Entwurf eines Frameworks zur Unterstützung von Reproduzierbarkeit für die OpenEO Plattform

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Bernhard Gößwein

Matrikelnummer 01026884

an der Fakultät für Informatik

der Technischen Universität Wien

Betreuung: Ao.Univ.Prof. Dipl.-Ing. Dr.techn. Andreas Rauber
Mitwirkung: Dr. Tomasz Miksa

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Bernhard Gößwein   Andreas Rauber

Designing a Framework gaining Repeatability for the OpenEO platform

DIPLOMA THESIS

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Bernhard Gößwein

Registration Number 01026884

to the Faculty of Informatics

at the TU Wien

Advisor: Ao.Univ.Prof. Dipl.-Ing. Dr.techn. Andreas Rauber
Assistance: Dr. Tomasz Miksa

Vienna, 1ˢᵗ January, 2001

_____   _____
Bernhard Gößwein   Andreas Rauber

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Bernhard Gößwein
Vorderer Ödhof 1, 3062 Kirchstetten

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Kurzfassung

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Abstract

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Introduction

1.1 Motivation

Over the last decades remote sensing agencies have increased the variations of data processing and therefore the amount of resulting data. To preserve the data for further usage in the future it is necessary to have citable data and processes on the data to ensure repeatability in a long-term.[30] Reproducibility is discussed in many science areas such as computer science, biology and also in computational geoscience. According to [26] where the reproducibility and replicability of scientific papers in geoscience got tested, only half of the publications were replicable and none of them reproducible. In [18] a survey of geoscientific readers and authors of papers got executed, with the goal of finding reasons for the lack of reproducibility in earth observation sciences. One of the results is that even though 49% of the participants responded that their publications are reproducible, only 12% of them have linked the used code. The understanding of open reproducible research is different among the participating scientists in a way that the interpretation is more related to repeatability and replicability. The main reasons for the lack of reproducibility in computational geoscience are, according to [18], insufficiently method descriptions, persistence of data identifier, legal concerns, the general impression that it is not necessary and too time consuming. Reproducing geoscientific papers failed by the different individual interpretation of the approach and alternative software versions that produce unequal results. The vast majority of issues on reproducing results are required changes of code and a deeper understanding of the procedures. In some cases there occur system dependent issues related to the usage of random access memory and installation libraries of the operating system. [18]

1.2   Problem Description

The vast majority of data used in earth observation sciences are retrieved and provided via Service Oriented Architecture (SOA) interfaces. Data Provider like Google Earth Engine[1] and EODC[2] host an Web Application Programming Interface (API) for data download and processing data. Due to a different range of functionality and a difference between the endpoints of the providers it is great afford to create a workflow for more than one provider. The OpenEO project has the goal to be an abstraction layer above different EO data providers. The underlying structure of OpenEO consists of three parts:

- **Client Module**: Is written in the program language of the user and transfers the users commands to the backends.

- **Core Module**: A standard on how the communication should take place between client and backend.

- **Backend Module**: The provider of the data and the services, which gets the instructions from the clients and returns the results.

Further information on the software architecture of the project is defined in the project proposal ([27]) and in section 3. On the creation time of this thesis there is no consideration of repeatability in the OpenEO architecture. Verification of work-flows for users of OpenEO is not in the agenda of the OpenEO project. Generalized layers have the opportunity to be implemented in a way that makes processes and data scientifically verifiable and reproducible, because it handles data and processes on the data in a standardized way for different providers. Even though the range of functionality and the API endpoints are well-defined in the OpenEO core-API, the contributing content providers (OpenEO back ends) will have different underlying software execution environments. The used technology of an OpenEO back end will evolve in the future, hence it can lead to different results on the same workflow execution. Considering the following: A scientist runs an experiment using OpenEO as research tool and gets an arbitrary result. The same scientist runs the same experiment with the same input data some months later and gets a slightly different result. The question occurs, why are the results distinct? Has the used data changed, has the user accidentally submitted different code or has some underlying software inside the back end provider changed. Adding a possibility for the users of OpenEO to gain this information is an important feature for the scientific community. The aim of this thesis is to design an extension to OpenEO, so that users are able to retrieve provenance data about a job re-execution. [27]

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[1]https://earthengine.google.com
[2]https://www.eodc.eu

1.3 Aim of the Work

The expected outcome of this thesis is to discover and develop a possible framework for making repeatability conceivable in the OpenEO project. This enables users to re-execute work-flows and validate the result, so that differences on the process or data are visible for the users. To achieve this goal a model for capturing the provenance of the back ends within the project has to be discovered and implemented to evaluate the ability of the model. The solution shall then conclude recommendations for the OpenEO project on how to improve re-execution validation for the users and how it can be achieved. Considering the problem description and the recommendations above, the following research questions can be formulated:

- **How can an OpenEO job re-executed be applied like the initial execution?**

  - How can the used data be identified after the initial execution?
  - How can the used software of the initial execution be reproduced?
  - What data has to be captured when?
  - How can the result of a re-execution in future software versions be verified?

- **How can the equality of the OpenEO job re-execution results be validated?**

  - What are the validation requirements?
  - How can the data be compared?
  - How can changes of the OpenEO backend environment be recognised?
  - How can differences in the environment between the executions be discovered?

1.4 Use Cases

To validate the design proposed in this thesis, there are use cases defined in the following sections. They describe scenarios about stakeholders of the OpenEO project that are currently not possible, but may be accomplish-able with the solution of this thesis.

1.4.1 Re-Use of Input Data

The first use case is about the re-use of input data between job executions. Reproducible methods are especially important for the scientific community. Since scientists are likely to build on results or methods of publications, it is an opportunity for OpenEO to make the re-use simple. In this case a scientist creates a publication by using OpenEO and citing the method and data accordingly. Another scientist in a similar area of research wants to use the same input data but use a different approach of processing it. Hence
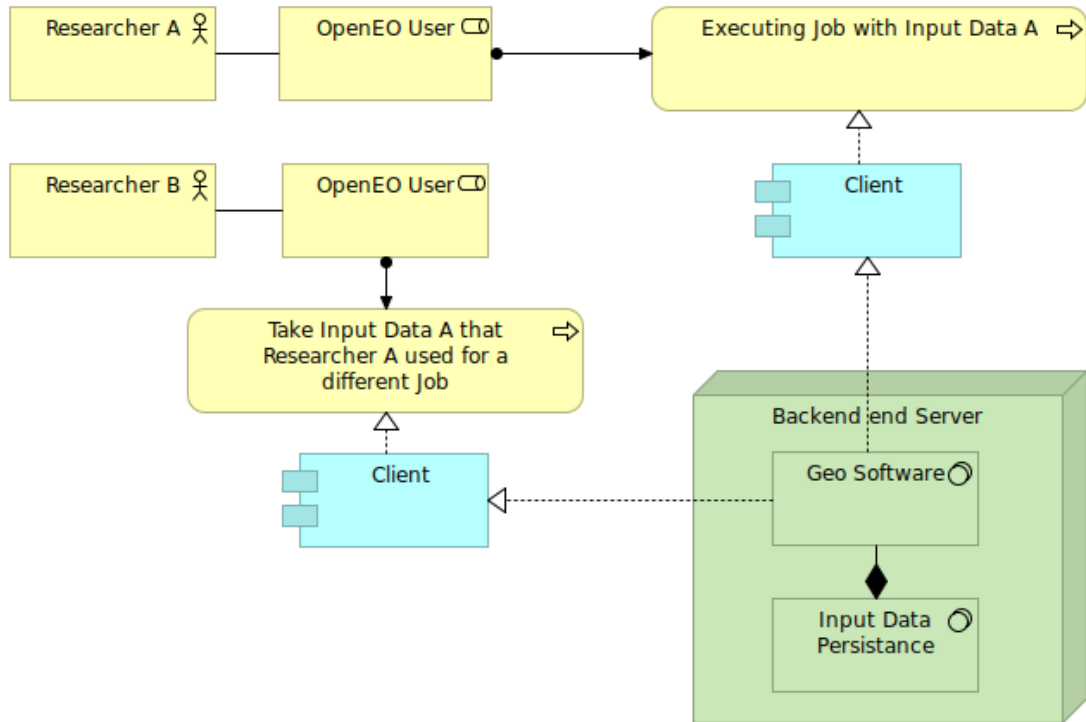
Figure 1.1: Overview of the first Use Case

there needs to be a possibility to cite the input data in a way, that another user can re-use it in a different processing chain. An overview of the architecture of the use case can be viewed in figure 1.1.

1.4.2 Providing Job Execution Information

This use case is like the first one, but is only about job dependent environment information. The back end provider can automatically get provenance data about the job execution, like used software packages and their versions. The user gets additional information on a job execution. Motivation for this is to add transparency of the job processing for the users, so that researchers can describe their processes in more detail. It can also help OpenEO users to understand why results differ from executions in the past. An overview of the architecture of the use case can be viewed in figure 1.2.

1.4.3 Compare different Job executions

The third use case is dedicated to the OpenEO users. The goal is to add a possibility for users of OpenEO to compare different jobs not only by their results, but also on the way they were executed. The comparison is between a job execution and another one on the same back end. Therefore, the processing and the input data has to be identifiable. To
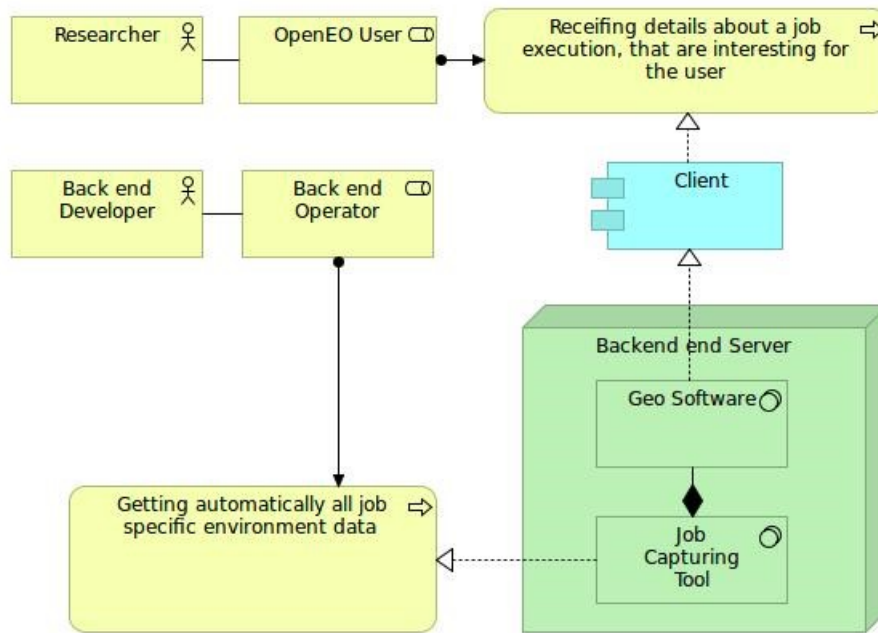
Figure 1.2: Overview of the second Use Case

make the comparison interesting to the users there also has to be additional information. For usability the comparison needs to be easy to apply and easy to understand, therefore accessible in the environment of the user at the OpenEO client. In addition to the previous conditions a visualization of the differences for the users can lower the access barrier for users to use the feature. An overview of the architecture of this use case can be viewed in figure 1.3.

1.5 Methodological Approach

The use cases defined in the previous section require specific changes to the components of OpenEO. In the following list parts of the suggested solution are briefly described.

1. **Data Identification** In order to accomplish the capturing of processing workflows described in the use cases in section 1.4, the input data has to be identifiable. In order to achieve this the recommendations of the RDA (see [31]) have to be implemented by additional versioning and query databases.

2. **Process Versioning** To accomplish the verification of different process executions, the process has to be identifiable. Therefore, a versioning of the process code can be used to persist different states of the code. The thesis is for an OpenSource project and the code of the back ends are published at Github, so Git is used as the tool to capture the code state.
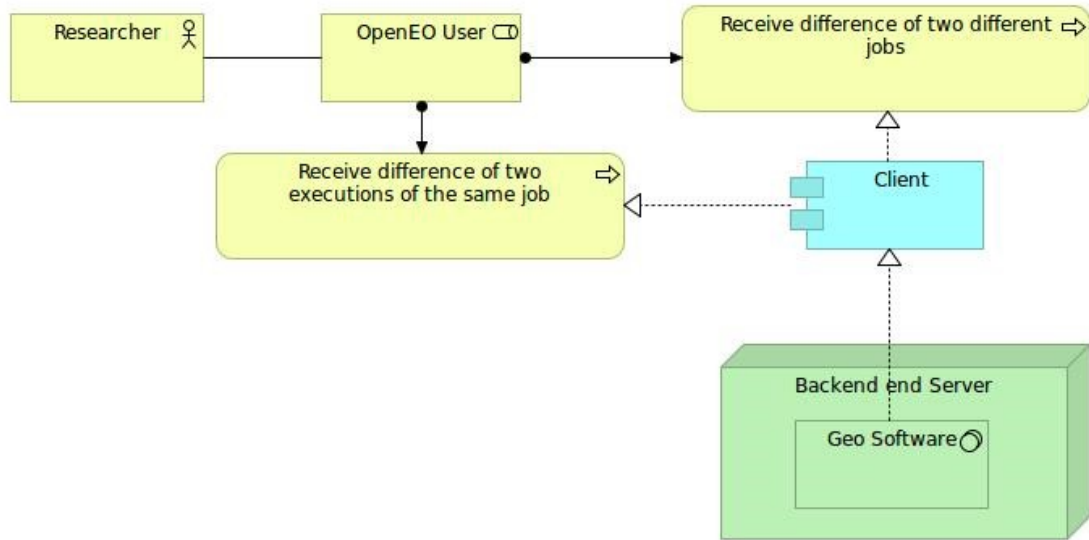
Figure 1.3: Overview of the third Use Case

3. **Additional Information** In order to gain an description of interest for users of OpenEO some additional environment information about the data and the code gets persisted. This information is forwarded to the user and visualized.

