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WOntoVLab: A Virtual Laboratory Authorship Process Based on Workflow and Ontologies

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***Abstract*—Virtual laboratories can be used by educational institutions to facilitate and enrich the learning of specific procedures. To provide an enviroment similar to the real one, it is recommended to create experiments that require the accomplishment of a protocol (guide) aiming to support the assessment of the students. Furthermore, it is important to stimulate the identification of different possibilities to the execution of a same task, considering similar materials and procedures. In this context, this paper describes WOntoVLab, a virtual laboratory authorship process that relies on workflow representation technology and ontologies in order to represent experiments based on semantic vocabulary and alternative steps. The framework developed, WOntoVLab Process Framework (WPF), is also detailed so that educational institutions can be able to define virtual laboratories according to the WOntoVLab process.**

***Index Terms*—Virtual Laboratory, XPDL, Workflow, Ontology, Alternative Protocol**

I. Introduction

Virtual laboratories enable the simulation of experiments on computers, providing an environment equipped with necessary apparatus for laboratorial practices with no need of a physical installation. In general, both educational institutions and companies employ virtual laboratories in order to support learning activities, demonstrations, testing and training.

When applying a laboratorial experiment in an educational context, students must accomplish a specific goal so that it is possible to analyze the strategies they have used to achieve it. To make such assessment in virtual laboratories, it is interesting to define experiments according to a protocol composed of a series of activities to be performed by students.

Aiming to correctly represent these protocols, some technologies can be applied to model experiments based on execution flow. In this sense, Cesarini *et al* [1] and Pongpech *et al* [2] employ workflows to represent e-learning environments that require a protocol to be followed. Therefore, workflow representation technology can also be used to model protocols in virtual laboratories in a standardized way. The XML Process Definition Language (XPDL) [3], recommended by the WfMC (*Workflow Management Coalition*) for workflow definition, can be adopted in order to provide experiment interoperability among different virtual laboratories.

In conventional laboratories, students usually handle situations that impede them from performing an experiment exactly as established by the default protocol. For example, the absence of a particular equipment or material. Moreover, students may apply other similar strategies to execute an experiment, achieving equivalent results. In order to reproduce these features in virtual laboratories, it is necessary to consider the several ways of performing an experiment, aiming to provide a richer learning process that explore student creativity and foster knowledge sedimentation. Thus, it is interesting to semantically describe possible procedures, materials and resources that are available to virtual laboratories, what can be accomplished by means of ontologies [4]. Ontologies can support the definition of protocols by representing concepts and tasks commonly related to specific experiments. Furthermore, reasoning over ontologies can help finding out alternative protocols adopted by students, by inferring procedures that are equivalent to each other.

In this context, we propose the WOntoVLab process to virtual laboratories, which supports authorship, implementation and execution of experiments concerning alternative protocols based on ontologies and workflow representation technology. WOntoVLab makes it possible to define experiments based on protocols and semantic information, encouraging students to explore several strategies to perform an experiment, as can be done in traditional laboratories. To explain the WOntoVLab process, this paper is organized as follows: Section II presents background concepts for understanding of the WOntoVLab process, which is further described in Section III. Section IV describes a real application of WOntoVLab, as a case study carried out in the molecular biology domain. Finally, Section V presents our conclusions and future work.

II. Background

In this section, we present some features of virtual laboratories researched in the literature. We also briefly introduce concepts related to the application of workflow and ontologies in virtual laboratories, which are necessary for comprehending the WOntoVLab process.

A. Virtual Laboratories

Conventional laboratories provide physical infra-structure, but may have room limitations, scheduling and financial issues.

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Remote laboratories, such as *DSP-based remote control laboratory* [5], *Weblabs* [6] and *The microelectronics WebLab 6.0 iLab* [7], can be used to overcome some of these limitations, but problems related to schedule and space restrictions still remain. Hence, there is a strategic interest in virtual laboratories, the main focus of this research, as they provide a powerful environment for experimentation and teaching. Moreover, they allow students to perform experiments anytime and anywhere [8], with less capital investment when compared to physical and remote laboratories.

Among the virtual laboratories researched in the literature, some of them provide an environment where the student pre-configures the parameters of needed resources and then waits until the laboratory performs the experiment. In this case, the student does not interact during the experiment execution, as he only performs the pre-configuration and collection of results. The *BVL System* [9] follows this approach, by providing an environment composed of agents for simulation and behavior analysis. Other laboratories [10] [11] [12] [13] propose environments for experimentation, but they do not support the execution of experiments that require a protocol. Among the virtual laboratories researched, *ViroLab* [13] can be highlighted, since it uses ontologies to support complex queries over both data and provenance repositories, considering the domain of infectious diseases. However, *ViroLab* does not apply ontologies during experiment definition and execution steps. Thus, there is no recommendation of similar apparatus or procedures, neither inference of alternative protocols, which could enhance the learning process.

