

Build and Execution Environment (BEE): an Encapsulated Environment Enabling HPC Applications Running Everywhere

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Abstract—Variations in High Performance Computing (HPC) system software configurations mean that applications are typically configured and built for specific HPC environments. Building applications can require a significant investment of time and effort for application users and requires application users to have additional technical knowledge. Linux container technologies such as Docker and Charliecloud bring great benefits to the application development, build and deployment processes. While cloud platforms already widely support containers, HPC systems still have non-uniform support of container technologies. In this work, we propose a unified runtime framework – Build and Execution Environment (BEE) across both HPC and cloud platforms that allows users to run their containerized HPC applications across all supported platforms without modification. We design four BEE backends for four different classes of HPC or cloud platform so that together they cover the majority of mainstream computing platforms for HPC users. Evaluations show that BEE provides an easy-to-use unified user interface, execution environment, and comparable performance.

Index Terms—high performance computing; cloud computing; container.

I. INTRODUCTION

High Performance Computing (HPC) systems have become critical infrastructures for science and industry. For example, domain experts use HPC systems to run large-scale physical simulations, big data analysis, multi-layer artificial neural networks, molecular dynamics experiments, and DNA sequencing.

As different HPC systems typically have customized software environments, HPC users must often configure and build their application for each specific machine, which is time consuming and can become a bottleneck to productivity. Moreover, in some cases, years- or even decades-old legacy applications still serve as key components in the process of scientific or industry research. These legacy applications may have no active support and often require specific deprecated versions of libraries and/or hardware in order to make them run correctly. It may be hard to find or build library implementations that meet the requirement of legacy applications while remaining compatible with current HPC systems. These requirements impose great challenges for HPC users.

Due to availability of shared computing environment, users may need to frequently switch between computing systems.

This can be among different HPC platforms or even cloud platforms. Differences in software environments may impede users when choosing a platform that has different software/hardware configurations. A consistent execution environment is also important for HPC application developers. Consistency between developing, testing, and production environments can greatly save developers' time on fixing compatibility issues, that can significantly accelerate the development process.

Virtualized environments, and particularly virtual machines (VMs), have been thoroughly investigated for HPC systems to provide more consistent, isolated, and secure environments [1], [2]. For example, Huang, et al. [3] built a virtualized HPC environment using Xen-based VMs. By leveraging high performance I/O passthrough [4], VMs can achieve near-native performance when running HPC benchmarks. In [5], Zhang, et al. illustrated that current resource managers in HPC systems cannot well supervise VMs and associated critical resources, so they proposed Slurm-V, that extends Slurm with virtualization-oriented capabilities. Huang, et al. and Tikotekar, et al. [6], [7] characterized the performance of running multiple kinds of applications on virtualized HPC clusters. In [8], Huang, et al. proposed Inter-VM Communication (IVC), a VM-aware communication library to support efficient shared memory communication among computing processes on the same physical host and then they built an MPI library that was IVC enabled.

However, managing application specific VM images is not trivial, given that VM images need to contain files of the operating system, dependent libraries/packages, user applications, and input/output data, that may take several gigabytes of disk space. Migrating images between HPC systems or distributing images among compute nodes can consume a lot of time. On the other hand, Linux containers are more lightweight. Many implementations of Linux containers have been proposed e.g., Docker [9], Charliecloud [10], Shifter [11], and Singularity [12]. They provide consistent execution environments for development, build, and deployment. By using Linux containers, developers only need to build their application once in the container on their local machine, and then the application can run on any supported machine. For doing that, one only needs to transfer the container image to the target execution machine.

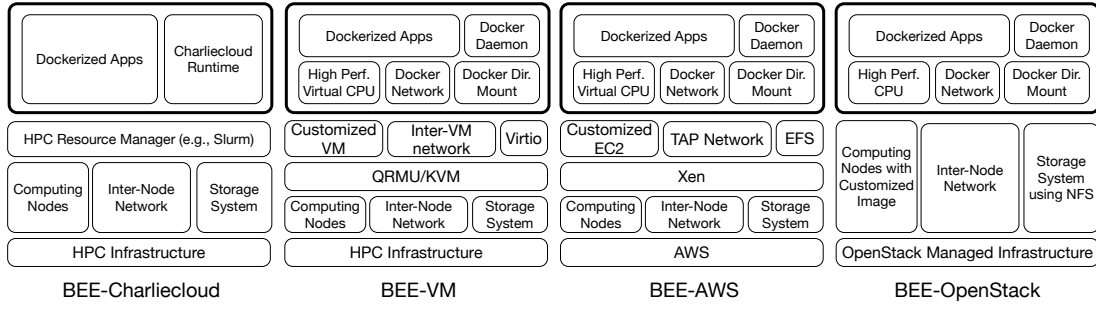


Fig. 1: BEE Backends

The container image usually only contains minimal operating system composition, application-dependent libraries/packages, and user applications, with much less space requirement than VM images [13]. Also, since Linux containers allow the guest application to share much of the host operating system including the Linux kernel, the performance penalty is small [14], [15].

It can be of great benefit to bring the advantages of Linux containers, as realized in the cloud, to HPC users; however, HPC systems have support of Linux containers in a non-uniformed fashion. Some systems can natively support widely used Docker containers; Some systems run incompatible older Linux kernels that make them unable to support Linux containers [16]. Some systems cannot support Docker containers but can support other Linux container implementations e.g., Charliecloud [10], Shifter [11] and Singularity [12]. This is challenging for HPC users who want to take the benefits of Linux containers and who already have their HPC applications running in Linux containers on one system and need to migrate to another one, since different Linux containers/runtimes are not mutually compatible with each other. Even on an HPC/cloud system where a certain kind of Linux container is supported, running HPC applications still needs complicated configuration, since Linux containers, by their nature, are built for isolation, that is contrary to the sharing fashion adopted by HPC applications.

In this work, we design a unified build and execution environment that overcomes the challenges when running containerized applications in HPC systems. We call it Build and Execution Environment (BEE).

- 1) **Docker image support:** Among all kinds of Linux container implementations, Docker is one of the most widely used implementations in the HPC community. With the support of Docker image, current HPC users can deploy their Dockerized application using BEE with no modification.
- 2) **Reproducibility:** BEE aims to build up similar HPC-friendly execution environments across different platforms, allowing Dockerized applications to behave consistently. This is accomplished through a series of specially design modules – BEE backends. Different BEE backends target different classes of platform, but they can build up execution environments with similar hardware configuration and software stack.