4. **User Endpoints** The interface for the user has to be implemented so that the use cases can be executed by the users. Therefore, the OpenEO client and core API has to be modified. The adapted client in this thesis is the python client.

1.6   Structure of Work

The following sections are structured as follows:
Chapter 2 gives an overview of related scientific activities in the area of reproducibility in the earth observation sciences and reproducibility in other areas with similar objectives.
Chapter 3 describes the technologies and concepts that are used in the implementation of this thesis. This chapter also provides an overview of the EODC back end used for the implementation.
Chapter 4 provides the concept to address the research questions defined in section 1.3. This is the theoretical definition of what has to be implemented in the OpenEO project.
Chapter 5 has a detailed explanation to the proof of concept prototype implementation and how the concept of chapter 4 was realized for the EODC back end.
Chapter 6 dives into the evaluation of the implementation by applying the use cases to the implementation of chapter 5.
Chapter 7 summarizes the outcome of the implementation and evaluation. It contains a discussion about possible flaws and future work.

CHAPTER 2

Related Work

2.1 Reproducibility

According to [40] reproducibility is defined as the re-run of an experiment by a different researcher in the manner of the original experiment. Repetition on the other hand is the re-run of the exact same experiment with the same method, same environment and very similar result. Reproducibility is a common problem in all scientific areas. It is an issue of the whole scientific community to produce results that are reproducible. Therefore in [34] there are ten rules defined to gain a common sense about reproducibility in all science areas. They consist of the basic idea that every result of interest has to be associated with a process and data used. External programs have to be persisted as well as custom script versions. The usage of version control is recommended. In addition there is a rule defined to make the scripts and their results publicly available. [34] Reproducibility is also the key element of The Fourth Paradigm published in [13]. It leads to the term eScience, which has the aim of bringing science and computer technologies closer together. The general concept is to enable scientific procedures in the new information technologies used by data intensive sciences. The expected result of eScience is to get all scientific papers publicly available including the necessary data and processes so that scientists are able to have a fast interaction with each other. [13] eScience has the potential to enable a boost in scientific discovery by providing approaches to make digital data and work-flows citable. In [33] is a common way of reaching the goal formulated above. It describes an approach to look at whole research processes, other than only data citation by introducing Process Management Plans. The capturing, verification and validation of the input data for a computational process is also demonstrated within the paper.[33] Computer sciences have the issue of a high amount of published papers that are not provided by enough information to make them reproducible. The problem will not be solved by the scientists that need to do additional afford to make reproducibility possible, but by providing new tools for scientists that allow it automatically as stated in [22].

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There are some additional issues on reproducibility in computer science like that the used software technologies are deprecated and not available any more. Therefore persisting the execution context is critical to make a re-execution of the experiment possible. One proposed concept of doing so is the VFramwork described in in more detail in the method section 3.

Data citation is a key issue of reproducing results of past experiments. Preserving the exact process without persisting the original data is no real gain for the scientific community. If the data used in an experiment is not available anymore, or not specified explicit enough then there is no chance of reproducing it no matter how much information about the execution was persisted. In earth observation persisting the data for reproducibility in the future is an issue discussed in [30].Gaining data identification in digital sciences has an official working group named Working Group on Data Citation (WGDC), which created 14 recommendations on data citation further explained in section 3.4.

2.1.1   PROV-O

In 2003 the World Wide Web Consortium published the PROV model as a standard for provenance definitions. It is defined by twelve different documents. In the context of this thesis the PROV Ontology (PROV-O) is the most relevant. [2] PROV-O is a standard language used to describe OWL2 Web Ontology. It is designed as a lightweight concept to be used in a broad spectrum of applications.
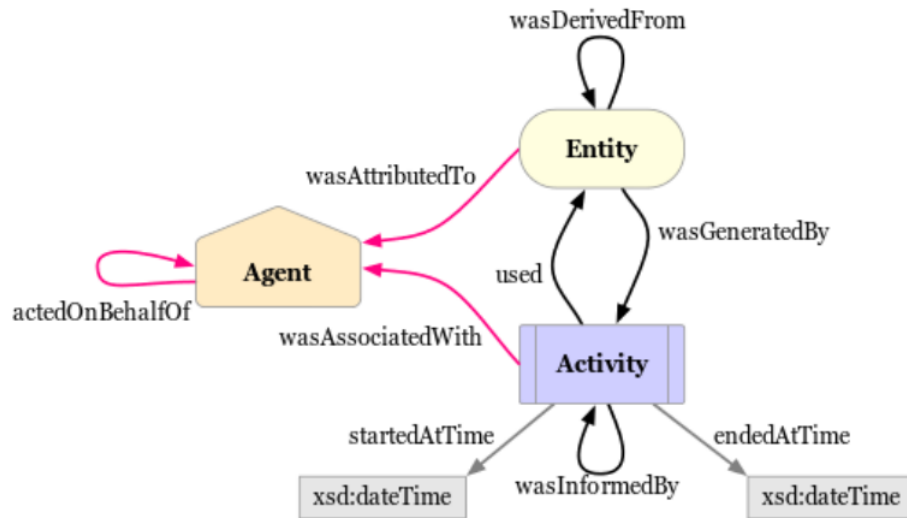
Figure 2.1: Overview of the main components of PROV-O [3]

In figure 2.1 there is the basic setup of the PROV concept. It consists of three main elements. The Entity is any physical, digital, conceptual thing. Provenance records describe Entities that can consist of references to other Entities. Another element is the Agent, which is responsible for Activities and that they are taking place. Examples for Agents are software, persons or organizations. The association of an Agent to an

Activity defines the responsibility of the Agent to the Activity. An Activity describes what happened that the Entity has come to existence and how attributes of an Entity changed.[2] In this thesis the PROV-O standard is not implemented, but since it is a reasonable extension it is mentioned in the future work section 7.2.

2.2 Earth Observation Science

Reproducibility is a well discussed topic of the computational geoscience. The high amount of earth observation data leads to complex research programs and therefore high complexity in the papers. According to [26] where the reproducibility and replicability of scientific papers in geoscience are tested, only half of the test group publications are replicable and none of them reproducible. There are publications to address this lack of reproducibility in the earth observation science. The sections below summarize some examples of earth observation communities progresses in terms of the lack of reproducibility.

2.2.1 Vadose Zone Journal (VZJ)

In order to face the issue of lacking reproducibility in geoscience the Vadose Zone Journal (VZJ) started a Reproducibility Research (RR) program in 2015. [38] The earth observation science is a big part of VZJ publications and most of them are not conform with the open computational science guidelines. The main reasons are behaviors of scientists that do not see the overall benefit of putting effort into documentation. Therefore the VZJ started an RR program to publish alongside the scientific paper also the code and data used by the scientists for evaluating the publication. This shall lower the access barrier for scientists to publish their research work entirely. Aim of the project is to create a community of researchers with a common sense of reproducibility and data citation on the platform and to animate other scientists to join the approach.[38]

2.2.2 The Geoscience Paper of the Future (GPF)

The geoscience paper of the future (GPF) is according to [11] a proposed standard to help geographical scientists by making reproducible publications. It defines recommendations on data management and software management, by introducing the reader to available repositories. The gain of it is applying concepts of open science and reproducibility to earth observation papers. A GPF needs to apply the following requirements:

- **Reusable data** in a public repositories and persistent identifiers.

- **Reusable software** (including software for preparing and post editing of the data) in a public repositories and persistent identifiers.

- **Documenting the computational provenance of results** in a public repositories and persistent identifiers.
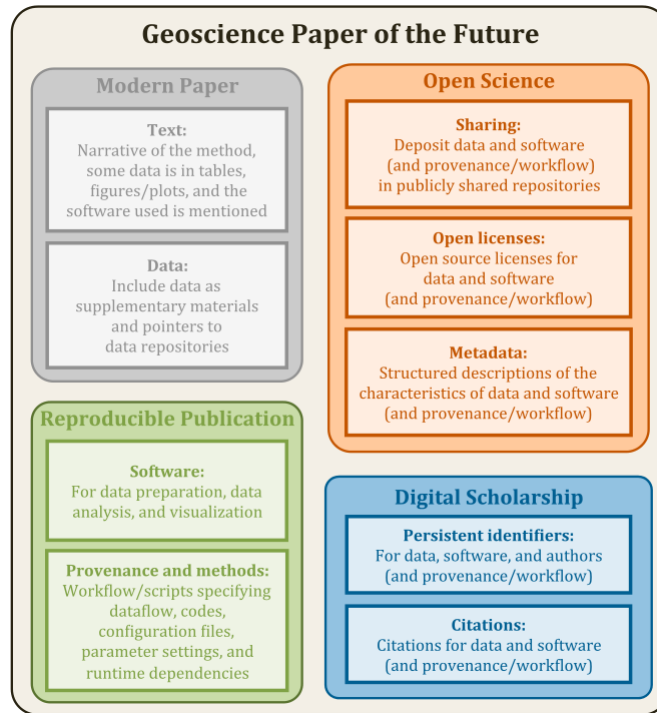
Figure 2.2: Comparison between reproducible publications and geoscientific papers of the future [11]

In figure 2.2 the differences with a reproducible paper gets visualized. In addition to the characteristics of the reproducible paper the GPF focuses on publishing the data publicly with open licenses with citable persistent identifiers. The GPF consists of a set of 20 recommendations for geoscientists regarding data accessibility, software accessibility and also provenance information.

2.2.3   Climate Change Centre Austria (CCCA)

The Climate Change Centre Austria (CCCA) is a research network for Austrian climate research online available since 2016 and has 28 members. The main tasks are the provision of climate relevant information, the inter-operable interfaces and long term archiving of scientific data. In 2017 the NetCDF data citation was added to the project. The set up of the data service and the technology used in the background is similar to the set up of the EODC back end. Therefore the process of enabling data identification was similar to this thesis. The concept used for gaining data citation was the RDA recommendations defined in [32] and can be viewed in figure 2.3. The main difference is the more complex architecture of the CCCA service compared to the EODC back end used for the OpenEO project. File formats also differ, because EODC uses GeoTiff instead of NetCDF at their back end. Nevertheless the concept of enabling data identification is similar in both projects.[36] CCCA is Open-source and available at GitHub, see [35].
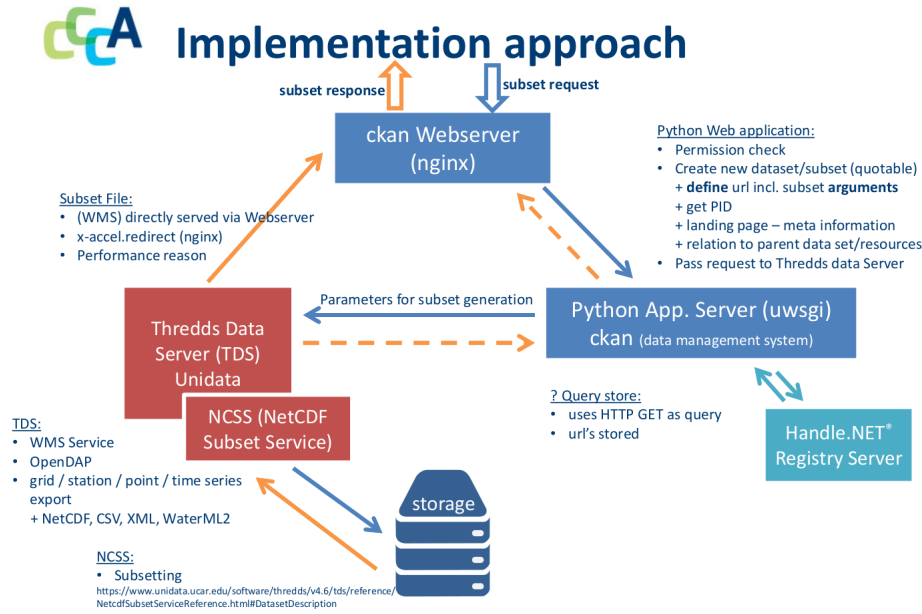
Figure 2.3: Concept of the CCCA NetCDF Cata Citation [36]

2.3 Existing Tools

In this section tools that are designed to solve similar problems like this thesis get summarized and described further. There is also an explanation why the specific tool was not used for the solution of this thesis.

2.3.1 Noworkflow

Noworkflow is introduced in [23] as a script provenance capturing tool with the aim to not influence the way researchers implement experiments. As proof of concept the noWorkflow command line tool got implemented for python. The provenance is captured in a SQLite database by different trials. A trial represents the environment information about one execution of the experiment.The main benefits of noWorkflow is that it does not instrument the code and it automatically captures the definition, deployment and execution provenance in a local SQLite database. The stored meta-data can be accessed via the command line interface of noWorkflow. In addition to just retrieving the information about the execution environment there is also analyses features added.[23]

The noWorkflow framework got improved regularly after the first announcement. In [29] an additional feature of tracking the evolution of the experiment execution is added. It improves the possibility to compare different trials of an experiment and to visualize the history of past executions. In [28] the fine-graned provenance tracking extension of noWorkflow is implemented. With it the execution of the python script can be viewed as a set of execution lines. It also adds a visualization of all called functions
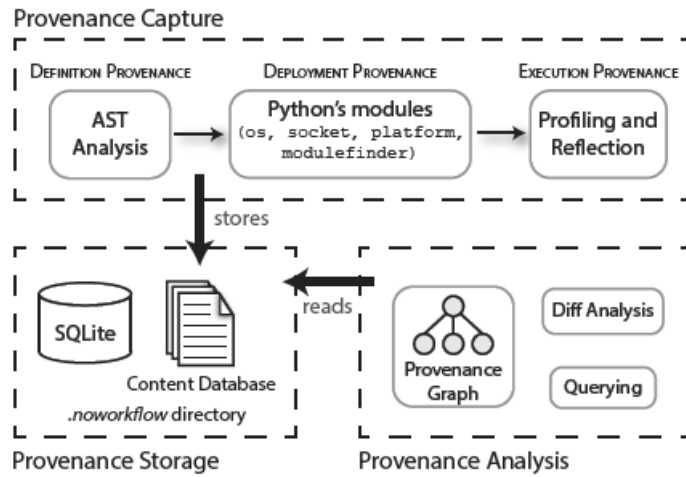
Figure 2.4: Architecture of noWorkflow [23]

with some limitations on multiple function calls in one line, dictionaries and lists. In [4] the provenance capturing of noWorkflow in combination of yesWorkflow, which gathers information about the provenance using comments and annotations (see [20]), got combined. The combination enabled a broader provenance information, querying and visualizations. In this thesis noworkflow is used in an alternative attempt of the implementation described in section 5.3.3, but is not part of the final solution due to reasons provided in 6.3.

