workflow** can represent any number of activities (it is often an entire sub-workflow), a given **Conceptual Link** can represent any number of data flows (*i.e.* data is transferred from the source to the target) and or any number of ordering constraints (*i.e.* the target starts after the source is done). Figure 8 in Section 3.1 will illustrate that, after the definition of data flows and ordering constraints in our model.

Because in-silico experiments are inherently very data-driven, Conceptual Links will most often translate to a set of data flows. Even then, a Conceptual Link should not be confused with a Data Link, since it restrains neither number nor types of data transferred.

Let H be the set of Conceptual Workflows and R be the binary relation of Conceptual Link, the relation R is transitive: $\forall x, y, z \in H, xRy \wedge yRz \Rightarrow xRz$.

2.2 Application to VIP use case

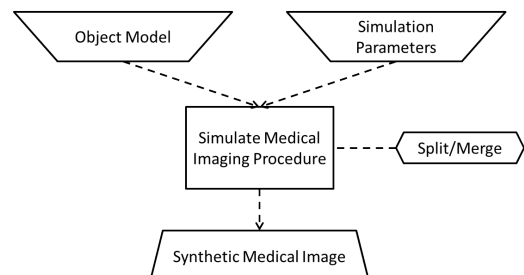


Figure 4: High-level Conceptual Workflow - Generic VIP simulator

To provide end-users with an interface that eases the extension of the platform to new simulators, it is necessary to identify common ground between the VIP simulators already in place, at the level of elements as well as at the structural level. While the four simulators considered initially were developed independently and do not show much resemblance at first glance, they share a common high-level structure modeled as a Conceptual Workflow in Figure 4:

- the **Object Model (OM)**: what is scanned by the medical imaging procedure (*e.g.* a brain, a lung),
- the **Simulation Parameters (SP)**: procedure’s details (*e.g.* probe orientation, scanner dimensions),
- from those inputs, the system produces a **Synthetic Medical Image (SMI)** by performing the action **Simulate a Medical Imaging Procedure (SMIP)**
- and the simulation is optimized by splitting the data over many processing resources then merging the results, hence the cross-cutting non-functional concern **Split/Merge**, captured in a Pattern (see Section 4.1).

This workflow seems generic enough to serve as a basis not only for the four simulators initially included in the platform, but also for those that will be added later on.

3. TRANSFORMATION PROCESS

Conceptual Workflows can be used on their own, as a way to formally describe in-silico experiments at the level of the end-user’s domain, but the execution is the ultimate goal of any Scientific Workflow and thus their true use is through conversion to Abstract Workflows that can be delegated to existing Scientific Workflow frameworks. To that end, Conceptual Workflows must embed enough information to enable their transformation into Abstract Workflows.

While the conversion Abstract → Concrete takes place between a framework and an infrastructure and thus has to be entirely automated, the conversion Conceptual → Abstract has to rely on much user knowledge and decision-making and therefore is semi-automated at best. We will discuss how in Section 5.

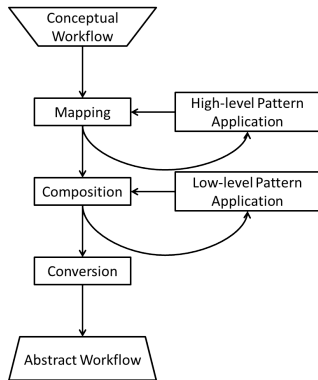


Figure 5: From Conceptual to Abstract Workflow

The conversion is done in 3 major steps, shown in Figure 5:

1. **Mapping** is the step where the scientific functions (*e.g.* **Align Gene Sequence**) are mapped to processing units (*e.g.* grid services) that fulfill them.

2. **Composition** is the step where the units found at the previous step are inter-connected.
3. **Conversion** is a step of translation from our model to an existing Abstract Workflow language such as *GWENDIA* [14] or *Taverna’s SCUFL* [9].