- 3) **Multiple platforms support:** We design four BEE backends that support four different classes of systems. For HPC systems, instead of using Docker container runtime, we choose to use Charliecloud, a Linux container implementation with much less usage requirement than Docker and its runtime supports running Docker images. Charliecloud only needs execution systems to have Linux user namespace enabled, and it is usually enabled by default on many current and new HPC systems. Using Charliecloud, we build our first BEE backend for HPC systems – BEE-Charliecloud. For older HPC systems that do not have Linux user namespace support, BEE provides another BEE backend – BEE-VM. It can run Dockerized HPC applications through Docker runtime via a specialized VM. In addition to HPC systems, we also design two BEE backends to support running HPC applications on cloud systems. These allow users to run HPC applications when cloud platforms are preferable computing resources for users. Specifically, BEE provides BEE-AWS that allows Dockerized HPC applications to run on Amazon Web Services (AWS) platform and BEE-OpenStack for OpenStack-based HPC or cloud infrastructures.

- 4) **End-to-end automation:** BEE provides end-to-end automation that hides all launching details from users. Users only need to provide a BEE task description file (beefile), Docker images, and run scripts in order to launch a task on BEE. BEE will handle all the complications including: connecting to the remote platform, setting up suitable computing environment, configuring network and storage, and launching applications.
- 5) **Flexibility:** BEE provides a unified user interface, so together with BEE backends, BEE users have the flexibility to switch between different platforms, as their needs require, with no modification to their applications and minimum modification to the task description file.

The rest of this paper is organized as follows: We discuss the BEE framework design in section II. The designs of four BEE backends are discussed in section III - VI. Performance is evaluated in section VII. We showcase VPIC, a real HPC application running in BEE in section VIII. In section IX, we discuss related works and how BEE is unique. Finally, we make our conclusion in section X.

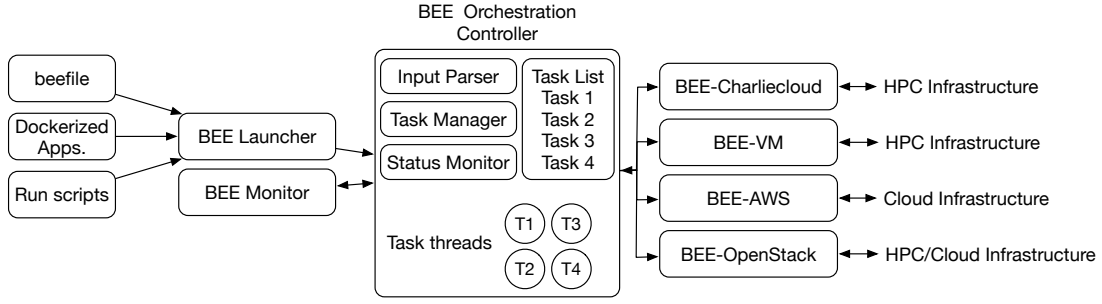


Fig. 2: BEE Framework

II. BEE DESIGN OVERVIEW

The goal of BEE is to enable unified experience for users when launching HPC applications across different platforms. This is manifested in two ways: (1) A unified user interface that only requires minimum configuration to launch applications on a platform or switch between different platforms; (2) Similar execution environments for applications on different platforms that enable consistent application execution behavior.

A. User interface

The unified user interface consists of three inputs when launching an application using BEE:

- 1) A Docker image containing the application;
- 2) Run scripts;
- 3) Task description file – `beefile`;

The first input is the Docker image containing the application. Then, to run the application when it is deployed on a platform, users need to provide run scripts. Depending on the application, the scripts can be in many forms e.g., Shell scripts, Python scripts, etc. Both the Docker image and run scripts do not need to be modified when switching between different execution platforms. Finally, to hide most complications and still provide enough capability of customization, we propose to use a simple JSON-format task description file (`beefile`) to handle all the communications between users and BEE.

Listing 1 shows the template of a `beefile`. Users need to select the suitable execution platform (line 3), provide general sequential run scripts (line 5 - 9) and MPI parallel run scripts (line 10 - 14), information about Dockerized application (line 16 - 20), and finally provide necessary platform-specific information (line 21 - 26) e.g., node list, credential information. Note different Docker containers, by default, do not share a file system at runtime, but many HPC application processes running on different nodes need to have a shared directory to share data, so BEE needs users to specify a directory inside the container (line 16) that will be mounted to a shared host filesystem at runtime. When switching between platforms, users only need to make modifications to the `beefile`.

B. Execution environment

To build similar execution environments on different platforms that can lead to consistent application execution behavior, BEE backends are proposed. A BEE backend is

Listing 1: Template of `beefile`

```

1  "task_conf": {
2    "task_name": <task name>,
3    "exec_target": bee_cc | bee_vm | bee_aws |
      bee_os,
4    "general_run": [
5      { "script": <script 1> },
6      { "script": <script 2> }, ...
7    ],
8    "mpi_run": [
9      { "script": <script 1> },
10     { "script": <script 2> }, ...
11   ],
12 },
13 "docker_conf": {
14   "docker_img_tag": <docker image>,
15   "docker_username": <username>,
16   "docker_shared_dir": <dir>
17 },
18 "exec_env_conf": {
19   "bee_cc": { ... } or
20   "bee_vm": { ... } or
21   "bee_aws": { ... } or
22   "bee_os": { ... }
23 }

```

a module in BEE framework that can automatically build up an HPC-friendly execution environment on a specific class of platforms. We design different BEE backends for different classes of platforms that can build up similar execution environment. As for now, there are four BEE backends: BEE-Charliecloud, BEE-VM, BEE-AWS, and BEE-OpenStack. These are built aiming at four different classes of platforms: BEE-Charliecloud supports current and later HPC systems that have Linux user namespace support; BEE-VM supports older HPC systems; BEE-AWS supports AWS cloud platform; BEE-OpenStack supports OpenStack-based HPC or cloud platforms.