2.3.2   ReproZip

ReproZip is a packaging tool to enable the reproducibility of computational executions of any kind. It automatically tracks the dependencies of an experiment and saves it to a package that can be executed on another machine by ReproZip. It is even capable of letting the re-executor modify the original experiment. It was developed for the SIGMOD Reproducibility Review. In figure 2.5 the architecture of ReproZip is shown in detail. It traces the system calls to create a package defined in the configuration file. So that a single file with the extension ".rpz" gets produced. These type of files can then be unpacked on a different machine and re-executed. The aim of ReproZip is to make reproducible science easy to apply for single experiments. [5] The reason why it is not used in the solution of this thesis, is that the capturing is very fine granulated and takes too much performance from the back ends, which is a key selling point for back end providers. The payment for users of OpenEO, depending on the back end, may have to pay by the duration time of the processing. Another issue with ReproZip in the context of this thesis is that it is not possible to capture the big data of the back ends within the package, because it would take too much space.
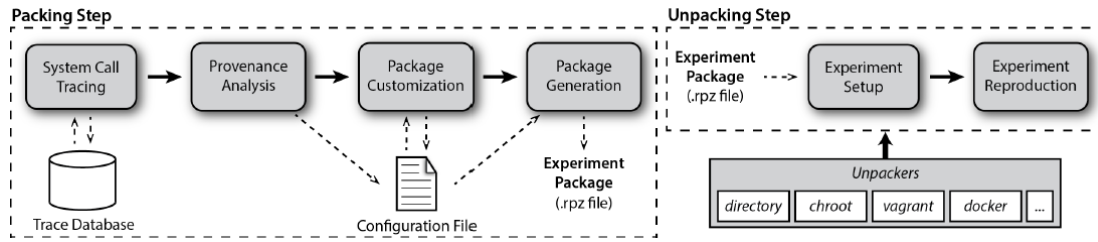
Figure 2.5: Overview of the ReproZip concept. [5]

2.3.3 Docker / Smartcontainer

Docker containers are very common in geoscience executions. The advantages on reproducible research and cost savings by using docker containers is discussed in [17] for the Geographic Object-Based Image Analysis (GEOBIA). The docker implementation of the image analysis was implemented with a docker image including a user interface that can be used by non-experts. There are experiments for the more general Object-Based Image Analysis (OBIA) with docker containers presented in [16]. Conclusion of the previous mentioned paper is very positive with only little shortcomings in the usability. The two papers mentioned above are using the docker images to make it easy to re-run an experiment on the OBIA system. Remaining question is how the docker configuration can be preserved in a manner so that it can be reproduced in different environments. The aim of [9] is to answer this question by introducing in addition to the Docker description file a workflow record saving the environment and entities involved. A SPARQL query got introduced to create the possibility to use the container as a repository of metadata. Another approach of preserving a docker container are smart container introduced in [14]. The aim of smart container is an ontology and software to preserve docker metadata. It uses the PROV-O standard to define the provenance. Docker containers are not part of the solution of this thesis, because the impact of the implementation shall not be too big for the back end providers. The solution has to be simple and general to be applied on all different back ends. Other back end implementations may use docker containers to apply the defined context model in 4.

Methodology

In this chapter the methodology used in the development of the solution of the thesis gets presented. In the following the reader gets informed about basic concepts used in the prototype implementation. The information is structured in subsections, where each is presenting different technologies or concepts.
In the first two sections there are technologies presented that are crucial for the concept of the design in section 4.
After that there are two sections presenting concepts used in the solution of this thesis. The last section of this chapter describes the OpenEO project further and more specifically the EODC back end, which is used for the proof of concept implementation.

3.1 Version Control Systems

Version control systems (VCS) became a very important part in all computational sciences. It enables to persist versions of code and the possibility to head back to a certain version of it. Before that programmers tend to have multiple directories to version the code. The basic idea of VCS is that via a command line interface it is possible to set a version of the current state of the code. These versions can be accessed in future, without changing other versions of the code and without multiple folders. [19] In this thesis Gitorious (Git) is used as version control system. Versions in git are defined as commits and are stored locally, but can be published to an external server, where, depending on the user rights, they are accessible for other users. The commits are stored locally and remotely. [1] In OpenEO Git is defined as the used versioning tool and GitHub is used as the publicly available server. Since OpenEO is an open source project, the code of every back end, core API and client is available at GitHub. In this thesis the Git commit and the GitHub repository is used as the identifier of code versions running at the back end.

3.2 Hash

Hash functions are used to validate the data without having to save the whole data. They have three important properties to work properly. First it has to be difficult that two different inputs have the same hash outcome. Second is has to be difficult to recreate the original input data from only the hash information. Last but not least it needs to be hard to find a message with the same hash value as an already known message. The properties described above makes the hash functionality a common tool to identify data without having to save the original one. [39] There are different hash functions available. In this thesis the SHA-256 is used for the metadata of the context model, mostly to compare differences in data outcomes.

3.3 VFramework

The basic concept of the VFramework is that the execution is done with parallel capturing of provenance data. During the original execution evidence gets collected into a repository. All of which is persisted in the context model of the execution. A re-execution can then be verified and validated using the provided provenance data in the context model of the original execution and the context model of the re-execution. The provenance data is divided into static and dynamic data. Static data defined in the VFramework is data that is not dependent on the execution of the experiment. The static environment information is therefore independent from the set up and the configuration of the execution. Dynamic data on the other hand has to be captured during the execution of the original experiment. It is the information specific for the workflow. [21] In figure 3.1 there is an overview of the VFramework concept.
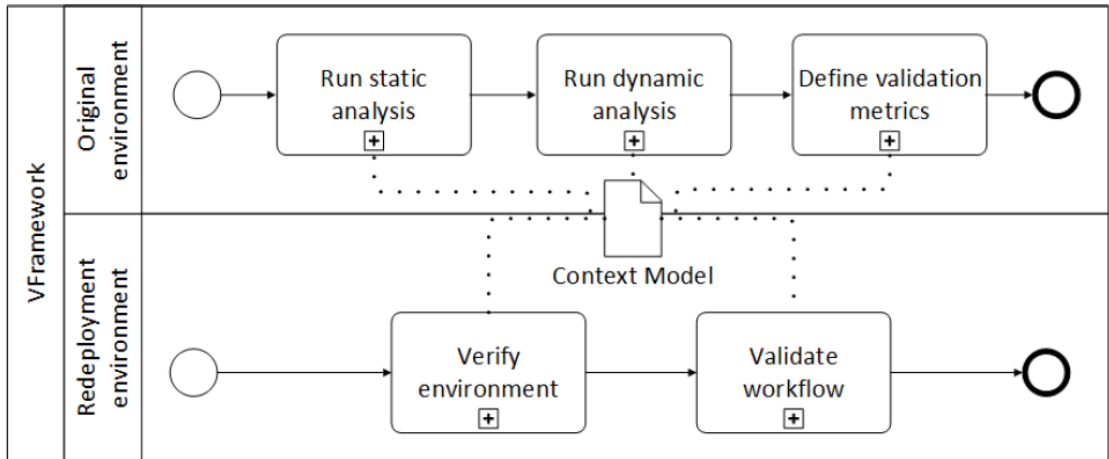

Figure 3.1: Overview of the Concept of the VFramework [21]

3.4 Data Identification

Data identification and citation is a main concern in many computer relying sciences. For the aim of this work, the input data is a key element of the capturing. If the input data can not be identified correctly, the capturing of the processing on it does not gain useful information. Therefore the identity of the data has to be guaranteed. The Research Data Alliance (RDA) presents general solutions to achieve data identifications. There are 14 recommendations defined to achieve the identification of an exact version and subset of input data. The recommendations are independent of the type of data and database. In the following the most important recommendations for this thesis get briefly introduced.[32]

- **R1: Data Versioning**
  Changes on a data record needs to result in new versions of the data record and the persistence of the deprecated data records. All data record versions need to be identifiable and accessible.

- **R2: Timestamping**
  All changes to the database have to be comprehensible via timestamps. So every time changes are applied to the data, there needs to be a timestamp when it happened.

- **R3: Query Store Facilities**
  There needs to be a query store implemented at the data provider to store queries including their metadata to be able to re-execute them in the future. The database has to store, according to [32] the following things:

  - The original query as posed to the database
  - A potentially re-written query created by the system (R4, R5)
  - Hash of the query to detect duplicate queries (R4)
  - Hash of the result set (R6)
  - Query execution timestamp (R7)
  - Persistent identifier of the data source
  - Persistent identifier for the query (R8)
  - Other metadata (e.g. author or creator information) required by the landing page (R11)

- **R4: Query Uniqueness**
  Since there should not be equal queries with the same result stored at the query store, there needs to be a normalized query that can be directly compared to other queries. Hence there needs to be a programming logic to normalize the queries and to enable their uniqueness.

- **R5: Stable Sorting**
  The sorting of the resulting data needs to be unambiguous and therefore reproducible.

- **R6: Result Set Verification**
  To ensure that the resulting data of the query is comparable there needs to be a checksum or hash key of it.

- **R7: Query Timestamping**
  There needs to be a timestamp assigned to every query in the query store, which represents the last update of the entire database or the query dependent data of the database.

- **R8: Query PID**
  Every query record in the query store needs to have a Persistent Identifier (PID). There must not be a query with the same normalized query and the same result checksum.

- **R9: Store the Query**
  The data described in previous recommendations have to be persisted in the query store.

- **R10: Automated Citation Texts**
  To make the citation of the data more convenient for researchers, there shall a generation of the citation text snipped including the query PID.

- **R11: Landing Page**
  The PID need to be resolvable in a human readable landing page, where all the data mentioned in the previous recommendations is provided to the scientist.

- **R12: Machine Actionability**
  Providing an API landing page so that not only humans, but also machines can access the metadata by query re-execution.

- **R13: Technology Migration**
  If the database where the query store is implemented needs to be mi grated to a new system, the queries need to be transferred too and have to be updated according to the new setup.

- **R14: Migration Verification**
  There shall be a service so automatically verify a data and query migration, to prove that the queries in the query store are still correct.

The implementation of the recommendations for the purpose of this thesis is described in section 5.1.

3.5 OpenEO

The OpenEO project contains of three modules, the client module written in the programming language of the users, the back end drivers that enables for every back end to understand the calls from the clients and the core API that specifies how the communication takes place. The core API is a standard that the back end providers accepted to implement on their systems. The back end drivers are the translation of the client calls to the back end specific API. This architecture decouples the clients from the back ends so that every client can connect to every back end that applies to the OpenEO core API standard see figure 3.2 . An example of a workflow would be that a scientist wants to run an experiment on the EODC back end and defines the processing with the python client in pure python code.[27]
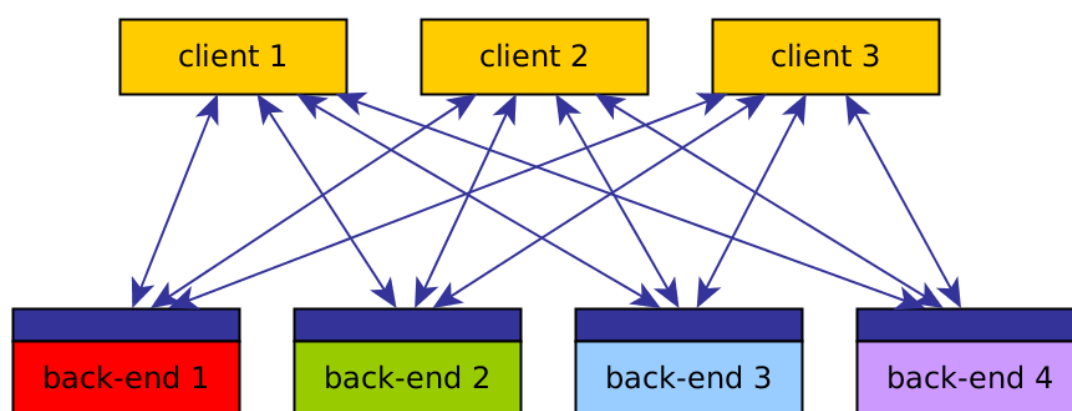
Figure 3.2: Overview of the OpenEO architecture. [24]

The communication is specified as an OpenAPI description, which is a way of defining RESTful communication in a standardized way. The definition consists of the possible end points at the back end and also the requests and the responses. The whole communication protocol is specified with OpenAPI.[37] In the following the relevant RESTful request types in OpenEO and the policy of choosing between them gets introduced.[24]

- **GET Request**
  GET requests are used to retrieve data from the back ends. The functionality is limited to read operations on the data records.
  (e.g. GET /collections returns a list of available collections at the back end.)

