Automatizing experiment reproducibility using semantic models and container virtualization

Maximiliano Osorio [a], Idafen Santana-Perez [b] and Carlos Buil-Aranda [a,*]

[a] *Departamento de Informática, Universidad Técnica Federico Santa María, Avda España 1680, Valparaíso Chile*
E-mails: mosorio@inf.utfsm.cl, cbuil@inf.utfsm.cl

[b] *Ontology Engineering Group, Universidad Politécnica de Madrid, Campus de Montegancedo, Madrid, Spain*
E-mail: isantana@fi.upm.es

Abstract.
Experimental reproducibility is a major cornerstone of the Scientific Method, allowing to run an experiment to verify its validity and advance science by building on top of previous results introducing changes to it. In order to achieve this goal, in the context of current in-silico experiments, it is mandatory to address the conservation of the underlying infrastructure (i.e., computational resources and software components) in which the experiment is executed. This represents a major challenge, since the execution of the same experiment on different execution environments may lead to significant result differences, assuming the scientist manages to actually run that experiment. In this work, we propose a method that extends existing semantic models and systems to automatically describe the execution environment of scientific workflows. Our approach allows to identify issues between different execution environments, easing experimental reproducibility. We have evaluated our approach using three different workflow management systems for a total of five different experiments, running on a container virtualization system (i.e. Docker). That showcases the feasibility of our approach to both reproduce the experiments as well as to identify potential execution issues.

Keywords: experiment reproducibility, semantic models

1. Introduction

Looking at the International Vocabulary of Metrology from the ACM [1], experiment reproducibility is achieved when the measurement from a experiment can be obtained with stated precision by a different team, a different measuring system, in a different location on multiple trials. For computational experiments, this means that an independent group can obtain the same result using artifacts which they develop completely independently. Similarly, according to [2], experiment reproducibility is the ability to run an experiment with the introduction of changes to it, getting results that are the same with the original one. Introducing changes allows to evaluate different experimental features of that experiment since researchers can incrementally modify it, improving and re-purposing the experimental methods and conditions [2]. To allow experiment reproducibility it is necessary to provide enough information about that experiment, allowing to understand, evaluate and build it again. Commonly, experiments are described as scientific workflows (representations that allow managing large scale computations) which can be executed on distributed computing systems. To allow reproducibility of these scientific workflows it is necessary to address a workflow conservation problem, which implies the conservation of the underlying infrastructure (i.e. computational resources such as the hardware infrastructure and software components) in which the scientific workflow is executed. Experimental workflow conservation refers to the process of obtaining the same result from an ex-

*Corresponding author. E-mail: cbuil@inf.utfsm.cl.

periment in a different environment [3]. Experimental workflows need to guarantee that there is enough information about the experiments so it is possible to build them again by a third party, obtaining the same results without any additional help from the original author. In the context of experimental conservation and reproducibility for digital objects, physical conservation is usually defined as the process keeping a copy of the environment that is able to mimic the original infrastructure and that can be enacted without intervention or modification, as opposed to logical conservation, which focus on describing how the environment can be reproduced [3].

To achieve that conservation, the research community has focused on conserving workflow executions by conserving data, code, and the workflow description, but little work has been done in conserving the underlying infrastructure. The work in [4] or the Timbus project[1] [5], which focuses on business processes and the underlying software and hardware infrastructure, provided some advances in the problem of conserving the experiment infrastructure.

Other approaches, such as Reprozip [6], propose to describe an environment using a packaging tool. Reprozip runs the experiment and generates package file which contains the experiment itself and a description of the inputs, outputs, environment variables and everything needed to run the experiment. Finally, it is possible to generate a Docker image from the experiment by using these descriptions. However these descriptions use the internal Reprozip structure and they do not have any ontology describing them. Furthermore, Reprozip suffers from the same problem than the Timbus project since it needs to run the experiment to obtain that information. However, these approaches either leave out of the scope the physical conservation of the workflow computational environment (relying on the chosen infrastructure) or that conservation is done almost manually.

One way to solve the physical conservation problem is the use of Virtual Machines (VM), as described in [4]. However there are several problems associated to the use of VMs, such as the use of large amounts of space to distribute any scientific workflow. A VM is an entire Operating System on which all packages needed to run a workflow are installed. Whereas this generates a cohesive package for distributing and experiment, it highly difficulties the portability and distribution of software that need specific configuration. Moreover, scientific communities are moving from VM-based approaches to using lightweight solutions to solve the computational needs, including a more collaborative and agile approach. To solve these problems, the scientific community started to use operating-system-level virtualization. This technology, also known as containerization, refers to an Operating System (OS) feature in which the OS kernel allows the existence of multiple isolated user-space instances called containers. It is thus not a complete OS virtualization, since it depends on the host OS. Also, containers are architecture-dependent, and thus it is not possible to run a container in a different system architecture from the one it was built on. However, the containers on which the experiments run are around 1/10 of a VM, making containers a more suitable scenario to distribute experiments, taking into account the previous considerations. One of the most popular container-based virtualization technologies is Docker[2].Docker Containers can be seen as lightweight virtual machines that allow the assembling of a computational environment, including all necessary dependencies, e.g., libraries, configuration, code and data needed, among others. Docker containers are used intensively in both industry and science, mostly to preserve the execution environment of software applications and also to preserve the physical environment of an experiment. We claim that containers not only are lightweight but more importantly, they are easier to automatically describe so we will improve the process of documenting scientific workflows. Using Docker, the users can distribute these computational environments through software images using public repositories such as DockerHub[3]. In order to achieve logical conservation, we have developed an annotator system for Docker Images that describe the workflow management system, as well as their dependencies. In this way, we aim at improving the container's limited physical conservation they provide, adding the annotations as context of the execution environment. To validate our solution we reproduce 5 different computational experiments. These experiments span different systems, languages and configurations, showing that our approach is generic and can be applied to a wide range of representative computational experiments. We run these experiments, we describe them logically and next we

[1] http://www.timbusproject.net/

[2] https://www.docker.com/

[3] https://hub.docker.com/

reproduce them based on the logical descriptions we obtained before. To validate the approach we compare the outputs obtained from the reproduced experiments to the original ones.

2. Scientific workflows using containers

Scientific communities are following container-based approaches more and more often for conducting their empirical studies. Even when their main goal is not necessarily experimental reproducibility, the fact that these communities, which are mainly IT-oriented [7], are embracing such paradigms shows that lightweight virtualization techniques are a suitable environment for computational science. We now briefly introduce Docker and how Docker images are built.