Fig. 1 shows the hardware and software stack of the four BEE backends. The bold rectangle on the top row of each BEE backend indicates the execution environment that each BEE backend provides. Below that are different technolo-

gies that are used to enable consistent execution environment. Further below are the three components that are most critical to HPC applications: *computing*, *network*, and *storage*. Each BEE backend is designed to provide similar computing, network, and storage environment for the runtime environment that runs Dockerized HPC applications. This makes sure that applications do not need to be modified to run on another BEE backend and preserving the same execution behavior. We will discuss the design details of each BEE backend in the following sections.

C. Components in BEE framework

Finally, we introduce other components in the BEE framework that help connect the user interface with BEE backends. **Fig. 2** shows the framework of BEE. The BEE Launcher is the BEE frontend for users to launch a task on BEE-supported platforms, using the three inputs mentioned earlier. The core part of BEE is the BEE Orchestration Controller, that is responsible for connecting the BEE frontend and the four BEE backends. It takes the task launching requests from BEE Launcher and initiates task launching process through BEE backends. BEE Orchestration Controller uses different threads to manage different tasks at the same time. It also keeps track of the status of each launching process.

III. BEE-CHARLIECLOUD

Charliecloud [10] is a Linux container runtime based on Linux user namespaces. It offers all the necessary runtime functionalities for HPC applications. It has three major benefits that make it the ideal runtime for BEE on HPC systems: First, it takes standard Docker images as input via the built-in image flattener, so it helps maintain the same user interface as the other three BEE backends. Second, Linux user namespaces only bring minor performance overhead, full exposure of host hardware resources, and no requirement of privileged operations or daemons. Third, Linux user namespaces is widely supported by default on current HPC systems, making BEE a highly usable framework. So, using Charliecloud we design BEE-Charliecloud for HPC platforms.

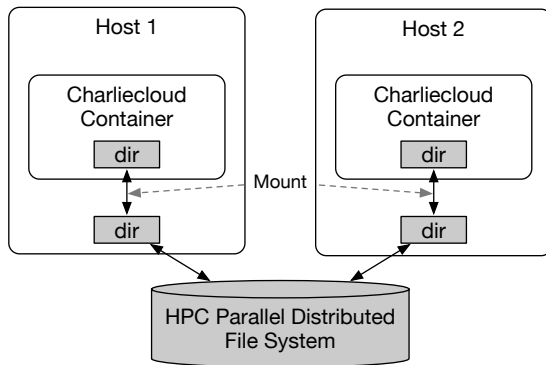


Fig. 3: Shared Storage Design using Virtual IO

When designing a BEE backend, one problem is identifying the suitable balance point between sharing and isolation of the runtime environment. Charliecloud offers comparable

runtime isolation to Docker, that enables the user to pack all dependencies and tools in the image, avoiding additional application-specific configuration in the runtime environment. On the other hand, HPC applications usually require some degrees of data sharing: *sharing via network* and *sharing via storage*.

A. Network Design

Sharing via network means processes running on different containers need to be able to share data via network. Charliecloud by default exposes all hardware network interfaces to its container runtime environment. Since HPC systems usually have interconnected networks between nodes, processes running in Charliecloud can communicate through the network interfaces on each node and get the benefits of any available network technology e.g., Infiniband. So, in BEE-Charliecloud we choose to keep the default network settings.

B. Storage Design

Sharing via storage is not natively supported by Charliecloud. By default each container only mounts the filesystem in the flattened input image. To enable sharing via storage, we use the `--bind` option at container launch time to mount an user-specified host directory to a shared directory inside the container as mentioned in the user interface section. Since HPC systems usually have shared filesystem among nodes, processes can share data via the shared directory inside each container as shown in **Fig. 3**. After each container is configured, BEE-Charliecloud automatically executes user's runscripts via the Charliecloud command `ch-run`. When initiating MPI parallel jobs, BEE-Charliecloud wraps `mpirun` command outside `ch-run` together with necessary MPI launching options. When deployed on HPC systems with Slurm resource manager, BEE-Charliecloud can interact with Slurm frontend to configure computing resources automatically. **Algorithm 1** shows the launching logic of BEE-Charliecloud.

Algorithm 1 BEE-Charliecloud launching logic

Require: Dockerized application (Docker image/Dockerfile)

Require: BEE configuration file (beefile)

Require: Run scripts

```

1: pull/build_docker(beefile)
2: flattened_tar_file ←
   ch-docker2tar(docker_image)
3: flattened_filesystem ←
   ch-tar2dir(flattened_tar_file)
4: compose_ch-run_options()
5: for each sequential run script in beefile do
6:   slurm_allocate_resources()
7:   ch-run(script)
8: end for
9: for each parallel run script in beefile do
10:  slurm_allocate_resources()
11:  mpirun_ch-run(mpi_script)
12: end for
```

IV. BEE-VM DESIGN

To support BEE on older HPC systems that do not have Linux user namespace enabled, we design a second BEE backend for HPC system - BEE-VM, so that together with BEE-Charliecloud they make BEE support majority of the current HPC systems. BEE-VM creates a VM layer on top of the host and then deploys Docker on the VM layer; as shown in Fig. 1. VM brings the isolation that enables us to run Docker even on a system with constraint. It utilizes Kernel-based Virtual Machine (KVM) (on by default in Linux), a hardware accelerated hypervisor, to provide bare-metal performance. As shown in Fig. 4, we run one VM per HPC host node and one Docker container per VM.

Similar to BEE-Charliecloud, besides running applications in isolated environment, another goal of the BEE-VM design is enabling two kinds of sharing, *sharing via network* and *sharing via storage*, between Docker container applications running on different machines.

A. Network Design

The network design of BEE-VM mainly targets two functions: (1) BEE needs to remotely login and control each VM via SSH; (2) MPI needs network to share data between processes.

In order to enable the SSH connection to the VM through the host, the hypervisor is configured to create dedicated virtual network interface card (vNIC) used for port forwarding that maps an unused port on the host to the SSH port on the VM. As for MPI, it cannot use the vNIC for SSH, since it usually uses a different (random) port for communication, so we cannot use port forwarding on a specific port. To handle this problem, we have two solutions. For a system with regular Ethernet, we create a second vNIC on each VM and connect all of them in a virtual subnet (i.e., multicast or P2P connection). We choose this over more straight forward approaches (e.g., bridging) because this approach does not require any administrative privilege to the system. For a system with InfiniBand, we adopt Single Root Input/Output Virtualization (SR-IOV) to connect all VMs. To connect all the Docker containers together, we choose to start the Docker container in 'host network' in which all network configurations are exposed to the container, so that each container has the same connectivity as VM.

