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Dynamic Virtualized Deployment of Particle Physics Environments on a High-Performance Computing Cluster

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Abstract Particle physics experiments at the Large Hadron Collider (LHC) need a great quantity of computing resources for data processing, simulation, and analysis. High-Performance Computing (HPC) resources provided by research institutions can be useful supplements to the existing World-wide LHC Computing Grid (WLCG) resources allocated by the collaborations. At the University of Freiburg, the shared HPC cluster NEMO has been made available to ATLAS and CMS users accessing it from external machines connected to the WLCG. To this effect, the full software environment corresponding to a WLCG center is provided in a virtual machine image. The interplay between the schedulers for NEMO and for the external cluster is ensured through the ROCED service. An OpenStack infrastructure is deployed at NEMO to orchestrate the simultaneous usage by bare metal and virtualized jobs. Through the setup, resources are provided to users in a transparent, automatized, and on-demand way. The performance of the virtualized environment has been evaluated for particle physics applications.

Keywords Virtualization · Particle Physics · Grid Computing

1 Introduction

This paper presents the concepts and implementation of providing a HPC resource to ATLAS and CMS users accessing external clusters connected to the World-wide computing grid (WLCG) with the purpose of running data production as well as data analysis on the HPC host system. For this purpose, the HPC cluster NEMO at the University of Freiburg is deploying an OpenStack instance to handle the virtual machines. The challenge is in provisioning, setup, scheduling, and decommissioning the virtual research environments (VRE) dynamically and according to demand. For this purpose, the schedulers on NEMO and on the external resources are connected through the ROCED service[2].

A VRE in the context of this paper is a complete software stack as it would be installed on a compute cluster fitted to the demands of ATLAS or CMS workloads.

2 Virtualization infrastructure

Virtualization has become mainstream technology over the last decade as it allows both to host more than one operating system on a single server and to strictly separate users of software environments. While widespread in computer center operation this technique is rarely applied in HPC.

2.1 Computing at the University of Freiburg

The computer center at the University of Freiburg provides medium scaled research infrastructures like cloud, storage and especially HPC services to cater to the needs of various scientific communities. Significant standardization in hardware and software is necessary for the operation of compute systems comprised of more than 1000 individual nodes with a small group of administrators.

The level of granularity of the software stack provided is not fine enough to directly support the quite

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special requirements of world-wide efforts like the ATLAS or CMS experiments. To utilize the system optimally and to open the cluster to as many different needs as possible without increasing the person power required for operation, novel approaches to the utilization of the installed hardware are necessary. Transferring expertise from the operation of the established local private cloud, the use of OpenStack as a cloud platform has been identified as a suitable solution for NEMO to provide a more flexible software deployment in addition to the existing software module system. This produced a couple of implications ranging from challenges in the automated creation of suitable virtual machines, their on-demand deployment and the scheduling on the cluster and virtual resources level.

2.2 Research Cluster NEMO

The research cluster 'bwForCluster NEMO' is a cluster for state-wide research in the scientific fields Elementary Particle Physics, Neuroscience and Microsystems Engineering. It started its operation on the 1st of August 2016 with then 748 nodes having 20 physical cores and 128 GiB of RAM each. The high speed network used is Omni-Path. The parallel storage is BeeGFS with 576 TB capacity. October 2017 the NEMO cluster was extended by scientific groups and has currently 900 nodes and a total capacity of 768 TB of parallel storage.

2.3 Separation of software environments

The file system of a virtual machine (or virtualized research environment (VRE) in the described use case) is a disk image presented as a single file. From the computer center's perspective this image is seen as a black box requiring no involvement or efforts like updates of the operating system or the provisioning of software packages of a certain version. From the researchers perspective the VRE is an individual (virtual) node where everything from the hardware level – at least to a certain degree like CPU or RAM – up to the operating system, applications and configurations can be controlled autonomously by the research groups.

To allow more flexible software environments the standard bare metal operation of NEMO is extended with a parallel installation of OpenStack components [12]. The NEMO cluster uses Adaptive's Moab Workload Manager [3] as a scheduler of compute jobs. Since OpenStack tries to schedule the virtual machines on the same nodes and resources itself, it is necessary to define a primary or master scheduler, who controls which jobs should run on which worker node. Moab and Openstack are unaware that there exists another scheduler within the cluster and no API exists so that both can communicate with each other. Since most users still use the bare metal HPC cluster Moab is used as the primary scheduler. It allows for detailed job description and offers sophisticated scheduling features like fair-share, priority-based scheduling, detailed limits and much more. Openstack will still schedule the virtual machines, but Moab will initially start the VRE jobs and the VRE job will instruct Openstack to start the virtual machine on the reserved resources and which flavor to use (resource definition in OpenStack).