2.1. Introduction to Docker

From a technological point of view, Docker is a solution that allows virtualizing a minimal version of an Operating System (OS), sharing the resources from the host machine by means of software images. On top of this virtualized OS image, dependencies can be deployed and applications can be executed. These new imagescan be easily published into Docker Hub[4], the canonical repository which also supports the maintenance and download of containers. Throughout this section, we introduce how Docker and its hub work, starting with how Docker images are created and stored in Docker Hub.

2.2. Docker repositories and files

Docker builds a software image by following the set of instructions, defined as steps, written in the Dockerfile. A Dockerfile is a text file that contains all commands to build a Docker image and run a container using this image. The Dockerfile usually have several lines, which are translated into image layers whereas Docker builds the image (one dockerfile line translates to one image layer). The first line in such files is the `FROM` keyword, which imports the base OS on which all software will be installed. These base OS are the so called parent images. In the building process, commands are executed sequentially, creating one layer at a time. These lines contain commands to be executed within the OS at the `FROM` line. When an image is updated or rebuilt, only the modified layers (i.e. modified lines) are updated. These explicit mentions to the commands to be executed, including their order and parameters, is what allows our system to extract the necessary information for annotating the computational environment, including the components and steps. Since various images can have common layers, the proposed annotation process analyses each layer of the image and not the resultant image. Thus, the system can reuse previous analysis.

[4]https://hub.docker.com/

2.3. Publishing and Deploying Docker images from Docker Hub

Docker Hub is an online registry that stores two types of public repositories, official and community. Official repositories contain public, verified images, from well-known companies and software providers, such as Canonical, Nginx, Red Hat, and Docker itself. At the same time, community repositories can be public or private repositories that are created by individual users and organizations, which share their applications and results.

By using that registry and a command line, it is possible to download and deploy Docker images locally, running the container in a host environment and then executing the software inside the image. Users are allowed to create and store images into the Docker Hub registry, by creating a Dockerfile or extending an existent one. This descriptor file describes all steps needed to build the Docker image, builds the image and finally uploads it to Docker Hub via command line. However, Docker Hub and the image do not control what packages are in the images nor whether the image will deploy correctly. It is worth noticing that to upload the new Docker image users need to use a set of command line tools provided by Docker and that the Dockerfile is not uploaded within the image.

These registries allow scientific communities to store and share, curating the content of the containers, as well as to check the identity of the publisher and retrieve the containers of interest. However, the information of the content of each repository is not always accessible in a clear manner. As most of the times only short descriptions of the containers is provided, it is not clear what components are installed on it. Even when Dockerfiles are available, these are not intuitive enough to follow and understand which packages are being deployed by each command. Also, some components might exist in the container that are not specified by the Dockerfile itself. To tackle this problem, we pro-

pose an automatic approach for analyzing the content of a Docker image and extract the information about the software components installed on them. This information is then converted to semantic data, codified as RDF under the set ontologies we have developed, as mentioned in Section 3.1.

2.3.1. Docker and Virtual Machines

As we have seen, the container architecture allows to store millions of images in a single place such as DockerHub. This is due to the use of the layered architecture of Docker images and the fact that these images are executed on top of a host operating system. Consider a 1 GB container image; for a user to run a VM for each experiment she would need to have 1 GB times the number of VMs she wants. With Docker and AuFS that user can share the 1 GB data between all the containers. If that user has 1,000 containers she still might only have a little over 1 GB of space for the containers OS (assuming they are all running the same OS image).

The Singularity container system. In the scientific community the most popular solution for allowing container-based reproducible experiments is Singularity [8]. Singularity main characteristic is that allows running containers without the need of using super user privileges since a Singularity container image encapsulates the operating system environment and all application dependencies necessary to run a defined workflow. If a container needs to be copied, this means physically copying the image. Since Singularity images are terated as standard files simplifies management and access controls to well known POSIX based file permission [8].

3. Reproducibility in scientific workflows using Docker Containers

In this paper, we mainly focus on the role that Docker plays for experimental reproducibility, which fundamentally happens once the experiment has been conducted and its results have been disseminated. The use of containers poses several benefits during the designing, development, testing and execution phases of a research process, before the publication of the results. As isolated environments, containers allow users, mostly researchers from different areas conducting computational simulations, to test new solutions without jeopardizing real, and costly, production infrastructures. Containers thus allow scientists to explore different configurations without hindering the performance and stability of the final computational infrastructure.

Moreover, as their evolution can be tracked along the development process, it is possible to rollback to previous Docker images in case new dependencies or modifications introduce errors. Thus, containers are being more and more commonly adopted by research communities, publishing them as part of the scholarly communication process, hosted on the aforementioned repositories. However, some work is still needed to use containers as key element for experiment reproducibility.

Here, we argue that the description of computational environments is necessary for achieving the reproduction of the experiment. Furthermore, the information must be enough to compare and detect differences between the original and the reproduced environments.

Since Docker images are isolated and independent environments, the installed software components within the container should only be related to a single experiment. This is considered a best practice in the software engineering community and we adhere to it. By making this assumption, we consider that the description of the environment is done without any noise from other tools or experiments.

To automatically annotate the software packages within the Docker images we propose a system which receives as input the repository name, queries the container's package system which software packages are installed and stores the annotations in our RDF repository.

3.1. Semantic models

In [4], the authors proposed The Workflow Infrastructure Conservation Using Semantics ontology (WICUS). WICUS is an OWL2 (Web Ontology Language) ontology network that implements the conceptualization of the main domains of a computational infrastructure. These are: Hardware, Software, Workflow and Computing Resources domain. Scientific workflow requires a stack of software components, and the researchers must know how to deploy this software stack to achieve an equivalent environment. The main drawback of these ontologies is that they do not consider OS virtualization techniques. The only ontology that considers that technology is [9], however it is not integrated with a provenance ontology such as WICUS. We extend these previous works to develop our ontology, named Dockerpedia, so we can annotate

scientific experiments using container virtualization. Following Ontology Engineering best practices, we start by importing some abstract classes, and relations from WICUS ontology: (1) `DeploymentPlan`, `DeploymentStep`, `ConfigurationInfo` and `ConfigurationParameter` classes describe the steps to deploy and configure the software, and (2) `SoftwareStack` and `SoftwareComponent` that model the software elements that must be installed and their dependencies. We extend the ontology with the specific classes and properties related to OS virtualization, generic to any virtualization system that uses deployment layers such as Docker or Singularity[5]. We define the new class `SoftwarePackage` as a subclass of `SoftwareComponent` so we are able to define the software packages installed by the underlying OS. Every `wicus:SoftwareComponent` has an object type relation to `dockerpedia:hasVersion` denoting the package version which was installed within the container.