B. Storage Design

To share data between processes in Docker containers, we need to first build a shared filesystem between different VMs. Here, we use the Virtio feature [17] in QEMU to map a host directory to a directory inside VMs. It only requires minimum configuration at VM boot time. Since HPC systems usually use shared filesystem (via NFS, Luster, etc.), each VM will also have the same file-sharing capability as long as they map to the same host directory. For data sharing in the Docker layer, we use the data volume mount feature in Docker to mount the shared folder inside VM to a directory in Docker. Since Docker runs as a process at the VM layer, mounting the data volume adds negligible overhead.

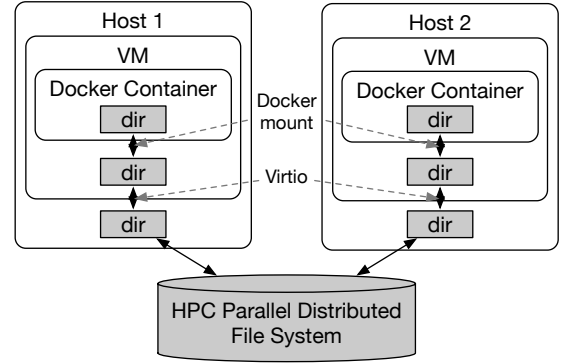


Fig. 4: Shared Storage Design using Virtual IO

C. BEE-VM Deployment

Algorithm 2 shows the launching logic of BEE-VM. Before using BEE-VM the first time, users need to use the image builder provided by BEE to build the base VM image. The image is customized for BEE-VM that includes pre-installed softwares and settings. It only need to be done once. After that each VM will only work on a copy of the base image without any modification to the base image. During launch, BEE-VM first deploys VM on each HPC node (line 1 - 6). Next, the hostfile on each VM is setup in order to let each VM communicate with each other without using complicated IP addresses. The virtio storage is mounted in line 14. In the next stage, depending on what the user provides, BEE-VM will either pull the Docker image from public/private registries or build a new Docker image from a Dockerfile loaded into the local VM. Finally, BEE starts the application by launching from the first node (i.e., master node).

V. BEE-AWS DESIGN

AWS is one of the most widely used commercial cloud computing platforms. It offers great configuration flexibility towards computing software/hardware environment, network, storage, and security. Many researchers from both HPC and cloud community use AWS to run large scale applications. However, configuring the desired computing environment on AWS is tedious and can impede experiment workflow, especially for users with less knowledge or experience on AWS. Although many tools offer the ability to automate the computing environment setup process, they usually cannot create an environment suitable for HPC applications. Even though tools such as StarCluster [18], do offer the capability of creating HPC-friendly environment on AWS, it suffers from two drawbacks. First, they do not offer the support of automatic Docker container deployment and execution. Users still need to manually deploy and run their applications. Second, they usually do not offer HPC/cloud cross-platform support.

Here we design BEE-AWS as another BEE backend. BEE-AWS enables the same end-to-end automation on AWS as provided in BEE-Charliecloud and BEE-VM on HPC systems. Most importantly, BEE-AWS offers the same user interface and execution environment as BEE-VM, so the user

Algorithm 2 BEE-VM launching logic

Require: Pre-built QEMU Img. (only need to build once)

Require: Allocated host nodes: H_1, H_2, \dots, H_k

Require: Dockerized application (Docker image/Dockerfile)

Require: BEE configuration file (beefile)

Require: Run scripts

```
1: for i in 1 to beefile.num_of_nodes do
2:   node_i.copy_img()
3:   node_i.compose_qemu_arg(storage_dir)
4:   node_i.compose_qemu_arg(network_conf)
5:   node_i.start_vm()
6: end for
7: wait_for_all_vm_to_become_ready()
8: for i in 1 to beefile.num_of_nodes do
9:   node_i.set_hostname()
10:  for j in 1 to beefile.num_of_nodes do
11:    node_j.setup_hostfile(node_i.ip())
12:  end for
13: end for
14: for i in 1 to beefile.num_of_nodes do
15:   node_i.mount_via_virtio()
16: end for
17: for i in 1 to beefile.num_of_nodes do
18:   node_i.pull/build_docker(beefile)
19:   node_i.conf_docker_storage(efs_mnt)
20:   node_i.conf_docker_network(host_mode)
21:   node_i.start_docker('ssh daemon')
22: end for
23: for each sequential run script in beefile do
24:   node_0.docker_exec(script)
25: end for
26: for each parallel run script in beefile do
27:   node_0.docker_exec(mpi_script)
28: end for
```

only needs to make minimum modifications to the BEE configuration file (beefile) in order to switch to AWS.

The computing resources are based on Xen-based VMs and they also known as EC2 instances. Since EC2 instances are VM-based, users are given full control inside each VM. So, here we configure them (via customized AMI) to enable Docker runtime. Users of BEE can specify desired instance type via BEE configuration file (beefile). Same as on the HPC platform, data sharing via network and storage also need to be handled.

A. Network Design

EC2 instances by default have network interconnect capability via the network in their infrastructures. However, they still need to be customized for HPC applications. First, as mentioned in BEE-VM design, MPI commonly uses random port for communication, so we need to create an EC2 security group that has a range of ports opened based on the MPI implementation specification. Second, for fast network interconnection, EC2 instances need to be placed in the same placement group. This makes sure the physical hardware

allocated for each EC2 instance are close to each other so that the network is optimized for low latency and high throughput. As for network interconnection between Docker containers, we follow a similar choice made using BEE-VM, that enables 'host network' mode at launch time.

B. Storage Design

By default EC2 instances do not share filesystems. To enable file sharing, we choose to create Elastic File System (EFS) and mount EFS to each EC2 instance. This design has better performance than the master-slave based Network File System (NFS) adopted in Starcluster. We use the volume mounting feature of Docker to enable file sharing between Docker containers similar to BEE-VM.

Algorithm 3 shows that launching logic of BEE-AWS. We use Boto API to remotely launch EC2 instances on AWS (line 7 - 15). After that we use SSH connection to control each instance.