When a VRE job is submitted to the NEMO cluster Moab will first calculate the priority and the needed resources of the job and then insert it into its queue. When the job is in line for execution and the requested resources are available, the job will start a script which then starts the VRE on the selected node within the resource boundaries. During the run-time of the VRE a monitoring script checks if the VRE is still running and exits the job if the VRE ends. When the job ends, OpenStack gets a signal to terminate the virtual machine and the VRE job ends as well. Neither Moab nor OpenStack can look into the VRE and so it cannot assess if it is actually active or idle. To solve this issue, a customized glue component called ROCED has been introduced (described in further detail in Section 4). It is used as a broker between different HPC schedulers translating resources, monitoring usage inside the virtual machine and starting and stopping VRE images on demand.

3 Generation of the image

The VREs in the use case described in this paper is simply a OpenStack container in the format of a compatible VM image. These images are provided in an automatized way allowing versioning and archiving of the environments captured in the images. The approaches used in the different groups are described in the following.

3.1 Packer combined with Puppet

One approach to generating the image is the open-source tool `packer`[8], interfaced to `puppet`[10]. `Packer` allows to configure an image based on an `.iso` file using a kickstart [9] file and flexible script-based configuration. It also provides an interface to `puppet` making it a convenient tool if an existing `puppet` role is to be used for the images. If the roles are defined according to the hostname of the machine as is conventional in `puppet` with `hieradata`, the hostname needs to be set in the scripts supplied to `packer`. Propagation of certificates require an initial manual start of a machine with the same hostname to allow handshake signing of the certificate from the `puppet` server.

Apart from these initial adjustments, `packer`'s interface to `puppet` allows a fully automated image generation with up-to-date configuration.

3.2 Image generation using the Oz toolkit

Another option to employ a fully-automated procedure is to use the OZ toolkit [4]. All requirements and configuration options of an image can be specified via an XML file, called template. The partitioning and installation process of the operating system is fully automated, as OZ will use the remote-control capabilities of the local hypervisor. After the installation of the operating system, additional libraries and configuration files can be installed. Once the image has been built, it is automatically compressed and uploaded to a remote cloud site. Using this technique allows to build images in a reproducible fashion, as all templated files are version controlled using git. Furthermore, existing template files are easy to adapt to new sites and experiment configurations.

4 Interfacing batch systems and virtual resources using ROCED

While virtualized HPC systems and commercial cloud offerings provide the necessities to acquire computing and storage capacity by dynamic resource booking, the computing needs of High-Energy Physics research groups additionally require workflow management systems which are able to manage thousands of running jobs. While some cloud providers, for example Amazon with AWS Batch [5], provide a service for workflow management, these offerings are often limited to one specific cloud instance. To dynamically distribute batch jobs to multiple sites and manage machine life-time on specific sites, a combination of a highly-scalabe batch system and a virtual machine scheduler is desirable.

4.1 ROCED

Many capable batch systems exist today and they can be interfaced to virtualization providers using the cloud meta-scheduler ROCED (Responsive On-demand Cloud Enabled Deployment) which has been developed at the KIT since 2010 [2]. ROCED is written in a modular fashion in python and the interfaces to batch systems and cloud sites are implemented as so-called *Adapters*. This makes ROCED independent of a specific user group or workflow. It provides a scheduling core which collects the current requirement of computing resources and decides if virtual machines need to be started or can be stopped. One or more Requirement Adapters report the current queue status of batch systems to the central scheduling core. Currently, Requirement Adapters are implemented for the Slurm, Torque, HTCondor and GridEngine batch systems. The Site Adapters allow ROCED to start, stop and monitor virtual machines on multiple cloud sites. Implementations exist for Amazon EC2, OpenStack, OpenNebula and Moab-based virtualization at HPC centers. Special care has been put into the resilience of ROCED: it can automatically terminate non-responsive machines and restart virtual machines in case some machines dropped out. This allows VM setups orchestrated by ROCED with thousands of virtual machines and many tens of thousands of jobs to run in production environments.