In order to progressively transform Conceptual Workflows into Abstract Workflows, we have to enrich the model with low-level elements that pertain to abstract workflows, if not in a fully detailed and readily executable way, at least in a precise enough manner that the link between conceptual and abstract levels remains clear.

Those needed low-level elements are detailed in the next section. As for the application of patterns, mentioned on Figure 5, it will be described in Section 4.1.

3.1 Model

As of now, we have found necessary to describe the following elements that are commonly found in **Abstract Workflows** (though under various names):

- **Activities** are processing units such as *Web services, grid jobs, tasks* or sub-processes.
- **Input (resp. Output) Ports** are the arguments (resp. products) of Activities.
- **Inputs (resp. Outputs)** are the arguments (resp. products) of the workflow itself.
- **Data Links** are data transfers between 3 possible pairs of elements:
 - Input → Input Port,
 - Output Port → Input Port or
 - Output Port → Output.
- **Order Links** are ordering constraints between activities, ensuring the target does not start until the source activity is finished. We have not included other types of control flows in our model yet, but we plan to at least include conditionals.

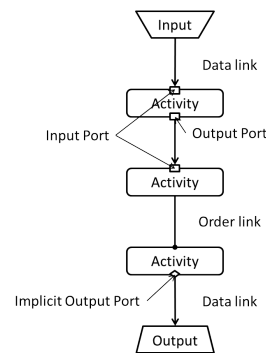


Figure 6: Graphical Convention - Low-level elements

All those elements are shown on Figure 6 and their relationships are described in UML³ on Figure 7 (default cardinality is * (many)).

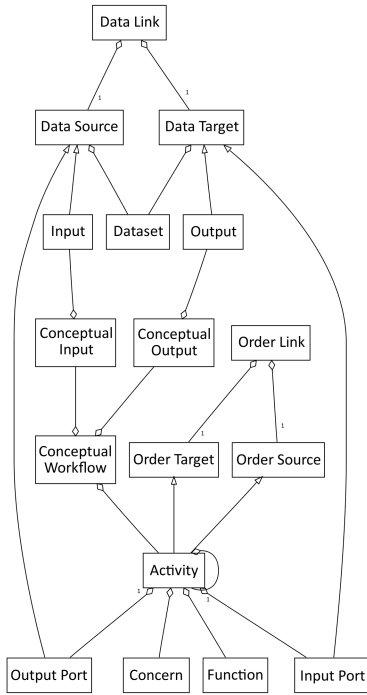


Figure 7: Meta-model - Low-level elements

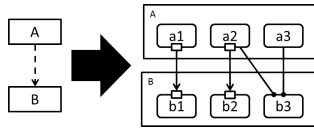


Figure 8: Conceptual Links Expressiveness

As mentioned in Section 2.1 and as shown on Figure 8, Conceptual Links can represent any number of Data Links and/or Order Links.

Like Conceptual Workflows, Activities are nested so as to provide encapsulation. Like their equivalents in Abstract Workflows, Activities are black boxes: they might be atomic processing units like Web services or grid jobs, but they might as well be entire sub-workflows.

Occasionally, data transfers between activities are done implicitly: if an activity A produces data at a specific location where the activity B retrieves it, or if the Scientific Workflow Framework handles the transfer transparently (so that each activity processes local data), then it is an implicit data transfer in the sense that it does not appear on the Abstract Workflow.

For such a transfer to take place successfully, knowledge of it must be present at some level. For instance, the user might know that all activities must be fed the same path as input for the entire process to work, or the *service descriptors* might contain information about the implicit data that is interpreted by the *Enactor* (the software that deploys and controls the workflow's execution) transparently for the user.

In both cases, the knowledge is required but not explicit on the workflow itself and thus it hinders both reading and sharing. To alleviate this problem, we introduce the concept of Implicit Port that denotes the implicit production or consumption of data by an Activity.

