# A Backend Platform for Supporting the Reproducibility of Computational Experiments

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#### Abstract

In recent years, the research community has raised serious questions about the reproducibility of scientific work. In particular, since many studies include some kind of computing work (for instance, executing an algorithm encoded using some programming language), reproducibility is also a technological challenge, not only in computer science, but in most research domains.

Replicability and computational reproducibility are not easy to achieve, not only because researchers have diverse proficiency in computing technologies, but also because of the variety of computational environments that can be used. Indeed, it is challenging to recreate the same environment using the same frameworks, code, programming languages, dependencies, and so on.

In this work, we propose an Integrated Development Environment allowing the share, configuration, packaging and execution of an experiment by setting the code and data used and defining the programming languages, code, dependencies, databases, or commands to execute to achieve consistent results for each experiment. After the initial creation and configuration, the experiment can be executed any number of times, always producing exactly the same results. Furthermore, it allows the execution of the experiment by using a different associated dataset, and it can be possible to verify the reproducibility and replicability of the results. Our platform aims to allow researchers in any field to create a reproducibility package for their science that can be re-executed on any other computer.

To evaluate our platform, we used it to reproduce 25 experiments extracted from published papers. We have been able to successfully reproduce 20 (80%) of these experiments achieving the results reported in such works with minimum effort, thus showing that our approach is effective.

### 1 Introduction

Reproducibility is the ability to replicate the results of a study using the original methods, materials, and data. It is paramount for science and is widely considered to be a precondition of scientific advancement [6, 17]. Replicability is the capacity to obtain the same results using new methods, materials, and data and/or consistent conditions with the original study [6, 17].

In recent years, many concerns have been raised related to the reproducibility of today's computational work. A significant amount of scientific research is nowadays supported by some kind of computational experiment. Thus, reproducible research is now more than ever a technological challenge in many research domains.

Computational reproducibility should be easily achievable since it is possible to specify detailed information about the computational environment being executed. This should enable the reproduction of the computation environment in the same way. But in practice, this does not happen (see section 3). The complexity of today's software makes the reproducibility process more difficult [32]. Research in many fields (e.g., chemistry, climate change, biology) is supported, in several studies, by computational experiments [32]. However, many of these researchers are not experts in software development. Thus, although they may be able to create the necessary code for their experiments (e.g., scripts in Python or R), they may find it difficult to create reproducible computing experiments. In fact, this is even the case for computer science conferences (section 3).

To keep research reproducible, it is essential to investigate, perform, analyze, and rerun the experiments associated with that research in order to obtain corresponding results as before. For this to be possible, when working with a computational experiment, it is necessary to rebuild the original computing environment using the original code and its dependencies, the same data, and the same script-based workflow [45, 5].

Describing all the dependencies used and which versions are used is not a trivial task. Package management tools of each programming language (PL), such as pip<sup>1</sup> for Python or npm<sup>2</sup> for JavaScript, have integrated commands which can build a file with the dependencies needed for an experiment. However, these files do not have all the information to enable computational reproducibility. Moreover, researchers without a computer science background may not know how to use such tools [32]. There are tools to aid researchers in making their computational experiments reproducible such as Open Lab [53], SciInc [62], CDE-SP [48], Encapsulator [47], A Framework [43], CARE [33], VisTrails [24], Binder [7], RenkuLab [37], Whole Tale [4], ReproZip [10, 12, 11], or RunMyCode [54]. However, these approaches are limited to a set of PLs, do not allow the use of more than one PL per project, do not allow the use of databases, or do not allow researchers to specify which commands should be executed to achieve the experiment results. The Association for Computing Machinery (ACM) has motivated researchers to build a reproducibility package by creating a virtual machine. However, again this is not easy for many researchers. In section 8 we further discuss related work.

To assess the use of reproducibility tools, we defined the following research question (RQ), which we answer in section 3:

#### **RQ1**: What is the adoption of reproducibility tools among researchers?

To answer this RQ we designed and distributed an online survey. Although the aforementioned approaches allow the reproducibility of experiments, just one of the 38 researchers answering our survey acknowledged to have used one of these platforms to save and reproduce computational experiments.

Thus, with our work, we mainly seek to answer the following RQ (section 4):

# **RQ2:** To which extent can we propose a platform that helps to make computational experiments from different fields reproducible?

To answer this RQ, we propose an Integrated Development Environment (IDE) that allows the share, creation, configuration, (re-) execution and packaging of computational experiments, which also includes the validation of reproducibility and replicability of the results. Researchers need to associate a dataset to each experiment, however, it is possible to execute using a different dataset. In this way, researchers can compare the results achieved with the results of previous runs by using the associated data or different data.

For now, we focus our work on the backend of the platform, not providing a user interface (which we plan to design and build in future work). Our platform is developed to support a variety of experiments, including Artificial Intelligent (AI) experiments. For these experiments, we make researchers aware of the importance of making the experience reproducible, helping them associate the possible seed used with the project. In addition, Furthermore, our approach can be used to create a capsule of the research experiment containing the code and its dependencies, the data and databases, the process, and the commands to achieve the experiment results. Our main goal is to support the researchers in developing, executing and sharing the code they produce for their experiments, allowing them to manage the data and code associated with that experiment,

<sup>&</sup>lt;sup>1</sup>https://pypi.org/project/pip/ <sup>2</sup>https://www.ppmig.com

without the need to manage dependencies, compilers, and other variables. The proposed platform can handle many PLs, databases, and other data files. It can also automatically infer information from the experiment, such as PLs and dependencies, creating the proper environment for the execution. The researcher can then easily export a reproducibility package that can be executed on any computer just by double-clicking a single file, making the experiment easily sharable and re-executable.

To evaluate our platform, we selected a set of experiments included in already published papers and tried to recreate them using our platform. In particular, we seek to answer the following RQ (section 5):

#### **RQ3:** What kinds of experiments can supported?

To answer this RQ, we collected experiments from related work, from major conferences, and some others from Zenodo so we could have a variety of experiments. We collected 31 experiments from fields such as computer science, medicine, or even climate change science. We were, in general, successful in reproducing the experiments, achieving the same published results, and were able to create a reproducibility package that anyone can re-execute just by executing a single file.