- **POST Request**
  POST requests are used to create new data records at the back end.
  (e.g. POST /jobs creates a new processing job at the back end.)

- **PATCH Request**
  PATCH requests are used to update an existing record at the back end.

(e.g. /PATCH /job/job_id modifies an existing job at the back-end but maintains the identifier.)

- **DELETE Request**
  DELETE requests are used to remove existing data records from the back end.
  (e.g. /DELETE /job/job_id removes an existing job from the back end.)

3.5.1 Job Execution

The job execution workflow in OpenEO starts at a client application that let the user define what has to be processed in the client specific programming language. The main part of the job execution definition is based on the description of what input data shall be used, which filters have to be applied and the processes that should be executed on the data. Therefore, OpenEO introduces the process graph, which is defined as a tree structure describing the processes with their data and the input data identifier. The input data id is back end specific. The process graph has a JSON format and gets generated by the clients in the background without users noticing it directly. In figure 3.3 there is an example of a process graph.

```json
{
    "process_id":"min_time",
    "args":{
        "imagery":{
            "process_id":"/user/custom_ndvi",
            "args":{
                "imagery":{
                    "process_id":"filter_daterange",
                    "args":{
                        "imagery":{
                            "process_id":"filter_bbox",
                            "args":{
                                "imagery":{
                                    "product_id":"S2_L2A_T32TPS_20M"
                                },
                                "left":652000,
                                "right":672000,
                                "top":5161000,
                                "bottom":5181000,
                                "srs":"EPSG:32632"
                            }
                        },
                        "from":"2017-01-01",
                        "to":"2017-01-31"
                    }
                },
                "red":"B04",
                "nir":"B8A"
            }
        }
    }
}
```

Figure 3.3: Proof of Concept process graph of the EODC back end for the OpenEO core API version 0.0.2 . [25]

The back ends interpret the process graph from inside out. In figure 3.3 the element in the center of the process graph defines the input data identifier in the "imagery" block, with the "product_id". In this case the "s2a_prd_msil1c" is chosen as input data identifier. After reading the input data id, the back end iterates one step up in the hierarchy of the process graph and calls the process "filter_bbox" with the parameters "left", "right" and so on. Every process beginning with "filter_" is a filter operation that specifies the selection of the input data. The output data of the previous process is the input data of the next process. In figure 3.4 the same process graph is visualized from the back end point of view, so the order of how it gets executed.

> Maybe change picture to 0.3.0 version if that is used in the future and update the text below
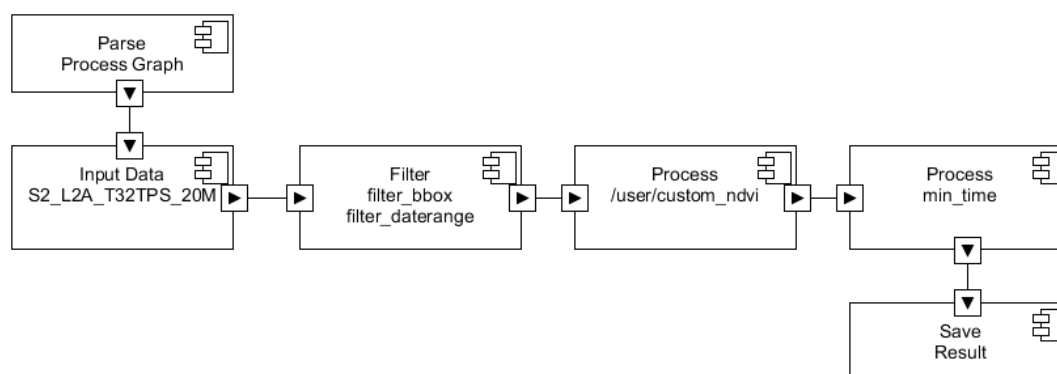

Figure 3.4: Action chain of the back end after receiving the process graph of figure 3.3

There are two different kinds of process executions depending on the back ends capabilities, synchronous and asynchronous calls. Synchronous calls are directly executed after the back end receives them and the user has to wait until the job is finished. For example on the python client the program waits after sending the process graph to the back end until the back end returns the result, which is directly returned to the user. An asynchronous call does not get executed until the user starts the execution on the back end through an additional endpoint call. When the processing is finished the user can download the result at another endpoint of the back end. For asynchronous calls there is also the possibility to subscribe to a notification system on the back end, so that the user gets notified when the job execution finished. The processes are defined at the OpenEO core API and therefore independent of the back end they get called at, other than the data identifier, which is different for every back end.

The previous example shows a process graph that only uses predefined processes and data. Within the OpenEO project there is the possibility to define individual processes and execute them on the back end. In the project they are called "user defined functions" and are at the writing of this thesis still not well-defined, but are basically code written by the OpenEO user that gets sent to the back end and executed there at a secure environment. The user can define processes and can run them with the data provided at the back end, using the infrastructure of the back end. Every back end has to individually define what

Table 3.1: List of all back end providers of the OpenEO project

Organisation	GitHub
EODC	`https://github.com/Open-EO/openeo-openshift-driver`
VITO	`https://github.com/Open-EO/openeo-geopyspark-driver`
Google	`https://github.com/Open-EO/openeo-earthengine-driver`
Mundialis	`https://github.com/Open-EO/openeo-grassgis-driver`
JRC	`https://github.com/Open-EO/openeo-jeodpp-driver`
WWU	`https://github.com/Open-EO/openeo-r-backend`
Sinergise	`https://github.com/Open-EO/openeo-sentinelhub-driver`
EURAC	`https://github.com/Open-EO/openeo-wcps-driver`

the restrictions on user defined functions are. [10]

3.5.2 Back end Overview

Even though the back ends implement the OpenEO core API standard, they are still diverse behind this abstraction layer. Some back ends have already an API, where the OpenEO calls have to be adapted to. There are 7 partners within the OpenEO project that are implementing a back end driver. The back ends have to manage the translation of the process graph to the actual code that executes the defined process chain. The billing of the users can be completely different on every back end. In table 3.1 there is an overview of all contributing OpenEO back ends and the related GitHub repository.

3.5.3 EODC Back End

The EODC back end is one of the contributing back end providers of the OpenEO project. It is in general a python implemented back end that uses virtualisation technologies for the job execution. The overlaying technology is OpenShift (using Kubernetes) [12], which is capable of scaling docker containers and handles the execution of them. In the docker containers the python code for the processing gets executed. The docker description files and the python code is available on GitHub[1]. In this thesis the latest version of the EODC back end provided in GitHub with the version 0.0.2 is used. In this version every process of the OpenEO process graph is represented by an own docker container and python code of the processing. The service layer for accessing the back end is accomplished by the python library Flask. Even though EODC has a lot of already processed data, it only uses data from Sentinel 2 and Sentinel 1 in OpenEO. The provided data are satellite images from the European Space Agency (ESA), which gets the raw data coming directly from the Sentinel satellites.

The data management of EODC is file-based, so every image data is stored in a unique directory and filename combination. Meta-data is provided at via a PostgreSQL database

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[1]https://github.com/Open-EO/openeo-openshift-driver/tree/release-0.0.2

including the PostGIS[2] plug-in. The provided query tool for EODC users is the OGC standard interface CSW[3]. In figure 3.5 an overview of the EODC meta-database is displayed. The structure is retrieved from the github repository of the EODC back end [10], where every database entity is defined. Every Process entity can have parameters desribed by the Parameter entity. The ProcessNode is representing one node in a process graph and is therefore related to exactly one ProcessGraph entity. Every Job has a related process graph, there may be jobs that use the same process graph, but in the current set up they are persisted both in the database.
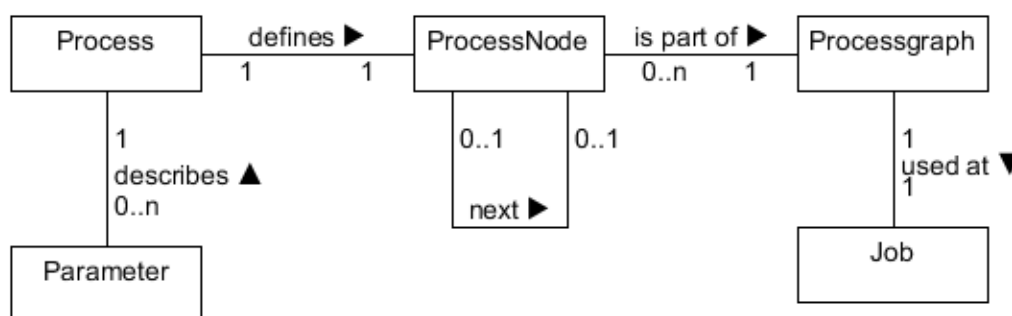
Change github link and text if switch to version 0.3.0

Figure 3.5: Overview of the EODC meta-database structure.

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[2]https://postgis.net
[3]http://cite.opengeospatial.org/pub/cite/files/edu/cat/text/main.html

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Design

In this chapter the design of the provenance capturing in the OpenEO project gets described. The aim of this chapter is to explain the general concept of how to gain reproducibility in the OpenEO project. The chapter is structured in six parts. In the first part an overview of the concept gets presented. In the next three sections the main components presented at the overview are described in detail. These are the Data Handler, the Job Capturing and the Result Handler. The next section defines the resulting context model. In the last section of this chapter defines the user interfaces needed to use the data of the context model from an OpenEO user perspective. The following chapter 5 shows a proof of concept implementation of the design.

4.1 Overview

In this section an overview of the concept is presented and in figure 4.1 visualized. In this figure the workflow that every OpenEO back end driver needs to implement in the white components. The green elements in the diagram are the proposed extensions of this thesis design. The typical job execution work-flow is described in the following steps.

1. **OpenEO Client**
   The user defines the input data, the filter operations and the processes that need to be executed at the back end via the OpenEO client. Then the user orders the job to be executed, therefore the client creates a process graph. The user identification and the process graph is sent via the RESTful endpoint defined in the OpenEO coreAPI to the back end driver.

2. **Data Query**
   The Data Query component receives the process graph and parses the data identifier and the filter operations out of it to query for the input data records needed for the job. These are forwarded to the Process Execution component.
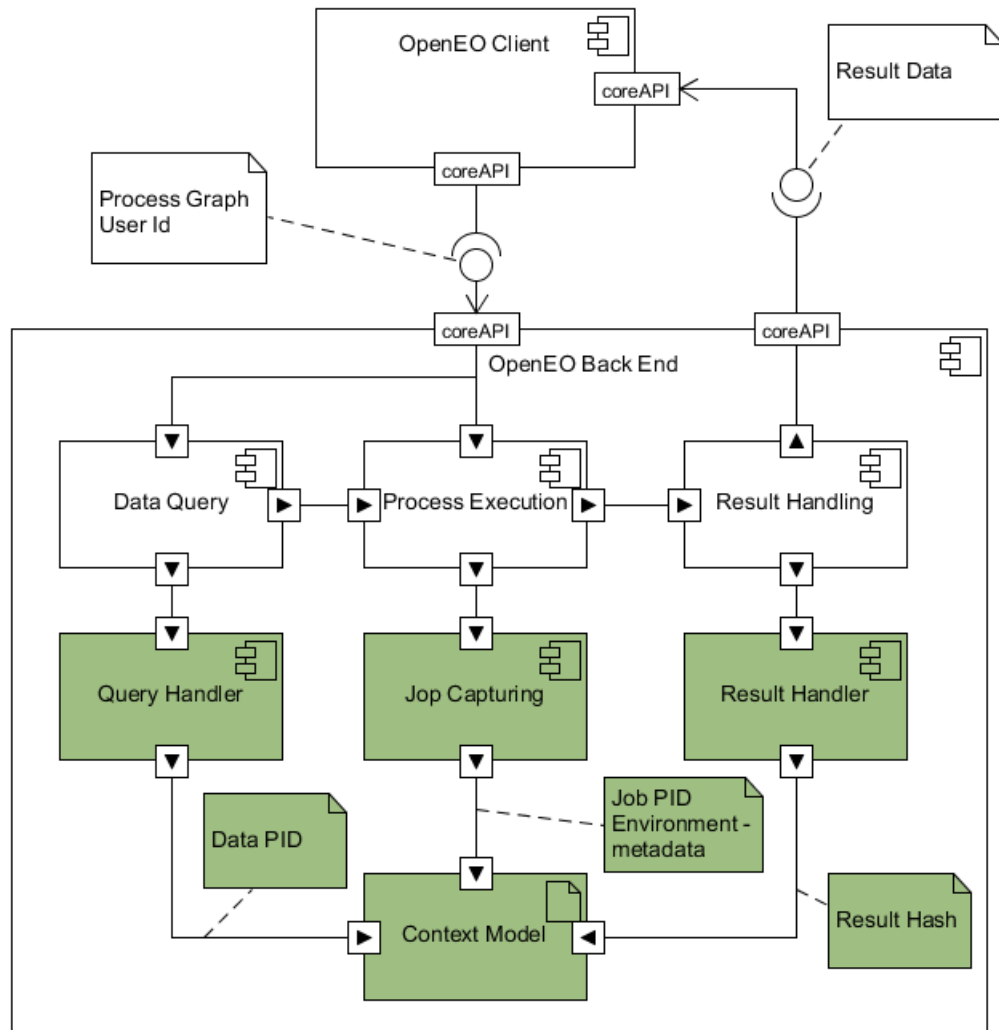
Figure 4.1: Overview of the Design

3. **Process Execution**

   The Process Execution component receives the process graph and the input data from the Data Query component. It parses the processes from the process graph and executes them in the order of appearance. After every process defined in the process graph got executed, the resulting data is forwarded to the Result Handling component.

4. **Result Handling**

   The Result Handling component receives the results from the Process Execution component and persists all meta-data about the job and the result. In the meantime

the resulting data is sent back to the OpenEO client, if the job was not a batch job. If it is a batch job the user has to actively order the results from the back end.