VI. BEE-OPENSTACK DESIGN

OpenStack is a cloud operating system that is able to manage large pools of computing, storage, and network resources. It has been widely deployed in both research facilities and cloud computing environments. To bring the same unified execution environment and end-to-end automation to OpenStack, we build BEE-OpenStack as another BEE backend.

Unlike AWS, the computing sources of OpenStack can be either bare-metal machines or VM. In either case, users are given full control inside the operating system. So, similar to BEE-AWS we enable Docker runtime inside each OpenStack instance.

A. Network Design

On our OpenStack test environment (Chameleon Cloud), network interconnects are enabled by default between instances. So, we do not need to further configure it. For OpenStack infrastructures that need customized network, BEE will configure it automatically to ensure network interconnect capabilities between instances. The detail is omitted here. Similar to before, we use 'host network' mode for Docker containers.

B. Storage Design

Similar to AWS, by default, OpenStack instances do not share filesystems. On our OpenStack test environment (Chameleon Cloud), there is no OpenStack-managed storage system. So, we adopt NFS based file sharing between master instance (first instance) and worker instances. We use the volume mounting feature of Docker to enable file sharing between Docker containers similar to BEE-VM and BEE-AWS

Algorithm 4 shows the launching logic of BEE-OpenStack. Here we first use OpenStack CLI client to launch a pre-built Stack template for BEE, and then use SSH to control each instance.

Algorithm 3 BEE-AWS launching logic

Require: Pre-built AMI (only need to build once)

Require: Dockerized application (Docker image/Dockerfile)

Require: BEE configuration file (beefile)

Require: Run scripts

```
1: if user given EFS name not exist then
2:   request_creating_efs(efs_name)
3:   while efs_status(efs_name) != active do
4:     sleep()
5:   end while
6: end if
7: initialize_ec2_service_connection()
8: bee_sg = create_security_group()
9: bee_sg.authroize_ingress('tcp', '22')
10: bee_pg = create_placement_group()
11: for i in 1 to beefile.num_of_nodes do
12:   bee_ec2_i = create_ec2(bee_sg,
13:     bee_pg)
14:   bee_ec2_i.start()
15: end for
16: wait_for_all_instance_to_become_ready()
17: for i in 1 to beefile.num_of_nodes do
18:   bee_ec2_i.set_hostname()
19:   for j in 1 to beefile.num_of_nodes do
20:     bee_ec2_j.setup_hostfile(bee_ec2_i.ip)
21:   end for
22: end for
23: for i in 1 to beefile.num_of_nodes do
24:   bee_ec2_i.create_efs_mount_point()
25:   bee_ec2_i.mount_to_efs(efs_name)
26:   bee_ec2_i.pull/build_docker(beefile)
27: end for
28: for i in 1 to beefile.num_of_nodes do
29:   bee_ec2_i.pull/build_docker(beefile)
30:   bee_ec2_i.conf_docker_storage(efs_mnt)
31:   bee_ec2_i.conf_docker_network(host_mode)
32:   bee_ec2_i.start_docker('ssh daemon')
33: end for
34: for each sequential run script in beefile do
35:   bee_ec2_0.docker_exec(script)
36: end for
37: for each parallel run script in beefile do
38:   bee_ec2_0.docker_exec(mpi_script)
39: end for
```

VII. EVALUATION

We evaluate the four BEE backends on four different platforms: For BEE-Charliecloud and BEE-VM, we test them on the bare-metal environment on Chameleon Cloud at Texas Advanced Computing Center (TACC). Each node is equipped with two Intel Xeon E5-2670 v3 CPU (clock frequency at 2.30 GHz) with 128 GB DRAM. Each node is connected with Mellanox ConnectX-3 Infiniband card with peak transfer speed at 10 Gbps. For BEE-AWS, we choose to use c3.4xlarge EC2 type at AWS Oregon region. Each node is equipped with Intel Xeon E5-2680 v2 CPUs and 30GB

Algorithm 4 BEE-OpenStack launching logic

Require: Pre-built OpenStack Img. (only need to build once)

Require: Dockerized application (Docker image/Dockerfile)

Require: BEE configuration file (beefile)

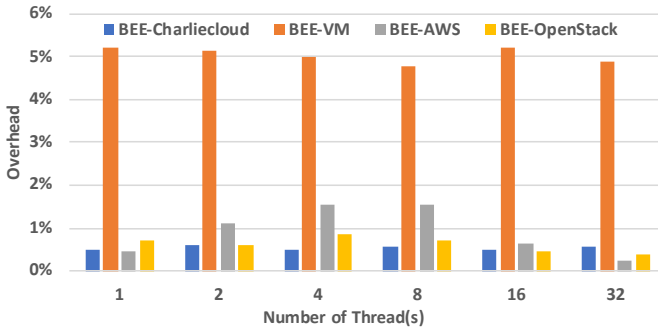
Require: Run scripts

```
1: initialize_nova_service_connection()
2: create_new_sshkey()
3: launch_bee_stack(beefile)
4: wait_for_all_instance_to_become_ready()
5: for i in 1 to beefile.num_of_nodes do
6:   bee_os_i.set_hostname()
7:   for j in 1 to beefile.num_of_nodes do
8:     bee_os_j.setup_hostfile(bee_os_i.ip)
9:   end for
10: end for
11: bee_os_0.create_nfs_mount_point()
12: for i in 1 to beefile.num_of_nodes do
13:   bee_os_i.mount_to_nfs(bee_os_0.ip())
14: end for
15: for i in 1 to beefile.num_of_nodes do
16:   bee_os_i.pull/build_docker(beefile)
17: end for
18: for i in 1 to beefile.num_of_nodes do
19:   bee_os_i.pull/build_docker(beefile)
20:   bee_os_i.conf_docker_storage(nfs_mnt)
21:   bee_os_i.conf_docker_network(host_mode)
22:   bee_os_i.start_docker('ssh daemon')
23: end for
24: for each sequential run script in beefile do
25:   bee_os_0.docker_exec(script)
26: end for
27: for each parallel run script in beefile do
28:   bee_os_0.docker_exec(mpi_script)
29: end for
```