Based on these RQs and our answers to them, the main contributions of this work are:

- a set of principles that a reproducibility platform should follow (section 2);
- an initial overview of the perspectives of researchers about reproducibility difficulties and tool usage (section 3);
- the backend of a reproducibility platform tackling the reproducibility principles and the researchers' perspectives that can cope with experiments from very different scientific fields (section 4);
- a list of several reproducibility packages for existing scientific publications (section 5);

Before we introduce our platform, in section 2 we discuss in more detail the challenges of reproducing computational experiments, and we define a set of principles a platform supporting computational reproducibility must follow to be successful. This may help future researchers proposing other approaches for reproducibility.

# 2 Challenges in Reproducibility

The digital transformation of science has made available new publication channels for research data. These publications come from specialized data repositories, large centralized or decentralized platform infrastructures, or commercial application providers to traditional self-hosted web server downloads. Some examples of these platforms are CKAN<sup>3</sup>, DSpace<sup>4</sup>, EUDAT<sup>5</sup>, GitHub <sup>6</sup>, the Harvard Dataverse<sup>7</sup>, Zenodo<sup>8</sup>, and derived systems.

Nowadays, these platforms provide ways to upload and publish research datasets with an institutional, disciplinary focus, or general purpose. Such platforms also need to fill the needs of different stakeholders in a variety of usage scenarios [39, 36].

Although these platform help spread science, they are not enough to make it reproducible. Researchers need to expose their results, but also other artefacts, such as code and data, and explain how to use them to achieve the published results. However, these platforms do not provide means to make the code easily reproducible.

Based on previous work, we summarize a set of challenges a researcher needs to take into consideration when intending to make an experiment easily reproducible:

<sup>&</sup>lt;sup>3</sup>https://ckan.org/

<sup>&</sup>lt;sup>4</sup>https://dspace.lyrasis.org/

<sup>&</sup>lt;sup>5</sup>https://www.eudat.eu/

<sup>&</sup>lt;sup>6</sup>https://github.com/

<sup>&</sup>lt;sup>7</sup>https://dataverse.harvard.edu/

<sup>&</sup>lt;sup>8</sup>https://zenodo.org/

C1: Software In the research process, the software has a high impact on the reproducibility of experiments [14].

When someone tries to reproduce an experiment but uses the wrong software, the wrong version, or even the wrong dependencies, the experiment may produce different results from the original one. It is known as Code Rot [3]. The management of the software to use is difficult as even newer versions of software that claim to be compatible with the previous ones, may have unintended differences that can affect reproducibility. To allow reproducibility, all the information related to the software should be identified to ensure a consistent behavior [32].

The term Dependency Hell refers to a common issue in software development where multiple packages share a dependency, but depend on different and incompatible versions of that dependency. As only one version of a dependency is allowed in a project's environment, resolving these conflicts and finding a compatible solution can be challenging [48].

Another potential problem with reproducibility is when the libraries are unavailable. To get these libraries, it is necessary to find them which hinders reproducibility.

Software is the tool that helps the researcher in the reproducible process (create, configure, run, encapsulate and re-run), however, it is not easy to find easy-to-use and complete solutions [25, 64].

C2: Command It is crucial to make available the commands to execute the code, along with the file to execute and all the values of the parameters needed to reproduce the experiment. Some researchers prefer not to use parameters on the command, but this approach makes it difficult for those who intend to extend or explore the research. So using parametrization is an important method for extension, as it could give both the original researcher and other researchers the ability to easily extend the approach, explore the parameter space, and validate results [32].

However, using a single command with too many parameters can be very confusing for other researchers to extend the experiment. To make the extension exploration and reproducibility easier, it is better to simplify the command and break it into smaller commands and smaller workflows. In the end, it is necessary to explain what each command does and organise them in a general workflow [59, 42, 32].

Furthermore, the expected result should be available for comparison, because there is no guarantee that the same command applied by a different user on a different machine will get the same result. This can happen due to the differences in the dependencies installed, the software, the data used, and the dependencies implicitly provided by the system [32].

**C3:** Data Making available all the data is another important element to allow reproducibility [41]. Most researchers use some kind of input as starting data as well as the final generated results of their experiments. These inputs sometimes are in remote locations, so security or privacy issues can occur during the data download.

Some data files may contain private information, that is normally omitted from the publication, but without it, the experiment is not reproducible. Receiving this information as an input parameter can identify the need for the information without publishing the delicate data, enhancing reproducibility [32].

Furthermore, researchers intend to find and reuse existent data, but the existing platforms and approaches do not include sufficient metadata (e.g., title, authors, version, PLs, software description, Uniform Resource Identifier/DOI and execution requirements) to find and reuse data [55].

C4: Hardware Enabling reproducibility using the same performance, scalability, and efficiency is another challenge because the same hardware should be used (e.g., the same computing power such as RAM, CPU, GPU, and storage). However, in this work, we will not take into consideration experiments that may have hardware requirements.

From the challenges C1, C2, and C3 we just discussed, we identify a set of principles a reproducibility platform should follow. We also introduce principles that are orthogonal to the challenges.

#### From C1

**P1** Such a reproducibility platform should allow researchers to define the PLs used in the experiment, the compilers, the dependencies, and the libraries, as well as the correct version of each.

**P2** It should allow saving all the dependencies needed to execute the experiment together with the code.

#### From C2

**P3** The platform should support the configuration of the commands for the execution of the experiment.

**P4** It should allow the validation of the computational reproducibility using the results of previously performed experiments as a means of comparison.

#### From C3

**P5** Such a platform should provide mechanisms that allow researchers to manage the data of the experiment.

#### **Orthogonal principals**

**P6** It should be able to deal with the diversity of PLs (and their dependencies) used by researchers.

**P7** It should support all types of experiments, from the execution of simple scripts to the execution of more complex experiments (e.g., involving databases or several PLs).

P8 The platform should support researchers with little knowledge of computing.

**P9** It should enable the sharing of the experience easily.

**P10** It should facilitate the re-execution of the experiment even for users outside the research domain.

In this section, we have synthesized the challenges already identified in the literature. However, we also want to have some more insights from the researchers themselves. Thus, in the following section, we present a small survey about the views of researchers on reproducibility.

# 3 Researchers' Experience with Reproducibility

We performed a survey<sup>9</sup> in which the main goal was to gather some information related to the familiarity of researchers with the concept, the challenges, requirements, and the main difficulties of computational reproducibility. Furthermore, it is important to know which platforms researchers use/know to reproduce experiments. Note that this survey is not intended to be complete, but rather to give us a more informed view about researchers' perspectives on reproducibility.