To make the whole workflow reproducible, the single components have to be identifiable. Hence, the following elements get introduced as additions to the back end.

- **Query Handler**
  The Query Handler component is responsible for applying data identification to the back end. The query and the resulting data generated by the Data Query component needs to be persisted and identifiable by a Persistent Identifier (PID). The Query Handler is described in more detail in section 4.2.

- **Job Capturing**
  The Job Capturing component is responsible for enable code identification of the used processing at the back end. Therefore, a PID of the code used for the processing has to be introduced. In addition, meta-data of the job execution environment gets captured, to gain feedback information for the users. The Job Capturing component is described in more detail in section 4.3.

- **Result Handler**
  The Result Handler component is responsible for creating a comparable result checksum or hash. The data created by the OpenEO back end can be too big to be persisted in the future, hence there need to be a checksum or hash to be at least capable of confirming equal results. The Result Handler component is described in more detail in section 4.4.

- **Context Model**
  The Context Model is not a component, but a data set that consists of all the meta-data mention in the previous components. One context model is related to one job execution. The details about the Context Models can be found at section 4.5.

4.2 Query Handler

The input data of the processing is crucial for the outcome of the job execution. Even though the process graph already contains an identifier for the input data that has to be unique for the specific back end, changes to this data might not result in a new identifier. So jobs called later in time might use another version of the input data than the previous jobs. To prevent this the input data has to be persisted according to the 14 steps of data provenance defined by the RDA [32]. Every back end is responsible for applying data identification. In the design chapter it is assumed that the back ends preserve the data as described in 4.2. The Query Handler is the module where the data persistence is implemented and depends highly on the structure and architecture of the back end. Therefore, no common definitions can be made for all back ends in this section. In chapter 5 there is

a proof of concept implementation on the EODC back end. The context model elements of the job executions are specified with a "J" in the beginning for readability reasons. Elements of the back end environment context model are specified with a "B" in the beginning.

J1: Input Data Persisted Identifier
The output of the Query Handler is the PID of the input data of a job execution. Every job execution has input data that has already assigned a PID or where a new PID needs to be created. Therefore the PID is added to the job dependent context model.

4.3   Job Capturing

The aim of this section is to describe the job execution capturing and a description of data that shall be captured. The meta-data provided by the job capturing can be categorized in static and dynamic data. Where static data is defined as not dependent on job properties and dynamic data is defined as job dependent information. In the following two sections the static data (in this thesis called back end provenance) and dynamic data (in this thesis called job dependent provenance) are further described.

4.3.1   Back end provenance

The scope of this part of the context model is to get the static environment of where the job execution at the back end takes place. It contains the provenance data that is independent of a job execution, so does not change regardless of how many jobs were processed. It can only change from inside of the back ends by their maintainers. In the OpenEO project there are a great variety of different back end providers with very distinct setups, so the challenge of this part is to make it as simple and generic as possible. The data captured in this part of the context model is not meant to be shown to the user directly, because of security issues. The following meta-data is suggested for the back end provenance. The context model elements of the back end environment are specified with a "B" in the beginning for readability reasons. Elements of the job dependent context model are specified with a "J" in the beginning.

> Check meta-data after implementation

B1: Code Identification
Since the OpenEO project is open source, every back end has a GitHub repository were at least the basic setup is stored. The aim of this strategy is to get other back ends with similar settings to reuse the already working setups of the running back ends. Therefore every back end provider has a GitHub repository were the code is public-ally available. This information is added to the back end provenance by saving the git repository URL, the used branch, the used commit and local changes to the repository. This information can be used to identify the used code at the back end.

B2: Used Folders
The back end will most probably not only use the GitHub repository for the processing,

so that other folders are involved. For example configuration files may not be persisted in GitHub for security reasons. This information is also crucial for the job execution and therefore needs to be stored. Changes of this directory have to be detected and stored in the context model. Therefore, a checksum or hash key of the additional folders are created and persisted in the context model.

B3: OS and packages
The operating system can also have an impact on the processing and so it has to be stored to the context model too. Not only the information about the operating system, but also the installed packages are added to the context model. If the whole processing is done in a virtual container the operating system of that container shall be stored. If the whole processing is done in a docker container, the docker description file can be used for the environment data.

B4: Core API Version
The back ends core API version is the version of the OpenEO core API it currently is capable of. In the productive usage of the OpenEO project it can happen, that the versions of the clients and the back ends differ, so that the behavior might not be compatible. So the back end server configuration depends on the core API version of OpenEO, hence it shall be added to the context model.

B5: Back End Version
The captured data described in the previous sections will result in a back end version. The back end version shall be an identifier (e.g. a number) that gets updated on every change of the backend considering the provenance data described above.
To provide long term stability of the capturing, it is a good idea to implement a tool to automatically capture the provenance data and persist it in a back end context model. Every change on any of the previously described back end meta-data has to be detected automatically and have to result in a new back end version.

4.3.2   Job dependent provenance

In this section the job dependent provenance of the context model gets described. The data captured is tied to a specific job execution, so for every job execution a new job context model gets created. The process graph is already a description of the processes that run at the back end. So sending the same process graph to the same back end again shall result in the same outcome. To assure that the process graph can be re-executed in the same way as the original execution, meta-data about the original execution gets captured. The single parts of the capturing are described more in detail in the following subsections.

Process Environment

In this section the capturing of the process itself gets described. As mentioned above the process is described with the incoming process graph, but to be certain that the same process id results in the same code, the code version is added to the context model. To be able to identify code from different versions a source control management needs to be installed. An example of doing so is persisting the back end source code on a public platform like GitHub. The way of executing a specific process graph is not only related to the code running it, but also by the dependencies of the code. Therefore the programming language version and the additional used libraries of it are persisted in the context model. To gain more meta-information about the processing the start time and end time can be added to the context model via timestamps. This leads to the following capturing elements in the job context model.

J3: Programming Language
The programming language of the code that is used for the processing. In addition the version of the programming language has to be included in this information.

J4: Installed packages of the programming language
To identify the environment of the code execution, the installed packages of the programming language can be captured and added to the context model. The version of the packages have a high influence on the outcome, hence can also be included in the context model. For example in python the installed modules can be added with their versions to the context model.

J5: Start and End time of process execution
On the beginning of the process execution a time-stamp can be created and at the end of the process execution. These timestamps can then be persisted in the context model.

Back end provenance

The back end provenance described in 4.3.1 defines the version of the code that is executed and therefore has to be added to the job context model. Over time the back end provenance will get updated so that every job need to persist the original back end configuration at the execution time. There are two possible solutions to achieve this. First the identifier of a specific version of the back end gets added to the context model. In this case the data of the back end provenance versions have to be persisted and accessible. The second solution is to put the whole back end provenance of the current version into the job execution context model.

J2: Back end provenance / Code Identifier
The version of the back end provenance during the job execution. Since for every change on the back end a new version will be applied, the back en version is the code identifier of the execution. If the back end environment is not persisted properly at the back end, the whole back end provenance can be added to the context model.

4.4 Result Handler

The output data of the processing has to be captured as well to be able to compare job execution outcomes. In the OpenEO project the results can be rather big, that is why a simple generated hash value of the output result is enough in the context model defined in this thesis. The output data does not have to be identifiable within the scope of this thesis, but just comparable with other executions. Therefore a hash of the output data is sufficient. The aim of the output data capturing is not to add the possibility to find differences between results, but to be able to see that the results differ.

J6: Result Hash
The output result of the job need to be verifiable and therefore need to be persisted. An easy way to achieve this is to take the hash value over the sorted output files.

4.5 Context Model

The context model is the data record that saves the provenance of a job execution. The type of storage is defined by the infrastructure of the back end provider. It can be stored in a relational database or in a file-based system as a file on the file system. It has to be added to the meta-data database of the back end. There are two different context models that need to be persisted at the back ends.
First the back end environment context model that saves job independent provenance and results in a back end version. The mandatory element of the back end environment is the back end version that defines the state of the back end in a specific time. The back end version need to be resolvable to the specific code version that was present in a past execution. In addition meta-data about the back end can be added. The elements (B1-B5) defined in section 4.3.1 are suggestions of elements in the back end environment context model.
Second the job execution context model that includes all information that is dedicated to a specific job. There are three mandatory elements in the job context model. The input data identifier has to be persisted in the context model, so that it can be identified and used in future job executions. The used version of the back end for the execution has to be included in the context model, to be able to re-execute it with the same code in the future. The output hash has to be added to the job dependent context model, so that different results can be detected. In section 4 the elements (J1-J6) are recommendations of these data and suggestions on additional job specific meta-data.

4.6 User Interface

In this section the information for the users and how it is provided gets described. The capturing described in the previous sections consists of information about the back ends that shall not be completely passed to the users in detail. For example it can be a security risk to provide specific programming language packages. On the other hand the users

need to be able to see the differences of job executions and get environment information about the back ends. Therefore there has to be a filter on which data can be shown to the users and what not. Every captured information is also not necessarily interesting for the users. Data that is not secure to the user has to be defined by the different back ends themselves. The OpenEO project has a very diverse set of back ends and every one has an unique company security guideline.

Provenance information need be provided to the user. Therefore there have to be additions to the core API specification. Additional endpoints for the users to get information about the back end has to be created for the core API, back end and client. The following points summarize the set of needed additions, they are structured with a "U" in the beginning to add readability through the thesis.

U1: Back end version
There has to be an endpoint for users to retrieve back end specific information especially the current version. The aim of it is to present the users with information about the current state of the back end and to help OpenEO users to decide, which back end they want to use. There is already an endpoint defined in the OpenEO core API specification for the capabilities of the back end, where the back end information can be added.

U2: Detailed Job Information
There is already an endpoint to get detailed information about the job status. But the provenance of the job is not in there yet, so it has to be specified in the API what information from the job context model is provided there. At least the resolvable persisted identifier of the input data, the back end version and the result set hash has to be added to the view for comparison reasons. To make it human readable e.g. the resolvable identifier URL of the input data and the GitHub repository and commit identifier can be provided.

U3: Comparing two Jobs
The API has to add an end point for making it possible to compare two different jobs. There does not exist an endpoint for this in the current(version 0.0.2) core API specification. The response of the comparison request consists of the differences in the context model between two jobs.

U4: Re-use of Input Data
The current core API version (v0.0.2) is not capable of letting the user choose, which version of data the user want to use. Hence, there has to be an addition to the process graph so that product identifier has an additional time-stamp. So every input data identifier has now a time-stamp for when the data was retrieved. The meaning of the time-stamp is to tell the back end that the user wants to use the data at the time of the time-stamp. This gives the back ends the possibility to design their own strategy of applying a version to the data. It has to be persisted, which version of the data was available on what date and time. In addition the API can allow to include the use of an input data PID in the process graph. So that users can include cited data directly in a new created job.

update version if
needed

Implementation

In this chapter the prototype of the concept described in 4 gets presented on the EODC back end. The implementation consists of all suggested changes that need to be made to the OpenEO workflow including parts of the back end, core API and the clients. Thus all three parts of the OpenEO project architecture get modified in the presented solution. There are several different back ends and clients implemented in parallel, which are all compatible with each other. One of each of the clients and the back ends is used for the proof of concept of this thesis. The python client[1] is modified for the purpose of this thesis. The EODC back end[2] gets used for the back end part. Since python is the most common programming language at the contributing back ends of the OpenEO project, these implementations get used. Both of the chosen implementations are using python as their main programming language. The adaptations described in 4 are implemented for the usage of the python client accessing the EODC back end. Both of the solution implementations are open source and can therefore be used by other back end providers with a similar setup.

The implementation can be divided in four independent parts. In the following four sections these parts are described in detail. First the data identification implementation gets described, so the implementation of the RDA recommendations on the EODC back end. The next section is about the implementation of the automated back end provenance tracking tool that captures data defined in section 4.3.1. After that there is a section about the job execution provenance as defined in 4.3.2. The last section is about the implementation of user interface additions defined in 4.6.

