Development and demonstration of a proof-of-concept for the integration of programming frameworks for high performance computing into a container-based workflow orchestrator.

2. Project Paper

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Abstract:

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List of abbreviations

AI Artificial Intelligence

k8s Kubernetes

ML Machine Learning

HPC High Performance Computing

CC Cloud Computing

CI/CD Continuous Integration/Continuous Delivery

IaC Infrastructure as Code

PoC Proof of Concept

HPE Hewlett Packard Enterprise

CNCF Cloud Native Computing Foundation

CLASP Cloud Application Services Platform

CWL Common Workflow Language

SME Subject Matter Expert

TCP Tightly Coupled Problems

LCP Loosely Coupled Problems

SMART Simple Multiattribute Rating Technique

WSM Weighted Sum Model

MAUT Multi-attribute Utility Therory

SMART-ER SMART Exploiting Ranks

ROC Rank order centroid

RS Rank Sum

RR Rank Reciprocal

PFS Pachyderm File System

PV Persistent Volume

VM Virtual Machine

CNI Container Network Interface

FAM Fabric Attached Memory

SSO Singele Sign On

IP Interlectual Property

UDP User Datagram Protocol

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1 Introduction

In this section, the underlying motivation of this project is explained. Furthermore, the problems which will be addressed by this project are described, which serve as the basis for the research questions which will guide this project and ultimately result in solutions and further questions which are listed in the contributions section and discussed in the conclusion.

1.1 Motivation

The proliferation of "Big Data" has led to the need to compute, analyse, and visualize ever-increasing amounts of datasets, which themselves are getting more and more complex, has led to an ever increasing demand for more efficient and quicker ways to process data.

Both the High Performance Computing (HPC) and the Cloud Computing (CC) community have been working on solutions to distribute and parallelize computations for decades, both with their own approaches and solutions to their respective problems.

While the HPC community has been putting a lot of effort into developing new and extremely efficient ways to parallelize computations, the CC community has been focusing on improving the flexibility, scalability and resilience of their solutions as well as improving the ease of use for their developers and users.

Both used to be very distinct and separate communities due to their very different usecases, while the HPC community was mostly concerned with scientific computing and simulations of physical phenomena, the CC community is mostly concerned with providing a reliable and easily up and down scalable infrastructure for the industry and businesses.

Now with the advent of Machine Learning (ML) and Artificial Intelligence (AI) the two communities are starting to converge, as the ML and AI community is adopting the tools and techniques of both communities to solve their problems as they see fit.

But this convergence of the two is not without its problems, being developed in two coexisting and separate communities, the tools and techniques of both communities are not always compatible with each other, the goal of this project is to find a way to bridge this gap and to find a way to combine the best of both worlds.

1.2 Problem Statement

The following key problems have emerged from the convergence of High Performance Computing (HPC) and Cloud Computing (CC) communities, especially in the context of Machine Learning (ML) and Artificial Intelligence (AI) research:

- **Workload Resilience and Fault Tolerance in HPC:** HPC systems often lack mechanisms to recover from task failures within larger jobs, running for an extended time. When a component task fails, it can invalidate the entire computation, requiring a restart from scratch. This need for resilient failover and verification strategies as well as the need to avoid computational wastage is a key challenge for HPC systems, especially with every increasing system sizes and complexity.[3]

- **Environment/Package Management in HPC:** HPC systems are notorious for their complex package management systems. As having a shared infrastructure between many users each with their own specific needs and requirements of different versions of packages, libaries and software, all the while sharing a common environment. Many solutions to this problem have been developed, each with their own advantages and disadvantages.[4][5][6][7]

- **Portability Issues with HPC:** Tieing in with the previous point, HPC systems are often designed to be optimized for specific hardware as well as having a very specific software stack. This makes the portability of applications between different HPC systems very difficult and often infeasible.[8] This lack of portability contrasts sharply with the more platform-agnostic nature of CC environments, where the containerization of applications has become the norm for ensuring portability.

- **Scalability and Flexibility in HPC:** Due to its direct access to the hardware and very specific hardware needs, HPC systems are often hard to dynamically scale and inflexible. while CC systems are designed to be easily scalable and flexible and are often designed to be hardware agnostic and abstract away the underlying hardware. This becomes especially relevant in the context of heterogeneous hardware, where the hardware is not uniform and consists of different types of hardware, which is becoming more and more common in the context of ML and AI research.

- **Lack of Interconnected Problem Solving in CC:** The workloads traditionally deployed on CC systems are often independent of each other, like load balancing, web hosting, etc. This is in stark contrast to the interconnected nature of HPC workloads, where each part of the input data is dependent on the other parts of the input data, such that all nodes of the system need to be able to communicate with each other.

[3] Egwutuoha et al. 2013
[4] Dubois/Epperly/Kumfert 2003
[5] Bzeznik et al. 2017
[6] Gamblin et al. 2015
[7] Hoste et al. 2012
[8] Canon/Younge 2019, p. 50

- **Provenance and Reproducibility:** Another need that is becoming more and more important in the context of ML and AI research is the need for provenance and reproducibility of results. Being able to tell which data was used to train the model, is of ever increasing importance as the influence the resulting models have on our lives increases as well as the data used to train the model. This is especially important since it is crucial to ensure that the data is not biased, outdated, or otherwise flawed, which could lead to incorrect predictions, decisions, or recommendations. in addition various data sources, from images to text, may have copyright restrictions that, when overlooked, can lead to significant legal complications.
- **Versioning Limitations:** The dynamic nature of ML and AI research necessitates robust versioning solutions for data, configurations and code. While CC has developed many solutions to this problem over the years, making them their own subsection of the ecosystem, namely Continuous Integration/Continuous Delivery (CI/CD) tools for the testing and deployment of applications aswell as Infrastructure as Code (IaC) tools for the deployment of infrastructure. While many solutions have been developed for the one-off deployment of HPC systems, the dynamic nature of CC systems necessitates a more robust solution to this problem, from which the HPC community could benefit aswell.

1.3 Research Questions

To address the aforementioned problems, to bridge the gap between the two paradigms and to combine the best of both worlds, an integration of the two paradigms is needed. This was accomplished by integrating a HPC framework called 'Arkouda[9]' into a container based CC workflow management tool called 'Pachyderm'[10] and integrating both with the supporting infrastructure the CC system enables us to use. This process of integration and prototyping as well as the explanation of the underlying concepts and technologies will be the focus of this project.

- **RQ1:** *How can a high-performance computing framework be effectively integrated into a container-based workflow management tool?*
- **RQ2:** *What are the opportunities for improving the integration of high-performance computing frameworks with container-based workflow management tools?*

[9] Merrill/Reus/Neumann 2019
[10] **pachydermPachyderm**

1.4 Contributions

In order to address the problems stated above, find answers to the research questions and to bridge the gap between the two paradigms, the following contributions were made:

- **C1:** *An analysis of the problem space and existing solution, within the constraints of time, resources and businesses needs.*
- **C2:** *A prototype implementation combining the 'Arkouda' framework with the Kubernetes (k8s) based workflow orchestrator 'Pachyderm'*
- **C3:** *Further integrations of tools from both sides of the spectrum, addressing many of aforementioned pain-points*

2 Methodology

2.1 Prototyping

Needs to have a methodology from the Spectrum of Methodologies for Business information systems[11]

Argumentation why this project is centrally a Prototyping project:

- The research questions are directly inspired bt the needs of the customer
- The limitations and the scope are both defined by the available resources of the business unit as well as the time constraints of the project and the available know-how
- Based[12] can be classified as a presentation prototype in which we do a does a vertical integration of many different sysytems, according to budde this can be described as a vertical interface, as it reaches through the entire stack of technological abstraction[13]
- to create this prototype we will be using Which will be using spiral modle[14]

[11] Wilde/Hess w.y.
[12] Budde et al. 1992, p. 91
[13] Budde et al. 1992, p. 94
[14] Boehm 1988

2.2 Decision Making

As previously described, the methodology of Prototyping benefits from a very tight loop of iterations between the different phases of the project. While this is highly effective in producing a good end result, it can also take many iterations and a lot of experimentation until an adequate tool or solution has been found. Given the constraints of a limited time frame for this project, it becomes crucial to use this time as efficiently as possible. Sometimes, when the time does not permit a thorough exploration of

To ensure that the decisions made are the most optimal within the constraints of the available information, adopting a systematic, replicable, and transparent decision-making process becomes essential. Over the years, various frameworks have been crafted to guide decision-making, particularly when information is complex and multi-dimensional.

2.2.1 Weighted Sum Model

Evangelos Triantaphyllou suggests that the Weighted Sum Model (WSM) is in practice the most used and most relevant decision-making framework[15]. The WSM method, by design, mandates the assignment of specific weights to each criterion based on its relevance. Subsequent to this, every alternative is evaluated based on these weighted criteria, resulting in a cumulative score. The alternative with the highest score is therefore the optimal choice.

$$A_i^{WSM-score} = \sum_{j=1}^{n} w_j a_{ij} \quad for\ i = 1, 2, 3, \ldots, m.$$

Abb. 1: Formula for calculating the WSM score[16]

Where:

- !TODO! add explanations of variables

This method, despite its simplicity and direct approach, isn't without limitations. One notable drawback is its dependence on dimensionless scales. For the weights to properly reflect the criteria's importance, the scores need to be on a common, dimensionless scale, a detail not always feasible or convenient in practice.