3.2 Application to VIP use case

All four simulators share the high-level Conceptual Workflow shown on Figure 4, but the transformation process yields different results depending on the target application. The step-by-step transformation process of each simulator is outside the scope of the present article. To illustrate the transformation process, we shall focus on the **PET simulator (Sorteo)**, for it showcases most of the optional steps.

Sorteo simulates a PET procedure through a *Monte Carlo algorithm* [15]. It is done in three steps:

1. `generateJobs` effectively splits data, so that different chunks are processed in parallel,
2. *singles* (short for single photons) are generated with one call per job to `sorteo_singles` and then merged through one call to `sorteo_single_end`
3. and then one call per job to `sorteo_emission` compute *emissions* from the singles and, finally, the emissions are merged by one call to `sorteo_emission_end`.

The Object Model is mapped to a file called `fantome_v`, the Simulation Parameters to `text_protocol` and the Synthetic Medical Image to `sinogram`.

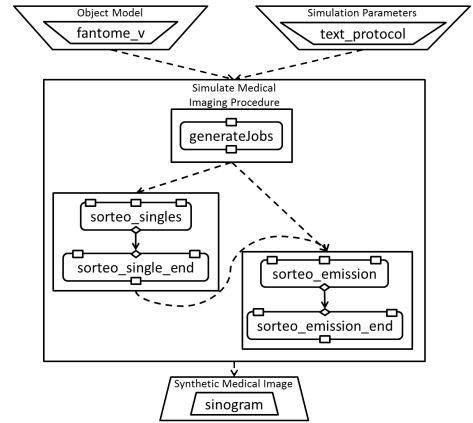


Figure 9: Sorteo - Mapping

The result of the Mapping phase is shown on Figure 9.

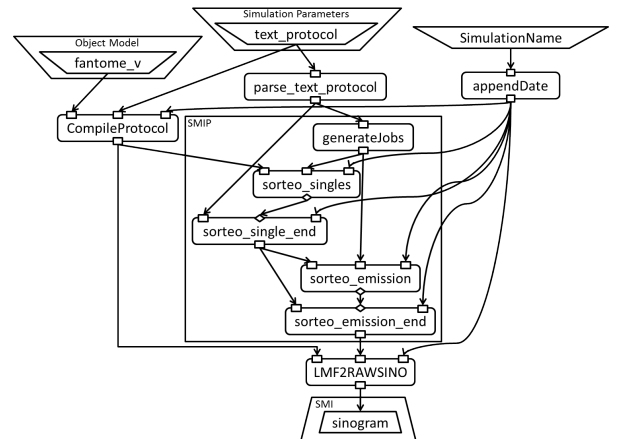


Figure 10: Sorteo - Composition

When trying to compose the activities mapped at the previous step, we encounter many type mismatches:

- as its name suggests, `text_protocol` is not in binary format, as expected by `sorteo_singles`, and the activity `CompileProtocol` will remedy that,
- `sorteo_single_end` and `generateJobs` expect the total number of jobs, an information that is contained in `text_protocol` but must be extracted through the script `parse_text_protocol`,
- and the final output is supposed to be of type `raw SINO`, but `sorteo_emission_end` produces an `LMF` file, the conversion of which is done by the converter activity `LMF2RAWSINO` (which in turn also requires the binary protocol produced by `CompileProtocol`).

Having resolved those mismatches, we are left with 6 yet unattached input ports and all of those expect the name of the output directory, produced by the activity `appendDate`. The plugging of `appendDate` in so many places in the same workflow makes the final result, shown on Figure 10, slightly difficult to read. Fortunately, we can use Patterns, that we will introduce in Section 4, to alleviate this issue.