5.1 Data Identification

As defined in section 4.2, implementing the RDA recommendations needs to be done | add concept discussed with Andi

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[1]https://github.com/Open-EO/openeo-python-client
[2]https://github.com/Open-EO/openeo-openshift-driver

by every back end provider individually. In this section the data identification solution on the EODC back end is presented. Other OpenEO back end provider can use the presented approach as well to enable data identification on their back end setup.
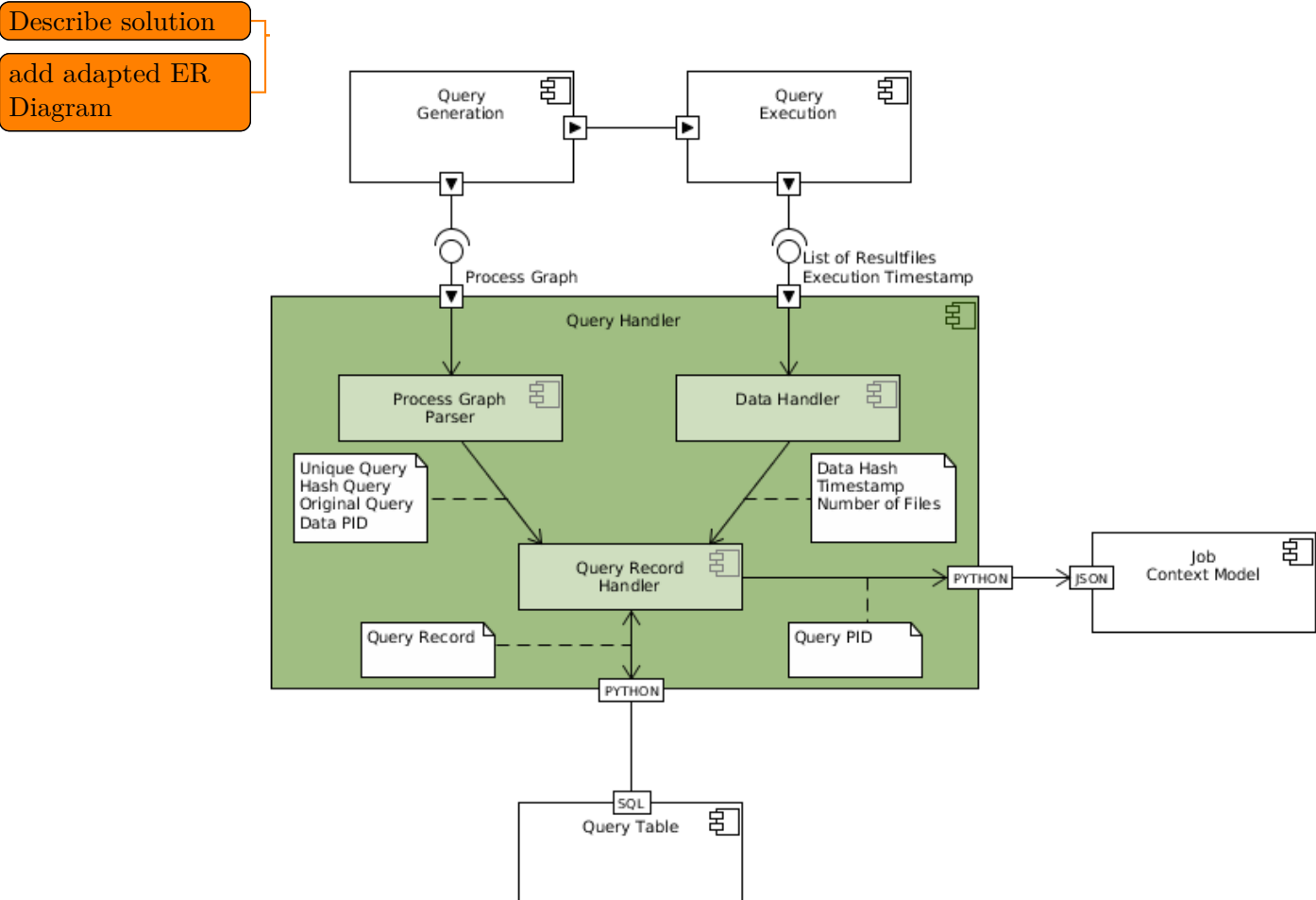
Describe solution

add adapted ER Diagram

Figure 5.1: Overview of the proposed data identification workflow at the EODC back end

5.2   Back end provenance

The aim of the automated back end provenance computation is to make an easy to implement approach to capture all changes of the back end that have an influence on the back end processing results. In addition to this the implementation generates a back end version automatically on changes at the back end. The proposed tool can be used by every OpenEO back end with a Linux system. It is completely independent of the existing back end services, so it is an additional tool that has to be executed at the back end. In this section the implemented tool is called "BackendMonit".
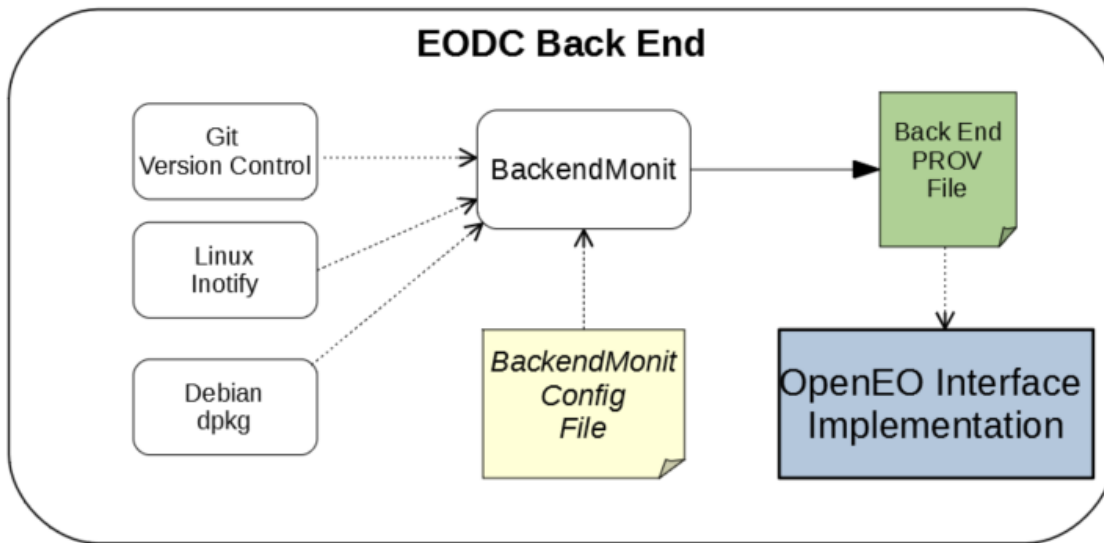
Maybe merge with Job provenance

Figure 5.2: Overview of BackendMonit inside of the EODC back end

BackendMonit is a stand alone capturing tool that gets called periodically as a cron job (see [6]) by the back end hosting machine. EODC uses python as their default programming language on a Debian Linux based system, therefore the capturing tool is written in python and uses linux and debian tools. It is implemented in a way that other linux based back ends can use it to capture back end changes too, with some minor changes. The back end provenance tool uses a command line interface (CLI) and a configuration file as a parameter. The workflow of running BackendMonit is as follows:

1. **Install Requirements**
   BackendMonit requires for the execution a view linux packages. First the tool runs on Python 3.6 hence it has to be installed on the system. There are no additional python packages necessary for it. Another requirement is inotify and dpkg, or any other packet management system for a Linux distribution. The version control system Git is also a requirement on the back end, since every back end has its own GitHub repository it is most probably already installed.

2. **Setup Configuration File**
   To make BackendMonit adaptable for other systems there needs to be a configuration file to configure the behaviour of it. The tool comes with a default configuration file, which the back end provider has to adapt to the back end. All paths to the tools described in the previous point is in the config file specified. Additionally, the path to the GitHub Repository used for the local back end repository is set in the configuration file and a list of folders, which are used by the back end provider for the execution of jobs, excluding temporary folders.

3. **Starting Service**
   After the configuration is done, BackendMonit is executed in daemon mode, where it starts all processes of inotify to run in the background. To start the tool in daemon mode the "–init" parameter has to be set on execution.

4. **Start Cronjob**
   Now that inotify is configured and started as a service, BackendMonit has to check periodically if something changed on back end side. Therefore, the tool needs to be started every minute adding the "–check" parameter. Every time that happens it compares the current state of the back end with the current context model and if it differs it adds a new back end version with all metadata to the context model JSON file.

Provenance Repository

The context model of the back end provenance is a single JSON file that consists of all versions of the back end and their meta-data described below. In figure 5.3 there is an example snipped of the provenance repository.

```
{
    "backend_version": 1,
    "git_repos": [
        {
            "branch": "release-0.0.2",
            "commit": "177d082e45b211f18f3b1ae55c3a65e45c96cf89",
            "diff": "E5C2D5FAB26EE11BAECC91294A4E519FC8B688992E66696ECD34B36D4470D7E6",
            "url": "https://github.com/Open-EO/openeo-openshift-driver.git"
        }
    ],
    "working_dir_changes": "9F86D081884C7D659A2FEAA0C55AD015A3BF4F1B2B0B822CD15D6C15B0F00A08"
}
{
    "backend_version": 2,
    "git_repos": [
        {
            "branch": "release-0.0.2",
            "commit": "177d082e45b211f18f3b1ae55c3a65e45c96cf89",
            "diff": "E5C2D5FAB26EE11BAECC91294A4E519FC8B688992E66696ECD34B36D4470D7E6",
            "url": "https://github.com/Open-EO/openeo-openshift-driver.git"
        }
    ],
    "working_dir_changes": "C66769040CF7EB5EBE0141C91B1C34B4FFD01908979849A5F0B299375B63542B"
}
```

Figure 5.3: Example snipped of the provenance repository of the EODC back end.

In the following it is explained how the in section 4.3.1 defined provenance data points are read from the system by BackendMonit.

B1: Github Repository

To capture the github repository, all folders that consists of github repositories have to be added to the configuration file. Git shall be installed at the back end and the path to the Git command has to be added to the configuration file as well. The monitoring tool will add the GitHub URL, the branch, the commit and a hash of all local differences to

the context model. If there are any changes to the previous model there will be a new back end version.

B2: Used Folders

Used folders by the back end have to be specified in the configuration file, excluding temporary folders and files. The tool daemon will check these folders on changes and will update the context model if anything changed at this folders. The tool used for this is inotify (see [15]), this tool can be used to call a command if any changes on the file system in specific folders occur. The changes can be further specified by 12 different operations on the filesystem like IN_DELETE, IN_ACCESS. For the purpose of capturing changes to the used folder only write access on the folders trigger inotify.

```
inotifywait −d −e modify −e attrib −e moved_to −e create −e delete DIR
                    −o outfile.log
```

B3: OS and packages

The linux operating system the eodc back end runs on is a debian based[7] operating system therefore the operating system release information and the packages can be retrieved with the debian packaging system (dpkg [8]).

```
dpkg −−get−selections
```

B4: Core API Version

The core API version will be added updated manually from the back end developers. Therefore the core API version is also read from the back end "GET /version" endpoint of the back end that returns the currently supported core API version.

B5: Back End Version

The back end version begins with 1 and gets incremented on every change of the above described data. On every call of the cron job BackendMonit capture all above points and compares them to the most recent context model. If there are differences the version gets incremented by one and persisted in the context model.

5.3 Job dependent provenance

The capturing of the job dependent data is limited to the job execution modules of the EODC back end. The EODC back end of the release version "0.0.2" transforms the process graph into separate docker containers. For every process in the process graph there is a docker container created that runs python code with the input of the previous process. The first process docker container has the input data as input value. The result gets into a temporary folder separated by the different process result. Every process has its own temporary output directory until the whole process graph got executed, after that the temporary folders get deleted and only the result is saved and persisted. To achieve the job provenance data capturing described in chapter 4.3.2 the processes have to provide information about the input, output data and the processing itself. Two different

39

Table 5.1: Relation of context model definition and JSON context model.

Context Model Definition	JSON Key
J1: Source Input Data Identifier	input_data, process_details
J2: Process Code Identifier	code
J3: Programming Language	code_env
J4: Installed packages of programming language	code_env
J5: Start and End time of process execution	process_details
J6: Result Hash	process_details, output_data
J7: Back end provenance	backend_env

implementations were created to achieve the job dependent provenance capturing. The first implementation uses the python code wrapper noworkflow [23]. So instead of calling the processing with python, it gets called with the noworkflow wrapper that automatically creates a meta-data database about the python execution. The second implementation adds the specific information of interest to the logging of the processing and reads the logging files to generate the context model. The second implementation is in plain python. As described in the chapter 4.3.1 the programming language of the back end shall be used for the implementation of the capturing tool. So the solutions use python to retrieve the needed provenance data. Both implementations have the same functionality and cover the full implementation of the described data of the Design section.

5.3.1   Provenance Repository

There is a context model for each executed job, if the job gets re-executed, the context model gets replaced by the new context model. The job re-execution is internally handled as a new job with the same process graph. The functionality of letting the same job be re-executed without creating a new job id got dropped from the agenda of the OpenEO project in version 0.0.2 [27]. The context model get persisted as a JSON file in the job execution directory. After the job carried out in the EODC back end the results are saved in a folder named after the unique job identifier. There the context model JSON file gets created by the implementations described below. The JSON file has the following structure:

> **Update figure 5.4 input_data identifier to the query store PID**

In figure 5.4 there is an example context model of a job execution. It consists of all points described for the context model in the Design section. In the following table there is the mapping between the context model definition defined in section 4 and key of the JSON context model file.

> **update table with the new numbers defined in DE-SIGN**

The mapping described in the table above is implemented by both solution systems.

40

```json
{
    "backend_env": { ...
    },
    "code": "edd1a0d3ddca9992ba6221ff5332bf900625754292098800ed490330ff800139",
    "code_env": [
        "alabaster==0.7.11",
        "apted==1.0.3",
        ...
        "python-dateutil==2.7.3",
    ],
    "input_data": [
        "gb5511fce256cb2985699a82249d4133kj9b7875b0b7b67fd7f379fh6740039f"
    ],
    "job_id": "example",
    "openeo_api": "0.0.2",
    "output_data": "c448e6f8cd027bf0af70bab8d8372b339e70858ffc9f19854d5ea38bf401b856",
    "process_details": {
        "0_filter_bbox": {
            "output": "89ad98f264cfde64c086a3c314fcdfeb8896b0112276611be7596fce0e660fba",
            "timing": {
                "end": "2018-10-21 11:27:47,552",
                "start": "2018-10-21 11:27:46,33"
            }
        },
        ...
        "3_min_time": {
            "output": "c448e6f8cd027bf0af70bab8d8372b339e70858ffc9f19854d5ea38bf401b856",
            "timing": {
                "end": "2018-10-21 11:27:47,653",
                "start": "2018-10-21 11:27:47,644"
            }
        }
    },
    "process_graph": {
    ...
    }
}
```

Figure 5.4: Design Overview of capturing the job context model.