[15]Triantaphyllou 2000, p. 1
[16]*Weighted Sum Model* 2022

2.2.2 Simple Multi-Attribute Rating Technique

In contrast to the WSM , which predominantly utilizes a direct mathematical approach to rank alternatives based on their weighted sum scores, the Simple Multiattribute Rating Technique (SMART) methodology offers a more comprehensive approach to multi-criteria decision-making. While WSM is primarily concerned with simple weighted arithmetic sums, the SMART method dives deeper, ensuring that diverse performance values—both quantitative and qualitative are harmonized and placed on a common scale.

The SMART method, grounded in Multi-attribute Utility Theory (MAUT), provides a structured framework that encompasses more than just the weighting of criteria. It involves:

1. Discernment of vital criteria pertinent to the decision in focus.
2. Weight allocation to each criterion in accordance to its significance.
3. Evaluation of each potential alternative against the identified criteria, culminating in a score.
4. Aggregation of these individual scores via their associated weights, yielding a total score for every alternative.

By adhering to the SMART framework, alternatives can be sequenced based on their aggregated weighted scores. This systematic approach equips decision-makers to choose solutions that align closely with their objectives. The computational formula integral to the SMART method is:

$$x_j = \frac{\sum_{i=1}^{m} w_i a_{ij}}{\sum_{i=1}^{m} w_i}, \quad j = 1, \ldots, n.$$

Abb. 2: Formula for calculating the SMART score[17]

Where:

- x_j Is the overall utility socre for alternative j. The higher the score, the better the alternative, in comparison to the other alternatives.
- a_{ij} Is the utility score for alternative j for the criterion i.
- w_i Is the weight of criterion i.

This method's emphasis on utility functions ensures a more nuanced and adaptable approach to decision-making compared to models like WSM, making it suitable for complex scenarios where criteria and alternatives are diverse in nature[18].

[17] Taken from Fülöp 2005, p. 6
[18] Fülöp 2005, p. 6

2.2.3 SMART Exploiting Ranks

The SMART Exploiting Ranks (SMART-ER) method is a variant of the SMART method that attempts to alleviate the largest issue of the original SMART method, namely the problem of a somewhat arbitrary ranking of the options if no numerical values can be derived.

This method addresses the issue by letting the decision maker simply ranking the different criteria in relation to each other and then normalizing the weights[19]. They propose the different weighting curves.

$$w_i(ROC) = \frac{1}{n}\sum_{j=1}^{n}\frac{1}{j}, \quad i = 1, \ldots, n.$$

Abb. 3: Formula for the ROC weights

The ROC takes the centroid of the rank order and uses the reciprocal of the rank as the weight.

$$w_i(\ RS\ ) = \frac{n+1-i}{n(n+1)/2}, \quad i = 1, \ldots, n.$$

Abb. 4: Formula for the RS weights

The RS uses linear curve where weights are normalized by dividing them by the sum of all weights.

$$w_i(RR) = \left(\frac{\frac{1}{i}}{\sum_{j=1}^{n}\frac{1}{j}}\right),\ rank\ i = 1, \ldots, n,\ option\ j = 1, \ldots, n$$

Abb. 5: Formula for the RR weights

The RR emphasizes the most important criteria by using the reciprocal of the rank as the weight, then normalizing each weight by the sum of all reciprocals.

[18] *Multi-Criteria Decision Analysis for Use in Transport Decision Making* 2014, p. 26
[19] Roberts/Goodwin 2002, p. 296

3 State of the Art

3.1 Containerization

Container Solutions

Software defined Infrastructure

Large Scale Container Orchestration

3.2 High Performance Computing Frameworks

3.2.1 Loosely Coupled Problems

Loosely Coupled Problems (LCP) also known in the industry as "embarrassingly parallel"[20] problems are problems that can be broken up into smaller independent tasks that can be executed in parallel.

tools like Mapreduce and Spark

3.2.2 Tightly Coupled Problems

In contrast to LCP problems, Tightly Coupled Problems (TCP) problems are problems that can not be broken up into smaller independent tasks that can be executed in parallel, instead of working independently, each atomic task needs to communicate at least with one other task. A good example of a TCP problem are the n-body problems, where the position of each body is dependent on the position of all other bodies.

tools like MPI, OpenMP and Chapel

[20]**smtn**

4 Creation of the Artifact

4.1 Initial Goals

As this project was first and foremost a project, designed to interactively explore the problemspace from the perspective of the HPC community, all the while being contained by business requirements and time constraints, the initial goals of this project were very broad and open ended. At first the initial goal was simply to create a Proof of Concept (PoC) of a realistic workflow engine using the "Arkouda" project, in order to present the Customer with a easily graspable example of its capabilities.

While we are approaching the problem from the perspective of the HPC community, the intended enduser of this tool are the data scientists and Subject Matter Expert (SME)s that are working with the HPC systems, and therefore the tool needs to be designed and selected with the fact in mind that the enduser will most likely not be knowledgeable in the field of HPC or the underlying infrastructure.

In the first iteration of the project a preselection of possible Workflow management tools was given from the business side, with the option to increase the scope if the presented tools were not sufficient.

Therefore the goals of the first iteration of this project was twofold, first to determine which, if any, of the presented tools were suitable for the task at hand, and to determine what would make an adequate PoC for the customer.

The following iterations are split into the tree main aspects of the project and will be discussed in their own subsections. While these steps where happening concurrently, they each address a different aspect of the project and therefore underwent their own iterative processes.

4.2 Overall Structure

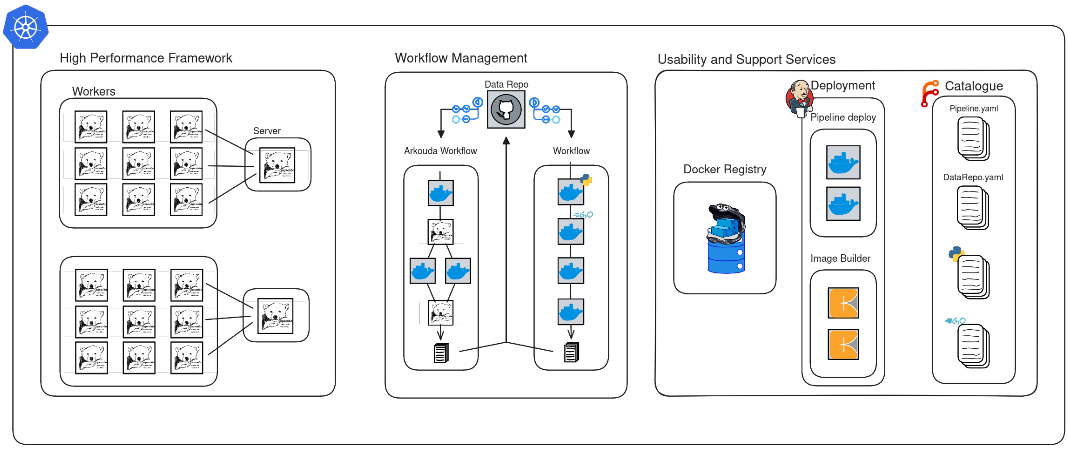

Abb. 6: Pachykouda high level infrastructure diagramm

As can be seen in figure 6, the artifact is composed of 3 main components, the **Central Workflow Engine** which is responsible for the orchestration of the workflows (center) and interfaces directly with the underlying infrastructure, the **HPC Framework** which is responsible for the execution of TCP workloads (left) and the **Supplementary Services** which aim at improving the usability and accessability for the enduser (right).

All this is build ontop of a hardware agnostic k8s cluster, which is responsible for the orchestration of the different components and the underlying infrastructure.

4.3 Selection of Workflow Management Tools

As described in section 4.1, the first iteration of this project was to determine which, if any, of the presented tools were suitable for the task at hand. The following section will describe the process of selecting the tools and the criteria that were used to evaluate them. Because the time frame does not allow for a full integration and testing of all the presented tools in depth we will be using a decision making framework to evaluate the tools, as described in the Methodologies 2.2 to determine which tools will be most suitable for an initial PoC and will serve as a good starting point for the project and future iterations.

- **Pachyderm:** A k8s based Workflow manager, written in go which was recently aquired by Hewlett Packard Enterprise (HPE).
- **Argo:** A k8s based Workflow manager , written in go, which is a Cloud Native Computing Foundation (CNCF) project[21].
- **Cloud Application Services Platform (CLASP):** An in-house developed workflow manager, written in Java, utilizing Serverlet to execute workflows[22].
- **Snaplogic:** A commercial low-code/no-code workflow manager with a focus on data integration and data engineering[23].

But given that it was possible to select projects outside of the initial selection, the following projects also need to be considered:

- **Airflow:** A Python-based workflow manager under the CNCF umbrella, known for its easy-to-use interface and extensibility[24].
- **Kubeflow:** A k8s-native platform for deploying, monitoring, and running ML workflows and experiments, also a CNCF project, streamlining ML operations alongside other Kubernetes resources[25].
- **Knative:** An open-source k8s-based platform to build, deploy, and manage modern serverless workloads, simplifying the process of building cloud-native applications[26].
- **Luigi:** An open-source Python module created by Spotify to build complex pipelines of batch jobs, handling dependency resolution, workflow management, and visualization seamlessly[27].

[21] *Argoproj/Argo-Workflows* 2023
[22] Sayers et al. 2015
[23] *iPaaS Solution for the Enterprise* 2023
[24] Haines 2022
[25] *Kubeflow* 2023
[26] *Home - Knative* 2023
[27] *Spotify/Luigi* 2023

- **Common Workflow Language (CWL):** An open-standard for describing analysis workflows and tools in a way that makes them portable and scalable across a variety of software and hardware environments, from workstations to cluster, cloud, and high-performance computing environments.