We annotate every line from the Docker file as a `wicus:DeploymentStep` and the Dockerfile as a `wicus:DeploymentPlan`. In summary, we annotate every installed software package on the container file system, not only those packages in the Dockerfile. This allows us to reproduce any experiment as long as it uses a container virtualization system and imports and build their tools using their configuration files (such as with multi-stage builds[6]).

Our final ontology, which is available online under its namespace URI[7], is depicted in Figure 1.

3.2. Annotator

The annotation service implements a REST interface which receives as input the Docker image in which the scientific workflow will run. By scanning it, the system can describe the software components that support such the filesystem of the image and the building steps needed to run it. The whole annotation process is the following: First, the system downloads the Docker image and mounts it (without running it). Next, we scan the image searching the software packages installed, and finally, the system creates the RDF data from the scan process and link these data to external RDF resources such as the Debian package repository and the Common Vulnerabilities and Exposures database[8]. We show the overall architecture of the annotator, available as part of the project[9], in Figure 2.

3.2.1. Building steps annotations

Docker builds an image by either reading a set of instructions from a Dockerfile or just deploying that image on a host in case the Dockerfile is nor present. Thus, to identify what packages are going to be installed within the docker image we either read that Dockefile and execute it or we deploy that image and run an analysis over it. In case of the latter, we have to extract the information from the Docker image by using the image's manifest file, which is always available for a given image in the image manifest file (available in every Docker image). This file contains the image's internal configuration and the set of layers from which the image is built. According to the official documentation [10], the most important attributes of the manifest file are:

name: name of the image's repository
history : the list of the layers composing the current image layer. This field contains its ID and its parent layers ID's. It is the history of how the current image is constructed. More in detail, for each layer the history field contains:

Id: the layer's ID;
Parent: *string* the parent's ID;
ContainerConfig: the layer's build command;
Author: the author's name and email.

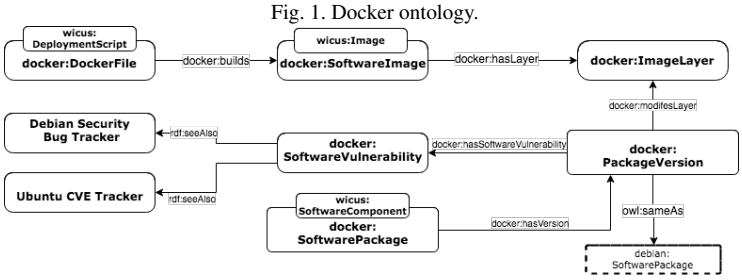
With all these information provided by either the Docker file or the manifest file within the Docker image we are able to reproduce the Docker image only deploying it, and thus without modifying any parameter in the image. In the next section we describe how we annotate the software components within the Docker images.

3.2.2. Software Components annotations

Each Docker image layer installs or removes software packages. To be able to describe the execution environment of a scientific experiment we need to describe the software components that are installed within the experiment image. To do that we rely on

[5]https://singularity.lbl.gov/
[6]https://docs.docker.com/develop/develop-images/multistage-build/
[7]https://dockerpedia.github.io/ontology/release/0.1.0/index-en.html
[8]https://cve.mitre.org/
[9]https://github.com/dockerpedia/annotator
[10]https://docs.docker.com/registry/spec/manifest-v2-2/

Fig. 1. Docker ontology.



the installation process done by the software package managers of the image's operating system. A package manager system is a collection of software tools that automate the process of installing, upgrading, configuring, and removing software components. We classify the package managers in two types: system and general. System package managers are the managers of the operating system (e.g., apt by Debian Family, yum by RedHat Family) and general package managers are custom package manager, which generally are used to install a specified language package (e.g., pip, conda, npm).

A common approach for finding the software components is to search the lines that use the package manager. For example, Listing 1 shows the command to install the TensorFlow software package.

```
apt-get install -y --no-install-recommends \
        build-essential \
        curl \
        libfreetype6-dev \
        libhdf5-serial-dev \
        libpng12-dev \
        libzmq3-dev \
        pkg-config \
        python \
        python-dev \
        rsync \
        software-properties-common \
        unzip
```

Listing 1: Ubuntu command to install the TensorFlow software

The main problem of this approach is that there is no information about the software packages versions nor the software dependencies installed. Also, this command installs 184 packages which the scientist may not be aware of.

We use Clair[11], a tool designed for the analysis of vulnerabilities in docker containers, to identify which packages the container virtualization system installs. Clair is an open-source tool from CoreOS designed to identify known vulnerabilities in Docker images. It has been primarily used to scan images in the CoreOS private container registry, Quay.io[12], but it can also be used to analyze images from DockerHub. Clair downloads all layers of an image, mounts and analyzes them, determining the operating system of the layer and the packages added and removed from it. As a result from the analysis, Clair downloads all layers of an image, mounts and analyzes them, determining the operating system of the layer and the packages added and removed from it. Clair is compatible with several of the most common system package managers, such as Ubuntu, Debian, Alpine, RedHat, CentOS, and Oracle. Thus, our implementation supports experiments that run over those well-known Linux distributions. Due to the popularity of the Conda[13] management tool in the scientific community and as a generalization proof, we extend Clair in our system to detect the packages and dependencies installed by this package manager[14].

3.3. Comparing different versions of execution environments

One of the most common problems when reproducing an experiment is to ensure that the execution environment is not the problem if the results obtained from a latter execution are different. Using our approach it is possible to check that two execution environments are the same. The process to ensure that is the following:

1. Annotate execution environment 1 (e.g. Pegasus workflow) using the annotator and store the annotations.

[11] https://coreos.com/clair
[12] http://status.quay.io
[13] https://conda.io/docs/
[14] https://github.com/dockerpedia/clair

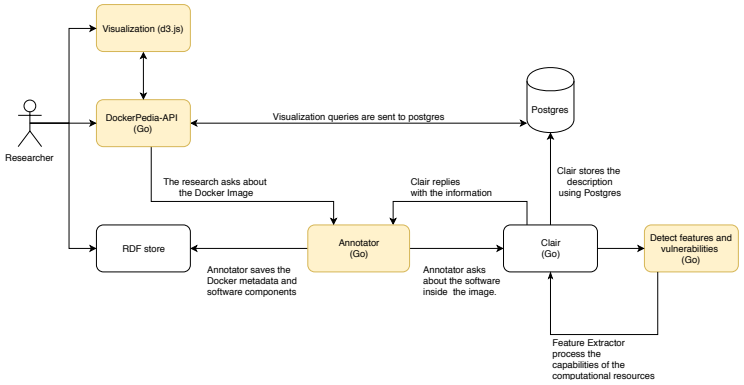


Fig. 2. This Figure shows the general architecture of the Annotator system. The Annotator provides researchers an API which receives as input a Docker image URL from DockerHub. The annotator will describe that image using the semantic model depicted in Figure 1 and it will also search for software vulnerabilities. The system also provides a visualization tool of the components within each Docker image. These components are highlighted in yellow.