5.3.2 Benchmarking Mode

As defined in section 4.3.2 there is also the optional possibility to capture not only the overall process, but also every process and the data in between for comparison reasons. If the process executed is not the first one and the benchmarking capturing mode is on, the input data identifier gets replaced by the output hash of the previous process. The scope of the benchmarking is just to make it able to see differences in the executions, but not to be able to identify the differences. Hence, a hash of the previous output data is sufficient. The hash gets created after the execution, by creating the hash of the execution at temporary output directory of the previous process. The EODC back end creates for each process execution a temporary folder where the output data of every process is stored, after the execution the temporary folder gets deleted. Between the finished execution and the deletion of the temporary folders a self provided python function gets called to make an SHA-256 hash over the results. In the benchmarking mode not only the data gets captured between the processes but also the timing of the single process executions. This is done by adding logging messages for the start and end of the process

may not be implemented... –> Future work

execution. The logging file is afterwards parsed and the timestamps are copied to the context model. Last but not least the identifier of the code is captured, by reading the git information out of the back end provenance. For the user convenience the url of the process code on GitHub with the currently checked out commit is added to the context model. Both implementations have the benchmarking realized as described before.

```
{
    "process_details": {
        "0_filter_bbox": {
            "code_id": "https://github.com/Open-EO/openeo-openshift-driver/tree/177d082e45b211f18f3b1ae55c3a65e45c96cf89/operations/filter-s2",
            "output": "89ad98f264cfde64c086a3c314fcdfeb8896b0112276611be7596fce0e660fba",
            "timing": {
                "end": "2018-10-21 11:27:47,552",
                "start": "2018-10-21 11:27:46,33"
            }
        },
        "1_filter_daterange": {
            "code_id": "https://github.com/Open-EO/openeo-openshift-driver/tree/177d082e45b211f18f3b1ae55c3a65e45c96cf89/operations/filter-s2",
            "output": "89ad98f264cfde64c086a3c314fcdfeb8896b0112276611be7596fce0e660fba",
            "timing": {
                "end": "2018-10-21 11:27:47,552",
                "start": "2018-10-21 11:27:46,33"
            }
        },
        "2_NDVI": {
            "code_id": "https://github.com/Open-EO/openeo-openshift-driver/tree/177d082e45b211f18f3b1ae55c3a65e45c96cf89/operations/ndvi",
            "output": "9003ad2c78f982c30ee63552a7c04488e22199514ad10a4c376c7eeb0523af52",
            "timing": {
                "end": "2018-10-21 11:27:47,644",
                "start": "2018-10-21 11:27:47,552"
            }
        },
        "3_min_time": {
            "code_id": "https://github.com/Open-EO/openeo-openshift-driver/tree/177d082e45b211f18f3b1ae55c3a65e45c96cf89/operations/min-time",
            "output": "c448e6f8cd027bf0af70bab8d8372b339e70858ffc9f19854d5ea38bf401b856",
            "timing": {
                "end": "2018-10-21 11:27:47,653",
                "start": "2018-10-21 11:27:47,644"
            }
        }
    }
}
```

Figure 5.5: Example of an benchmarking mode snipped out of the process graph.

In the following two sections the process of capturing the context model in two different implementation approaches get explained further. First the approach of using noworkflow as capturing tool and second the implementation with plain python and logging.

5.3.3 Noworkflow Implementation

Noworkflow is a python module used to capture the provenance of a python script execution. The main aim of it is that the program itself does not have to be changed, it only has to be executed with the noworkflow interpreter instead of python. It then automatically creates a provenance database on every execution of the script called "trial". Every execution creates a new trial. A trail in the past can be re-executed with the same conditions and the trails itself can be easily compared and visualized with noworkflow [23]. Noworkflow and its capabilities are described in section 2.3.1. For the purpose of the job dependent provenance capturing described in the Design section, only parts of the provenance capturing functionality that noworkflow offers gets used.

J1: Source Input Data Identifier
The source input data identifier is the id for the input data and query provided by the EODC query store described in section 5.1.

J2: Process Code Identifier

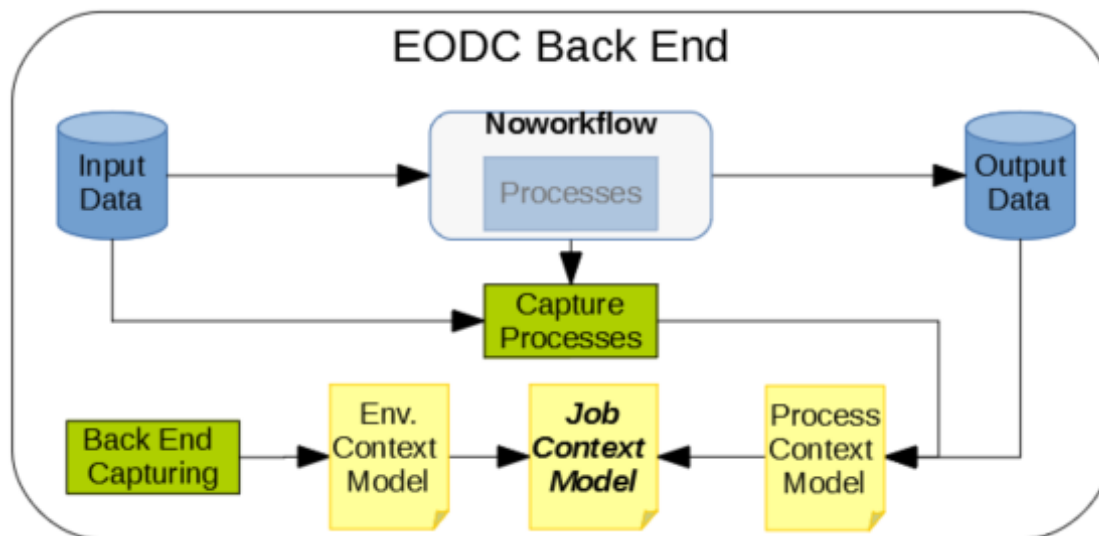> Move to "additional implementation" and describe it a little bit less

Figure 5.6: Overview of the noworkflow implementation.

The job identifier is defined by the back end version, which includes the current state of the locally checked out GitHub repository.

To make a more detailed comparison possible there gets also the hash of the executed code added to the context model.The job execution runs with noworkflow and for every execution there is a noworkflow trial created that consists of the hash of the executed code. The hash from the database of noworkflow gets retrieved via the command line interface. It contains the command "show" (see code block below), which returns the data of a specific trial. The code hash gets extracted from the output and added to the context model for easy comparison reasons.

```
now show −−dir=JOB_DIR
```

J3 and J4: Programming Language and Installed packages of programming language

The programming language gets captured with the modules of the python packages in the noworkflow database. To retrieve the modules the command line interface is used with the command "-m" (see code block below) that returns all used python modules including the version of python used to execute the code. In the context model the python version is in the list of used python tools returned by the noworkflow command. The data is restructured to fit in the JSON output file and represented by a list.

```
now show −m −−dir=JOB_DIR
```

J5: Start and End time of process execution

The start and end time of the processes gets captured through the logging of the processes. Every process writes to a logging file the start and end time of the execution. The data is human readable to provide the user retrieving the context model more comfort. The

used format is "yyyy-MM-dd hh:mm:ss". The seconds have three digits for more precise time stamps. All log files are in the job execution folder, where the data gets persisted. After the execution when the context model gets created the timestamps are read from the log file and added to the context model of the processes.

J6: Result Identifier

The result identifier consists in the common capturing mode of the output data of the whole process graph execution. It is a SHA-256 hash of the resulting sorted output files, which are placed in the results folder of the job execution directory. The order id is a counter that starts with zero and increments for each process executed. It describes in which order the processes get executed. It is used in the context model to get feedback about the execution order of the processes.

J7: Back end provenance

The back end provenance is read from the BackendMonit context model JSON file at the back end described in section 5.2. Provenance of the latest back end version gets copied to the context model. The whole back end provenance get included to the context model so that the environment is independent of the persistence of the back end provenance file.

5.3.4 Python Implementation

The noworkflow tool needs some additional requirements to the back end provider and slows down the processing, because the granularity of the code capturing is much higher than needed. These are the reasons why back end provider might not want to use the provenance tool in a productive server. The EODC implementation proposed by this thesis is an example for other back ends and hence needs to be easy to implement. So another solution for capturing the processing is implemented in pure python. The python solution uses logging messages to transfer the needed data from the process execution program to the capturing tool that reads the logs after the job is finished. This needs no additional python packages and the execution can stay the same. The only changes to the original server implementation is the new logging messages that have to be added to the already existing logging framework at the EODC back end. An overview of the logging and capturing process of this solution can be viewed at figure 5.7.

J1: Source Input Data Identifier

The source input data identifier is the id for the input data and query provided by the EODC query store described in section 5.1.

J2: Process Code Identifier

The job identifier is defined by the back end version, which includes the current state of the locally checked out GitHub repository.

To make a more detailed comparison possible there gets also the hash of the executed code added to the context model. In the python solution a SHA-256 hash gets generated over the whole source code used for the job processing.

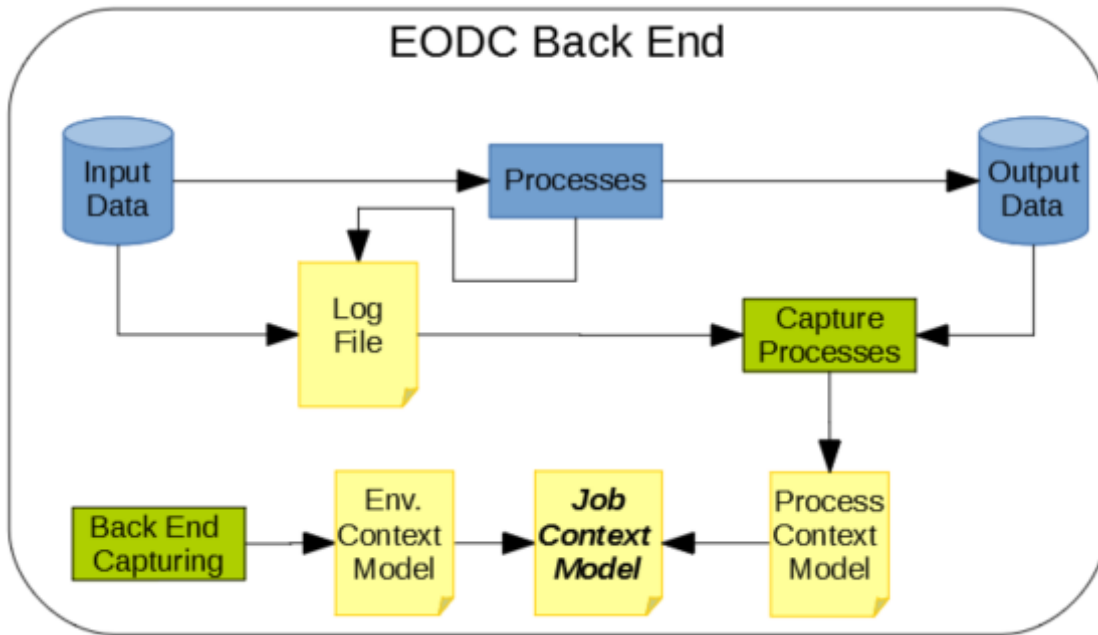**J3 and J4: Programming Language and Installed packages of programming language**

Figure 5.7: Overview of the python implementation.

The programming language of the EODC back end is python and also the capturing tool is written in python. To list all installed packages in python "pip" can be used. With the python module "pip" the installed python modules can be managed. The EODC back end GitHub repository has a python environment file to automatically install all needed dependencies of python via "pip". A feature of that tool is the "pip freeze" call, which returns all installed python packages including their versions. This gets translated to a JSON list object and saved to the context model. In addition to this the python version gets captured by the "sys.version" call of the python capturing tool.

J5: Start and End time of process execution
The start and end time capturing is the same as described in the noworkflow implementation see section 5.3.3.

J6: Result Identifier
The result identifier is implemented in the same way as the noworkflow implementation see section 5.3.3

J7: Back end provenance
The back end provenance information is implemented in the same way as the noworkflow implementation see section 5.3.3

5.4   User Interface

The user interface implementation is done by adding endpoints to the existing OpenEO core API version 0.0.2 and applying the additional endpoints to the python client and the EODC back end. The relevant additions defined in section 4.6 are implemented in the following way:

U1: Back end version
Retrieving additional information about the back end was added into a new defined end point of the API. The new endpoint is a GET request called "/version". The user does not have to be logged in to access this endpoint. Response of the version endpoint is in the implementation the whole job independent provenance information of the back end, like defined in section 5.2. In a productive version the data may be filtered for information marked as a security risk. This endpoint was added to the EODC back end and to the python client so that the user can call a method in the python client called "version()" to retrieve the information of the back end directly in the python environment.

U2: Detailed Job Information
There is already an endpoint to get detailed information about the job status. It is the existing "GET /jobs/<job_id>" endpoint of the core API, which by the version of 0.0.2 only contains the execution state of the job and the job id. In addition to the already available information the whole job dependent provenance gets added to this endpoint in the implementation of this thesis. The python client got also changed to match the end point changes described before.

U3: Comparing two Jobs
The comparison of two jobs is not defined in the version 0.0.2 of the core API, hence there does not exist any. So a new one has to be defined in a manner of the existing endpoint definitions. For the purpose of this thesis the endpoint "POST /jobs/<job_id>/diff" gets introduced. In the url of the request you define the base job id that has to be compared with other jobs. In the body of the request the job ids that the base job shall be compared with are defined in a JSON list. After getting the request from the user, the back end compares the context models of the base job with every job in the request body list. The result consists of for every item in the base job context model the term "EQUAL", if the item is the same in both jobs, "DIFF", if the items are not the same in both jobs, or "MISSING", if the item is in the base job, but not in the target job of the request list. This can occur if the context model was modified in the future and some additional fields of it are not in the context models of the past or in the benchmarking mode if one process graph has mode processes defined than another one. The response consists of the context model of all jobs with one of the previously described three states inside of every items value. In the python client this feature was added and in addition there got an visualisation implemented to make the differences of the context models more visible to the users.