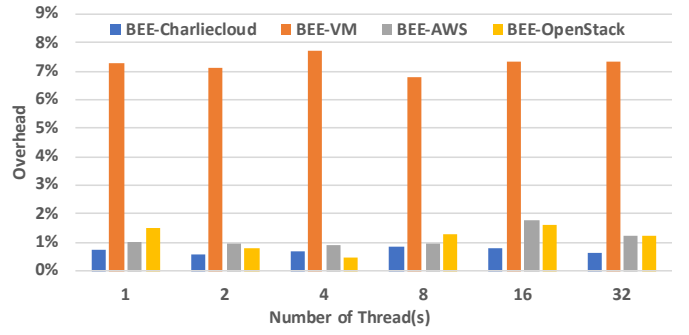
DRAM. On BEE-OpenStack, we choose the OpenStack environment at Chameleon Cloud@University of Chicago. We focus on evaluating three kinds of performance that are most important for HPC applications: *computation*, *storage*, and *network*. For each test, the comparison baseline is the native performance provided on each platform without using BEE or any additional encapsulated runtime system. Note: all platforms, except AWS, provide access to the bare-metal hardware, so baseline performance is the native performance on the hardware. For AWS, its Xen-based VM is an inseparable part of the platform and the underlying physical hardware is inaccessible to general users, so its baseline is the performance inside VMs.

A. Computational Performance

Computational performance of a platform is one of the most important capabilities for HPC applications. In this section, we compare the computational performance of all four BEE backends with the baseline. We choose one compute intensive benchmark test and one memory intensive benchmark test from the OpenMP version NAS Parallel Benchmarks



(a) Compute intensive workload (BT)



(b) Memory intensive workload (IS)

Fig. 5: Performance overhead compare with native performance provided on each corresponding platform.

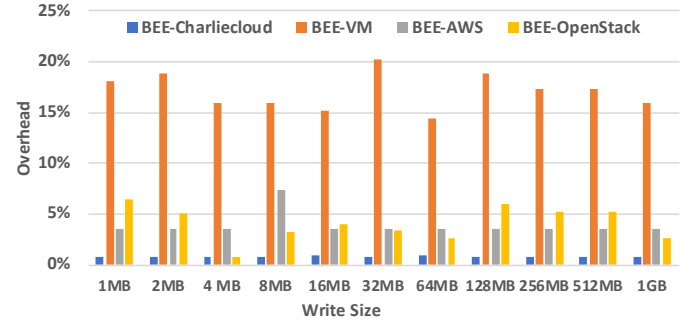
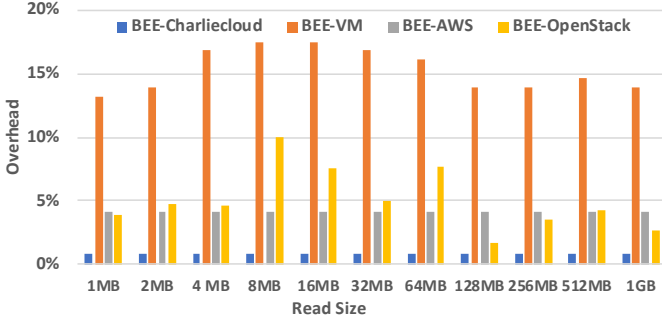


Fig. 6: Storage I/O read/write speed overhead compare with native speed provided on each corresponding platform.

(NPB)[19] in our evaluation. We test each benchmark running one to 32 threads (cores) to further show the computational performance on multi-thread environment.

1) *Compute intensive workload*: For compute intensive workload, we choose Block Tri-diagonal solver (BT) benchmark test with input matrix size of 102^3 (problem size: class B).

As we can see in **Fig. 5(a)**, for compute intensive workload, all four BEE backends have low performance overhead: BEE-Charliecloud 0.4% - 0.6% (avg. 0.5%); BEE-VM 4.8% - 5.2% (avg. 5.0%); BEE-AWS 0.2% - 1.6% (avg. 0.8%); BEE-OpenStack 0.3% - 0.9% (avg. 0.6%).

2) *Memory intensive workload*: For memory intensive workload, we choose Integer Sort (IS) test suit with 134217728 input integer (problem size : class C).

As we can see in **Fig. 5(b)**, for memory intensive workload all four BEE backends also have low performance overhead: BEE-Charliecloud 0.6% - 0.9% (avg. 0.7%); BEE-VM 6.9% - 7.7% (avg. 7.1%); BEE-AWS 0.9% - 1.8% (avg. 1.1%); BEE-OpenStack 0.5% - 1.7% (avg. 1.0%). In addition, both kinds of workload also exhibit similar speedup comparing with their baseline counterparts when we increase the number of threads.

B. Storage I/O

Storage I/O is another key component for many HPC applications. For example, large-scale simulations often need to first load large datasets before computation and frequently dump checkpoints during computation and once the simulation has concluded. Later, these results may be used for other simulations or for analytics. I/O performance plays an important role for the overall performance of HPC applications.

To evaluate the storage I/O performance of the four BEE backends and compare with the baseline performance, we use the Linux built-in command - dd. Specifically, to benchmark write performance, we use the dd command to write a file with data from /dev/zero. As for read performance, we use the dd command to read out the file just saved and write to /dev/null. To avoid reading from cache, we use `echo 3 > /proc/sys/vm/drop_caches` command to force the system to clear all cached data between each write and read. Usually this file is read-only inside a container, so we issue the command outside the container, achieving the same cache flushing effect. The file used for write and read is placed in the directory that is shared between instances or containers. We test different file sizes ranging from 1 MB to 1 GB. To eliminate noise and variation, we repeat each test 1000 times. **Fig. 6** shows the read and write performance on the four BEE backends comparing with the baseline (i.e., the IO performance on each platform without using BEE). As we can see, BEE-Charliecloud produces negligible read and write overhead (0.08%). BEE-VM uses both VM and Docker, so it produces relative higher overhead, 13.1% - 17.5% (avg. 15.2%) for read and 15.1% - 20.1% (avg. 17.1%) for write. BEE-AWS produces steady 0.4% overhead for read and 0.3% overhead for write. BEE-OpenStack produces 1.7% - 7.6% (avg. 5.0%) for read overhead and 2.7% - 6.4% (avg. 4.1%) for write overhead.