Selection Criteria

Due to this extensive list of diverse tools, a set of criteria was established to determine which tool would be the most suitable for the task at hand. The following list of criteria was established to evaluate the tools:

- **Ease of use:** As the inted endusers of the tool are not primarily HPC experts, the tool needs to be easy to use and understand, and should not require the enduser to have a deep understanding of the underlying infrastructure. While we can expect that the administration of the infrastructure will be done by adequately trained personnel, the enduser should be spared having to adapt to the underlying infrastructure as much as possible.
- **Extensibility:** One significant constraint of the project is the restricted number of available work-hours. Given that the project's environment predominantly centers around HPC (High Performance Computing) workloads, it's essential for the tool to be easily expandable without requiring extensive modifications to the underlying system. Ideally this property would be transferred to the enduser, allowing them to easily extend the developed tool further to their needs.
- **Community, Support and Documentation:** It is not enough that the software technically permits extensibility, the software also needs to be adequately documented and a support framework needs to be in place. Be it a community of users or a dedicated support team, the enduser and the developers need to be able to rely on the software being maintained and updated as well as being able to find expert help in case of problems.
- **Maturity:** With the boom of AI and ML in recent years[28], the number of tools and frameworks has exploded, and while this is a good thing it also means that a lot of these tools are still paving their way and are developing rapidly. While this is not necessarily a bad thing, it does mean that the tool might not be ready for production use and might not be able to provide the stability and reliability that is required for a production environment or are lacking in documentation and support.
- **Strategic alignment with HPE:** As this project is being developed within the context of HPE, it is important to consider the strategic alignment of the tool with HPE. HPE has is a large company with a diverse portfolio of products and services, and this project

[28] *24 Top AI Statistics & Trends In 2023 – Forbes Advisor* 2023

intersects with many different parts of the company. Therefore it is important to consider the strategic alignment of the tool with HPE and its products and services.

- **License:** While this PoC is not a commercial product in itself but rather an exploration of the problem space and a demonstration of what a final commercial product might be like, it is important to consider the licenses of the tools that are being used. Having to strip out a tool later on because of licensing issues would be a significant setback and therefore needs to be considered.

- **Cost:** Time is not the only constraint of this project, as the project is being developed within the context of HPE it is important to consider the cost of the tools that are being used.

Weigting of the Criteria

An integral part of the SMART methodology is the weighting of the criteria, as described in section 2.2. In order to rank the criteria themselves, as they are quite hard to quantify, We will be using the weighing methodology as described in the SMART-ER methodology 2.2.3.

The first step of which is the ranking of the criteria from most important to least important.

1. **Extensibility** As this is first and foremost a prototyping project, the actual development it at least for the first couple steps of the highest importance.

2. **Community, Support & Docs** This also applies for the external support available to the development team as if they are stuck, no developed can proceed, no matter the other factors.

3. **License** This criterion has to weighted carefully, as a highly restrictive license might be a dealbreaker, but a license that is too permissive might conflict with the strategic alignment with HPE.

4. **Strategic alignment with HPE** As this is developed by and for HPE their requirements need to be consider aswell.

5. **Ease of Use** While the ease of use is important as this should eventually become a product, for now the central aspect is to create a PoC therefore the usability is a priority, but not the highest.

6. **Cost** As this is a PoC and not a commercial product, the cost is not the highest priority as this will be of small scale and therefore the cost will be negligible in most cases.

7. **Maturity** While the maturity of the tool is important, as this is a PoC and not a commercial product, if the maturity of the tool does not impact the extensibility of the tool or the development process, it is not the highest priority.

As all these criteria are quite important, the weighting function selected for the criteria is the RS function, as described in section 2.2.3, as it does not rank the criteria too harshly. The lookup tables for the weighting function can be found in the appendix **??**.

Criteria	**Weight**
Extensibility	0.2500
Community, Support and Documentation	0.2143
License	0.1786
Strategic alignment with HPE	0.1429
Ease of use	0.1071
Maturity	0.0714
Cost	0.0357

Tab. 1: Weighting of the criteria

Evaluation of the Tools

Now that we have established the criteria aswell as their weighing, we can beginn to evaluate the tools based on the criteria. Here we will be using a mix of Methodologies, as some of these criteria can simply be indexed via analogous values, while others are of a more non specific nature. The discussion of which values will be used on which weighing scale for the tools comparison can be found in the apendix under

Criteria	**Pachyderm**	**Argo**	**CLASP**	**Snaplogic**
Ease of use	TBD	TBD	TBD	TBD
Extensibility	TBD	TBD	TBD	TBD
Community, Support & Docs	TBD	TBD	TBD	TBD
Maturity	TBD	TBD	TBD	TBD
Strategic alignment	TBD	TBD	TBD	TBD
License	TBD	TBD	TBD	TBD
Cost	TBD	TBD	TBD	TBD

Tab. 2: Evaluation of the suggested tools

The following table shows the evaluation of the tools which where chosen for their relevance to the problem space, based on the criteria and the weighting of the criteria:

Criteria	**Airflow**	**Kubeflow**	**Knative**	**Luigi**	**CWL**
Ease of use	TBD	TBD	TBD	TBD	TBD
Extensibility	TBD	TBD	TBD	TBD	TBD
Community, Support & Docs	TBD	TBD	TBD	TBD	TBD
Maturity	TBD	TBD	TBD	TBD	TBD
Strategic alignment	TBD	TBD	TBD	TBD	TBD
License	TBD	TBD	TBD	TBD	TBD
Cost	TBD	TBD	TBD	TBD	TBD

Tab. 3: Evaluation of the additional tools

Conculsion of the Selection Process

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

4.4 Implementation of the Artifact

This section will describe the iterative process of implementing the larger artifact and is broken up into 3 subsections. While these steps where happening concurrently, they each address a different aspect of the project and therefore underwent their own iterative processes.

4.4.1 Infrastructure

First iteration - Minikube

As the decision of the Workflow management tool was made, it was obvious that a dedicated k8s infrastructure was needed to run the tool[29]. The Pachyderm documentation gave two recommendations for setting up an initial development environment, preferably Docker Desktop or alternatively Minikube[30]. Due to the exclusive license of Docker-Desktop[31], which prevents large companies free usage of the product[32] the choice fell on Minikube for an initial test setup.

In addition to the underlying k8s Pachyderm also needs an external S3 Storage Bucket for its Pachyderm File System (PFS) for which we used MinIO, a self hostable S3 compliant object storage[33], which was also based on recommendations by the Pachyderm documentation.

The persistent storage requirements for the Pachyderm itself was fulfilled by manually creating two Persistent Volume (PV)'s on the hosts local harddrive. Using the Helm packagemanager[34] for k8s the at that point newest version 2.6.4 was installed from the official Artifacthub repository[35].

[29] *Pachyderm Docs - On-Prem Deploy* 2023
[30] *Pachyderm Docs - Local Deploy* 2023
[31] *Docker Terms of Service | Docker* 2022
[32] *Docker FAQs | Docker* 2021
[33] Inc 2023
[34] *Helm Docs Home* 2023
[35] *Artifacthub Pachyderm 2.6.4* 2023

The hostsystem of this iteration was a single ProLiant DL385 Gen10 Plus running Ubuntu 22.04.3 LTS x86_64. During the setup every step was diligently noted and put into a repository[36], alongside the needed scripts. The instructions can be found in the appendix at 3.

Learnings from the first iteration

The shortcomings of this naive first iteration became apparent very quickly, which was to be expected, as the goal of this iteration was to create a minimal working example to get a better understanding of the toolings and the underlying infrastructure.

The first and foremost issue where the limitations imposed by Minikubes reliance on an Internal Virtual Machine (VM), during testing the inability to on the fly increase the resources of the VM became a significant bottleneck. At some point during the testing of 4.4.2 the VM was so overloaded that the installation was irreparably damaged which was seen as a sign to move on to the next iteration.

Another more subtle issue was the discrepancy between the experience a small scale k8s installation within Minikube and a large scale k8s cluster like the one that would be used in later steps of the project. Therefore it was decided that a more realistic k8s cluster would be needed for the next iteration, which became the Heydar cluster.

Second iteration - Heydar Cluster

Improving upon the shortcomings of the first iteration, the second iteration was based in the attempt to create a more realistic k8s cluster. To achieve this 20 ProLiant DL360 Gen9 Servers, running Ubuntu 22.04.3 LTS x86_64 where used to create a bare metal k8s cluster, using kubeadm as it provides deep integration with the underlying infrastructure[37].

But a bare metal cluster also comes with its own set of challenges, as the cluster needs to be provisioned and configured manually. In order to automate this process, the Ansible automation tool was used to set up all the nodes in praralel and to ensure that the all the nodes are in the same state. Ansible is a declarative tool which allows for the automation of the provisioning and configuration of the cluster[38], by specifying the desired state of the cluster in a playbook and then applying it to the cluster. The Ansible playbook used for the setup of the cluster can be found at Appendix 4/1.

Which unknowingly caused conflict between the Ansible playbook and the maintenance scripts of the cluster as the Heydar machines. As k8s needs very specific configurations on the underlying infrastructure like the deactivation of swap space[39].

[36] Eckerth 2023
[37] *Creating a Cluster with Kubeadm* 2023
[38] *Ansible* 2023
[39] *Installing Kubeadm* 2023

This was resolved by consulting with the maintainer of the cluster and adjusting the Ansible playbook as well as the maintenance config for the cluster nodes accordingly, after we had identified the issue.