2. Run the experiment and verify the results from execution environment 1.
3. Annotate execution environment 2 using the annotator and store the annotations
4. Run the experiment and verify the results from execution environment 2.
5. If any execution fails or the results differ, we can run one or more SPARQL queries to check the differences.

These queries can be used to check which layers of the environment are different. In Listing 2 we depict the SPARQL query used to identify the software components contained in the latest version of Pegasus.

Listing 2: SPARQL query obtaining the software packages installed in the latest Pegasus version

```
PREFIX vocab:
<http://dockerpedia.inf.utfsm.cl/vocab#>

SELECT * WHERE {
  pegasus_workflow_images%3Alatest
        vocab:containsSoftware ?p .
      }
```

In case there was any problem reproducing the execution environment of an experiment we can also compare the differences between two images. For example, the query in Listing 3 shows the query to compare two versions of the Pegasus image.

Listing 3: SPARQL query comparing two the software packages installed in two different Pegasus versions

```
SELECT * WHERE {
  pegasus_workflow_images%3Alatest
        vocab:containsSoftware ?p .
  pegasus_workflow_images%3Apegasus-4.8.5
        vocab:containsSoftware ?p
      }
```

4. Experimentation Process

In this section we evaluate our approach for allowing scientific experiment reproducibility. We reproduce five different experiments which run in different workflow systems (SoyKB and Montage on Pegasus, Internal extinction and Seismic Ambient Noise Cross-correlation on Dyspel4Py, and Modflow on WINGS). These workflows run over Java and Python and we deployed them on three different execution environments (Google Cloud, Digital Ocean and on a local machine) to guarantee that our approach is IaaS independent.

This section is organized as follows: we first describe how we execute the experiments we use to evaluate our approach (i.e. how we build the experiment images, how and where we store them, how we describe them and how we compare the results from the different experiment executions). When evaluating our approach, we first introduce the workflow system we use for next introducing the experiments that will run on that workflow system. Before continuing to the next workflow system and scientific experiments we show and compare the results from the workflow executions

Resource	Digital Ocean	Google Compute	Local
CPU (Arch)	64 bits	64 bits	64 bits
OS	Centos 7	Debian 9	Fedora 27
Docker version	17.05	17.05	17.05

Table 1
Image appliances characteristics.

with the existing state of the art results for the same experiments, showing the feasibility of our approach.

4.1. Building and storing the images

We built one Docker image for each workflow system so a researcher can import that image and install on it the software components needed to run the scientific data workflow. We did that by using the FROM instruction in the Dockerfile. For example, the SoyKB experiment uses the Pegasus workflow manager, thus the SoyKb image uses as base image the Pegasus software image at DockerHub. The SoyKB workflow needs to install other software packages besides the Pegasus system, which we also incorporated into the Dockerfile describing the container image. These files are available on our repositories for each workflow [15]. We also describe the workflow images using the Container description vocabulary developed by the Open Container Initiative[16].

4.2. Running the experiments

We rely on Docker Images stored on DockerHub for the physical conservation. Thus, the first experiment is to test if the Docker images are capable of packaging the software components of the selected experiments. The images that we are using in our experimentation are publicly available on DockerHub[17]. Moreover, we published the images with the corresponding Dockerfiles so that any user can inspect and improve them. Finally, we use two different infrastructure providers (DigitalOcean and Google Cloud) and a local machine to evaluate the reproducibility using physical conservation. Table 1 shows the hardware characteristics of these three environments.

The Docker version tested for this experimentation is compatible with CentOS 7, Debian 10/9/8/7.7, Fedora 26/27/28, Ubuntu 14.04/16.06/18.04, Windows 10, macOS El Capitan 10.11 and newer macOS releases. The installation process can be found https://docs.docker.com/install/

We include in each Docker image a README file with the instructions to run the experiment showing how to run the container. To illustrate this, Listings 4, 5 and 6 show the instructions to run the SoyKB workflow. First, we run the container the image, Next, the user must enter the container. The user can confirm that you are inside the container by the prompt. Finally, the user runs the workflow.

Listing 4: Download and run the SoyKB image

```
docker run -d --rm -it --name soybean \
mosorio/pegasus_workflow_images:soykb
```

Next, the user must enter the container. The user can confirm that you are inside the container by the prompt.

Listing 5: Run the shell bash and use it

```
root@docker-instance:~# docker exec \
-ti -u workflow:workflow soybean bash
workflow@a0f861e6fbc4:~
```

Finally, the user runs the workflow.

Listing 6: Run the workflow

```
workflow@a0f861e6fbc4:~/soykb \
./workflow-generator --exec-env distributed
```

4.3. Describing the components of the environment

As described in Section 3.2, we annotate the aforementioned workflows using the set of semantic models we have extended. The annotations are grouped by building steps and software components. In order to get the annotations from the containers, we use and extend Clair, as depicted in Figure 2, which shows the main steps of the process. Overall, the annotation process works based on the following phases.

1. The user queries the DockerPedia annotator API, using a Docker image at DockerHub as input.

[15] https://github.com/dockerpedia
[16] https://www.opencontainers.org/
[17] https://hub.docker.com/u/dockerpedia/

2. The DockerPedia annotator uses our extended version of Clair to analyze the image. Clair downloads all layers of an image, mounts and analyzes them, determining the operating system of the layer and the packages added and removed from it. In parallel, the annotator reads the building steps, labels, architecture and manifest from DockerHub.
3. Finally, the annotator combines all the gathered information and codifies and stores it in RDF, using the semantic models we developed.

4.4. Is the reproduced environment similar?

To evaluate if the original and reproduced environments are the same, we compare both annotated images using SPARQL to query the annotations. We have tested this in a real scenario, where one image was able to execute a workflow, whereas the other could not. More in detail, recently Pegasus updated to version 4.9 and required Java version 1.8 while the SoyKB workflow requires Java version 1.7 making thus incompatible the new Pegasus version with the workflow. With the result of the SPARQL query included in Listing 7 it is possible to spot the differences between both execution environments clearly.