C. Network

Finally, we evaluate the network performance of the four BEE backends. We use the HPCBench [20] to measure the bandwidth and latency when transferring data of different sizes between two processes in containers or on the plat-

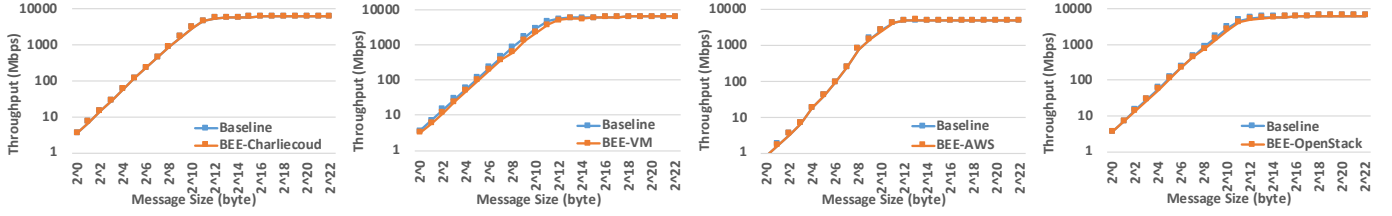


Fig. 7: P2P Network Throughput Comparison

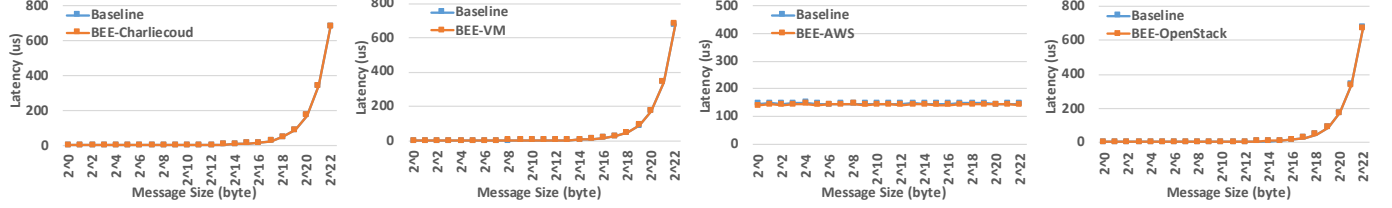


Fig. 8: P2P Network Latency Comparison

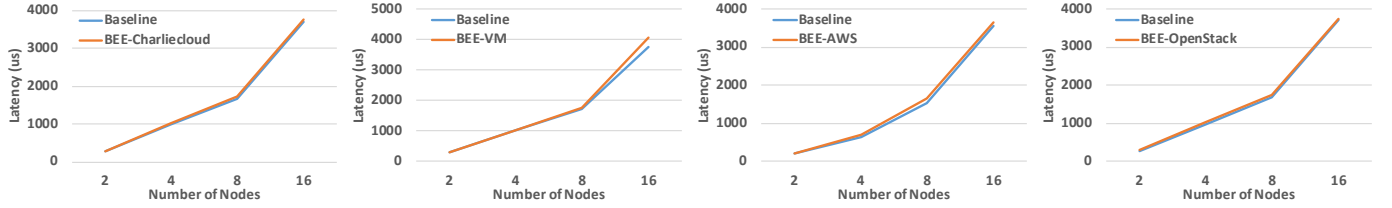


Fig. 9: All-to-all Network Latency Comparison

form without using BEE. BEE-VM and BEE-OpenStack use the Infiniband (IB) on Chameleon Cloud via SR-IOV. BEE-Charliecloud and BEE-AWS use the Ethernet connection. **Fig. 7** and **Fig. 8** show the point-to-point (P2P) network performance. MPI communication function calls between two nodes (one process per node) were used to test the average throughput and latency when transferring different message sizes. It can be seen that all four BEE backends can provide similar network bandwidth and latency compared to the baseline. **Fig. 9** also show the latencies of all-to-all collective communication in MPI. It shows that all four BEE backends still provide similar network performance large scale.

VIII. VECTOR PARTICLE-IN-CELL CASE STUDY

In this section, we showcase a widely used HPC application, Vector Particle-In-Cell (VPIC) plasma physics code [21], [22], [23], on the four BEE backends. VPIC is a general purpose particle-in-cell plasma simulation code for modeling kinetic plasmas in multiple spatial dimensions. VPIC is a memory bound application that runs on multiple nodes using MPI and pthreads. It has been optimized for modern computing architectures by using short-vector, single-instruction-multiple-data (SIMD) instructions and cache optimization. Before the simulation begins, VPIC needs to load an input deck and user configuration files. When computation is finished, VPIC writes the output. With flexible checkpoint-restart semantics, VPIC allows checkpoint files to be read as input for subsequent simulations. Moreover, VPIC has a native I/O format that

interfaces with the high-performance visualization software Ensign and Paraview.

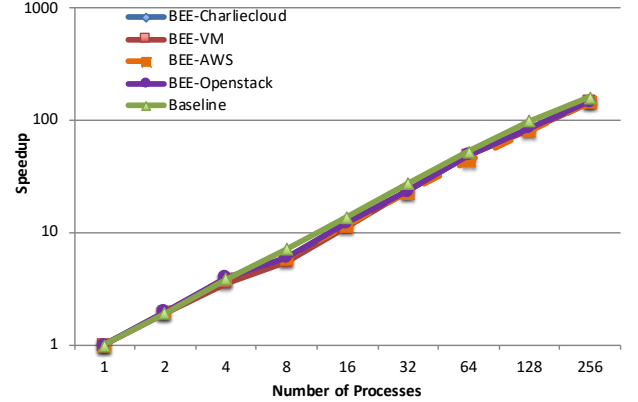


Fig. 10: VPIC scale up test

We test VPIC on different BEE backends using 1 to 256 processes. As shown in **Fig. 10**, all four BEE backends exhibit similar speedup compared with the baseline i.e., the speedup we can get on the bare-metal environment on Chameleon Cloud at Texas Advanced Computing Center (TACC).

IX. RELATED WORK

A. StarCluster

StarCluster [24] is an open source cluster launching tool for AWS that aims to automation the process of creating a HPC cluster-like computing environment on AWS. It uses a configuration file to let users specify desired configuration of

the cluster e.g., number of instances. Similar to BEE-AWS it uses BOTO APT [25] to communicate to AWS regards creating and launching EC2 instances and other resources. Although it offers automation, it suffers from three major drawbacks. First, it does not offer automatic deployment of Dockerized application. Current Docker users still need to manually copy Dockerized application to EC2 instances, configure the network and storage of each Docker container, then launch the application. Second, even not using Docker, users still need to manually login to the EC2 instances to deploy and launch their applications. Finally, it does not have HPC/cloud cross-platform portability.