[margin note: explain in detail what info was included here and how it got captured]

[margin note: explain in detail what info was included here and how it got captured]

[margin note: Maybe also add image of REST request & response.]

[margin note: Add image of the client visualisation]

In addition to the implementations defined before, a translation tool for the context model got implemented. It transforms the job dependent context model into a PROV-O specified file. This is only realized in the benchmarking mode of the back end and it describes the job execution steps. The mapping of the context model to the PROV-O standard is as follows.

describe PROV-O export of Context Model

add image of the PROV-O export

5.5 Implementation Overview

5.5.1 Changes to Client

5.5.2 Changes to Core API

5.5.3 Changes to Back end

Add the big picture of all components and their additions

CHAPTER 6

Evaluation

In this chapter the implementation gets tested and evaluated. By running the use cases it gets evaluated if the implementation reaches the aim of the thesis. First the RDA data identification recommendations are checked with the implementation and how they apply or not need to apply. Then the two implementations are compared with each other. The last section in this chapter is testing the in section 1.4 defined use cases against the implementation.

6.1 Data Identification

Describe Test Cases, introduce new Use Cases

- **R1: Data Versioning**

- **R2: Timestamping**

- **R3: Query Store Facilities**

- **R4: Query Uniqueness**

- **R5: Stable Sorting**

- **R6: Result Set Verification**

- **R7: Query Timestamping**

- **R8: Query PID**

- **R9: Store the Query**

- **R10: Automated Citation Texts**

- **R11: Landing Page**

- **R12: Machine Actionability**

- **R13: Technology Migration**

- **R14: Migration Verification**

Compare imple-
mentation with the
recommendations.
So how it was and
how it is.

Test Cases

6.2   Use Cases

In this section the use cases introduced in section 1.4 are tested against the python
implementation. The setup of the evaluation is on the back end side the EODC python
implementation described in section 5.3.4. To communicate with the back end the
modified python client gets used. The modifications to the python client are described
in 5.4. The use cases get evaluated by trying to apply them on the original OpenEO
setup (version 0.0.2) and comparing it to the implemented additions described in section
5. The release-0.0.2 OpenEO set up is named original set up for convenience reasons and
the OpenEO set up with all, in this thesis described, changes is called modified set up.
An Overview of the evaluation is visualized in figure **??**

Explain set up
in more Detail
(EODC Back end
, python client,
maybe github urls)

6.2.1   Re-Use of Input Data

The first Use Case can be seen from two perspectives. From the back end providers point
of view and from the users point of view. The user wants to get information about the
back ends provenance and the current version. The back end provider wants to have an
automated tool to capture the provenance data and to create automatically back end
versions. This is done in the implementation by running the BackendMonit tool described
in section 5.2. The back end provider has just to start the service of BackendMonit and
the capturing and back end version creation will be done automatically. Users will use
an OpenEO client to access the back end. Therefore, in the following the use case gets
visualized by the view of an OpenEO user using the python client:

Original Setup

Modified Setup

Run Test case 1
and show how it
was and how it is
now. + Python
Client Results

6.2.2   Capturing job dependent environments

Run Test case 2
and show how it
was and how it is
now. + Python
Client Results

Original Setup

Modified Setup

6.2.3 Getting differences of job executions

Original Setup

Modified Setup

> Run Test case 3 and show how it was and how it is now. + Python Client Results

6.3 NoWorkflow vs Python Implementation

The two implementation approaches are implementing the same features, even though there are major differences between them. In this sections the different implementations get compared and the advantages and disadvantages of them get discussed. Therefore three categories get confronted by both implementations. First the effort of applying the implementation gets compared, then the performance of the python and the noworkflow implementation is compared. The last comparison is about the maintenance and the extensibility of the solutions.

6.3.1 Implementation Effort

The implementation of this thesis applies the purposed reproducibility context model creation only for the EODC back end. There are six other back end providers in the project were there needs to be a solution too. Therefore the effort of the implementation gets graded so that other back end providers can decide, which solution they want to implement.

noWorkflow
The implementation of noworkflow is by the definition of noworkflow itself quiet easy. The EODC back end is a python implemented back end and therefore just the call of the python scripts has to be changed to the noworkflow command line interface, which is a wrapper around python. That was everything that has to be done on the code provenance capturing part. The created database has to be moved to the job output folder. To get the provenance data the command line tool has to be called, so there is some effort to find the needed data in the documentation of the tool. After finding the information it has to get parsed for the information needed for the context model, which takes some effort, but can be done in a view hours.

Python
The python implementation does not affect the processing code of the EODC back end, but adds some additional logging calls to it. So that the actual code has to be modified, which takes longer than the noworkflow implementation. After the logging calls are added to the code the capturing part is done. For retrieving the information of the logging file it has to get parsed to transfer it to the context model of the job. This is easily done, because the added logging messages are only the needed information and it is self formatted so that the parsing is easy to implement.

Table 6.1: Performance comparison between noworkflow and python implementation

original execution	noworkflow solution	python solution
4069 ms	11900 ms	4074 ms

noWorkflow vs Python
The implementation effort of both solutions are very similar, the noworkflow solution has the advantage, that the capturing does not require changes in the code. The downside of noworkflow is that it captures much more provenance information than needed for the context model and the needed information has to be extracted from the database in case to get it.

6.3.2   Performance

Most of the OpenEO back end provider have customers that pay by the length of the execution time and therefore the provenance capturing addition has to affect performance as little as possible. Therefore the performance of the two implementations get compared.

noWorkflow
Due to the wrapper around the python interpreter, the performance after applying the solution was very low. The execution time a bit more than three times the original execution without capturing. The fact about the bad performance of noworkflow is the reason for the implementation of the python solution.

Python
The python implementation adds almost no overhead to the execution. The parsing of the log file is the only part of the python code that has an real effect on the performance. Hence, the execution duration using the python solution is only a view milliseconds longer compared to the unmodified execution.

noWorkflow vs Python
The python implementation is by far much more efficient when it comes to performance. The main reason is the wrapper around python and the high amount of captured data in the noworkflow solution of data that is not needed in the context of this thesis. In the table below the timings of the proof of concept execution is recorded. The timing in the table is the time between sending the request and getting response from the server about the finished processing.

6.3.3   Maintenance and Extensibility

OpenEO is still involving and will be in the future due to the rapidly changing earth observation market. So in this section the extensibility and the maintenance of the solutions gets compared.

noWorkflow
NoWorkflow is already capturing much more information about the execution. It also

comes with a high amount of features to query the provenance data and to visualize it. NoWorkflow is also still evolving and new features may be added to it in the future. On the other hand the noworkflow solution is depending on the external maintenance of noworkflow, which is not guaranteed. So it can happen, that noworkflow does not work with a new python version, or if the back end provider switches to another programming language noworkflow can not be used any more. In addition to this disadvantages it is hard to add additional provenance data that is not already captured by noworkflow, because then noworkflow has to be adapted.

Python
The python solution is only capturing exactly the information that the back end provider wants it to capture. On fine granulated capturing and parsing the additional effort can be quite high. The advantage on this implementation is that the tool is easy extensible by just adding more logging information. Since logging is a simple feature of python it can be assumed that it will not change much in the future. If the back end provider decides to switch to a different programming language it can easily switch by adapting the code parsing to the new language and add the logging messages to the new back end implementation.

noWorkflow vs Python
Noworkflow comes with more features, especially for the back end provider to query and visualize the provenance data, but it is much harder to add information to the provenance capturing mechanism. So the python solution is much more flexible on changes and more independent from the environment than the noworkflow implementation.

CHAPTER 7

Conclusion and future Work

7.1 Conclusion

5. Summary of thesis 6. Describe limitations 7. Describe noworkflow and python implementation differences 8. Describe possibilities 9. Describe improvements

7.2 Future Work

In this thesis a concept for applying reproducibility in the OpenEO project is purposed. Still there are major issues to be addressed in the future of the OpenEO project. There are several ways to improve the concept and many open questions, which are open for the future.

OpenEO is still evolving until the project end 2021 and also afterwards. There are a lot of features that have to be defined and may interfere with the concept proposed in this thesis. User defined functions are part of the project and to be capable of reproduce them can lead to adaptations to the concept. Another main issue of the OpenEO project is the billing concept that has to be apply-able to a diverse set of back ends. Since the capturing process and the generation of the context model takes time it has to be considered in the billing plan of the back ends. The growing diversity of the back ends applying the OpenEO standard is a huge challenge to the design of the context model of this thesis.

The storage of the context models in JSON files was used in this thesis , but has definitely limitations that have to be addressed in the future e.g. the querying over the data sets. In the solution of this work the data is captured for identifying how jobs are executed and to be able to identify how the job was executed. An addition to this can be a way to automatically apply the reproduction of an executed jobs of the past. To achieve this a method of validating the output of a job execution needs to be introduced. The possibility to get automated data and process citation to researchers of OpenEO interfaces is also a

possible future work. Special users may need a finer granularity of the process capturing, leading to a definition of scalability of the processing capturing.

Talk about PROV-O

Benchmarking Mode

So far only the capturing of a single process, including input and output data, are described, but not how the whole process graph shall be captured. The general idea of the job dependent provenance capturing is to capture the input data of the process graph, the whole process graph and the output of the process graph like described in the sections above. This is a common concept the back end providers can agree on and is not affecting the back end providers implementations much. It is also capable of giving the OpenEO user a simple overview of how the results are generated and what are differences between different job executions. To make the comparison of different execution behaviors more informative, the granularity of the capturing can be improved.

update the picture

That is how the bench marking context model gets introduced. The idea is that not only the input data the whole process and the output data gets captured, but also every data in between of every process in the process graph. So for every process in the process graph the input, output data gets captured and the code executing the process. This makes it easier for users to see were the execution actually changed. But it also comes with higher implementation costs at the back end side. It also will affect the performance of the execution more than the common context model. The possibility of the implementation of such a granularity is also highly dependent on the back end implementation. Not every back end might be able to implement this into the back end due to execution optimization where the execution and results of the single processes in the process graph are not distinctable. Nevertheless in theory the granularity does not have to stop there, the data and code could be captured for every line in the code. This flexibility of capturing makes it also a context model that can be adapted to different use cases in the future.
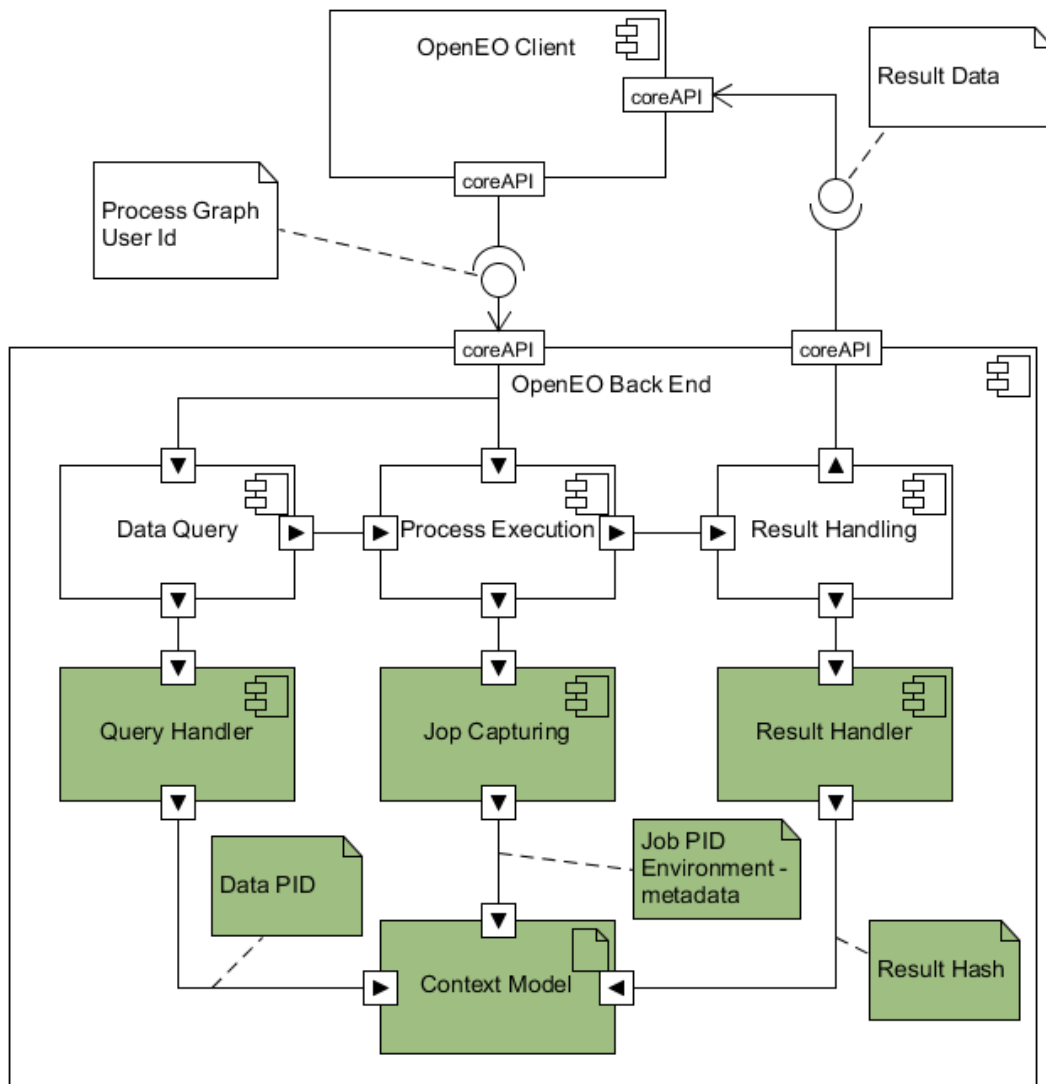
Figure 7.1: Design Overview of capturing the job context model in bench marking mode.

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