Listing 7: What are the different components between two images?

```
PREFIX vocab:
<http://dockerpedia.inf.utfsm.cl/vocab#>
PREFIX DPimage:
<http://dockerpedia.inf.utfsm.cl/resource
/SoftwareImage/>

SELECT ?p WHERE {
  DPimage:dockerpedia-pegasus_workflo
  w_images_latest
  vocab:containsSoftware ?p .
  MINUS{
    DPimage:dockerpedia-pegasus_workflow
    _images-4.8.5
    vocab:containsSoftware ?p
  }
}
```

In summary, for each of the experiments described in the next Section, we perform the following steps:

- Build a Docker image for each of the scientific workflows.
- Annotate each of the previous Docker images.
- Reproduce the environment from the annotations obtained by our approach.
- Compare both execution environments.
- Evaluate and compare the size between virtual machine image and container image.
- Run the experiments and compare their execution results with the original workflow execution results. If the results are the same we managed to successfully reproduce the experiment.

4.5. Pegasus

Pegasus [10] is a Workflow Management System (WMS) able to manage workflows comprised of millions of tasks, recording data about the execution and intermediate results. The Pegasus package has been obtained from the official repository [18] and the Pegasus images used in this work are available on DockerHub [19].

4.5.1. Soybean Knowledge Base

The SoyKB workflow [11] is a genomics pipeline that re-sequences soybean genes for desirable traits such as oil, protein or root system architecture. The workflow analyzes in parallel several samples of soy genes and executes operations over the resulting data such as de-duplicate data, and merge and filter results. The workflow instance used in this paper is based on a sample dataset that requires less memory than a full-scale production workflow, however it carries out the same process and requires the same software components.

Figure 3 shows the SoyKB main software dependencies for running the workflow on Pegasus are classified in self-dependencies (in yellow) and third-party dependencies (in purple). The main components in these dependencies are `bwa`, `gatk` and `picard` while the main third-party dependency is an unknown version of Java.

We evaluated the results obtained manually, as in [4], since the scientific workflow execution is non-deterministic, due to some of its steps being probabilistic, as they were originally designed. We compared the structure of the resulting data, file sizes, number of lines and the absence of errors. The workflow outputs a VCF file containing genomic data, which is the

[18] http://download.pegasus.isi.edu/wms/download/debian

[19] https://hub.docker.com/r/dockerpedia/pegasus_workflow_images/

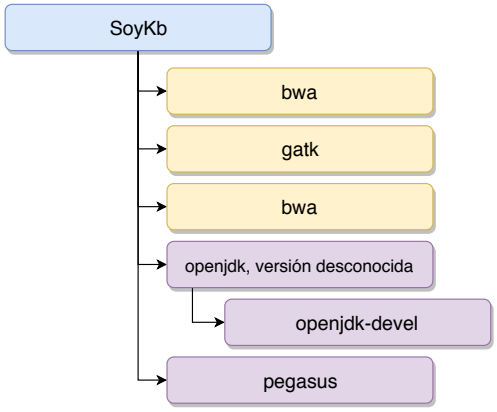


Fig. 3. Pegaqsus's SoyKB Workflow representation.

same data available in the official Pegasus repository in GitHub [20], thus we can conclude that the outputs are equivalent and that the workflow was reproduced successfully. Both the SoyKB workflow image and the workflow execution results are in DockerHub [21].

4.5.2. *Montage*

The Montage workflow [12] was created by the NASA Infrared Processing and Analysis Center (IPAC) as an open source toolkit that can be used to generate custom mosaics of astronomical images in the Flexible Image Transport System (FITS) format. In a Montage workflow, the geometry of the output mosaic is calculated from the input images. The inputs are then re-projected to have the same spatial scale and rotation, the background emissions in the images are corrected to have a uniform level, and the re-projected, corrected images are co-added to form the output mosaic. Figure 4 illustrates a small (20 node) Montage workflow. The size of the workflow depends on the number of images required to construct the desired mosaic. Each of the nodes in the workflow is a binary software that contributes to the final image generation. Since the software is only provided in its binary format (not packaged), we downloaded it and added it as a dependency in our DockerFile [13].

We use a perceptual hashing tool [22] to compare the outputs from the original Montage workflow execution provided by Pegasus and our reproduced Pegasus environment. We obtain as result a similarity factor of

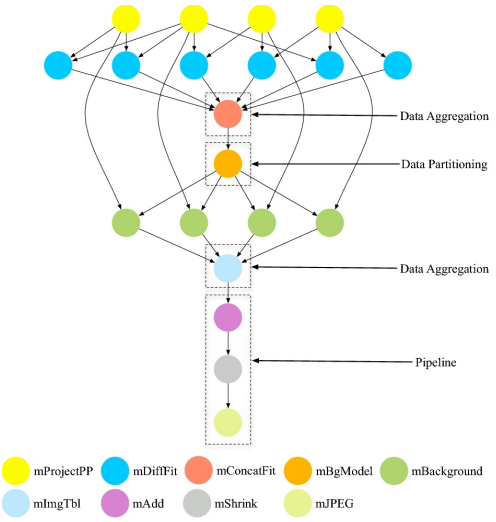


Fig. 4. Workflow representation provided by Pegasus. Each of the nodes is an operation executed by different software components. This shows the complexity of the execution environment needed to run the experiment.

1.0 (out of 1.0). Figures 5a and 5b show both resulting images.

4.6. *dispel4py*

dispel4py [14] is a Python library for describing workflows. It describes abstract workflows for data-intensive applications, which are later translated and enacted in distributed platforms (e.g. Apache Storm, MPI clusters, etc.). The dispel4py images are available at DockerHub [23]. To install the packages needed to run the workflows we use Conda, a package, dependency and environment manager for Python-based execution environments. To freeze the version of the packages that will be installed, we include the complete list of installed packages on the GitHub repository.