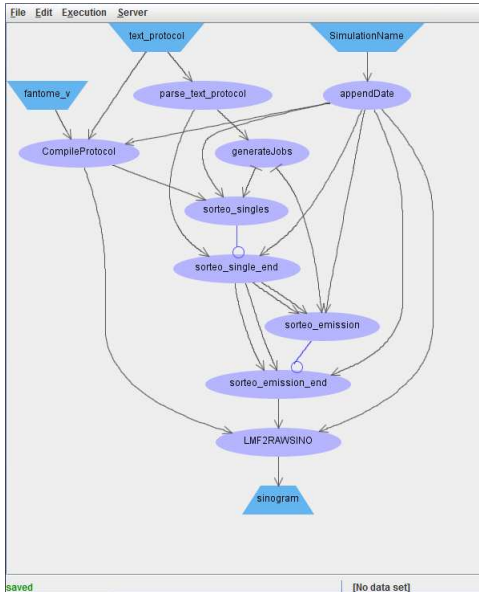


Figure 11: Sorteo in GWENDIA/MOTEUR2

The last conversion step, to an actual Abstract Workflow, is a matter of conversion from our system’s internal model to the target language of the platform (*i.e.* GWENDIA [14]). Figure 11 is a screenshot of the GWENDIA Sorteo workflow edited in MOTEUR2. Among other things, we need to make sure that all activities are fed the same directory name and that merge activities (*i.e.* `sorteo_single_end` and `sorteo_emission_end`) are appropriately synchronized. The former issue is solved through the use of Patterns, as described in the following section. The latter issue is one commonly found when translating implicit data links (*i.e.* links between implicit ports): in GWENDIA, inserting control links ensures proper synchronization.

4. REUSABLE COMPONENTS

Encapsulation on its own (through nesting of Conceptual Workflows and Activities) does not provide enough flexibility to untangle concerns and ease sharing and reuse for two main reasons.

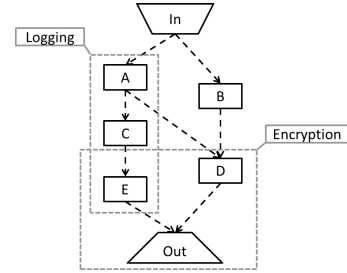


Figure 12: Cross-cutting concerns

On the one hand, components are often used multiple times inside the same parent workflow. Sub-workflows are impractical in that case, because they cannot be cleanly reused inside a given workflow: they are either duplicated and instantiated as many times as they are used (lowering performance and legibility) or they make the graph harder to draw and read with many unnecessary edges. On the other hand, cross-cutting concerns that impact the structure of the base process (*e.g.* logging) simply defy encapsulation as soon as they are tangled, like on Figure 12.

Taking inspiration from *Aspect-Oriented Programming*, we propose the notion of **Patterns**, reusable fragments that are woven into the base process dynamically during either the Mapping phase if they are high-level Patterns (*i.e.* Patterns that contain only high-level elements) or the Composition phase if they are low-level Patterns, (*i.e.* Patterns that contain low-level elements such as Activities).

The Patterns of our Conceptual Workflow Model are not to be confused with the famous *Workflow Patterns* [?] identified systematically in business workflows to evaluate the expressivity of workflow languages.

4.1 Model

Patterns are themselves **Conceptual Workflows**, special in that they feature **Join Points**.

Join Points are placeholders in a **Pattern** that are replaced with elements of the base process during application.

A **high-level Pattern** is one that features only high-level elements, namely: Conceptual Inputs, Conceptual Workflows, Conceptual Outputs and Conceptual Links. If a Pattern features low-level elements such as Activities and Data Links, then it is a **low-level Pattern**.