B. Workflow and Virtual Laboratories

To represent experiments that involve protocols, some researchers [1] [2] apply workflow representation technologies in an educational context. In this case, workflows are used to manage an activity flow that students must follow in an e-learning environment. One of the most popular technologies to represent workflows is the *XML Process Definition Language* (XPDL) [3], proposed by the *Workflow Management Coalition* (WfMC). XPDL contains elements to represent each step that composes an experiment, its execution order, the apparatus needed in each step and their properties. Section III describes more information on how WOntoVLab process employs XPDL.

C. Semantics for Virtual Laboratories: Ontologies

In computer science, an ontology consists of a set of representational primitives that aim to model a domain of knowledge [14]. These primitives are typically classes, attributes and relationships. Ontologies have been widely used in several applications for semantic information processing between both humans and computer systems, as they represent semantic constructions and support reasoning of new knowledge.

Specifically, regarding to virtual laboratories, ontologies can be used to describe concepts, relationships and instances associated with the experiments performed by students. For this purpose, *domain ontologies*, which express conceptualizations of specific domains [4], are appropriate to semantically represent concepts and relationships related to resources, instruments and materials used in experiments. Thus, it is possible to recommend similar concepts to the experiment designer, based on inferences over the domain ontology.

When representing semantics related to experiments, it is essential to describe their procedures and respective interdependencies. Such information can be represented by *application ontologies*, which describe concepts concerning a domain and a particular task [4]. For virtual laboratories, an application ontology can be used to represent the steps that constitute a particular task, prerequisites and required resources, as well as the several alternatives to execute the experiments.

Once we have described the basic concepts related to virtual laboratories, workflow and ontologies, next section presents the WOntoVLab process, which proposes the use of workflow and ontologies in order to support well defined experiments, involving alternative protocols.

III. The WOntoVLab Process

Aiming to deal with the drawbacks of virtual laboratories pointed out in Section II, we propose the WOntoVLab process, which relies on *workflow representation technology*, *domain* and *application ontologies* to support definition and execution of experiments. This process provides a model for building virtual laboratories, making it possible to recommend semantically similar apparatus and infer alternative protocols. In WOntoVLab, experiments can be designed independently of domain, demanding only the modification of the ontologies used for the domain and application required. Figure 1 presents the proposed process, detailing its steps: experiment authorship (creation), execution and assessment.

The authorship step (*Create Experiment* - Item 1 of Figure 1) assists the designer (or teacher) in outlining the experiment protocol. Firstly, the designer should gather the required data related to the experiment. Afterwards, he begins the selection of the apparatuses needed for each step of the experiment, supported by the domain ontology (Item 3). For each chosen apparatus, inferences are made over the ontology in order to recommend similar resources to the designer. These recommendations are useful to select the appropriate vocabulary related to the experiment, but they are not mandatory, the designer decides whether or not to accept them.

For each created step, the designer should link it to its correspondent task represented in the application ontology (Item 2). This ontology represents the semantics of the experiments by specifying procedures and their interdependencies. By linking steps and tasks, it is possible to verify if students had performed protocols that are different from the original one proposed by the designer, but that achieve the same result. This process is successively repeated until the creation of all experiment steps. Ending the authorship step, an authorship workflow is created (Item 4) to represent the defined protocol in XPDL. XPDL language elements formally model the required resources, their configuration, the sequence