We made available this survey to all the authors of the 2022 edition of the International Conference on Software Engineering since we used some of these works in our evaluation (see section 5). From the 700 contacted authors, we got 38 responses. Moreover, we spread the same survey on social media platforms (Twitter, Facebook, and LinkedIn) through public posts, and also distributed the survey through our contacts via email, for which we got 38 responses too.

Our sample is composed mostly of Ph.D. students (46%), followed by faculty members (33%) and researchers (11%). They are from Portugal (46%), China (16%), and the USA (13%). Furthermore, 90% of the respondents have more than two years of research experience.

 $<sup>\</sup>label{eq:product} ^9 A vailable at {\tt https://docs.google.com/forms/d/e/1FAIpQLScUtalm-7X0BwjKbNtpam5WDywQ8wWVTzf03sfE8K0yA0c1EQ/viewform.}$ 

The "computational reproducibility" term is familiar to 84% of the surveyed, and 79% tried to reproduce experiments performed by others. However, most of them, 66%, had difficulties in doing so.

As we can see, only a few researchers did not find it difficult to reproduce others' works.

The main challenges in computational reproducibility found in this survey are "Missing information to execute the experiment" (34%), "Data not available" (25%), "Code not available" (24%), and "Installation not successful" (17%).

Only 11% of the surveyed know a reproducibility platform, namely Binder, while all the others do not know any. Only 8% of the surveyed reproduce their experiments using docker<sup>10</sup>, 8% of the surveyed publish the code on Zenodo, and 5% on GitHub.

Finally, we asked what requirements were considered necessary to allow computational reproducibility. The answers were "Make available the data" (29%), "Make available the code" (28%), "Make available the description of all the dependencies used and its versions" (24%), and "Make available the PL used and its version" (18%).

To conclude, the answers to this survey show us that the term computational reproducibility is a term well-known in the research community. However, researchers usually have difficulties when trying to reproduce experiments performed by others. Although with this small survey, we do not have a complete view of the researchers' perspectives on reproducibility, we can conclude that, although there are already some proposals to aid in reproducing computational experiments (see section 8), the researchers that answered this survey still do not use them at scale, which also motivates our own work.

# 4 Design and Implementation of a Reproducibility Platform

Based on the principles defined in section 2 and the data collected from the researchers described in section 3 in this section, we present our design and implementation of a backend of a platform that gives support to the creation and execution of computational experiments. Notice we focus our work on the software environment and assume the hardware does not influence the outcome of the experiments (although in some kinds of experiments that are actually intended, we will not consider such cases). In this work, we do not provide a user interface, which we plan to design and build in future work.

The methodology that researchers should follow to create a reproducibility package using our platform can be formulated in the following chronological order:

- 1. Researchers create a new project, choose the type of the project and fill in some fields (e.g., project name, description, etc.). For now, we only support the execution of scripts with a database integrated and AI experiments. However, the latter is necessary to make researchers aware of the reproducibility of the experiment, so we force researchers to associate the seeds used in the code with the project (Step 1 in fig. 1);
- 2. They upload the experiment files (e.g., code and datasets) or reuse a pre-existent project by providing its remote location. This functionality enables the uploading of individual or zip files, which can contain all the needed files of the experiment (Steps 2 and 3 in fig. 1).
- 3. They can manage the files within the platform (e.g., create some missing files/folders, edit and delete some unnecessary files/folders loaded by mistake or no longer needed) (Step 4 in fig. 1);
- 4. They configure the execution of the project and associate the dataset of that execution (e.g., choose a specific version of the PL and configure the databases) (Step 5 in fig. 1); This functionality can infer important information such as the PLs, dependencies and their version, however, the researcher must validate that information. In addition, it allows the configuration of AI

<sup>&</sup>lt;sup>10</sup>Docker is a platform designed to help developers build, share, and run modern applications. Docker uses service virtualization at the operating system level (https://www.docker.com/).

experiments. These experiments cannot be reproducible if researchers do not define the seeds used. To try to solve this problem, we are making researchers aware that they need to define the seeds used in the project. Furthermore, the researcher can provide more information (e.g., commands to build the project, and the configurations of possible databases) to generate a container specification and build a container image of the experiment. In addition, researchers need to associate a dataset to each experiment, allowing them to execute the experiment using a different associated dataset. In this way, it is possible to verify the computational reproducibility and replicability. After the platform concludes this step, our approach will execute the experiment 2 times to verify the computational reproducibility (Step 5 in fig. 1);

- 5. Researchers execute the experiment using the dataset associated or a different dataset. This functionality enables the reusing of container images, generated in the previous step, to start a new execution. In addition, it allows adding a pre-existing container image to add a database to the run. All the executions which use the same container image reuse the same computational environment to execute the experiment, however, if needed, the user can use the same computational environment but using a different dataset. Furthermore, it is possible to specify which commands one would like to run (Step 6 in fig. 1);
- 6. Researchers get and visualize the results (Step 7 in fig. 1);
- 7. Validate the computational reproducibility or the computational replicability.Researchers can define the location of the output (e.g., console output, a file, etc.), however, if it is not defined, we will compare all files changed and the console output (Step 8 in fig. 1);
- 8. Researchers build a reproducible package of the experiment. It allows building a reproducible package, which contains all the information needed to execute the experiment, that can be run on Windows, Mac OS or Unix operating systems. It reuses the container image previously generated and adds all the necessary information, including the commands executed when running the experiment (Step 9 in fig. 1).

fig. 1 presents an activity diagram formalizing this process.

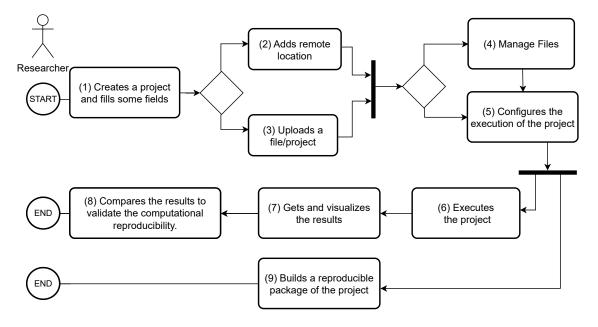


Figure 1: The activity diagram of a researcher using our approach

### 4.1 Architecture

Our platform has three main components, namely "Data Management", "Computational Environment", and "Code Execution". Furthermore, we have a database, which saves some required information. fig. 2 represents the components' diagram of this approach. In the following, we explain in detail each one.