4.2 Using HTCondor as front-end scheduler

The open-source HTCondor project provides a workload management system which is highly configurable and modular [6]. Batch processing workflows can be submitted and are then forwarded by HTCondor to idle resources. HTCondor maintains a resource pool, which worker nodes in a local or remote cluster can join. Once HTCondor has verified the authenticity and features of the newly joined machines, computing jobs are automatically transferred. Special features to connect from within isolated network zones, for example via a Network Address Translation Portal, to the central HTCondor pool are available. The Connection Brokering (CCB) service [7] is especially valuable to connect virtual machines to the central pool. These features and the well-known ability of HTCondor to scale to O(100k) of parallel batch jobs makes HTCondor well suited as a workload management system for the use cases described in this paper.

The virtual machines spawned for the CMS user group of the KIT come with the HTCondor client (`startd`) pre-installed and this client is started after the machine has fully booted and connects to the central HTCondor pool at the KIT via a shared secret. Due to HTCondor's dynamic design, new machines in the pool will automatically receive jobs and the transfer of the job configuration and meta-data files is handled via HTCondor's internal file transfer systems.

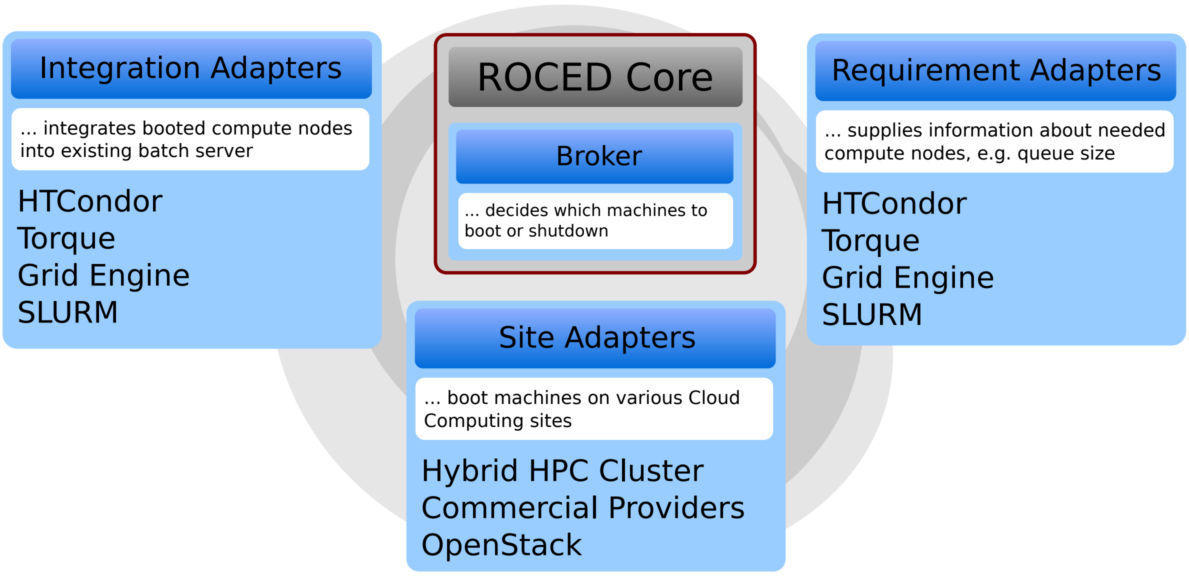

Fig. 1 Overview of the ROCED modular design. The ROCED Core contains the Broker which decides when and on which sites new virtual machines are booted. The Requirement Adapters report about the utilization and resource requirements of the attached batch systems. The Site Adapter is responsible to manage the lifetime of virtual machines on an cloud site and the Integration Adapter ensure that newly booted machines are integrated into the batch system.

4.3 Using SLURM as front-end scheduler

Alternatively to the approach in Sec. 4.2, the scheduler Slurm has been incorporated into the ROCED setup by the ATLAS group at University of Freiburg. While Slurm provides a built-in functionality for dynamic startup of resources in the *Slurm Elastic Computing* module[11], this has been found to be unsuitable for resources which are not expected to be available within a fixed time period, in this case due to the presence of a queue in the host system which may postpone the start of a resource by a significant, varying period. In addition the transfer of information, such as error states, from one scheduler the the other, and therefore to the user, is very limited. Therefore, ROCED has been chosen as the interface between the Moab scheduler on the host system and the Slurm scheduler on the submission side.