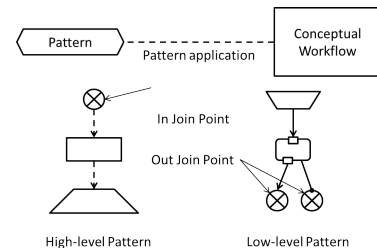


Figure 13: Graphical Convention - Patterns

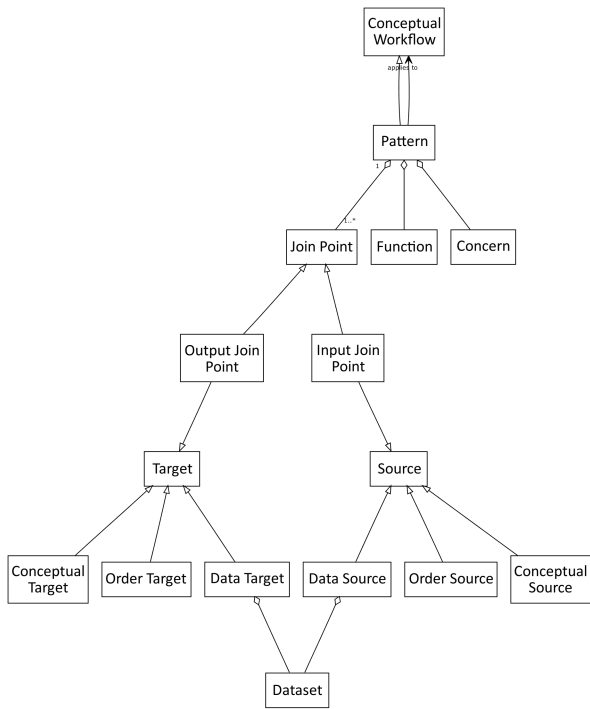


Figure 14: Meta-model - Patterns

Both levels of Patterns are shown on Figure 13 and the part of the meta-model concerning Patterns is described in UML³ on Figure 14 (default cardinality is * (many)).

To apply a Pattern to a Conceptual Workflow means to merge the two by mapping each Join Point in the Pattern to a compatible element in the Conceptual Workflow. Each Join Point is connected to the rest of the Pattern it belongs to by at least one link and those links restrain compatibility: a Join Point must be replaced with an element that is compatible with its links. For instance, if a given In Join Point is connected to the rest of the Pattern by a Data Link, then it is replaced by a Data Source; Conceptual Sources and Order Sources will not do. Table 1 details all cases.

4.2 Application to VIP use case

The **Split/Merge** concern, *i.e.* the optimization by splitting data, can be implemented in very different ways, depending on the process it applies to as well as the activities the process maps to. For instance, the main activity of the MRI simulator (SIMRI) (*i.e.* a legacy program called `simri_calcul` wrapped as a Web service), uses *MPI* to process data chunks in parallel and thus already fulfills the **Split/Merge** concern. None of the other three simulators handle that concern internally.

Because it affects the very structure of a process, the pattern we defined to capture the **Split/Merge** concern is a high-level one. As shown on Figure 15, applying the **Split/Merge** pattern to a Conceptual Workflow boils down to weaving two additional steps into the process: a pre-processing step to split input and a post-processing step to merge output. Both steps must then be mapped like any other Conceptual Workflow.

When a conceptual workflow has been mapped to two or more activities, weaving becomes less straightforward. There are two main cases (shown on Figure 16):

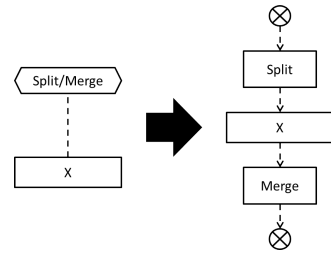


Figure 15: Pattern - Split/Merge

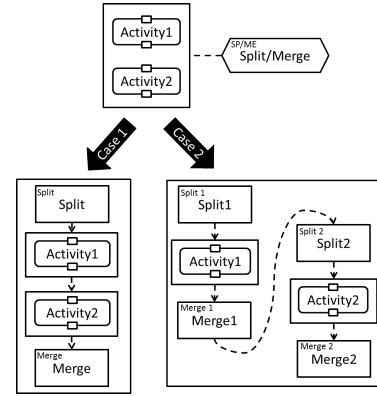


Figure 16: Split/Merge cases

- **Case 1:** data independence is valid throughout the processing chain and thus data is split only once at the very beginning and merged only once at the very end of the chain.
- **Case 2:** data independence is only valid at the scale of each activity and thus data must be merged after each processing step in the chain.