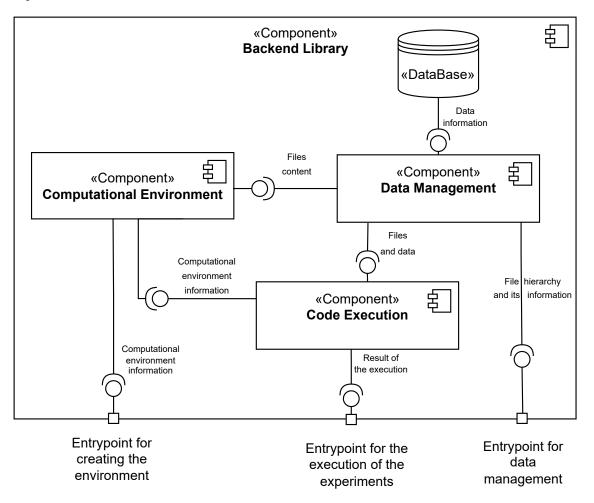


Figure 2: The components' diagram of our platform

#### 4.1.1 Data Management

This component is responsible for managing all the data of the platform, such as adding, editing and deleting files and folders. The researcher can use this component to upload all the necessary files on a project (e.g., code, datasets, etc.), and the Data Management Component saves on the database all the information of each file/folder.

This component complies with the principle P5 from section 2.

#### 4.1.2 Computational Environment

The function of this component is to build a computing environment able to deal with the diversity of development stacks (e.g., a variety of PLs, dependencies and, if needed, databases integrated) used by researchers and make that information available to the Code Execution Component (section 4.1.3) which executes the experiment.

The diversity of available computing environments is a challenge in general software development and is being tackled by using *containers* [13, 49], a technology that allows automatically building an environment based on a specification. A specification file for a container, also known as a container specification, is a document, like a template, that outlines the configuration and requirements of a containerized application or service. It describes the resources, environment, dependencies, and other necessary information for the container to run consistently across different environments [13, 49]. One of the most used containerization technologies is Docker<sup>11</sup> [49]. For instance, one may define a specification of an environment with Python 3, PostgreSQL 15.1 and Apache 2.4. By using the same specification, each member of a team works in the exact same environment as all the others. We build on this same principle to allow researchers to reproduce their experiments in a systematic way as the Computational Environment component is based on containerization.

This component complies with the P1, P2, P6 and P7 principles from section 2.

#### 4.1.3 Code Execution

This component is responsible for the execution of the experiment code/scripts, validating the reproducibility or replicability of results and building a reproducible package with all the information needed to re-execute the experience in the same way.

This component complies with the P3, P4, P9 and P10 principles from section 2.

#### 4.2 Implementation

In this section, we describe some relevant details of our implementation. We implement our approach in Python<sup>12</sup> and Node.js<sup>13</sup> and use a Neo4j<sup>14</sup> NoSql database, as well as Docker Hub.

The Data Management component is implemented in Node.js. We are using the Express<sup>15</sup> framework for communication. The information of all the files and folders of an experiment are saved on a Neo4j database.

The package responsible for the creation, configuration, execution and packaging of experiments is implemented in Python. We are using the Flask<sup>16</sup> framework for communication and we are also using Docker Hub as the containerization technology.

Our approach can build a variety of computing environments needed for researchers to execute their experiments. Our approach already supports a variety of PLs, namely C++, Perl, R, Java (maven), Python, Unix Shell and Jupyter Notebook. We have implemented a heuristics-based algorithm that allows the platform to infer the PLs of the project through file extensions. Moreover, our approach can also infer the dependencies to be installed, by constructing the project dependency graph.

The platform infers all the information needed to build the container specification, as the technology is Docker, this file is called dockerfile.

The platform performs all the steps of fig. 1, including building a reproducible package of the experiment. However, the execution of this reproducible package, which contains all the information needed to execute the experiment, is on the researcher's Windows, Mac Os or Unix operating system. The only requirement is to have Docker installed and running. This package can then simply be clicked and the experiment is executed.

It is easy to add another PL. For that to be possible, it is only necessary to do some updates to get a docker image of the wanted language from Docker Hub<sup>17</sup> and build a dockerfile with

 $<sup>^{11}</sup>$ www.docker.com

<sup>&</sup>lt;sup>12</sup>https://www.python.org/

<sup>&</sup>lt;sup>13</sup>https://nodejs.org/en/

 $<sup>^{14}</sup>$ https://neo4j.com/

<sup>&</sup>lt;sup>15</sup>https://expressjs.com/

<sup>&</sup>lt;sup>16</sup>https://flask.palletsprojects.com/en/2.2.x/

<sup>&</sup>lt;sup>17</sup>Docker Hub is the world's largest container image repository containing open source projects that are made available in containers (https://hub.docker.com/).

that information. However, we do not expect this to be done by researchers, but instead by a maintenance team of the tool.

Our approach supports databases, and it allows researchers to configure their setup. The databases currently supported are Mongo, SQLite MySql and PostgreSQL. As with PLs, it is easy to support another database technology.

# 5 Evaluation

We build an evaluation experiment to measure the capabilities of the platform. The main goal of this experiment is to reproduce a variety of experiments, from a simple script to experiments with integrated databases. We also considered experiments from different scientific fields. For that to be possible, we need to recreate the same environment using the same frameworks, code, data sources, the same PLs, dependencies, and the same version of the dependencies. After that, we execute the experiment and reproduce the results claims on the publication.

#### 5.1 Setup

We started by collecting experiments already published in scientific conferences. To do so, we used two different computer science research communities: software engineering through the conference IEEE/ACM International Conference on Software Engineering (ICSE), and databases through the conference International Conference on Very Large Databases (VLDB), three very well-known scientific events in their respective area. We analysed the first 30 articles of VLDB 2021<sup>18</sup> and the first 50 articles of ICSE 2022<sup>19</sup>. For each publication, we collected the link where the code of the publication is available. However, many of the publications do not have this information: for ICSE, only 32 papers have a link and for VDLB, only 19. From the ones with code, we selected five publications by randomly generating five numbers for each conference, each number representing one publication. For ICSE, we generated five numbers between 1 and 32 and achieved [1,9,12,13,23]; for VDLB, we generated five numbers between 1 and 19 and achieved [5,7,11,15,17].