4.6.1. *Internal extinction*

Internal Extinction of Galaxies The Virtual Observatory (VO) is a network of tools and services implementing the standards published by the International Virtual Observatory Alliance (IVOA) [24] to provide transparent access to multiple archives of astronomical data. VO services are used in Astronomy for data sharing and serve as the main data access point for astronomical workflows in many cases. This is the case of the workflow presented here, which calculates the

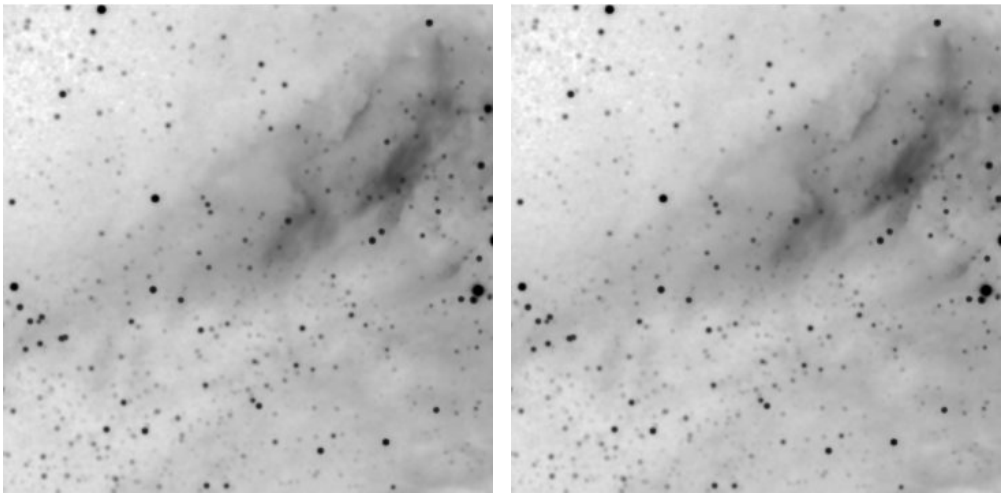
[20] https://github.com/pegasus-isi/PGen-GenomicVariations-Workflow

[21] https://doi.org/10.5281/zenodo.1889356,https://doi.org/10.5281/zenodo.1897809

[22] http://phash.org

[23] https://hub.docker.com/r/dispel4py/dispel4py

[24] http://www.ivoa.es



(a) Result from the Montage workflow execution on Pegasus

(b) Result from the Montage workflow execution on our reproduced Pegasus environment.

Fig. 5. The results from the Montage workflow execution using two different execution environments are exactly the same, validating our hypothesis.

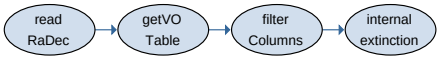


Fig. 6. Execution steps of the Internal Extinction scientific workflow

Internal Extinction of the Galaxies from the AMIGA catalogue [25]. This property represents the dust extinction within the galaxies and is a correction coefficient needed to calculate the optical luminosity of a galaxy.

The scientific workflow first reads the file containing the inclination and ascension rate of 1051 galaxies. Next, the workflow use these data values to to query the Virtual Observatory and obtains the results selecting only those values corresponding to the morphological type (Mtype) and the apparent flattening (logr25) features of the galaxies. Finally, the workflow calculates the internal extinction of the galaxy. Figure 6 shows the execution steps fo the workflow.

The main software dependencies needed to run such workflow are `requests`, `Python 2.7`, `numpy` and `astropy`.

Since the Internal Extinction workflow uses an online service, the input data may vary among workflow executions. Thus, we validated the different workflow execution outputs by verifying the results data structures, file sizes, number of lines and nonexistence of errors during the execution. Both executions (from the original and reproduced execution environments) were identical and we conclude that we were able to reproduce the experimental workflow. The Docker images and their results from these experiments are available at DockerHub [26].

4.6.2. Seismic Ambient Noise Cross-Correlation

Seismic Ambient Noise Cross-Correlation workflow (or xcorr workflow) is part of the project *Virtual Earthquake and seismology Research Community e-science environment in Europe* (VERCE). The goal of this workflow is to prevent damages by earthquakes and volcano eruptions. These natural events are preceded by changes in the Earth's geophysical properties such as wave speed.

The `xcorr` workflow has two stages, being the first a time series pre-processing of a seismic station data (which is done in parallel) and next each station correlates each pair. Figure 7 shows the workflow steps.

The main software dependencies are `Python 2.7`, `obspy` and `numpy`. Regarding the workflow execution, both executions on the original and replicated environment obtained the same results, thus concluding that we successfully reproduced the experiment. The output of `xcorr` is written to a file

[25] http://amiga.iaa.es

[26] https://doi.org/10.5281/zenodo.1889332,https://doi.org/10.5281/zenodo.1889328

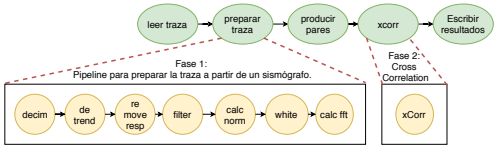


Fig. 7. Seismic Ambient Noise Cross-Correlation workflow representation. Each of the nodes has several operations executed by different software components, leading thus to multiple software versions that may cause problems when reproducing the experiment.

with the result of the cross-correlation calculations, which we compared for both executions.

The workflow images and results are available with persistend identiers in Zenodo[27].

4.7. WINGS

WINGS is a semantic workflow system that assists scientists with the design of computational experiments. A feature of WINGS is that its workflow representations incorporate semantic constraints about datasets and workflow components, and are used to create and validate workflows and to generate metadata for new data products. WINGS submits workflows to execution frameworks such as Pegasus and OODT to run workflows at large scale in distributed resources. Similarly, its main dependencies are `Git`, `Python 2.7`, `Java 1.8`, `Tomcat 8.5` and `Docker`. We also include the complete list of installed packages on the Dockerpedia GitHub repository[28].WINGS is the base WMS for executing MODFLOW-NWT.

4.7.1. MODFLOW-NWT

The USGS MODFLOW-NWT is a Newton-Raphson formulation for MODFLOW-2005 to improve solution of unconfined groundwater-flow problems. MODFLOW-NWT is a standalone program that is intended for solving problems involving drying and rewetting nonlinearities of the unconfined groundwater-flow equation. MODFLOW-NWT imports the Upstream-Weighting (UPW) Package for calculating intercell conductances, needs the Flow-property input for the UPW Package. The NWT linearization approach generates an asymmetric matrix. Figure 8 shows the three-step experiment workflow. The process starts by reading the MODFLOW-NWT model, next the workflow specifies in wich geographical zone the model is executed and finally the results are shown. Figure 9a and Figure 9b show the results generated by the original and reproduced execution environments respectively. The Docker images used for executing both workflows are available online [29].