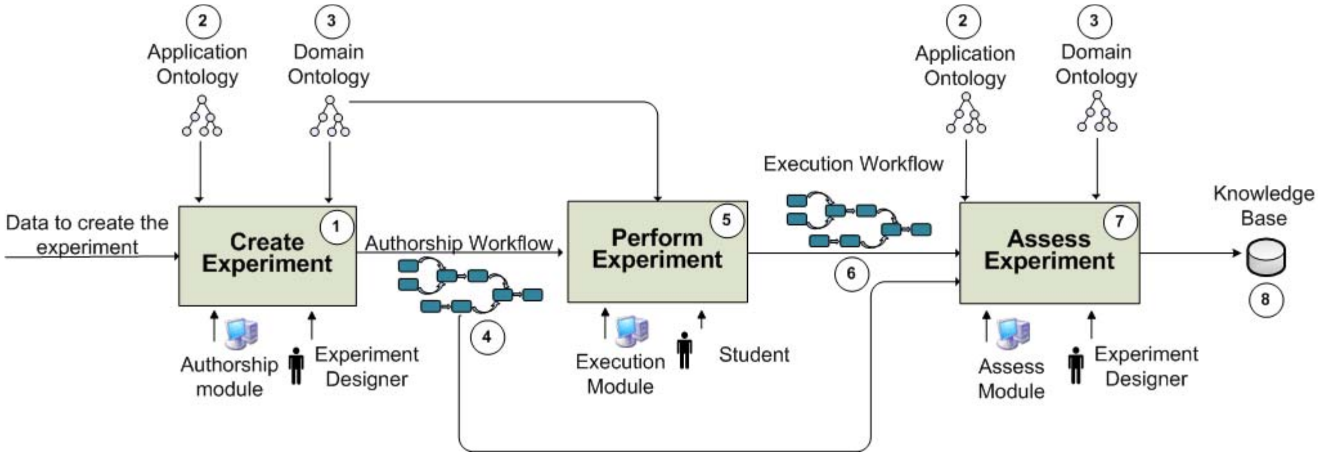

Fig. 1. WOntoVLab Process.

of experiment steps, and the association of each step with the application ontology. It is important to highlight that the designer is not supposed to know XPDL, since the virtual laboratory should provide a friendly interface that automatically generates the experiments in that language.

The next step of the WOntoVLab process (*Perform Experiment* - Item 5) comprises the execution module, which supports students in performing the experiment according to the protocol defined in the *authorship workflow* (Item 4). For each executed step, the student chooses required apparatuses (represented in the domain ontology). For each selected resource, similar apparatus are recommended, as well as it was done in the authorship step. Once the experiment execution has been completed, a *execution workflow* (Item 6) is generated in XPDL, describing all the steps performed by the student.

Finally, the last step corresponds to experiment assessment (*Assess Experiment* - Item 7), which aims to compare *execution* (Item 4) and *authorship* (Item 6) workflows. For each step in the execution workflow that has no identical correspondence in the authorship workflow, inferences are made over the ontologies (Items 2 and 3) to verify if there is a similar step in the authorship workflow. These inferences are validated by the designer, who is responsible for concluding the experiment assessment. The assessment module is adaptable and extensible, since step comparison strongly depends on the semantics of the domain that involves the experiments. At the end of the WOntoVLab process, all data regarding authorship, execution and assessment are persisted in a database (Item 8) to support future analysis, or even to assist further assessment processes.

It is important to emphasize that the WOntoVLab process can be applied in different domains, it is only necessary to replace the ontologies considering the required domain. As WOntoVLab employs XPDL to model workflows, it is possible to provide interoperability of experiments, because protocols are represented according to a standard language proposed by WfMC. Furthermore, WOntoVLab supports semantically alternative protocols in virtual laboratories, based on domain and application ontologies.

Regarding implementation issues, we have developed the *WOntoVLab Process Framework (WPF)* in order to provide functionalities for building virtual laboratories according to the WOntoVLab process. WPF methods implement the recommendation of similar resources and procedures based on ontologies, the comparison of authorship and execution workflows, among other functionalities. To develop this framework, we have used Java, Axis2 and Jena. Since there is a growing trend for making virtual laboratories available on-line, we have developed some WPF methods as web services. Hence, it is possible to increase visibility and accessibility for institutions who implement virtual laboratories following the WOntoVLab process. The Figure 2 illustrates three different virtual laboratories from different domains, accessing WPF functionalities through web services. A real-world application of WPF is illustrated in the next section, considering the molecular biology domain. Precisely, this case study applies WPF in a virtual laboratory focused on DNA extraction experiments.

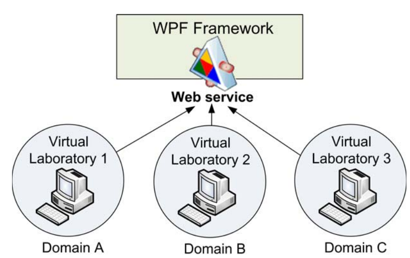

Fig. 2. Three virtual laboratories, from different domains, accessing WPF methods through web services.

IV. CASE STUDY: DNA EXTRACTION EXPERIMENT

To demonstrate a real application of the WOntoVLab process, we have developed a virtual laboratory prototype considering the molecular biology domain. For this purpose, we have modeled domain and application ontologies describing concepts, relationships and tasks related to DNA Extraction experiments, with support of domain experts. Figure 3 presents a portion of the domain ontology modeled. This ontology represents some apparatuses available in molecular biology laboratories, most of them are considered in this case study.