Moreover, we tried to find computational experiments in other areas through the Climate  $Change^{20}$  and Nature Climate  $Change^{21}$  journals, but the papers would not include information about the experiment setup, without which we could not reproduce the experiment. Although this was not an extensive study, it is yet another evidence that reproducibility is not yet fully tackled by many researchers. Regarding the query of medical, artificial intelligence and climate experiments, we only considered the first 100 results of each one. Once again, we randomly generated five numbers between 1 and 100 two times, five representing the medical repositories, five representing the artificial intelligence repositories and five representing the climate change repositories. We achieved the numbers [25, 38, 44, 58, 69] for medical repositories, the numbers [10, 24, 41, 64, 99] for artificial intelligence repositories and the numbers [14, 21, 31, 59, 78] for climate change repositories.

Furthermore, we have widened the range of experiences, and to do this, we have made two searches in the Zenodo repository. We searched by "Medical"<sup>22</sup>, "Artificial Intelligence"<sup>23</sup> and "Climate Change"<sup>24</sup> expressions, and we only considered software repositories.

We chose computer science conferences and medical, artificial intelligence and climate change experiments in the expectation that these papers would pose more complex challenges and a variety of experiences from various domains.

In addition, we performed all the experiments available in all the papers related to our approach (see section 8).

<sup>&</sup>lt;sup>18</sup>http://vldb.org/pvldb/volumes/15/

<sup>&</sup>lt;sup>19</sup>https://ieeexplore.ieee.org/xpl/conhome/9793835/proceeding?isnumber=9793541

<sup>&</sup>lt;sup>20</sup>https://www.springer.com/journal/10584/

<sup>&</sup>lt;sup>21</sup>https://www.nature.com/nclimate/

 $<sup>^{22} \</sup>tt https://zenodo.org/search?page=4\&size=20\&q=medical\&type=software$ 

<sup>&</sup>lt;sup>23</sup>https://zenodo.org/search?page=1&size=20&q=Artificial%20Intelligence&type=software

<sup>&</sup>lt;sup>24</sup>https://zenodo.org/search?page=1&size=20&q=climate%20change&type=software

```
1 {"languages": ["C++"],
2 "languagesVersion": {"C++":"gcc:8"},
3 "commandsToAdd": [
4 "g++ -03 ./src/bbfs_node.cpp -o out",
5 "g++ -03 /src/bbfs_edge.cpp -o out"]}
```

Listing 1: Request data of E3

We then proceeded to collect all the information relevant to reproduce the experiment, including the PL and version used, dependencies necessary to be installed, if a database was necessary, and which commands were executed to get the expected results. In table 1, we present the relevant information related to the set of experiments chosen from VLDB (experiments E1–E5), from ICSE (E6–E10), for climate change (E11–E15), for medical (E15–E20), for artificial intelligence (E21–E25) and from related work (E26–E31) (the entries in *Repository link* are clickable in the PDF version of the paper and lead to the repository available in the paper). Furthermore, we added a column called "Reproduced" in each table, which represents if we achieved reproducibility using our approach (more details in section 6).

Our own experiment environment is a personal computer with a 6-core CPU, and 16GB RAM, running Ubuntu 20.04.

### 5.2 Execution

Our approach is the backend of the platform, not providing a user interface, so we need to use its API on this execution. For each of the projects, we started by creating and populating with the corresponding code the projects (section 5.2.1). We then build the necessary environment (section 5.2.2) and execute the experiments (section 5.2.3). Finally, we create a reproducibility package (section 5.2.4).

#### 5.2.1 Create a project and upload its files

During this task, we used the "Data Management Component" described in section 4.1.1. The first step is to create a project and fill in some important fields, such as the project name and the project description. The response is the unique identifier of the project created. During the following tasks, we will need the returned unique identifier of the project.

The second step is to upload files to the project. We can upload a zip file or use a remote location (Git or DOI). At the end of this task, a new project is created in the platform.

#### 5.2.2 Build the environment for each experiment

The main goal of this task is to recreate the same computational environment of an experience. During this task, we used the "Computational Environment Component" described in section 4.1.2. We will exemplify the building process of two environments for two distinct experiments (E3 and E8).

The order in which the experiments are performed is irrelevant, and we could choose another experiment, but we consider that the first experiment we want to reproduce is the E3, and the second one is the E8. E3 uses C++, Python, Jupyter Notebook, and Unix Shell as the PLs. Furthermore, this experiment has only one Jupyter Notebook file. Python and Unix Shell files were not used in this execution, so we do not consider these PLs. The documentation of E3 indicates that to build the experiment, it is necessary to run the commands g++ -O3 ./src/bbfs\\_node.cpp -o out and g++ -O3 ./src/bbfs\\_edge.cpp -o out. For this task, we make use of the "Build a docker image" functionality of the "Computational Environment Component" (section 4.1.2). Our approach infers the PLs (C++) and inserts the commands to build the project. Listing 1 represents the request data after the user fills in all the information.

```
FROM ubuntu: 20.04
1
  RUN
       apt update &&
                        apt upgrade -y
\mathbf{2}
  RUN apt install -y gcc-8 make g++
3
  RUN update-alternatives --install /usr/bin/gcc gcc /usr/bin/gcc-8
4
     2000
  WORKDIR /files
\mathbf{5}
  COPY ./files .
6
  RUN g++ -O3 ./src/bbfs_node.cpp -o out
7
  RUN g++ -O3 ./src/bbfs_edge.cpp -o out
8
```

Listing 2: Dockerfile of E3

```
1 {"languages": ["python", "shell", "java"],
2 "languagesVersion":{"java":"openjdk-11", "python":"python:3.8"},
3 "commandsToAdd":["cd RLCheck/jqf/","mvn package","cd ../.."],
4 "hasRequirementsFile": "true"}
```

Listing 3: Request data of E8

After receiving this request, the server generates a dockerfile, builds a docker image and returns an identifier (ID) that represents that docker image. In Listing 2, we can see the dockerfile generated for the E3. The directory "files" contain all the files of the experiment.

E8 is a more complex experiment than E3 as it needs three PLs to execute (Python, Java and Unix Shell). The authors of the experiment mentioned that the prerequisites are "Java 8-11, Apache Maven and Python 3". Furthermore, all the Python dependencies that are necessary to install are in a file in the repository. To conclude, it is necessary to execute the following commands cd RLCheck/jqf/, mvn package, and cd ../... Our approach needs to replace cd command to WORKDIR in the generations of the dockerfile because the cd command has no effect after the execution of that command, and WORKDIR command changes the working directory for future commands. Thus, the request type to generate a dockerfile is the same as E3, but the content of the request data is different and is represented in Listing 3.