Any other case is a composite of those two and suggests that the conceptual workflow should itself be split or detailed through encapsulated sub-workflows.

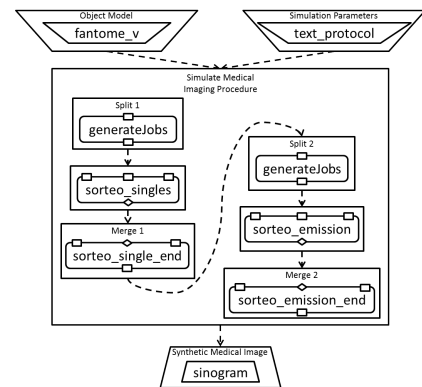


Figure 17: Sorteo - Mapping (with Patterns)

Sorteo is an example of the Case 2, as shown on Figure 17, which is the result of Mapping Sorteo after applying the **Split/Merge** Pattern. The `generateJobs` activity appears twice, but it is fairly easy to determine that it is the same instance during the Composition phase.

Table 1: Compatibility between Links and Sources/Targets

Abstraction Level	Link type	Source type	Target type
High-level	Conceptual Link	Conceptual Source	Conceptual Target
Low-level	Data Link	Data Source	Data Target
	Order Link	Order Source	Order Target

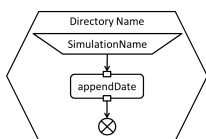


Figure 18: Pattern - Directory Name

All simulators expect the name of the output directory. There is a naming convention sub-workflow that is respected throughout the platform and it is captured in a Pattern called **Directory Name**, shown on Figure 18.

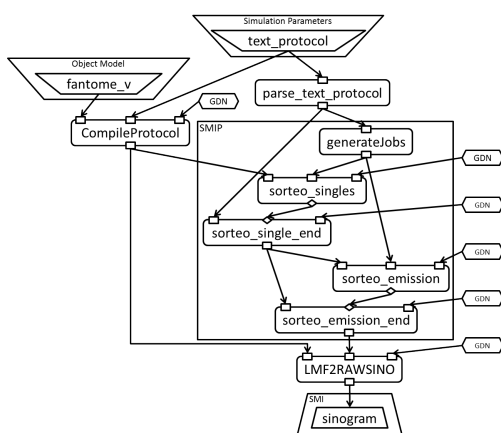


Figure 19: Sorteo - Composition (with Patterns)

Figure 19 shows the result of using the **Directory Name** pattern (abbreviated **GDN** on the figure) when composing Sorteo: the reuse itself becomes obvious and the overall readability is much improved.

5. PROCESS SEMI-AUTOMATION

Conceptual Workflows allow scientists to model their in-silico experiments directly at the domain level, but the transformation process into executable Abstract Workflows implies lowering the abstraction level and using technical and non-functional knowledge and know-how.

The transformation process from Conceptual to Abstract workflow defined in Section 3 was performed manually in the case presented in Section 3.2, but our goal is to provide tools for workflow designers to ease reuse, repurposing and ultimately sharing of Scientific Workflows. It is therefore critical to assist end-users through the transformation process as much as possible.

5.1 Resources

To achieve our goal implies handling multi-domain knowledge in a computer-legible way. As elaborated in [8], *Semantic Web technologies* were created and are developed

precisely to tackle that challenge.

An *ontology* is the formal definition of concepts and relationships between them. The standard language, recommended by the *World Wide Web Consortium*⁴ (*W3C*), is the *Web Ontology Language*⁵ (*OWL*). Ontologies have two main uses: (1) to describe a domain in a formal and standardized way (2) and to reason about *entities* (instances of the classes defined in the ontology) in order to infer new information based on what has been asserted. For instance, if it is stated that `:Man rdfs:subClassOf :Mortal` (men are mortal) and it is asserted that `:Socrates a :Man` (Socrates is a man), then an *inference engine* can infer that `:Socrates a :Mortal` (Socrates is mortal).