One important aspect of a production like cluster is the networking, as k8s does not natively manage communication on a cluster level, but instead relies on so called Container Network Interface (CNI)s to manage and abstract the underlying network infrastructure[40].

Here we where spoiled for choice once again, as there are a multitude of different CNIs available, each with their own advantages and disadvantages. The Kubernetes documentation provides a non exhaustive list of 17 different CNIs[41], which all fulfill this essential task in different ways. As the needs regarding the network plugin where not very specific at this point, the choice fell on Calico, as surface level research showed that it was a popular choice for bare metal clusters[42], provided security and enterprise support as well having a wide range of features[43]. But Calico proved to be more difficult to setup than expected, after consulting with a college who set up a different cluster with Calico, it was decided to use Flannel as a CNI instead. Flannel turned out to be much easier to setup and configure, as it is a very lightweight CNI which is designed for bare metal clusters[44], and foregoes the more advanced security features of Calico.

The Flannel configuration used for the cluster can be found at Appendix 4/2 it is closely based on the example configuration provided by the Flannel documentation[45].

Learnings from the second iteration

The second iteration was a significant improvement over the first iteration, as it provided a much more realistic environment for the development of the artifact. But it also came with its own set of challenges, as the bare metal cluster needed to be provisioned and configured manually, which was a significant time investment.

What became apparent very quickly was that the solution for the provisioning of the PV was no where near scalable, as it relies on the local harddrive of the host machine and therefore must host the container on the same machine as the PV which defeats the purpose of a multi node cluster in the first place. Therefore a more scalable solution needs to be implemented for the next iteration. A possible solution could be the use of distributed storage solutions like Ceph[46] or GlusterFS[47] in combination with the Rook project[48]. which will need to be explored in future iterations.

[40] *Cluster Networking* 2023
[41] *Kubernetes CNI Plugins* 2023
[42] *Explore Network Plugins for Kubernetes* 2023
[43] Mehndiratta 2023
[44] *Flannel* 2023
[45] *Flannel Install Config* 2023
[46] *Ceph.Io — Home* 2023
[47] *Gluster* 2023
[48] *Rook* 2023

As described in section XXX a service hosting Fabric Attached Memory (FAM) will be needed in future iterations aswell.

4.4.2 Tightly Coupled HPC Workloads

As described in section 3.2.2 TCP problems are a large part of the HPC world, but seem to lack native support in Pachyderm. Pachyderm as it exists as of writing this thesis, is centralized around LCP problems, as it is designed to work with large amounts of data but with each so called "datum" being independent of each other. This is a very good fit for LCP problems, and ties into their concepts of data lineage, versioning and providence.

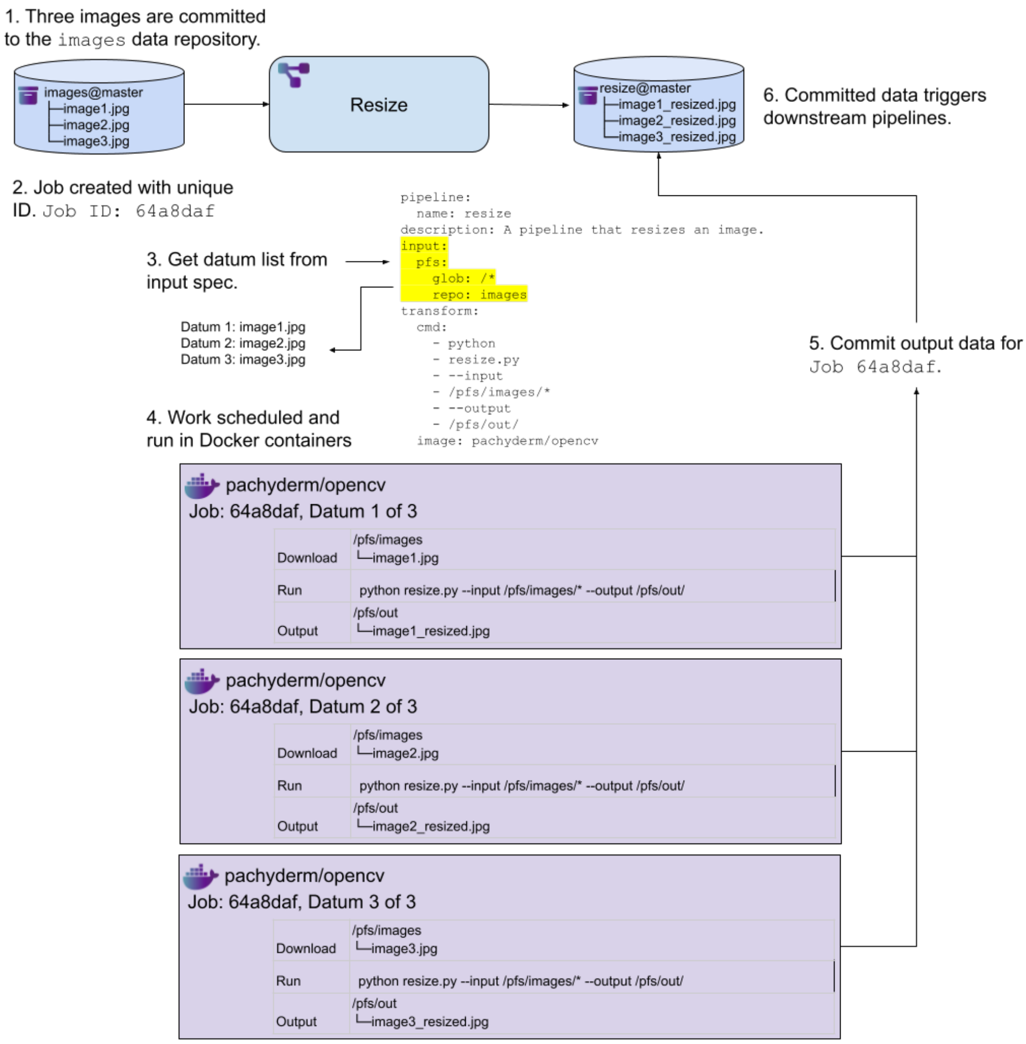

Abb. 7: Pachykouda datum distribution amongst workers [49]

Diagram 7 shows Pachyderms approach to distribute their datums amongst workers, given an already defined pipeline. Once Data files are added to the input repository, Pachyderm will

[49]Taken from: *Intro to Pipelines* 2023

determine Based on a glob pattern wether the files are relevant datums for the pipeline. If the newly added data fits the pattern each of the files will be supplied to its own instantiation of a worker, all originating from the same image, which will then process the data concurrently and independently of each other. After the worker has finished its task, the resulting datums are then collected in their own repository of data. A more detailed swim lane diagram of this process can be found in the appendix at Appendix 2/1.

This approach is very well suited for LCP problems, as the datums are independent of each other and can be processed in parallel without any issues. But it is not well suited for Large TCP problems, if the computation of the data can not be split into distinct independent datum files, or the computation is reliant on the intercommunication of the datums. If the datasets are small enough, this does not really present a problem as one can simply take all the data into a single workernode and process it there. But as a single worker node can only utilize the resources of a single physical compute node, this does not scale well with the size of the dataset and defeats the purpose of a distributed system in the first place.

So our goal for this section is a way to find a way to enable pachyderm to pool the entire resources of the cluster, in oder to solve a TCP problem.

First iteration - PachyKouda

As a first attempt to address this issue, it was decided that the integration of a TCP framework into Pachyderm on the container level would be the best approach. So the first iteration is based on the idea of a Pachyderm conforming client container, which is able to interface with an external TCP framework, which can handle the reception of the data, the distribution of the data amongst the workers and the collection of the results to reintegrate them into the PFS.

The first iteration of this idea was called PachyKouda, as it was based on the Arkouda TCP framework[50], which itself is a python binding for the Chapel programming language[51].

For that step an Arkouda worker was installed bare metal on the headnode of the Heydar cluster, in order to verify the feasibility of the idea, with the goal of moving the worker into the cluster in the next iteration.

The client container was based on the official User Datagram Protocol (UDP)-based build by the Arkouda team[52]. The container was then modified to be able to communicate with the Arkouda worker on the headnode of the cluster, it can now send data to the worker and receive the results.

[50] *Arkouda Gituhb Repository* 2023
[51] *Chapel-Lang* 2023
[52] *Arkouda-Contrib/Arkouda-Docker at Main · Bears-R-Us/Arkouda-Contrib* 2023

Learnings from the first iteration

4.5 Evaluation of the Artifact

5 Conclusion

6 Summary and Outlook

6.1 Summary

6.2 Outlook

Appendix

Appendix Index

Appendix 1: Discussion of Tool Evaluation and Weighing

Appendix 1/1: Extensibility

Appendix 1/2: Community, Support & Docs

Appendix 1/3: License

As discussed in section 4.3 the tools in consideration should not be to restrictive. To evaluate the criteria we will employ a 3 bucket system, where tools with an acceptable license get a value of 1, tools where the licensing is ideal get a 2, and tools which have a not acceptable license get weighted with 0.

- **Pachyderm** The licensing model of Pachyderm follows a model which has similarities with the "Open Core model"[53]. Which means that while the core functionalities are published as the "COMMUNITY EDITION" with a permissive source-available License (Apache License 2.0)[54]. Functionality like Singele Sign On (SSO) or the ability to create more than 16 pipelines are part of a different distribution under a Commercial License.

  But in our case this is of no concern, as the startup behind the Pachyderm softwarem, including its Interlectual Property (IP) was aquired by HPE. Giving us a free hand to modify without needing to worry.