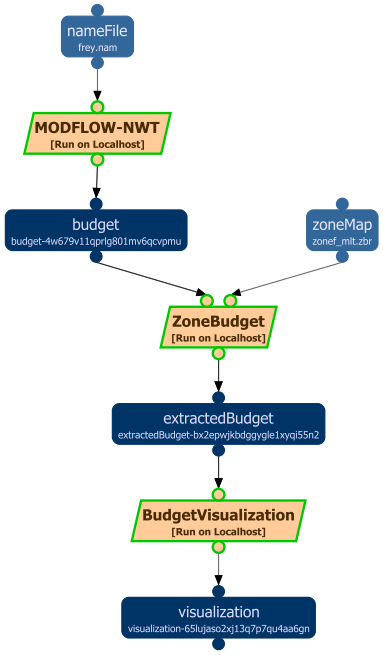


Fig. 8. MODFLOW-NWT workflow representation which we run locally. The workflow we run is identical to the existing in [15] and each workflow node executes an action for which different software components are needed. Descriptions are needed to ensure correct workflow reproducibility.

4.8. Results and discussion

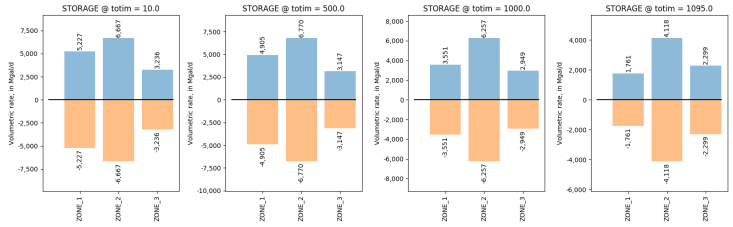
We executed the images for the workflows over their corresponding platforms, and each one of them used a different Docker version. Nonetheless, Docker guarantees that software will always run the same, regardless of underlying infrastructure and the Docker version.

All the executions were compared to their original one in a predefined VM image, where the execution environment was already in place. Results show that the container execution environments are able to execute their related workflows fully. To check that not only the workflows are successfully executed but also that the results are correct and equivalent, we checked their produced output data.

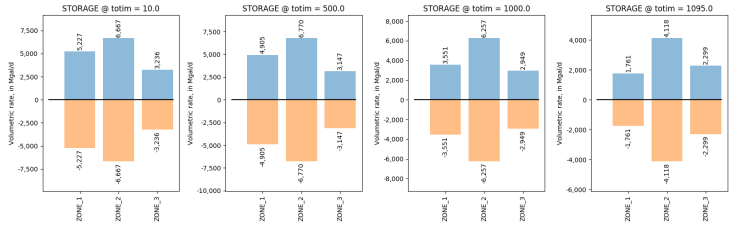
[27] https://doi.org/10.5281/zenodo.1889342, https://doi.org/10.5281/zenodo.1889336

[28] https://github.com/dockerpedia/wings-docker

[29] https://doi.org/10.5281/zenodo.1889348, https://doi.org/10.5281/zenodo.1889328



(a) This image shows the results from the MODFLOW workflow execution by the Information Sciences Institute (ISI)



(b) This image shows the results from the MODFLOW workflow execution in our local system.

Fig. 9. The results from executing the MODFLOW workflow at the ISI and on our local machine after using are identical. We managed to reproduce the original workflow by using our semantic model and container virtualization using Docker images.

In the case of Montage, which produces an image as output, we used a perceptual hash tool. The resulting image (0.1 degree image of the sky) against the one generated by the baseline execution, obtaining a similarity factor of 1.0 (over 1.0) with a threshold of 0.85.

In SoyKB and Internal Extinction workflows, the output data is non-deterministic due to the existence of probabilistic steps. In this case, the use of a hash method is unfeasible. Hence, we validated the correct execution of the workflow by checking that correct output files were actually produced, and that the standard errors produced by the applications did not contain any error message. In both cases the results obtained in each infrastructure were equivalent in terms of their size (e.g., number of lines) and content.

In the case of MODFLOW-NWT, which produces a histogram by zone, so we can compare it easily. The resulting histograms are the same between the original and reproduced environment.

Experimental results show that our proposal can automatically detect the software components, related vulnerabilities, building steps, and specific metadata of scientific experiments in the form of Docker images. Also, the results show that it is possible to extend Clair to annotate other package managers. In particular, we extended for Conda Package Manager.

The annotations generated by our approach allow comparing the software components between two or more environments. This feature can be used as a debug tool when a reproduced environment did not work.

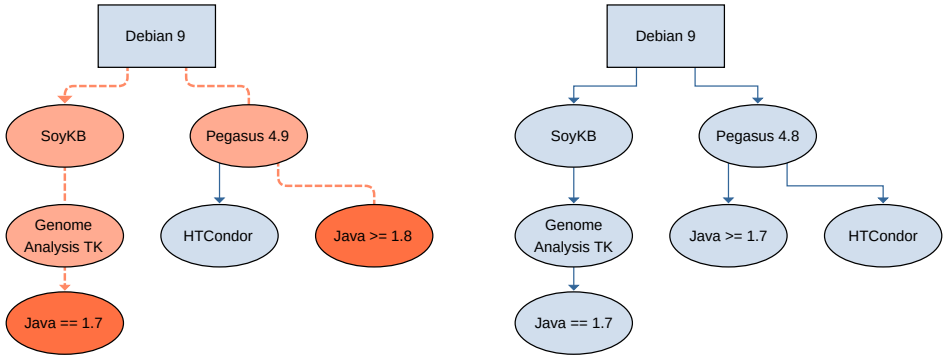
For example, On August 2018, we built the SoyKB workflow image, and we could execute the workflow successfully. However, we rebuilt a new image in November with the same DeploymentPlan and we were not able to run the workflow successfully.

We compared the software components inside both images and found the following differences:

- August image: Pegasus 4.8 and Java 1.7
- November image: Pegasus 4.9 and Java 1.8

Thus, we analyzed the SoyKB code and documentation and the Pegasus 4.9 dependencies obtaining the dependency graphs in Figures 10a and 10b. These graphs show that Pegasus 4.9 and the SoyKB experiment need different Java versions (Java 1.8 and 1.7 respectively), failing thus the execution of the experiment if one of these Java versions is used incorrectly. Building a new image with Pegasus 4.8 and Java 1.8 and SoyKB using Java 1.7 (Figure 10a) the experiment was executed correctly. Without the semantic descriptions provided a scientist would have had a hard time to spot that problem. Notice that the `latest` tag was not used in the Dockerfile to build none of the images. Simply an update operation caused that problem. This new image was named: `pegasus_workflow_images:4.8.5`

In summary, the results of our experiments are:



(a) Dependency graph Pegasus 4.9 and SoyKB (b) Dependency graph Pegasus 4.8 and SoyKB

Fig. 10. The orange nodes are the differences between the images

- Docker Images allow the execution the selected scientific workflows.
- Our annotator correctly obtained the software components installed by the supported package managers without install new components inside the image or execute the experiment.
- We could reproduce the environment for the five workflows using the annotations obtained by our approach.
- We can detect the similarities and differences between two versions of an image. Furthermore, we used the feature to detect and solve a issue.