B. Amazon Elastic Container Service

Amazon Elastic Container Service (ECS) [26] offers the capability of automating creating a cluster of EC2 instances on AWS and then deploying the Docker container on each instance. However, it does not create a shared file system automatically; users still need to manually configure EFS or S3 storage. In addition, it only targets AWS platform with no portability to other platforms.

C. Kubernetes

Kubernetes [27] is widely used open-source system for automating deployment of containerized applications. It supports many mainstream cloud platforms e.g., AWS, Google Compute Engine, Azure, IMB Cloud, etc. However, as discussed in [28], Kubernetes is designed for service-based workload on those platforms, so they are not suitable HPC applications. In addition, it has limited support on HPC systems.

X. CONCLUSIONS

In this work, we first discussed several workflow and productivity problems that current HPC users are facing. Then, we analyzed the potential of integrating commonly used Linux container technology into the existing HPC systems to build a consistent container environment for HPC users. Following this goal, we proposed a container-enabled framework, BEE, and four BEE backends for HPC and cloud systems that allow users to use the compute resources of both HPC systems and cloud computing systems with little extra configuration. Experiments show that BEE can achieve comparable performance. Finally, a case study on a widely used VPIC simulation tool was tested on BEE for performance comparison.

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REFERENCES

- [1] G. Vallee, T. Naughton, C. Engelmann, H. Ong, and S. L. Scott, "System-level virtualization for high performance computing," in *Parallel, Distributed and Network-Based Processing*, 2008. *PDP 2008. 16th Euromicro Conference on*, 2008.
- [2] A. Reuther, P. Michaleas, A. Prout, and J. Kepner, "Hpc-vms: Virtual machines in high performance computing systems," in *High Performance Extreme Computing (HPEC), 2012 IEEE Conference on*, 2012.
- [3] W. Huang, J. Liu, B. Abali, and D. K. Panda, "A case for high performance computing with virtual machines," in *Proceedings of the 20th annual international conference on Supercomputing*, 2006.
- [4] J. Liu, W. Huang, B. Abali, and D. K. Panda, "High performance vmm-bypass i/o in virtual machines," in *USENIX Annual Technical Conference, General Track*.
- [5] J. Zhang, X. Lu, S. Chakraborty, and D. K. D. Panda, "Slurm-v: Extending slurm for building efficient hpc cloud with sr-io and ivshmem," in *European Conference on Parallel Processing*, 2016.
- [6] S. Gugnani, X. Lu, and D. K. Panda, "Performance characterization of hadoop workloads on sr-io-enabled virtualized infiniband clusters," in *Proceedings of the 3rd IEEE/ACM International Conference on Big Data Computing, Applications and Technologies*, 2016.
- [7] A. Tikotekar, G. Vallée, T. Naughton, H. Ong, C. Engelmann, and S. L. Scott, "An analysis of hpc benchmarks in virtual machine environments," in *European Conference on Parallel Processing*, 2008.
- [8] W. Huang, M. J. Koop, Q. Gao, and D. K. Panda, "Virtual machine aware communication libraries for high performance computing," in *Proceedings of the 2007 ACM/IEEE conference on Supercomputing*, 2007.
- [9] "Docker," URL: <https://www.docker.com/>.
- [10] R. Priedhorsky and T. Randles, "Charliecloud: Unprivileged containers for user-defined software stacks in hpc," Los Alamos National Laboratory, Tech. Rep., 2016.
- [11] D. M. Jacobsen and R. S. Canon, "Contain this, unleashing docker for hpc," *Proceedings of the Cray User Group*, 2015.
- [12] G. M. Kurtzer, "Singularity 2.1.2 - Linux application and environment containers for science," 2016. [Online]. Available: <https://doi.org/10.5281/zenodo.60736>
- [13] C. Boettiger, "An introduction to docker for reproducible research," *ACM SIGOPS Operating Systems Review*, 2015.
- [14] D. Merkel, "Docker: lightweight linux containers for consistent development and deployment," *Linux Journal*, 2014.
- [15] B. Ruan, H. Huang, S. Wu, and H. Jin, "A performance study of containers in cloud environment," in *Advances in Services Computing: 10th Asia-Pacific Services Computing Conference, APSCC 2016, Zhangjiajie, China, November 16-18, 2016, Proceedings 10*, 2016.
- [16] A. S. Harji, P. A. Buhr, and T. Brecht, "Our troubles with linux kernel upgrades and why you should care," *ACM SIGOPS Operating Systems Review*, 2013.
- [17] R. Russell, "virtio: towards a de-facto standard for virtual i/o devices," *ACM SIGOPS Operating Systems Review*, 2008.
- [18] "Starcluster," URL: <http://star.mit.edu/cluster/>.
- [19] "NAS Parallel Benchmarks," URL : <https://www.nas.nasa.gov/publications/npb.html>.
- [20] "Hpcbench," URL: <http://hpcbench.sourceforge.net/>.
- [21] K. J. Bowers, B. J. Albright, B. Bergen, L. Yin, K. J. Barker, and D. J. Kerbyson, "0.374 pflop/s trillion-particle kinetic modeling of laser plasma interaction on roadrunner," in *Proceedings of the 2008 ACM/IEEE conference on Supercomputing*, 2008.
- [22] K. J. Bowers, B. Albright, L. Yin, B. Bergen, and T. Kwan, "Ultra-high performance three-dimensional electromagnetic relativistic kinetic plasma simulation a," *Physics of Plasmas*, 2008.
- [23] K. J. Bowers, B. J. Albright, L. Yin, W. Daughton, V. Roytershteyn, B. Bergen, and T. Kwan, "Advances in petascale kinetic plasma simulation with vplic and roadrunner," in *Journal of Physics: Conference Series*, 2009.
- [24] "StarCluster," URL : <http://star.mit.edu/cluster/>.
- [25] "Boto api," URL: <https://github.com/boto/boto3>.
- [26] "Aws container service," URL : <https://aws.amazon.com/ec2/>.
- [27] "Kubernetes," URL : <https://kubernetes.io/>.
- [28] "Hpc workloads unique challenges," URL : <https://kubernetes.io/blog/2017/08/kubernetes-meets-high-performance/>.