- **Argo** is licensed under the Apache License 2.0.[55] Apache 2.0 is quite a standard license for this kind of product, as it enables [....]

- **CLASP** is not a published software and therefore not under any specific license. But similar considerations as the ones of Pachyderm apply here aswell, as it is an internal project the IP also completely belongs to HPE

- **Snaplogic** is an entirely commercial product which does not provide insight into nor the right to modify their Software[56]. But as they might agree this is not a total knockout criterion for this entire project, but in regards to the licensing it will be weighted with 0.

- **Airflow** is licensed under the Apache License 2.0.[57]

- **Kubeflow** is licensed under the Apache License 2.0.[58]

- **Knative** is licensed under the Apache License 2.0.[59]

[53] *Pahcyderm -Pricing* 2022
[54] *Pachyderm/LICENSE at Master · Pachyderm/Pachyderm* 2023
[55] *Argo-Cd/LICENSE at Master · Argoproj/Argo-Cd* 2023
[56] *SnapLogic – Master Subscription Agreement* 2023
[57] *License — Airflow Documentation* 2023
[58] *Kubeflow/LICENSE at Master · Kubeflow/Kubeflow* 2023
[59] *Knative Docs/LICENSE at Main · Knative/Docs* 2023

- **Luigi** is licensed under the Apache License 2.0.[60]
- **CWL** is licensed under the Apache License 2.0.[61]

Appendix 1/4: Strategic alignment

Appendix 1/5: Ease of Use

Appendix 1/6: Maturity

Appendix 1/7: Cost

[60] *Luigi/LICENSE at Master · Spotify/Luigi* 2023
[61] *Cwl-Utils/LICENSE at Main · Common-Workflow-Language/Cwl-Utils* 2023

Appendix 2: Diagrams

Appendix 2/1: Pipeline Communication Swim Lane Diagram

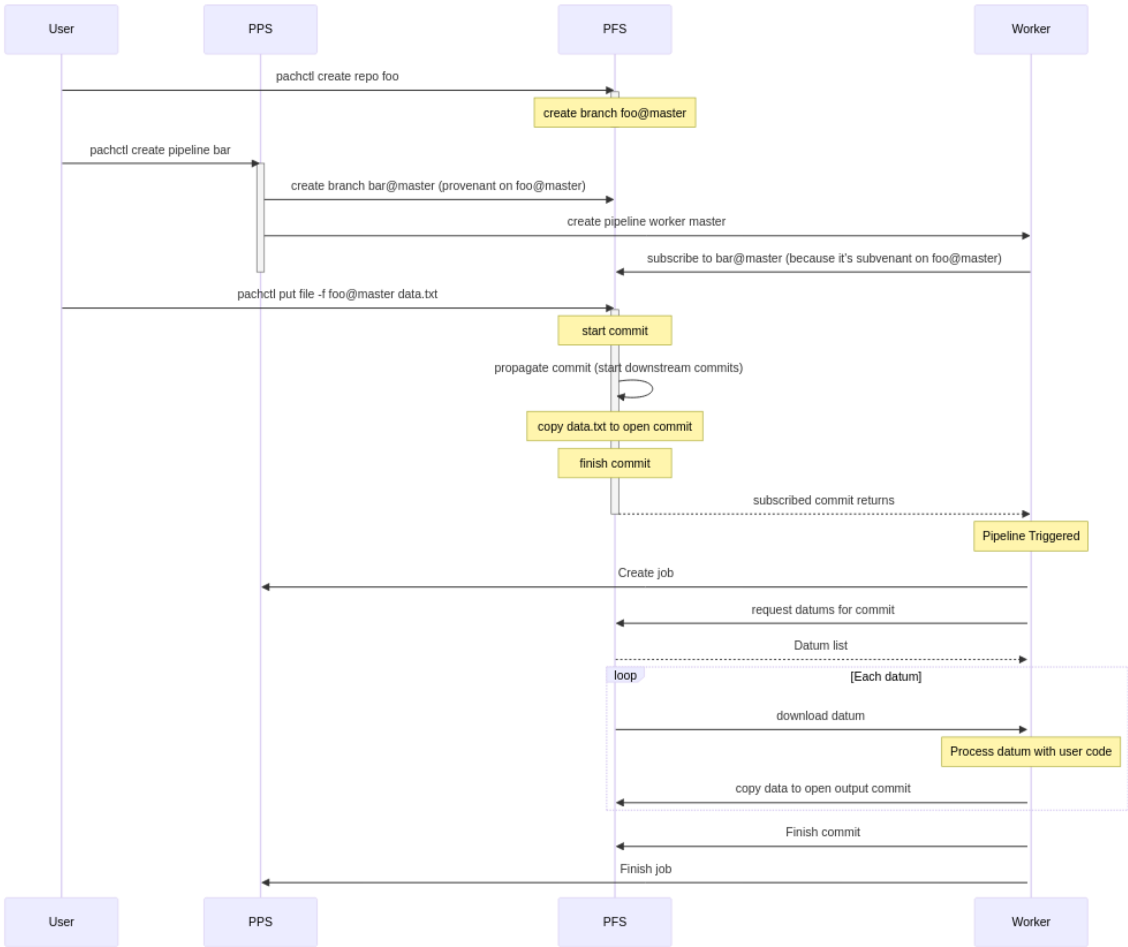

Abb. 8: Swimlane Diagram of the communication between the user and Pachyderm

Appendix 3: Minikube installation instructions

```
# Pachyderm

## Installation

These instructions are based upon the excellent guide by [Pachyderm](https://docs.pachyderm.com/latest/set-up/on-prem/)

### Proxy

If you are in the HPE internal network, you will need to set up the proxy.
```

[61]Taken from: *Intro to Pipelines* 2023

````
Simply execute the following command:

```bash
export HTTP_PROXY=http://web-proxy.corp.hpecorp.net:8080
export HTTPS_PROXY=http://web-proxy.corp.hpecorp.net:8080
```

If you want to make this permanent, add these lines to the `~/.bashrc` or equivalent file.

### kubectl

Simply following the instructions on the [kubernetes website](https://kubernetes.io/docs/tasks/tools/install-kubectl-linux/) should be sufficient.
But for the sake of completeness, here is what I did:

```bash
curl -LO "https://dl.k8s.io/release/$(curl -L -s https://dl.k8s.io/release/stable.txt)/bin/linux/amd64/kubectl"
sudo install -o root -g root -m 0755 kubectl /usr/local/bin/kubectl
```

If the proxy is giving you grief one can simply download the binary elsewhere and copy it to the target machine. (not recommended)

### Installing minikube

The same things apply for minikube as for kubectl.
The propper instructions can be found on the [minikube website](https://minikube.sigs.k8s.io/docs/start/)
But here is what I did anyway:

```bash
curl -LO https://storage.googleapis.com/minikube/releases/latest/minikube_latest_amd64.deb
sudo dpkg -i minikube_latest_amd64.deb
```

We can then test the installation by running:

```bash
minikube start
kubectl cluster-info
```

If you are getting an error stating that it is not able to connect to the cluster you might need to set the following environment variable:

```bash
export
````
````

````
    ↪ NO_PROXY=localhost,127.0.0.1,10.96.0.0/12,192.168.59.0/24,192.168.49.0/24,192.168.
```

### Installing [helm](https://helm.sh/docs/intro/install/)

Same procedure as every year...

```bash
curl https://baltocdn.com/helm/signing.asc | gpg --dearmor | sudo tee
    ↪ /usr/share/keyrings/helm.gpg > /dev/null
sudo apt-get install apt-transport-https --yes
echo "deb [arch=$(dpkg --print-architecture)
    ↪ signed-by=/usr/share/keyrings/helm.gpg]
    ↪ https://baltocdn.com/helm/stable/debian/ all main" | sudo tee
    ↪ /etc/apt/sources.list.d/helm-stable-debian.list
sudo apt-get update
sudo apt-get install helm
```

### [Persistent
    ↪ Storage](https://kubernetes.io/docs/tasks/configure-pod-container/configure-persis

We need to create a persistent volume for etcd and the postgres database.
Therefore we need to create a directory for each of them.

```bash
mkdir -p /mnt/pachyderm/etcd
mkdir -p /mnt/pachyderm/postgres
```

We then create the configuration files for the persistent volumes.

```yaml
apiVersion: v1
kind: PersistentVolume
metadata:
  name: etcd-pv
labels:
    type: local
spec:
  capacity:
    storage: 10Gi
  accessModes:
    - ReadWriteOnce
  storageClassName: manual
  local:
    path: /mnt/pachyderm/etcd

---

apiVersion: v1
````

````
kind: PersistentVolume
metadata:
  name: postgres-pv
labels:
    type: local
spec:
    capacity:
        storage: 10Gi
    accessModes:
        - ReadWriteOnce
    storageClassName: manual
    local:
        path: /mnt/pachyderm/postgres
```

And then the corresponding persistent volume claims.

```yaml
apiVersion: v1
kind: PersistentVolumeClaim
metadata:
  name: etcd-pvc
spec:
    storageClassName: manual
    accessModes:
        - ReadWriteOnce
    resources:
        requests:
        storage: 10Gi

---

apiVersion: v1
kind: PersistentVolumeClaim
metadata:
  name: postgres-pvc
spec:
    storageClassName: manual
    accessModes:
        - ReadWriteOnce
    resources:
        requests:
        storage: 10Gi
```

Then we add the storage class to the cluster.

```bash
kubectl apply -f filename.yaml
```

````
````

````markdown
We then take note of the storage class name because we will add it to the helm values file later. \
In this case it is `manual`.

### Installing [MinIO](https://min.io/docs/minio/linux/index.html)

We now install an S3 compatible storage system. Which one does not really matter, but I chose MinIO because it is easy to install and configure.

