Container Orchestration on HPC Systems

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Abstract—Containerisation demonstrates its efficiency in application deployment in cloud computing. Containers can encapsulate complex programs with their dependencies in isolated environments, hence are being adopted in HPC clusters. HPC workload managers lack micro-services support and deeply integrated container management, as opposed to container orchestrators (e.g. Kubernetes). We introduce Torque-Operator (a plugin) which serves as a bridge between HPC workload managers and container Orchestrators.

Index Terms—HPC Workload Manager; Orchestration; Containerisation; Torque; Slurm; Kubernetes; Singularity; Cloud Computing

I. INTRODUCTION

Cloud computing demands high-portability. Containerisation ensures compatibility of applications and their environment by encapsulating applications with their libraries and configuration files. Thus, enables users to move and deploy programs easily among clusters. Containerisation is a virtualisation technology. Rather than starting a holistically simulated OS on top of the host kernel as in a Virtual Machine (VM), a container only shares the host kernel. This feature makes containers more lightweight than VM. Containers are dedicated to run micro-services and one container mostly hosts one application. Nevertheless, containerised applications can become complex, e.g. thousands of separate containers may be required in production. Production can benefit from container orchestrators that can provide efficient environment provisioning and auto-scaling.

High Performance Computing (HPC) systems are traditionally applied to perform large-scale financial and engineering simulation, which demands low-latency and high-throughput. The typical HPC jobs are large workloads that are often host-specific and hardware-specific. HPC systems are typically equipped with workload managers. A workload manager is composed of a resource manager and a job scheduler. A resource manager allocates resources (e.g. CPU, memory), schedules jobs and guarantees no interference from other user processes. A job scheduler determines the job priorities, enforces resource limits and dispatch jobs to available nodes. Two main-stream workload managers are TORQUE and Slurm. Slurm includes both resource managers and job schedulers, while originally Torque only incorporates resource managers and later extends with job schedulers. Overall, HPC workload managers lack micro-service supports and deeply integrated container management capabilities in which container orchestrators manifest their efficiency.

We herein describe a plugin named Torque-Operator. It serves as a bridge between the HPC workload manager Torque and the container orchestrator Kubernetes. Kubernetes has been widely adopted, as it has a rapidly growing community and ecosystem with plenty of platforms being developed upon it. Furthermore, we propose a testbed architecture composed of an HPC cluster and a big data cluster where Torque-Operator enables scheduling container jobs from the big data cluster to the HPC cluster. The rest of the paper is organised as follows. Firstly, Section II briefly views the related work. Next, we describe the proposed architecture of our testbed and Torque-Operator in Section III. Followed, some preliminary results are given in Section IV. Lastly, Section V concludes this paper and proposes future work.

II. RELATED WORK

Torque-Operator extends WLM-Operator with Torque support. Both operators share similar mechanisms, i.e. schedule container jobs from cloud clusters to HPC clusters, nevertheless, their implementation varies significantly as Torque and Slurm have different structures and parameters.

WLM-Operator only allows submission of Slurm batch jobs wrapped in a Kubernetes yaml file from a cluster managed by Kubernetes. It invokes Slurm binaries i.e. sbatch, scancel, sacct and scontrol to transfer and manage Slurm jobs to a Slurm cluster. The operator creates virtual nodes which correspond to each Slurm partition, e.g. one virtual node corresponds to one Slurm partition and contains the information of its corresponding partition. Virtual node is a concept in Kubernetes. It is not a real worker node, however, it enables users to connects Kubernetes to other APIs and allows developers to deploy pods (a Kubernetes term) and containers with their own APIs. Jobs on the virtual node can be scheduled to the worker nodes. WLM-Operator creates a dummy pod on the virtual node in order to transfer the Slurm batch job to a specific Slurm partition. When the batch job completes, another dummy pod is generated to transfer the results to the directory specified in the submitted yaml file.