In Listing 4, we can see the dockerfile generated for E8.

#### 5.2.3 Run the experiments

After we have a docker image created, we only need to execute the experiment. For that to be possible, we need to insert the Id of the created docker image in the previous task and which command we intend to run. To do so, we make use of the "run an experiment" functionality of the "Code Execution Component" (section 4.1.3).

Listing 5 presents the request data to execute E3.

#### 5.2.4 Build the reproducible package

Finally, we created a reproducibility package for each of the experiments, which we make publicly available<sup>25</sup>.

We reuse the container image generated in the building of the computational environment task and reuse all the information provided on the execution of the experiment (commands) to encapsulate all that information in a folder along with the scripts needed to run the project. We built a reproducible package that can be run on Windows or Unix operating systems where the user just needs to have Docker installed and running. By clicking in "runExperiment" file, the experiment is executed automatically.

<sup>&</sup>lt;sup>25</sup>https://zenodo.org/record/8050716

```
FROM ubuntu: 20.04
1
  RUN
        apt update &&
                        apt upgrade -y
\mathbf{2}
  RUN apt install -y python3.8 python3-pip
3
  RUN update-alternatives --install /usr/local/bin/python python /usr
4
      /bin/python3.8 2000
  RUN update-alternatives --install /usr/bin/pip pip /usr/bin/pip3
\mathbf{5}
      2000
  RUN apt install -y openjdk-11-jdk openjdk-11-jre maven
6
  WORKDIR /files
7
  COPY ./files
8
  RUN mvn package
9
  WORKDIR RLCheck/jqf/
10
  RUN mvn package
11
  WORKDIR
           ../..
12
13
  RUN pip install -r requirements.txt
```

Listing 4: Dockerfile of E8

Listing 5: Request data for the execution of E3

# 6 Discussion

We chose 31 different experiments from published work in two research communities (ICSE and VLDB), in three research areas (Medical, Artificial Intelligence and Climate Change) and experiments executed in related work approaches.

Although 31 may not seem a significant number, making each one reproducible was quite challenging due to the diversity of experiments considered, encompassing different domains, and the variety of computational procedures involved. During the configuration of the computational environment, we needed to infer the information from the repository (e.g., PLs and dependencies used ) to try to fill in the parameters that were necessary to insert to build the same computational environment. This information was only sometimes clear. Our approach can infer the Python and R dependencies needed when the requirements file is missing. However, deducing the dependencies for other PLs is very difficult, so that information should be part of the project description. Although our backend already includes such a feature, we must design an easy way for researchers to have that information in the frontend.

We analyzed the articles on all the related work approaches. However, most methods do not have a validation section (Open Lab [53], Encapsulator [47], VisTrails [24], RenkuLab [37], Whole Tale [4], ReproZip [10, 12, 11], RunMyCode [54] and Binder [7]). It was thus not possible to compare our approach with those. An exception is CARE [33]. The authors selected seven significant applications (e.g., VLC, Firefox). However, they did not reproduce experiments but rather executed commands. Thus, there is no experiment to be reproduced. Nevertheless, our platform supports the PLs of that commands.

The authors of E26 and E27 presented two case studies of complex, high-energy physics applications and showed how their framework could be useful for sandboxing, preserving, and distributing applications [43]. Although the authors make available the case study link <sup>26</sup>, only one case study is actually available. Nerveless, it is impossible to reproduce the experiment because they only distribute a software package for enabling large-scale distributed computing, and there is no expected

<sup>&</sup>lt;sup>26</sup>https://curate.nd.edu/downloads/5712m615h8d

result, so we cannot compare our approach with this.

CDE-SP's authors described a pipeline, identified by E28, they conducted to determine the overall performance of CDE-SP [48]. However, they do not make available the experiment code, so we cannot reproduce the same experiment.

SciInc's authors selected three use cases for their evaluation (E29 [15], E30 [23], E31 [27]), and it is possible to access the repository [62]. We can install and execute E29 and E31, but it is not possible to verify the computational reproducibility because there is no information about the commands executed and the expected results. E30 does not have information about the experiment, but we tried to execute the "Main\_Shell\_Script.scr" file in the root of the project. However, it was impossible to reproduce that file since it tries to access information inside the cmd folder, but there is no such folder in the repository, so not all the files from this repository have been published.

The other three experiments we could not reproduce (E8, E10, E17 and E23) have different causes. For E8, the problem was due to not finding a Java class during the execution, E10 does not exchange information between the database and the functions of the experiment, for E17, the necessary dependencies have been installed, but the data needed to run the experiment is not available. We asked permission to access the CheXpert<sup>27</sup> portal; however, it was impossible to find the files inside the portal. For E23, there is no information about how to install the project, so we tried to install the project using "python setup.py install" command, however, during the installation, some files were missing.

Nevertheless, from the 31 chosen experiments, four of them are packages, and two do not have available the source code, so only 25 experiments are available to be reproduced. We were able to successfully install the required dependencies, execute, and create a reproducibility package for 20 of 25 (80%). Note that we were not even able to run E8, E10, E17, E23 and E30 on our computer (without the platform), and thus we feel confident stating that this was not an issue of our platform.

The execution of the experiments went smoothly. However, although the repositories included the command lines to execute the code, they did not have the expected results, so the verification of the reproducibility became more difficult, but we managed to compare our results with the claims of developments in the paper.

We are confident the challenges described in section 2 (C1, C2, C3) are well addressed by our approach.

Software (C1) is the biggest problem when addressing reproducibility. Our proposal allows users to build a complete container of the project, which will make it available for reuse by other researchers. In this way, it is possible to execute the same computational environment, even when some dependencies are not publicly available anymore. This addresses principles P1 and P2.

Command (C2) implemented in our approach allows researchers to configure the execution of experiments and execute the experiment with the same parameters. The results achieved by previous executions can be used as a means of comparison to validate the computational reproducibility. Principles P3 and P4 are tackled in this part of the work.

Data (C3) is handled in the platform by providing a mechanism to allow researchers to manage the data of the experiment. This was also our principle P5.

Our approach is able to deal with a diversity of PLs (and their dependencies) used by researchers. Furthermore, it supports a variety of experiments, from the execution of simple scripts to the execution of more complex experiments (e.g., involving databases or several PLs). Thus, we can say principles P6 and P7 are also addressed by our proposal.