```bash
wget https://dl.min.io/server/minio/release/linux-amd64/archive/minio_20230619195250.0. -O minio.deb
sudo dpkg -i minio.deb

mkdir -p /mnt/pachyderm/minio

# to manually start the server
minio server /mnt/pachyderm/minio --console-address :9001
```

The standard password is `minioadmin:minioadmin`

Then you can access the web interface at `http://localhost:9001` where you should login, change the password and create a bucket. \
The access credentials for the bucket will be added to the helm values file later, so take note of them.

### Installing [Pachyderm](https://docs.pachyderm.com/latest/set-up/on-prem/)

First we need to add the Pachyderm helm repository:

```bash
helm repo add pachyderm https://helm.pachyderm.com
helm repo update
```

We then get the values file from the repository and edit it to our liking.\
My setup is based on the version `2.6.4-1`, so it might be different for future versions.

```bash
wget https://raw.githubusercontent.com/pachyderm/pachyderm/2.6.x/etc/helm/pachyderm/val
```

#### MinIO

First we change the deploy target at line `L7`

```yaml
````
````

````
# Deploy Target configures the storage backend to use and cloud provider
# settings (storage classes, etc). It must be one of GOOGLE, AMAZON,
# MINIO, MICROSOFT, CUSTOM or LOCAL.
deployTarget: "MINIO"
...
```

This does not need to be set when using something else but with MinIO we also have to set `L544` to "MINIO"

```yaml
...
storage:
    # backend configures the storage backend to use.  It must be one
    # of GOOGLE, AMAZON, MINIO, MICROSOFT or LOCAL. This is set automatically
    # if deployTarget is GOOGLE, AMAZON, MICROSOFT, or LOCAL
    backend: "MINIO"
    ...
```

A little further down (`L635`) we find the MinIO configuration. We need to set the endpoint, access key and secret key.

This point was a little tricky as I had MinIO installed on the same machine as Pachyderm, but it would take no other value than the outward facing IP address of the machine.

```yaml
...
    minio:
      # minio bucket name
      bucket: "<bucket name>"
      # the minio endpoint. Should only be the hostname:port, no http/https.
      endpoint: "10.X.X.X:9000"
      # the username/id with readwrite access to the bucket.
      id: "<id>"
      # the secret/password of the user with readwrite access to the bucket.
      secret: "<secret>"
      # enable https for minio with "true" defaults to "false"
      secure: "false"
      # Enable S3v2 support by setting signature to "1". This feature is being deprecated
      signature: ""
      ...
```

#### Storage classes

Now we add the storage classes we created earlier to the Postgres at `L784`

```yaml
````

````
...
    # AWS: https://docs.aws.amazon.com/eks/latest/userguide/storage-classes.html
    # GCP: https://cloud.google.com/compute/docs/disks/performance#disk_types
    # Azure: https://docs.microsoft.com/en-us/azure/aks/concepts-storage#storage-classes
    storageClass: manual
    # storageSize specifies the size of the volume to use for postgresql
    # Recommended Minimum Disk size for Microsoft/Azure: 256Gi  - 1,100 IOPS https://azure.microsoft.com/en-us/pricing/details/managed-disks/
...
```

and for the etcd at around `L144`

```yaml
...

  # GCP: https://cloud.google.com/compute/docs/disks/performance#disk_types
  # Azure: https://docs.microsoft.com/en-us/azure/aks/concepts-storage#storage-classes
  #storageClass: manual
  storageClassName: manual

  # storageSize specifies the size of the volume to use for etcd.
  # Recommended Minimum Disk size for Microsoft/Azure: 256Gi  - 1,100 IOPS https://azure.microsoft.com/en-us/pricing/details/managed-disks/

...
```

#### SSL Certificates

My setup refuses to work without SSL certificates, so I had to generate some.

```bash
openssl genrsa -out <CertName>.key 2048
openssl req -new -x509 -sha256 -key <CertName>.key -out <CertName>.crt

kubectl create secret tls <SecretName> --cert=<CertName>.crt --key=<CertName>.key
```

We then edit the `values.yaml` file at around `L683` to use the certificates.

```yaml
...
  tls:
    enabled: true
    secretName: "<SecretName>"
    newSecret:
      create: false
````

````
    ...
```

### CLI

To directly interact with the cluster we need to install the Pachyderm CLI.

```bash
curl -o /tmp/pachctl.deb -L https://github.com/pachyderm/pachyderm/releases/download/v2.6.5/pachctl_2.6.5_amd6 && sudo dpkg -i /tmp/pachctl.deb
```

### Deploy

Now that the values file is ready we can install Pachyderm.

```bash
helm install pachyderm pachyderm/pachyderm \
  -f ./values.yml pachyderm/pachyderm \
  --set postgresql.volumePermissions.enabled=true \
  --set deployTarget=LOCAL \
  --set proxy.enabled=true \
  --set proxy.service.type=NodePort  \
  --set proxy.host=localhost \
  --set proxy.service.httpPort=8080

```

Now you might want to connect to the dashboard. This can be done by port-forwarding the service.

```bash
pachctl port-forward
```

:tada: Now we should be able to access the dashboard at `http://localhost:4000` :tada:
````
````

Appendix 4: Kubernetes setup scripts

Appendix 4/1: Ansible setup script

```
---
- hosts: heydar_nodes
  become: yes
  tasks:
    - name: Setting up environment variables
      lineinfile:
        path: /etc/environment
        line: "{{ item }}"
      with_items:
        - "https_proxy=http://proxy.its.hpecorp.net:80"
        - "HTTP_PROXY=http://proxy.its.hpecorp.net:80"
        - "http_proxy=http://proxy.its.hpecorp.net:80"
        - "NO_PROXY=localhost,127.0.0.1,10.0.0.0/8,172.16.0.0/16,10.93.246.68/28"

    - name: Update and install necessary packages
      apt:
        name: "{{ packages }}"
        update_cache: yes
      vars:
        packages:
          - apt-transport-https
          - ca-certificates
          - curl

    - name: Add Kubernetes apt-key
      shell: |
        curl -fsSL https://packages.cloud.google.com/apt/doc/apt-key.gpg | gpg --yes --dearmor -o /etc/apt/keyrings/kubernetes-archive-keyring.gpg
        echo "deb [signed-by=/etc/apt/keyrings/kubernetes-archive-keyring.gpg] https://apt.kubernetes.io/ kubernetes-xenial main" | tee /etc/apt/sources.list.d/kubernetes.list
        apt-get update -y
        apt-get install -y kubelet kubeadm kubectl containerd
        apt-mark hold kubelet kubeadm kubectl

    - name: Enable necessary kernel modules and sysctl parameters
      shell: |
        modprobe br_netfilter
        echo '1' > /proc/sys/net/bridge/bridge-nf-call-iptables
        echo '1' > /proc/sys/net/ipv4/ip_forward
        sysctl -p

    - name: Disable swap
      shell: |
```

```
        swapoff -a
        sed -i -e '/ swap / s/^/#/' -e '/\/swap.img/ s/^/#/' /etc/fstab # comments out swap in fstab

    - name: Join the Kubernetes cluster
      shell: |
        kubeadm join 10.93.246.87:6443 --token 0v7aoq.65ib2v0g70a6em49 --discovery-token-ca-cert-hash sha256:9cb5e62dd86cd7e94718c866575cd023c98cc89f2849dad3d25dfd75b13d1b72
```