The laboratory resources are modeled into three categories: *reagent and solutions*, *material* and *equipment*. This grouping was suggested by domain experts, who intended to best fit their needs regarding the experiments.

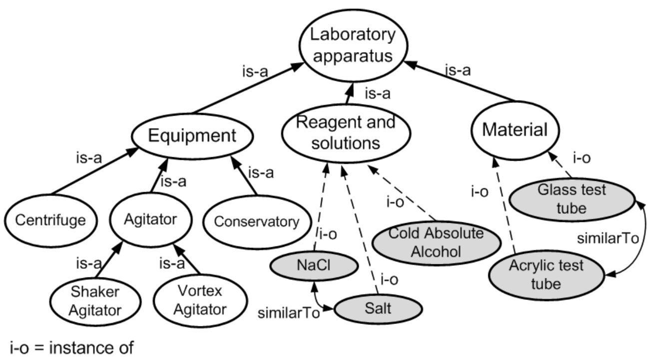

Fig. 3. Molecular Biology Domain Ontology Snippet.

According to the WOntoVLab process, in the first step (experiment authorship) the teacher gathers all data required to define a DNA extraction experiment. Afterwards, he/she begins outlining each experiment step. At this stage, WPF methods are accessed to retrieve the aparatuses modeled in the domain ontology, as well as their similar ones. WPF methods also obtain the tasks represented in the application ontology, so that the teacher can link them to each created step.

In order to illustrate how ontologies are handled in experiment authorship, we describe the step where it is requested to introduce cold absolute alcohol and salt in a test tube (step 11 from DNA Extraction Experiment). First of all, the teacher selects the apparatuses that composes this step, supported by WPF methods. After selecting 1mg of *NaCl*, the WPF performs inferences over the domain ontology to recommend *Salt* as a similar apparatus, but this recommendation was not accepted by the teacher. Next selected apparatus was *cold absolute alcohol*, which has no similar apparatus modeled in the ontology. Finally, the teacher accepted the recommendation of *glass test tube* apparatus, suggested by WPF after the *acrylic test tube* apparatus was selected. After choosing all resources, the teacher needs to associate this step with its respective task in the application ontology in order to support reasoning of similar steps. Therefore, step 11 is linked to the *AddSaltAlcoholTestTubeMethod1* task represented in the application ontology.

Having completed the creation of all steps, the authorship workflow is generated (Listing 1), in order to formally represent the experiment created. In line 2 of Listing 1, the attribute *id* assigns the identification *Step_11* to the previously described step. Line 5 contains its configuration, and line 6 depicts its goal. Note that Listing 1 also contains two types of extended attributes, *Name=Material* and *Name=ApplicationOntologyReference*. The first one links the apparatuses of the step 11 to their references in the domain ontology (lines 8 to 13), while the last one links the step 11 to its correspondent task in the application ontology.

Listing 1. XPDL Authorship Workflow code snippet

```
1
2 <xpdl:WorkflowProcess Id="DNAExtractionProcessId" Name="
      DNAExtractionProcess">
3 ...
4   <xpdl:Activities>
5     <xpdl:Activity Id="Step_11">
6       <xpdl:Description>Add cold absolute alcohol and salt
            in a glass test tube</xpdl:Description>
7       <xpdl:ExtendedAttributes>
8         <xpdl:ExtendedAttribute Name="Material"
9 Value="http://www.owl-ontologies.com/Ontology1251833905.owl
      #ColdAbsoluteAlcohol"/>
10        <xpdl:ExtendedAttribute Name="Material"
11 Value="http://www.owl-ontologies.com/Ontology1251833905.owl
      #Salt"/>
12        <xpdl:ExtendedAttribute Name="Material"
13 Value="http://www.owl-ontologies.com/Ontology1251833905.owl
      #GlassTestTube"/>
14        <xpdl:ExtendedAttribute Name="
              ApplicationOntologyReference"
15 Value="http://www.owl-ontologies.com/Ontology1258201595.owl
      #AddSaltAlcoholTestTubeMethod1"/>
16      </xpdl:ExtendedAttributes>
17      ...
```

Following the WOntoVLab process (Figure 1), next step is *Perform Experiment*, in which the student selects the apparatuses and configures their properties for each step. Note that this step is also supported by the WPF methods by recommending to the student similar resources represented in the domain ontology. Figure 4 shows the experiment execution screen taken from the prototype implemented in the TIDIA-AE e-learning environment [15].

