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Deployment of a programming framework based on microservices and containers with application to the astrophysical domain

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ABSTRACT

Scientific research is becoming increasingly global and has to address challenges that cannot be handled by small groups or individual researchers. Global research initiatives are often facing the lack of cooperative computing frameworks and storage resources. Such frameworks and resources are needed to address scientific problems at large scales. This paper investigates the potential of using container technologies over distributed computing infrastructure in the astrophysics domain. Due to the complexity of astrophysics applications, it is necessary to enable a parallelism pipeline for their execution. Such applications require High-Performance-Computing (HPC) environments to enable easy and reproducible deployment of astrophysics applications across multiple HPC cites "BRANE". BRANE provides easy and transparent access to end-users, allowing them to define their execution pipeline.[1] To validate the proposed solution, we considered an astrophysics application that uses the XSPEC package for spectral analysis from HEASoft. XSPEC software is used for spectral fitting of data from X-rays telescope observations. The Xrays data are very large that exceed 1Gb, and obtaining such a huge amount of data requires awesome time and human efforts. The conducted experiments have shown the usefulness, portability, and reproducibility of the proposed solution.

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1. Introduction

Porting parallel scientific applications to distributed computing infrastructures requires a significant effort from the domain scientific (in this case astrophysicists) and often requires background in computer science and computer systems (Heldens et al., 2020). Furthermore, data-driven science requires developing data-driven software systems, which should make it easy for the domain scientist to customize the application code to take advantage of the available computing resources, such as parallelization. High-Performance-Computing environments have played an important role in allowing scientists keep pushing further their research regardless of their local computing resources. In other terms, scientists should be able to use the power of HPC systems as a simple extension of the local workstation. For a domain scientist this is possible only if he/she provided with software environments that make hide the complexity of the infrastructure and make it easy to execute and monitor both the applications and data which is distributed across multiple HPC systems.

In the world of High-Performance-Computing infrastructures, the architecture models trend changed from software components-oriented architecture to service-oriented architecture. Therefore, using containers in high-performance computing systems will reduce the gap between local environments and HPC systems and will make the experiment more reproducible.

The adoption of containers (Bentaleb et al., 2021) has become the key enabling technology driving digital transformation. Furthermore, microservices architecture leads to speed up applications deployment, while insuring a good portability, fault isolation, and scalability features. During the last decade, scientific applications are shifting from the traditional monolith design to a microservice architecture. Microservices architecture decompose the monolithic systems into a collection of independent services that allow easier deployment, testing, and maintenance of a computing environment.

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[1] https://wiki.enablingpersonalizedinterventions.nl/user-guide/

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