Appendix 4/2: Flannel configuration

```yaml
apiVersion: v1
kind: Namespace
metadata:
  labels:
    k8s-app: flannel
    pod-security.kubernetes.io/enforce: privileged
  name: kube-flannel
---
apiVersion: v1
kind: ServiceAccount
metadata:
  labels:
    k8s-app: flannel
  name: flannel
  namespace: kube-flannel
---
apiVersion: rbac.authorization.k8s.io/v1
kind: ClusterRole
metadata:
  labels:
    k8s-app: flannel
  name: flannel
rules:
- apiGroups:
  - ""
  resources:
  - pods
  verbs:
  - get
- apiGroups:
  - ""
  resources:
  - nodes
  verbs:
  - get
  - list
  - watch
- apiGroups:
  - ""
  resources:
  - nodes/status
  verbs:
  - patch
- apiGroups:
  - networking.k8s.io
  resources:
  - clustercidrs
  verbs:
  - list
```

```
  - watch
---
apiVersion: rbac.authorization.k8s.io/v1
kind: ClusterRoleBinding
metadata:
  labels:
    k8s-app: flannel
  name: flannel
roleRef:
  apiGroup: rbac.authorization.k8s.io
  kind: ClusterRole
  name: flannel
subjects:
- kind: ServiceAccount
  name: flannel
  namespace: kube-flannel
---
apiVersion: v1
data:
  cni-conf.json: |
    {
      "name": "cbr0",
      "cniVersion": "0.3.1",
      "plugins": [
        {
          "type": "flannel",
          "delegate": {
            "hairpinMode": true,
            "isDefaultGateway": true
          }
        },
        {
          "type": "portmap",
          "capabilities": {
            "portMappings": true
          }
        }
      ]
    }
  net-conf.json: |
    {
      "Network": "172.16.0.0/16",
      "Backend": {
        "Type": "vxlan"
      }
    }
kind: ConfigMap
metadata:
  labels:
    app: flannel
    k8s-app: flannel
```

```
    tier: node
  name: kube-flannel-cfg
  namespace: kube-flannel
---
apiVersion: apps/v1
kind: DaemonSet
metadata:
  labels:
    app: flannel
    k8s-app: flannel
    tier: node
  name: kube-flannel-ds
  namespace: kube-flannel
spec:
  selector:
    matchLabels:
      app: flannel
      k8s-app: flannel
  template:
    metadata:
      labels:
        app: flannel
        k8s-app: flannel
        tier: node
    spec:
      affinity:
        nodeAffinity:
          requiredDuringSchedulingIgnoredDuringExecution:
            nodeSelectorTerms:
            - matchExpressions:
              - key: kubernetes.io/os
                operator: In
                values:
                - linux
      containers:
      - args:
        - --ip-masq
        - --kube-subnet-mgr
        command:
        - /opt/bin/flanneld
        env:
        - name: POD_NAME
          valueFrom:
            fieldRef:
              fieldPath: metadata.name
        - name: POD_NAMESPACE
          valueFrom:
            fieldRef:
              fieldPath: metadata.namespace
        - name: EVENT_QUEUE_DEPTH
          value: "5000"
```

```
        image: docker.io/flannel/flannel:v0.22.0
        name: kube-flannel
        resources:
          requests:
            cpu: 100m
            memory: 50Mi
        securityContext:
          capabilities:
            add:
            - NET_ADMIN
            - NET_RAW
          privileged: false
        volumeMounts:
        - mountPath: /run/flannel
          name: run
        - mountPath: /etc/kube-flannel/
          name: flannel-cfg
        - mountPath: /run/xtables.lock
          name: xtables-lock
      hostNetwork: true
      initContainers:
      - args:
        - -f
        - /flannel
        - /opt/cni/bin/flannel
        command:
        - cp
        image: docker.io/flannel/flannel-cni-plugin:v1.1.2
        name: install-cni-plugin
        volumeMounts:
        - mountPath: /opt/cni/bin
          name: cni-plugin
      - args:
        - -f
        - /etc/kube-flannel/cni-conf.json
        - /etc/cni/net.d/10-flannel.conflist
        command:
        - cp
        image: docker.io/flannel/flannel:v0.22.0
        name: install-cni
        volumeMounts:
        - mountPath: /etc/cni/net.d
          name: cni
        - mountPath: /etc/kube-flannel/
          name: flannel-cfg
      priorityClassName: system-node-critical
      serviceAccountName: flannel
      tolerations:
      - effect: NoSchedule
        operator: Exists
      volumes:
```

```
      - hostPath:
          path: /run/flannel
        name: run
      - hostPath:
          path: /opt/cni/bin
        name: cni-plugin
      - hostPath:
          path: /etc/cni/net.d
        name: cni
      - configMap:
          name: kube-flannel-cfg
        name: flannel-cfg
      - hostPath:
          path: /run/xtables.lock
          type: FileOrCreate
        name: xtables-lock
```

Appendix 4/3: Bash verification script

```bash
#!/bin/bash

# Define color codes
RED='\033[0;31m'
GREEN='\033[0;32m'
NC='\033[0m' # No Color

# Initialize error flag
error_flag=0

# Function to print info messages
info() {
    echo -e "${GREEN}[INFO] $1${NC}"
}

# Function to print error messages
fail() {
    echo -e "${RED}[ERROR] $1${NC}"
    error_flag=1
}

# Checking installation of necessary packages
dpkg -l | grep -qw apt-transport-https || fail "apt-transport-https is not installed"
dpkg -l | grep -qw ca-certificates || fail "ca-certificates is not installed"
dpkg -l | grep -qw curl || fail "curl is not installed"
dpkg -l | grep -qw kubelet || fail "kubelet is not installed"
dpkg -l | grep -qw kubeadm || fail "kubeadm is not installed"
dpkg -l | grep -qw kubectl || fail "kubectl is not installed"
dpkg -l | grep -qw containerd || fail "containerd is not installed"

# Check Kubernetes APT source list
grep -q "https://apt.kubernetes.io/ kubernetes-xenial main" /etc/apt/sources.list.d/kubernetes.list || fail "Kubernetes APT source list is not configured correctly"

# Check if swap is disabled
swapon --summary | grep -q swap && fail "Swap is not disabled"

# Check containerd configuration
grep -q 'SystemdCgroup = true' /etc/containerd/config.toml || fail "SystemdCgroup is not enabled in containerd configuration"

# Check sysctl parameters
[ "$(cat /proc/sys/net/bridge/bridge-nf-call-iptables)" == "1" ] || fail "bridge-nf-call-iptables is not enabled"
[ "$(cat /proc/sys/net/ipv4/ip_forward)" == "1" ] || fail "ip_forward is not enabled"

```

```
# Check proxy settings for services
[ -f /etc/systemd/system/containerd.service.d/http-proxy.conf ] || fail "Proxy
    ↪ settings for containerd service is not configured"
[ -f /etc/systemd/system/kubelet.service.d/http-proxy.conf ] || fail "Proxy
    ↪ settings for kubelet service is not configured"

# Check Kubernetes node status
if command -v kubectl &> /dev/null; then
    kubectl get nodes || fail "Failed to get Kubernetes nodes. Check if the
        ↪ node has joined the cluster successfully"
else
    info "kubectl command not found. Skipping Kubernetes node check"
fi

# Check status of services
if systemctl --all --type=service --state=active | grep -qw containerd; then
    systemctl is-active --quiet containerd || fail "containerd service is not
        ↪ running"
else
    info "containerd service not found. Skipping service status check"
fi

if systemctl --all --type=service --state=active | grep -qw kubelet; then
    systemctl is-active --quiet kubelet || fail "kubelet service is not running"
else
    info "kubelet service not found. Skipping service status check"
fi

# Print summary
if [ $error_flag -eq 0 ]; then
    info "All checks passed successfully."
else
    echo -e "${RED}Some checks failed. Please check the error messages
        ↪ above.${NC}"
fi
```

List of literature

24 Top AI Statistics & Trends In 2023 – Forbes Advisor (2023). URL: `https://www.forbes.com/advisor/business/ai-statistics/` (retrieval: 10/07/2023).

Ansible (2023). Ansible. URL: `https://github.com/ansible/ansible` (retrieval: 10/22/2023).

Argo-Cd/LICENSE at Master · Argoproj/Argo-Cd (2023). GitHub. URL: `https://github.com/argoproj/argo-cd/blob/master/LICENSE` (retrieval: 10/21/2023).

Argoproj/Argo-Workflows (2023). Argo Project. URL: `https://github.com/argoproj/argo-workflows` (retrieval: 10/07/2023).

Arkouda Gituhb Repository (2023). Bears-R-Us. URL: `https://github.com/Bears-R-Us/arkouda` (retrieval: 10/23/2023).

Arkouda-Contrib/Arkouda-Docker at Main · Bears-R-Us/Arkouda-Contrib (2023). GitHub. URL: `https://github.com/Bears-R-Us/arkouda-contrib/tree/main/arkouda-docker` (retrieval: 10/23/2023).

Artifacthub Pachyderm 2.6.4 (2023). URL: `https://artifacthub.io/packages/helm/pachyderm/pachyderm/2.6.4` (retrieval: 10/18/2023).

Boehm, B. W. (1988): A Spiral Model of Software Development and Enhancement. In: *Computer* 21.5, pp. 61–72. ISSN: 0018-9162. DOI: `10.1109/2.59`. URL: `http://ieeexplore.ieee.org/document/59/` (retrieval: 10/18/2023).

Budde, R./Kautz, K./Kuhlenkamp, K./Züllighoven, H. (1992): What Is Prototyping? In: *Information Technology & People* 6.2/3, pp. 89–95. ISSN: 0959-3845. DOI: `10.1108/EUM0000000003546`. URL: `https://doi.org/10.1108/EUM0000000003546` (retrieval: 10/02/2023).

Bzeznik, B./Henriot, O./Reis, V./Richard, O./Tavard, L. (2017): Nix as HPC Package Management System. In: *Proceedings of the Fourth International Workshop on HPC User Support Tools*. HUST'17. New York, NY, USA: Association for Computing Machinery, pp. 1–6. ISBN: 978-1-4503-5130-0. DOI: `10.1145/3152493.3152556`. URL: `https://dl.acm.org/doi/10.1145/3152493.3152556` (retrieval: 10/03/2023).

Canon, R. S./Younge, A. (2019): A Case for Portability and Reproducibility of HPC Containers. In: *2019 IEEE/ACM International Workshop on Containers and New Orchestration Paradigms for Isolated Environments in HPC (CANOPIE-HPC)*. 2019 IEEE/ACM International Workshop on Containers and New Orchestration Paradigms for Isolated Environments in HPC (CANOPIE-HPC). Denver, CO, USA: IEEE, pp. 49–54. ISBN: 978-1-72816-028-3. DOI: `10.1109/CANOPIE-HPC49598.2019.00012`. URL: `https://ieeexplore.ieee.org/document/8950982/` (retrieval: 10/04/2023).

Ceph.Io — Home (2023). URL: `https://ceph.io/en/` (retrieval: 10/22/2023).

Chapel-Lang (2023): *Chapel-Lang/Chapel: A Productive Parallel Programming Language*. URL: `https://github.com/chapel-lang/chapel` (retrieval: 10/23/2023).

Cluster Networking (2023). Kubernetes. URL: `https://kubernetes.io/docs/concepts/cluster-administration/networking/` (retrieval: 10/18/2023).