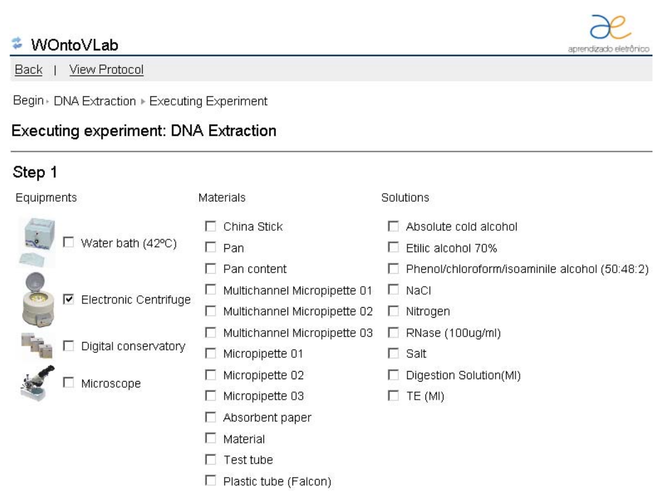

Fig. 4. Virtual laboratory prototype over TIDIA-AE environment.

Listing 2 represents the *execution workflow* generated after a student had performed the experiment. According to this listing, this student used the following apparatuses: *Salt*, *Cold absolute alcohol* and *acrylic test tube*. Note that the apparatuses used in the experiment execution are similar to apparatuses used in the authorship, except for *acrylic test tube*, represented in line 10 in listing 2.

Listing 2. XPDL Execution Workflow code snippet

```
1 ...
2   <xpdl:Activities>
3     <xpdl:Activity Id="Step_11">
4       <xpdl:ExtendedAttributes>
5         <xpdl:ExtendedAttribute Name="Material"
```

```
Value="http://www.owl-ontologies.com/Ontology1251833905.owl
     #ColdAbsoluteAlcohol"/>
         <xpdl:ExtendedAttribute Name="Material"
Value="http://www.owl-ontologies.com/Ontology1251833905.owl
     #Salt"/>
         <xpdl:ExtendedAttribute Name="Material"
Value="http://www.owl-ontologies.com/Ontology1251833905.owl
     #AcrylicTestTube"/>
      </xpdl:ExtendedAttributes>
      ...
```

Finally, the last step of WOntoVLab process is *Assess Experiment*. WPF provides methods to perform the comparison between authorship and execution workflows. These methods can be adapted or extended to suitable comparison algorithms depending on the experiment domain. According to the example of this case study, the *acrylic test tube* apparatus is different from those provided by the teacher. Then, in order to verify if the step that contains the *acrylic test tube* is similar to those ones proposed by the teacher, WPF performs the following analysis. Firstly, WPF queries the domain ontology to infer the similar apparatuses. Among the obtained ones, WPF checks if any of them is proposed in the authorship workflow. Considering the example, WPF inferred that the *glass test tube* apparatus is similar to *acrylic test tube*, so the step performed by the student corresponds to that one proposed by the teacher. If this analysis fails, WPF analogously performs inferences on application ontology in order to verify if the executed step had the same goal as that one proposed in the authorship workflow.

As a conclusion of this case study, we have observed that the methods provided by the WPF framework were successfully applied in a prototype of virtual laboratory related to DNA Extraction experiments. The feedback from domain experts was positive, and they envisage promising applications of WPF in several on-line virtual laboratories, as WPF provides its functionalities as web services.

Furthermore, domain ontology made it possible to semantically represent the experiment apparatuses, and inferences mechanisms supported the recommendation of similar apparatuses. Application ontology made it possible to semantically represent the step tasks, and also supported the inference of similar tasks. According to the domain experts, these semantic recommendations were useful not only to create the experiments but also to assess them.

Last but not least, XPDL language provided a formal and standard representation of the protocols that compose the experiments. Their use in conjunction with domain and application ontologies contributed to assess experiments performed by students, even when using protocols that were different from those initially proposed by the teacher.

V. Conclusion and Future Work

We have proposed the WOntoVLab process for virtual laboratory authorship, which enables the creation of experiments containing alternative protocols, based on workflow representation technology. Moreover, domain and application ontologies are considered in both experiment authorship and assessment steps, supporting the inference of similar apparatuses and procedures. Based on this process, it is possible to create an environment for virtual laboratories that explores student creativity and promotes knowledge sedimentation by considering alternative but equivalent execution flows.

As future work, we intend to improve the assessment process, by using Petri nets to represent workflows. We also plan to handle more workflow patterns such as *parallel split, synchronization, exclusive choice and simple merge*, besides the *sequence* pattern which is already considered in the WOntoVLab Process Framework. WOntoVLab Process should also be extended to remote laboratories, in order to support presetting recomendations [6]. Finally, we will evaluate the WOntoVLab Process in other domains, such as chemical and physics virtual laboratories.

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