In Kubernetes terminology, WLM-Operator creates a new object kind i.e. Slurmjob. The operator includes a service
program red-box that builds a gRPC proxy between Slurm and Kubernetes. gRPC proxy defines a service and implements a server and clients. The service defines the methods and their message types of responds and requests in a .proto format file. The server implements: 1) the interfaces 2) and runs a gRPC server which listens to the requests from clients and dispatches them to the right services. The client defines the identical methods as the server.

III. TORQUE-OPERATOR AND PLATFORM DESCRIPTION

We firstly illustrate the design of our platform architecture, then describe the structure of Torque-Operator. Torque-Operator is written in Golang programming language. Singularity [9] is the runtime container of our choice. Singularity is starting to be applied in many HPC centres [10], as it provides a secure means to capture and distribute software and computer environment. For example, execution of a Singularity container only demands a user privilege, while a Docker container [11], which is a container runtime widely adopted in cloud systems, requires root permission. Kubernetes supports Docker by default, though it can be adjusted to perform services for Singularity by adding Singularity-CRI [12]. Table I manifests the list of core applications that construct the testbed.

| Orchestrate         | Kubernetes, Torque          |
|---------------------|-----------------------------|
| Container runtime & its support | Singularity, Singulairy-CRI |
| Operator            | Torque-Operator              |
| Compiler            | Golang compiler              |

| TABLE I |
|---------|
| THE LIST OF CORE APPLICATIONS FOR THE TESTBED. |

A. Platform Architecture

The architecture of our platform is designed to serve as the testbeds for the EU research project CYBELE [1]. The platform is composed of an HPC cluster with Torque as its workload manager and a big data cluster with Kubernetes as its orchestrator. Its architecture is illustrated in Fig. 1. Noting that Fig. 1 is for illustration purpose, the number of nodes and the queues can vary in the testbeds.

In Torque, nodes are grouped into queues. Each queue is associated with resources limits such as walltime, job size. One node can be included in multiple queues. The HPC cluster is composed of a head node which controls the whole cluster nodes and compute nodes which perform computation. The Torque login node in Fig. 1 also serves as one of the worker nodes in the Kubernetes cluster. The Kubernetes cluster incorporates a master node which schedules the jobs and worker nodes which execute the jobs. A virtual node indicated in Fig. 2 transfers Torque jobs to the Torque cluster. The Torque job submitted from the Kubernetes login node is scheduled by Kubernetes master node to the virtual node. The virtual node transfers the abstracted Torque jobs to the Torque queue through the Torque login node. The merits of this architecture are: 1) it provides users with flexibility to run containerised and non-containerised jobs, 2) the containerised applications can be better scheduled to Torque cluster by taking advantage of the scheduling policies of Kubernetes.

B. Structure of Torque-Operator

The Torque job script is encapsulated into a Kubernetes yaml job script. The yaml script is submitted from a Kubernetes login node (in our case, the login node is also the master node). The PBS script part is processed by Torque-Operator. A dummy pod is generated to transfer the Torque job specification to a scheduling queue (e.g. waiting queue, test queue, which is a concept in the job scheduler). Torque-Operator invokes the Torque binary qsub which submits PBS job to the Torque cluster. When the Torque job completes, Torque-operator creates a Kubernetes pod which redirects the results to the directory that the user specifies in the yaml file.

As in WLM-Operator (Section II), Torque-Operator includes a service program red-box. Red-box generates a Unix socket which allows data exchange among the Kubernetes and Torque processes. Torque-Operator introduces a new object kind i.e. Torquejob (Slurmjob in WLM-Operator) and sets

1CYBELE: Fostering Precision Agriculture and Livestock Farming through Secure Access to Large-Scale HPC-Enabled Virtual Industrial Experimentation Environment Empowering Scalable Big Data Analytics https://www.cybele-project.eu/
A dummy pod to transfer the results from Torque to Kubernetes. Torque-Operator. Fig. 3 presents a Kubernetes yaml job script that encloses a PBS script.

The future work will focus on optimization of Torque-Operator that can offer more stable deployments. Performance evaluation will be carried out to compare efficiency of scheduling the container jobs by Kubernetes and Torque. The pilots of CYBELE project will be adopted as the benchmarks.

ACKNOWLEDGMENT

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement NO.825355.

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