For Slurm, it is necessary that each potential virtual machine is registered in the configuration at the time of start of the slurm server as well as the client. Slurm configurations also need to be in agreement between server and client. Therefore, a range of hostnames is registered in the configuration in a way that is mapped to potential IP addresses of virtual machines. These virtual machines have a fixed number of CPUs and memory and are registered under a certain Slurm partition. When a job is submitted to this partition and no other resource is available, information from the Slurm `squeue` and `sinfo` commands is requested and parsed for the required information.

Since the ATLAS Freiburg group comprises three sub-groups, each mapped to a different account on Moab/NEMO, special care is taken to avoid interference of resources used by another account to ensure fair share on NeMO, while allowing jobs from one group to occupy otherwise idle resources of another group.

ROCED determines the amount of VMs to be started and sends the corresponding VRE job submission commands to Moab. After the virtual machine has booted, the hostname is set to the IP dependent name which is known to the Slurm configuration. A cron job executes several sanity checks on the system. Upon successful execution of these tests, the Slurm client running in the VM starts accepting the queued jobs. After completion of the jobs and a certain period of receiving no new jobs from the queue, the Slurm client in the machine drains itself and the machine shuts itself down. The IP address as well as the corresponding hostname in Slurm are then released and can be used again.

5 Analysis of performance and usage

The approach described above has been implemented and put into production in the research groups at University of Freiburg (Physikalisches Institut) and Karlsruhe (... Institut). The following chapter presents the statistical analysis of the performance of the virtualized setup both in terms of job performance as well as usage statistics.

5.1 HEPSPEC benchmarks

The HEPSPEC standard defines benchmarking of CPU performance for High-Energy physics resources[13].

For an estimate of the performance of the virtual machines, machines with the same hardware configuration are compared which are either deployed via the existing Tier2/3 boot system ("bare metal") or via the NEMO OpenStack in virtual machines.

The results of the HEPSPEC benchmarks are presented in Fig. 2 which shows the HEPSPEC score determined per number of CPUs versus the number of CPUs. Different tests have been performed *bare metal*, where the benchmark code is run either with user rights ("realistic load") or with root privileges ("machine reserved"). The results illustrate that the bare-metal jobs are less performant than those performed in virtual machines on NEMO with machines under realistic load. Tests carried out in user space on the virtual machines are approaching *bare metal* tests with root permissions.

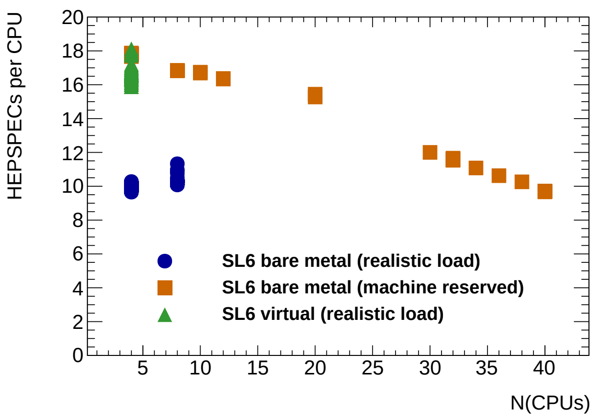

Fig. 2 Results of HEPSPEC benchmark tests: HEPSPEC per number of CPUs in dependence of number of CPUs.

As it is expected from first principles that the virtualisation reduces the CPU power available to the process, these results indicate non-optimal configuration of the bare-metal running. However it is reassuring for the use-case of running in the ATLAS environment on NEMO that the performance does not suffer.

5.2 Usage statistics

Figure 3 show the utilization of virtual machines which were orchestrated by ROCED depending on the re-

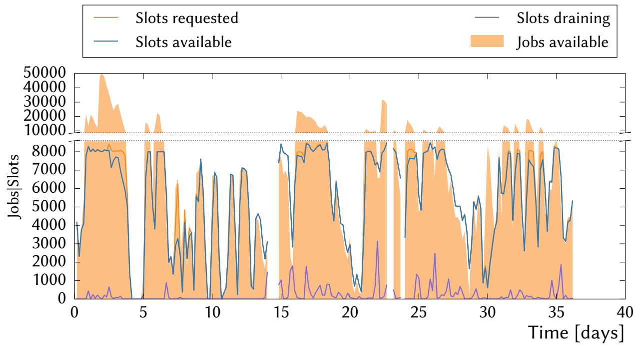

Fig. 3 Utilization of the shared HPC system by booted virtual machines. Up to 9000 virtual cores were in use at peak times. The fluctuations in the utilization reflects the patterns of the submission of jobs by our institute users. The number of draining slots displays the amount of job slots still processing jobs while the rest of the node's slot are already empty.