Moreover, the reproducibility package that can be obtained from the platform can be easily shared as it corresponds to a compressed file with just two files. By executing one, with a simple double-click, the entire experiment is executed. The only requirement is that docker, which is available both for Unix and Windows systems, is installed and running. Thus, we have reduced the problem of re-execution to having to install a single software tool, the most used for container management. Thus, principles P9 and P10 are also addressed.

<sup>&</sup>lt;sup>27</sup>https://stanfordmlgroup.github.io/competitions/chexpert/

Our approach is the backend of a platform, not providing a user interface. Thus, principle P8, which we consider a very important one, is not yet supported by our work. Nevertheless, we plan to design and build such an interface in future work [19].

# 7 Threats to Validity

The validation process has some threats divided into 4 sections [16, 60] addressed next.

## Conclusion validity

**Random heterogeneity of subjects** We tried to collect a variety of experiments, including experiments with only one PL and experiments with more than one, and with and without the use of databases. Moreover, we have selected experiments from different scientific fields, including climate change and medicine. Thus, our subjects are relatively heterogeneous and represent a sample of published scientific experiments.

### Internal validity

**Instrumentation.** The computational environment is only briefly described by the authors of the experiments we used, so it is more difficult to try to infer what dependencies and which versions were used in the execution of the original experiment. Thus, there is the risk that we have executed the experiments in slightly different conditions. Nevertheless, we were able to validate the results we obtained with the ones in the papers, and thus this risk is quite low.

### **Construct** validity

**Restricted generalizability across constructs.** Our approach improves computational reproducibility, however, for some experiments it is necessary to have more storage and computational power. Thus, we were not able to validate our approach with such demanding requirements. Nevertheless, most of the experiments we analyzed during this work did not have such restrictions and thus could potentially be executed within our platform.

### External validity

**Interaction of selection and treatment.** We collected a set of experiments from different computer science areas, however, we do not have experiments from domains other than computer science. Nevertheless, from experience, we know that at least in some areas it is not common to report the computational setting and thus it was not possible to find experiments from other domains. Moreover, the experiments we used are quite complex (e.g., in terms of (the number of) PLs used, databases, etc.) and thus we are confident that our platform can cope with experiments from other domains.

# 8 Related Work

There have been some tools proposed to aid researchers in making their computational experiments reproducible. We discuss them now based on their capabilities.

# 8.1 Supported PLs

Researchers perform experiments using a variety of PLs, so it is essential that the platform or the tool used can support such experiments. Some related works such as Encapsulator [47], Binder [7], RenkuLab [37], Whole Tale [4], Open Lab [53], VisTrails [24], RunMyCode [54] or the work by Haiyan [43] support only a limited set of PLs and are not extendable, so it is impossible to support

new PLs. However, CDE-SP [48], CARE [33], SciInc [62], and ReproZip [10, 12, 11] support an unlimited set of PLs.

#### 8.2 Automatic installation of dependencies

We see in section 2, that one of the main challenges in computational reproducibility is to install the required dependencies and library correctly. In this way, it is crucial that the platform can infer and install all the necessary dependencies and libraries to execute the code in the same way as the owner of the experiment.

ReproZip [10, 12, 11], VisTrails [24], CDE-SP [48], CARE [33], SciInc [62], and the work by Haiyan [43] can automatically track and identify all the required dependencies, binary files, code, data, and files needed to execute the code. Furthermore, Encapsulator [47] employs observed provenance capture to gather detailed provenance information and expose the underlying mechanisms of an analysis script. This process involves capturing fine-grained provenance data.

Binder [7], RenkuLab [37] and Whole Tale [4] are limited approaches because the researcher needs to install all the required dependencies in the platform.

#### 8.3 Supported databases

In general, computational experiments do not have databases integrated. However, complex experiments that involve databases are harder to reproduce, because reproducible tools do not support these experiments. ReproZip [10, 12, 11] is the only approach that supports experiments that have integrated databases.

#### 8.4 Configure the execution of the experiments

Making available all the information to allow computational reproducibility is essential to reproduce the same results; such information includes the values of the parameters used in the execution of the experiment.

One way to easily make this information available is to be possible to share the parameter spaces explored. Open Lab [53], VisTrails [24], Whole Tale [4], ReproZip [10, 12, 11], RunMyCode [54] are approaches that make it possible because the owner of the experiment can share the same parameter spaces explored with other researchers and making the process of the configuration of the experiment easier in the reproduction.

#### 8.5 Reproducible package

Docker offers greater reliability and flexibility, as well as being lightweight and capable of maintaining its own data and memory [3, 31]. By utilizing container images, Docker enables faster start-up times and efficient utilization of resources such as RAM and disk. This is due to the shared files and layered file systems that are inherent to containerization. By using this technique, it is possible to share a capsule with all the information needed to execute the experiment in the same way without the need to use another platform besides Docker.

Encapsulator [47], SciInc [62], ReproZip [10, 12, 11], CARE [33], VisTrails [24], CDE-SP [48], and the work by Haiyan [43] are approaches that automatically package everything required to execute the same experiment in another machine without the use of a specific platform.

Binder [7], RenkuLab [37] and Whole Tale [4] create a Docker image of the repository, but one needs the original platform to re-execute the code. Open Lab [53], RunMyCode [54] are approaches that, such as the previous one, it is necessary to re-execute the code on the platform, however, they do not use virtualization.

#### 8.6 Replicability of results

Replicability and reproducibility are two concepts that produce the same result, but using different methods, code or data. In all the related work approaches is not possible to mark or associate

a dataset to each execution, making the comprehension of the dataset used harder in future executions. In this way, all the related work approaches do not validate the replicability of results.

### 8.7 Validation of results

Validating the results stated in publications is hard work. Researchers have to run the experiment, read the results section, and compare the results obtained with the results stated in the publication. It was advantageous for the researchers to enter what the expected result was in the run and in each run this comparison was made in order to prove the reproducibility of results. However, the approaches in the related papers do not support this functionality.

#### 8.8 Supported operating system

Researchers build their experiments in their favorite Operating Systems (OS), so it should not be a limitation when we intend to reproduce an experiment. Binder [7], RenkuLab [37], Whole Tale [4], Open Lab [53], VisTrails [24], RunMyCode [54] and Encapsulator [47] are approaches that support all the Operating Systems, so it is not a limitation. However, Encapsulator [47], SciInc [62], CARE [33], ReproZip [10, 12, 11] and the work by Meng et al. (2015) are approaches limited to the Linux environment. This might prove problematic for many scientists who do not use Linux. Furthermore, CDE-SP [48] only supports Linux and Mac OS environments.