5. Related work

This work aims to allow scientists to reproduce their in-silico experiments. This is not the first work in trying to enable experiment reproducibility, and thus it is mandatory to look at the work done so far before starting our journey. For computational experiments to become reproducible, one needs to develop a system for linking scientific publications with computational recipes. These recipes (scientific workflows) need to be executed by data workflow systems [10, 16, 17], which run over commodity machines and make use of several other software components during its execution (i.e. the execution environment). All these experiment components need to interact to execute it, and they also have to run similarly if the experiment is reproduced by some other scientist in another environment. However, such component coordination is prone to errors, as the work in [18] pointed out. The authors studied the reproducibility of scientific workflows, showing that almost 80% of the workflows could not be reproduced. About 12% of the problems to reproduce these experiments were due to the lack of information about the execution environment. Furthermore, 50% of them were due to the use of third-party resources such as web services and databases that were not available anymore. Other studies have exposed the necessity of publishing adequate descriptions of the run-time environment of experiments to avoid replication hindering [19].

One way to allow experiment reproducibility is to use virtualization techniques by using a virtual machine (VM). In this way, the execution environment can be packed within a Virtual Machine and distribute it along with the experiment [20, 21]. However, the high storage demand of VM images remains a problem since a virtual machine needs to install the whole Operating System before installing any software component within it (consider that the minimal version of Windows is 4GB and 1GB for a Linux distribution). Also, the cost of storing and managing data in the Cloud is still high, and the execution of high-interactivity experiments through a network connection to remote virtual machines is also challenging. A list of advantages and challenges of using VMs for achieving reproducibility was exposed in [22]. VMs also introduce problems at the time of reproducing experiments: VMs work as black boxes, and even though is not strictly required to describe the experiment execution environment since we rely on the VM, it should be possible to know what components are installed within that VM, to be able to reproduce such environment outside the initial VM. In summary, even when VMs support reproducibility, they are too large and fixed, not being possible to

know what components are inside the VM and which of those are really needed to reproduce the execution of the in-silico experiment. In [23] the author presents a set of best practices to use Docker as a fundamental part for experiment reproducibility, however it is an early work describing some desiderata.

To solve the aforementioned problems, the community has adopted the use of Docker, contributions such as [24–26], so reviewers, interested readers, and future researchers can to reproduce the experiments within the same environment. Container solutions solve the problem of storage, however, the challenge of reproducing scientific contributions due to their high dependence on developed algorithms, tools and prototypes, quantitative evaluations, and other computational analyses that are not adequately documented still persists. It persists due to the containers working as black boxes in which the scientist cannot know easily what packages are installed, and thus making virtually impossible what software packages are required to run that experiment. In order to understand what is required to execute the experiment and what components might be causing issues when reproducing the experiment, additional information, in the form of well structured data, should be provided.

In the ReproZip project [6, 27] the authors present a work that allows researchers to automatically create a VM or a companion Docker container along with the experiment. What Reprozip does is to build a Docker image from the source code of a specific experiment. Using its package system, Reprozip stores an internal description of the scientific experiment and its environment, which can be recreated by on another machine having installed Reprozip. However, to use Reprozip it is still needed to install other software components, and the internal description used by Reprozip does not provide the features and flexibility provided by semantic descriptions, such as easily comparing two different execution environments or knowing which components are needed to run a specific part of a workflow.

The work in [4] addresses the problem of describing what is inside the VM image. To do that the authors solve the problem proposing a semantic modeling approach to conserve computational environments in scientific workflow executions. However, the annotation process is manual, and the high storage problem of the virtual machines persists. In the Timbus project[30] [5] the problem of logical conservation is addressed installing new software inside each environment (in this case, a virtual machine). However, this approach increases the complexity of the environment and requires to execute the computational environment.

In terms of ontological engineering for describing software components, the authors in [9] present the Smart Container ontology which extends the Provenance Ontology PROV-O [28] and models Docker in terms of its interactions for deploying images. Another related work [29] describes how to use RDF to represent Docker files. Similarly, a different approach in which software ontologies are used is to allow computational reproducibility [4]. In this work, the authors present a set of ontologies that model software and hardware components to allow the execution environment reproducibility.

As described in this section, several works have addressed the experiment reproducibility problem, providing frameworks in which virtualization techniques and structured knowledge representation are used. However, they either rely on VMs as black boxes, which are large and fixed environments that make the portability of such experiments not optimal or require a manual annotation process, which potentially hinders the quality and trust of the annotations, as the analysis of the dependencies is not always trivial to do for a human annotator. In the following section, we will describe our approach, which combines semantic descriptions and container-based virtualization to tackle these two problems.

6. Conclusion and future work

In this work, we proposed an automatic tool to annotate the software components of the computational environment of a scientific experiment. In this work we focus on container-based environments,combining them semantic capabilities of the annotations to conserve and reproduce computational environments of scientific workflow executions.

We conducted experiments to show the Docker Images are a lightweight unit and the images can be stored using public or private repositories such as DockerHub. Thus, we can ensure the physical conservation using these repositories. The utilization of Docker Images combined with our annotation process is a powerful approach to obtain the software components and building steps related to the environment. Moreover, we prove that the approach can be extended to other package managers such as Conda. In con-

[30] http://www.timbusproject.net/

clusion, this is a unique contribution which successfully addresses both physical and logical conservation of computational environments for scientific experiments. In regard to the reproducibility, our proposal can use these annotations, rebuild the computational environment and execute the related workflow automatically. Also, the results of our experimentation showed that these annotations can detect software components issues (e.g., incorrect versions).

In summary, this work adopts, modifies and implements new tools building a framework to automate the process of obtaining the requirements of the computational environment, to then store these annotations according to semantic models. Finally, this proposal concludes that the use of these annotations allows the reproduction and detection of problems in the computational environment of a scientific experiment.

As for the future work, this work could be extended to support other container-based virtualization solutions, such as Singularity [30]. Also, it would be possible to improve the software components descriptions by providing a visualization of the dependency graph and the installed files within the experiment. Finally, a much more challenging contribution would be to detect workflow execution events using *perf events*[31] from the Linux Kernel, allowing to identify which workflow steps are being executed and what files are being accessed so a more fine grained analysis could be done.

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