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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Dublin, October 4, 2023

Jon Eckerth

Abstract:

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. 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.

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List of abbreviations

AI	Artificial Intelligence
k8s	Kubernetes
ML	Machine Learning
HPC	High Performance Computing
CC	Cloud Computing

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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.[1]
- **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.[2345]
- **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. 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.

[1] Egwutuoha et al. 2013
[2] Dubois/Epperly/Kumfert 2003
[3] Bzeznik et al. 2017
[4] Gamblin et al. 2015
[5] Hoste et al. 2012

- **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 both data and computational processes. Both HPC and CC solutions often fall short in providing holistic versioning capabilities that cater to evolving research needs.

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[6]' into a container based CC workflow management tool called 'Pachyderm'[7] 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:** *To what extent does the use of a container-based workflow management tool affect the performance of the high-performance computing framework?*
- **RQ3:** *What are the opportunities for improving the integration of high-performance computing frameworks with container-based workflow management tools?*

[6]Merrill/Reus/Neumann 2019
[7]pachyderm 2023

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 afformentioned painpoints*

2 Methodology

2.1 Prototyping

Needs to have a methodology from the Spectrum of Methodologies for Business information systems[8]

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 - test

[8] Wilde/Hess w.y.

3 State of the Art

3.1 Containerization

3.1.1 General Containerization

3.1.2 Container Orchestration

3.2 Workflow Management Tools

3.2.1 Apache Airflow

3.2.2 Pachyderm

3.2.3 Kubeflow

3.2.4 Apache Oozie

3.3 High Performance Computing Frameworks

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3.3.2 MapReduce

3.3.3 Apache Flink

3.3.4 Dask

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4.1 Analysis of Userneeds

4.2 Design of the Artifact

4.3 Implementation of the Artifact

4.4 Evaluation of the Artifact

5 Conclusion

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6 Summary and Outlook

6.1 Summary

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6.2 Outlook

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