We conclude that the main platforms and approaches for sharing and computing research data are focused on specific domains and thus they are not able to reproduce complex experiments (using several environments, databases, etc.) or are not user-friendly platforms. In table 2 and table 3 we synthesize the characteristics of the methods and tools that we have just described.

## 9 Conclusion

Our approach is designed to support researchers in ensuring their research is reproducible and transparent during their study and in preparation for publication. One of the biggest obstacles to achieve this is creating the same computational environment, configuring it correctly, reproducing the experiment, and verifying its computational reproducibility.

We propose a solution to address these challenges and assist researchers in developing the experiment and preparing a reproducibility package to accompany their paper. This will enable reviewers and others to rerun the experiments. Our evaluation of the approach revealed that we successfully recreated and reproduced 20 out of 25 experiments, demonstrating that our methodology and backend platform can easily recreate, reproduce, and share experiments.

Currently, we are developing a frontend interface to enable researchers to create reproducible packages with ease [19]. Moreover, we plan to further study how to make the sharing of data among experiments easier for researchers, but also for the community in general [18].

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Publication	PLs	Database	Repository link	Dependencies description	How to execute	Repro- duced	Identifie
	Unix		<b>T</b> • • •	,		,	
Adnan et al. (2022)	Shel- l/Python	×	Link	1	1	1	E1
Bai and Zhao (2022)	Python	×	$\underline{\mathrm{Link}}$	×	1	1	E2
Chauhan et al. (2022)	C++/Pythor Unix Shell	×	Link	×	1	1	E3
Sun et al. (2022)	Python	PostgreSQL	Link	×	1	1	E4
Zhou et al. $(2022)$	Č++	X	Link	1	1	1	E5
Chen et al. (2022)	Python	×	Link	1	1	1	E6
	Java/Python						
Kukucka et al. (2022)	Unix Shell	×	Link	1	1	1	E7
Nguyen and Grunske (2022)	Python/Java	×	Link	1	1	×	E8
Xie et al. (2022)	Python	×	$\underline{\mathrm{Link}}$	$\checkmark$	1	1	E9
Zhang et al. $(2022)$	Java	MySQL	$\underline{\text{Link}}$	1	×	×	E10
Edwards (2022)	R	×	Link	1	Package	NA	E11
Hemes (2023)	R	×	$\underline{\text{Link}}$	1	×	1	E12
Jehn (2021)	Python	×	$\underline{\text{Link}}$	×	×	1	E13
Lin (2023)	Python	×	Link	×	1	1	E14
Qasmi and Ribes (2021)	R	×	$\underline{\mathrm{Link}}$	1	Package	NA	E15
Fries (2021)	Python	×	Link	×	1	1	E16
Han (2021)	Python	×	$\underline{\text{Link}}$	1	1	×	E17
Hoyt (2018)	Python	×	$\underline{\text{Link}}$	1	1	$\checkmark$	E18
Kailas et al. (2022)	Python/Unix Shell	×	Link	1	1	1	E19
Trueto (2021)	Python	×	$\underline{\mathrm{Link}}$	1	1	1	E20
Prezja (2023)	Python	×	$\underline{\text{Link}}$	1	Package	NA	E21
Santucci (2023)	Python	×	$\underline{\text{Link}}$	×	×	1	E22
Erickson (2019)	Python/Unix Shell/ C++	×	Link	$\checkmark$	1	×	E23
Coupette et al. (2022)	Python /Jupyter Notebook	×	Link	1	×	1	E24
Pala and García-Cuesta (2023)	Python	×	Link	1	×	1	E25
Tovar et al. (2023)	Python/ C/Unix Shell	×	Link	1	Package	NA	E26
Meng et al. $(2015)$	_	_	No info	_	_	NA	E27
Pham et al. $(2015)$	—	_	No info	_	_	NA	E28
Collins et al. $(2023)$	R	×	$\underline{\mathrm{Link}}$	1	1	1	E29
Essawy (2023)	Python/Uniz Shell	×	Link	×	×	×	E30
Hai (2023)	Python	SQlite	Link	×	×	1	E31

Table 1: Sample of reproducible experiments (NA stands for Not Applicable)

	Binder	Renku- Lab	Whole Tale	Repro- Zip	Open Lab Me	Vis- Trails	RunMy- Code	Our
Unlimited PLs	×	×	X	1	Х	Х	×	1
Researcher-friendly platform	1	×	1	×	1	1	1	×
Data management	1	1	1	$\checkmark$	1	1	1	1
Supports databases	×	×	×	1	×	×	×	1
Supports experiments from differ- ent fields	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	1
Automatically infers dependencies	×	×	×	1	×	1	×	$\checkmark$
Automatically infers PLs	×	×	×	1	×	×	×	$\checkmark$
Automatically installs necessary dependencies	$\checkmark$	$\checkmark$	$\checkmark$	1	×	1	×	1
Configures execution of experiments	×	×	1	1	1	1	1	1
Creation of reproducibility package	×	×	×	1	×	1	×	1
Reproducibility package executed anywhere	×	×	×	1	×	1	×	1
Validation of results	×	×	×	×	×	×	×	1
Supported operating system	All	All	All	Linux	All	All	All	All

Table 2: Comparison of characteristics of reproducibility tools with Graphical User Interface (GUI)

Table 3: Comparison of characteristics of reproducibility tools without GUI (only command line interface)

	CDE-SP	Encapsulator	[43]	CARE	SciInc	Our
Unlimited PLs	1	×	×	1	1	1
Data management	×	×	×	×	×	1
Supports experiments from differ- ent fields	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	1
Supports databases	×	×	×	×	×	1
Automatically infers dependencies	1	1	1	1	1	$\checkmark$
Automatically infers PLs	1	×	×	1	1	$\checkmark$
Automatically installs dependencies	$\checkmark$	$\checkmark$	1	1	1	1
Configures execution of experi- ments	×	×	×	×	×	1
Creation of reproducibility package	1	1	1	1	1	1
Reproducibility package executed anywhere	$\checkmark$	$\checkmark$	1	1	1	1
Validation of results	×	×	×	×	×	1
Supported operating system	Linux/Mac OS	All	Linux	Linux	Linux	All