The concepts the system will deal with can be divided into three classes: (i) domain concepts from the end-user scientific research area, (ii) technical concepts related to the execution of the experiment and (iii) non-functional concepts such as Quality of Service concepts. However, ontologies are not necessarily divided along those lines. For instance, in the context of the VIP project, the domain and technical concepts will come from the VIP ontology and we will build our own ontology dedicated to non-functional concerns.

The set of asserted information is generally called the *Knowledge Base*. In our system's case, it will be an actual *database* (called a *Triple Store* because it stores assertions as *Subject-Property-Object* triples).

Specific elements of our Conceptual Workflow model act as a bridge to the ontologies:

- **Functions** are domain or technical concepts describing processes and actions (*e.g.* `GenerateSingles`, `ConvertLMFtoRawSINO`),
- **Datasets** are domain or technical concepts describing data types or contents (*e.g.* `LungCancer`, `ZrawFormat`)
- and **Concerns** are non-functional concepts (*e.g.* `SplitAndMerge`, `Logging`).

As detailed in Sections 2.1, 3.1 and 4.1, Conceptual Workflows and Patterns are annotated with Functions and Concerns, Activities with Functions and Inputs/Outputs (of a Conceptual Workflow or of an Activity) with Datasets.

Ontologies and annotations form a graph whose vertices are entities and whose edges are properties; a *triple* is essentially an edge from a source vertex Subject to a target vertex Object, labeled by a Property. That graph is enriched through inference. Browsing those often huge graphs is somewhat akin to browsing *relational databases* and the standard *SPARQL Query Language for RDF*⁶ is itself an *SQL* look-alike. If we wanted to look for Conceptual Workflows that fulfill the `SplitAndMerge` concern, we would use a query that looks like Listing 1.

⁴<http://www.w3.org/>

⁵<http://www.w3.org/TR/owl-overview/>

⁶<http://www.w3.org/TR/rdf-sparql-query/>

Listing 1: SPARQL query example

```

SELECT ?cw
WHERE {
  ?cw a :ConceptualWorkflow .
  ?cw :fulfills ?concern .
  ?concern a :SplitAndMerge .
}

```

5.2 Towards automating transformation

At the start of the transformation process detailed in Section 3 and represented on Figure 5, we have the following information and tools at hand: a high-level annotated Conceptual Workflow that we want to transform, a Knowledge Base containing annotated Activities, Conceptual Workflows and Patterns as well as the ontologies the annotations refer to (*i.e.* theoretically, a domain ontology, a technical ontology and a non-functional ontology, though, as noted in the previous section, the distribution of concepts over ontologies might differ in practice).

During the **Mapping phase** of the transformation process, our system should suggest Activities, Inputs and Outputs matching the Functions, Datasets and Concerns that annotate the high-level Conceptual Workflow. Because perfect matches are unlikely, the system will have to look for partial matches (called candidates) - that is easily done through a SPARQL query - and rank them according to *similarity metrics* that take *semantic distance* (distance between concepts inside an ontology) into account. For instance, a `MonteCarloPETSimulator` with outputs `LmfFormat` like `Sorteo` is an imperfect but good match for a `PET-Simulator` that outputs `RawSINOFormat`.

During the **Composition phase**, our system should not only suggest composing elements found at the previous step, but also check every data link for consistency (and warn the user when a mismatch is found, like sending a **String** to a service expecting a **File**). When direct composition is not possible because of a mismatch, the system should try to look for converter activities or suitable chains of converter activities, up to a depth that does not impact performance too severely.

The **Conversion phase**, the final translation to a target Abstract Workflow language, ought to be fully automated. Each target language will warrant a dedicated translator. Our top priority is translation to the workflow language (GWENDIA) of the framework used on the VIP platform (*MOTEUR*), but we plan to work on other translators as well, especially one to *IWIR* (*Interoperable Workflow Intermediate Representation*), the multi-platform language of the *SHIWA*⁷ interoperability project.