Creating a Cluster with Kubeadm (2023). Kubernetes. URL: `https://kubernetes.io/docs/setup/production-environment/tools/kubeadm/create-cluster-kubeadm/` (retrieval: 10/18/2023).

Cwl-Utils/LICENSE at Main · Common-Workflow-Language/Cwl-Utils (2023). GitHub. URL: https://github.com/common-workflow-language/cwl-utils/blob/main/LICENSE (retrieval: 10/21/2023).

Docker FAQs | Docker (2021). URL: https://www.docker.com/pricing/faq/ (retrieval: 10/18/2023).

Docker Terms of Service | Docker (2022). URL: https://www.docker.com/legal/docker-terms-service/ (retrieval: 10/18/2023).

Dubois, P./Epperly, T./Kumfert, G. (2003): Why Johnny Can't Build [Portable Scientific Software]. In: *Computing in Science & Engineering* 5.5, pp. 83–88. ISSN: 1558-366X. DOI: 10.1109/MCISE.2003.1225867. URL: https://ieeexplore.ieee.org/abstract/document/1225867 (retrieval: 10/03/2023).

Eckerth, J. (2023): Installation Instructions Minikube Commit 69a05a755facc8d387e031ff5991c20d46dbe URL: https://github.com/Jo-Eck/ProjectPaper-2/tree/69a05a755facc8d387e031ff5991c20d46db project/Pachyderm (retrieval: 10/18/2023).

Egwutuoha, I. P./Levy, D./Selic, B./Chen, S. (2013): A Survey of Fault Tolerance Mechanisms and Checkpoint/Restart Implementations for High Performance Computing Systems. In: *J Supercomput* 65.3, pp. 1302–1326. ISSN: 1573-0484. DOI: 10.1007/s11227-013-0884-0. URL: https://doi.org/10.1007/s11227-013-0884-0 (retrieval: 10/03/2023).

Explore Network Plugins for Kubernetes (2023): Explore Network Plugins for Kubernetes: CNI Explained | TechTarget. IT Operations. URL: https://www.techtarget.com/searchitoperations/tip/Explore-network-plugins-for-Kubernetes-CNI-explained (retrieval: 10/19/2023).

Flannel (2023). flannel-io. URL: https://github.com/flannel-io/flannel (retrieval: 10/19/2023).

Flannel Install Config (2023). URL: https://github.com/flannel-io/flannel/blob/master/Documentation/kube-flannel.yml (retrieval: 10/19/2023).

Fülöp, J. (2005): Introduction to Decision Making Methods. In: *BDEI-3 Workshop, Washington*, pp. 1–15. URL: https://www.academia.edu/download/43447287/decisionmakingmethods.pdf (retrieval: 10/12/2023).

Gamblin, T./LeGendre, M./Collette, M. R./Lee, G. L./Moody, A./de Supinski, B. R./Futral, S. (2015): The Spack Package Manager: Bringing Order to HPC Software Chaos. In: *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. SC '15. New York, NY, USA: Association for Computing Machinery, pp. 1–12. ISBN: 978-1-4503-3723-6. DOI: 10.1145/2807591.2807623. URL: https://dl.acm.org/doi/10.1145/2807591.2807623 (retrieval: 10/03/2023).

Gluster (2023). URL: https://www.gluster.org/ (retrieval: 10/22/2023).

Haines, S. (2022): 'Workflow Orchestration with Apache Airflow'. In: *Modern Data Engineering with Apache Spark: A Hands-On Guide for Building Mission-Critical Streaming Applications.* Springer, pp. 255–295.

Helm Docs Home (2023). URL: https://helm.sh/docs/ (retrieval: 10/18/2023).

Home - Knative (2023). URL: https://knative.dev/docs/ (retrieval: 10/07/2023).

Hoste, K./Timmerman, J./Georges, A./De Weirdt, S. (2012): EasyBuild: Building Software with Ease. In: *2012 SC Companion: High Performance Computing, Networking Storage* *and Analysis*. 2012 SC Companion: High Performance Computing, Networking Storage and Analysis, pp. 572–582. DOI: 10.1109/SC.Companion.2012.81. URL: https://ieeexplore.ieee.org/abstract/document/6495863 (retrieval: 10/03/2023).

Inc, M. (2023): MinIO | MinIO for Kubernetes. MinIO. URL: https://min.io (retrieval: 10/18/2023).

Installing Kubeadm (2023). Kubernetes. URL: https://kubernetes.io/docs/setup/production-environment/tools/kubeadm/install-kubeadm/ (retrieval: 10/22/2023).

Intro to Pipelines (2023). URL: https://docs.pachyderm.com/latest/learn/intro-pipelines/ (retrieval: 10/23/2023).

iPaaS Solution for the Enterprise (2023). SnapLogic. URL: https://www.snaplogic.com/ (retrieval: 10/07/2023).

Knative Docs/LICENSE at Main · Knative/Docs (2023). GitHub. URL: https://github.com/knative/docs/blob/main/LICENSE (retrieval: 10/21/2023).

Kubeflow (2023). Kubeflow. URL: https://www.kubeflow.org/ (retrieval: 10/07/2023).

Kubeflow/LICENSE at Master · Kubeflow/Kubeflow (2023). GitHub. URL: https://github.com/kubeflow/kubeflow/blob/master/LICENSE (retrieval: 10/21/2023).

Kubernetes CNI Plugins (2023). Kubernetes. URL: https://kubernetes.io/docs/concepts/cluster-administration/addons/ (retrieval: 10/19/2023).

License — Airflow Documentation (2023). URL: https://airflow.apache.org/docs/apache-airflow/stable/license.html (retrieval: 10/21/2023).

Luigi/LICENSE at Master · Spotify/Luigi (2023). GitHub. URL: https://github.com/spotify/luigi/blob/master/LICENSE (retrieval: 10/21/2023).

Mehndiratta, H. (2023): Comparing Kubernetes Container Network Interface (CNI) Providers | Kubevious.Io. URL: https://kubevious.io/blog/post/comparing-kubernetes-container-network-interface-cni-providers (retrieval: 10/19/2023).

Merrill, M./Reus, W./Neumann, T. (2019): Arkouda: Interactive Data Exploration Backed by Chapel. In: *Proceedings of the ACM SIGPLAN 6th on Chapel Implementers and Users Workshop*. CHIUW 2019. New York, NY, USA: Association for Computing Machinery, p. 28. ISBN: 978-1-4503-6800-1. DOI: 10.1145/3329722.3330148. URL: https://dl.acm.org/doi/10.1145/3329722.3330148 (retrieval: 10/04/2023).

Multi-Criteria Decision Analysis for Use in Transport Decision Making (2014). Red. by Michael Bruhn Barfod/Steen Leleur. DTU Lyngby: DTU Transport.

Pachyderm Docs - Local Deploy (2023). Pachyderm Docs - Local Deploy. URL: https://docs.pachyderm.com/2.6.x/set-up/local-deploy/ (retrieval: 10/18/2023).

Pachyderm Docs - On-Prem Deploy (2023). Pachyderm Docs - On-Prem Deploy. URL: https://docs.pachyderm.com/latest/set-up/on-prem/ (retrieval: 10/18/2023).

Pachyderm/LICENSE at Master · Pachyderm/Pachyderm (2023). URL: https://github.com/pachyderm/pachyderm/blob/master/LICENSE (retrieval: 10/21/2023).

Pahcyderm -Pricing (2022). Pachyderm. URL: https://www.pachyderm.com/pricing/ (retrieval: 10/21/2023).

Roberts, R./Goodwin, P. (2002): Weight Approximations in Multi-Attribute Decision Models. In: *Journal of Multi-Criteria Decision Analysis* 11.6, pp. 291–303. ISSN: 1099-1360. DOI: 10.1002/mcda.320. URL: https://onlinelibrary.wiley.com/doi/abs/10.1002/mcda.320 (retrieval: 10/16/2023).

Rook (2023). URL: https://rook.io/ (retrieval: 10/22/2023).

Sayers, C./Laffitte, H./Reddy, P./Ozonat, K./Sayal, M./Simitsis, A./Singhal, S./Koutrika, G./Das, M./Aji, A./Bosamiya, H./Riss, M./Wilkinson, K./Lucio, J./Cantal, A./Carvalho, C. (2015): Cloud Application Services Platform (CLASP): User Guide, Introduction, and Operation. In: pp. 1–60.

SnapLogic – Master Subscription Agreement (2023). SnapLogic. URL: https://www.snaplogic.com/master-subscription-agreement (retrieval: 10/21/2023).

Spotify/Luigi (2023). Spotify. URL: https://github.com/spotify/luigi (retrieval: 10/12/2023).

Triantaphyllou, E. (2000): 'Introduction to Multi-Criteria Decision Making'. In: *Multi-Criteria Decision Making Methods: A Comparative Study*. Ed. by Evangelos Triantaphyllou. Applied Optimization. Boston, MA: Springer US, pp. 1–4. ISBN: 978-1-4757-3157-6. DOI: 10.1007/978-1-4757-3157-6_1. URL: https://doi.org/10.1007/978-1-4757-3157-6_1 (retrieval: 10/12/2023).

Weighted Sum Model (2022). In: *Wikipedia*. URL: https://en.wikipedia.org/w/index.php?title=Weighted_sum_model&oldid=1114224941 (retrieval: 10/16/2023).

Wilde, T./Hess, T. (w.y.): Methodenspektrum der Wirtschaftsinformatik: Überblick und Portfoliobildung. In.