GWENDIA is a hybrid workflow language (mostly data-driven but featuring control constructs such as loops, conditionals and order constraints) that handles data arrays explicitly [14]. Since GWENDIA is so expressive and our final workflow representation (*i.e.* the result of the Composition phase) is fairly close to it, the conversion will be straightforward but for a few advanced constructs that require further investigation.

⁷<http://www.shiwa-workflow.eu/>

5.3 Limitations

Between the Concrete level of execution, where the Enactor handles strings, files and Web services, and the Conceptual level of the user's domain, where semantics are formally defined by ontologies, there is always a gap of description where knowledge is present only implicitly. Try as we might, we will never completely fill that gap, neither by extending ontologies to ever finer-grained concepts (*e.g.* extending `:ImageFile` with `:PNGFile`), nor by extending the basic formats with higher-level information (*e.g.* tagging additional information inside the files).

From that gap will come false positives, where the composition of two activities will seem possible to the system, because they match at both the low level of types and the high level of concepts, but will not work for some unforeseen and/or out-of-scope reason.

Besides, annotations will likely be imperfect themselves and that entails false negatives: good candidates that will rank low or not be found at all, because either they themselves or the Conceptual Workflow they could be suggested for were not annotated properly.

For all those reasons, the transformation process can never be fully automated. Still, the more computer-aided it becomes, the better.

6. RELATED WORKS

Our approach is very similar to that of the Wings [?] project, but their aim is to build a self-contained solution on top of the Pegasus⁸ framework. While we see the benefits of a single unified system from high-level in-silico experiments all the way down to computing infrastructures, we hope that by defining our model upstream from all existing frameworks, it will be of use for users of existing systems and potentially become a basis of comparison between frameworks.

The well-known *myExperiment* project [5] is a Scientific Workflow sharing social website, leveraging the *Web 2.0* to ease workflow discovery. Workflows can be discovered by keywords, tags, authors and so on, but all those methods, save for pure *social sharing*, rely on additional metadata provided by the workflow authors. As for the reuse aspect of sharing, the *myGrid* team, behind Taverna as well as *myExperiment*, advocates for “*semantically rich aggregations of resources, that possess some scientific intent or support some research objective*” [?]: a definition we believe our Conceptual Workflows fit.

The *WOODSS* project [13], like our proposal, enhances reuse and sharing through the creation of knowledge base of annotated Scientific Workflows, but they provide no formal high-level description like Conceptual Workflows.

The *Kepler Project* [11] has always considered Separation of Concerns a top priority, going as far as isolating the *Model of Computation* (*i.e.* the exact same workflow can be executed in entirely different ways depending on which *Director* is selected, for instance in sequence or in parallel). Among works to improve reuse of Kepler workflows are [4], which introduces a separated control-driven layer in the data-driven Kepler, and [1], which captures technical and non-functional concerns as coarse-grained composable blocks. In both cases, the user is further shielded from the concrete technical decisions taken at runtime and, in the

⁸<http://pegasus.isi.edu/>

latter, Semantic Web technologies are also considered a viable tool to semi-automate instantiation (*i.e.* mapping) and wiring (*i.e.* composition). In neither case is the in-silico experiment formally represented at all.

7. CONCLUSION AND FUTURE WORKS

We have defined Conceptual Workflows and shown how they can be used to untangle concerns and improve readability, by emphasizing the scientific process itself, and thus ease reuse and repurposing. That formal model (including low-level elements akin to those found in Abstract Workflows), semantic annotations and a SPARQL query engine make it possible to semi-automate the transformation from an in-silico experiment (described as a high-level Conceptual Workflow) to an executable artifact (in an Abstract Workflow language).

In the future, we plan to investigate how much our Conceptual Workflow model and the system we are building on top of it can become useful not only for reuse and repurposing, but also for portability - using Conceptual Workflow as a go-between two different target Abstract Workflow languages - and to improve accessibility for end-users - through the improved readability and support of know-how transfer via computer-aided design.

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