source demands of the users of the KIT group. At peak times, up to 9000 virtual cores were filled with user jobs, which was at that time more than half of the 16.000 cores of the initial NEMO cluster.

The usage of the hybrid cluster model is shown in figure 4. The diagram shows the shared usage of NEMO's cluster nodes running either bare-metal or virtualized jobs. The part of the cluster which runs virtualized jobs or VREs changes dynamically from job to job, since the VREs are started by a standard bare-metal job.

At the beginning the cluster was only containing the operating system and some basic development tools, scientific software was added after the the cluster was already in production mode. Since the VRE for the CMS project was already available when the NEMO cluster started it could already use the whole cluster while other groups still had to wait for the research software to be deployed on the cluster. This explains the high usage by VREs in the first months of operation. With more and more software being available for bare-metal usage the amount of VRE jobs decreased. This figure is only an estimate because VRE projects are not forced to use VREs and therefore could run bare-metal jobs as well.

6 Conclusions and Outlook

A system for the dynamic, on-demand provisioning of virtual machines to run jobs in a High-Energy Physics context on an external, not dedicated resource as realized at the HPC cluster "NEMO" at University of Freiburg has been described. Reasons for the need for an interface between the schedulers of the host system and the external system from which requests are sent

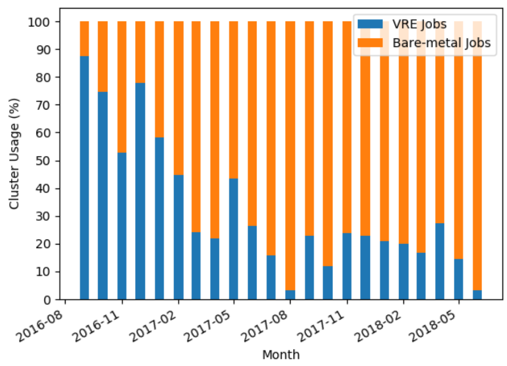

Fig. 4 Usage of the NEMO cluster in the time between September 2016 to June 2018. The blue bars indicate the usage by jobs running directly in the hosts' operating system, while the orange bars are jobs running in virtual machines.

have been explained. The performance and usage have been analyzed for two groups.

This approach can be generalized to other platforms and possibly also other forms of virtualized environments (containers).

The caveat is that there is a performance loss due to the virtualization overhead. However, this is perfectly acceptable if the benefits of virtualized research environments outweigh the loss in performance for an individual use case or an entire scientific work flow. General feasibility and provisioning of virtualized research environments for scientific computing.

Using virtualization inside an HPC system opens up the possibilities for several interesting features. While their implementation would require tighter integration between HPC scheduler and virtualization framework, they could solve several classic problems with HPC systems, especially those designated for novice HPC users.

Provided the virtualization basics snapshot and migration functionality for running virtual machine instances should become further features of a virtualized cluster. This means that running processes can be stopped, possibly moved to a different node in the virtualization cluster and then resumed. For an HPC system, this would be practical for two use cases. The first one concerns long running monolithic jobs. These are, for very practical reasons, non favored jobs in HPC environments, assuming they are permitted in the first place. However, the costs to adapt a particular workflow based on such monolithic tasks to a HPC system, e.g. by parallelizing and partitioning it manually, may sometimes exceed the practical use of the resulting solution. If the monolithic job could automatically be stopped, checkpointed and resumed at regular intervals, this might very well constitute a more economic procedure. In the second use case, if there is a mix of pleasingly parallel high throughput jobs (using only single cores or nodes) and massively parallel high performance jobs (using several nodes), the second class of jobs should be concentrated on nodes that share optimal high performance network communication paths. Typically this is accomplished by high investments in the network topology or sophisticated tuning of the job queue. However, if jobs could be moved around the physical machines (i.e. de-fragmented), optimal high performance network communication paths can be guaranteed by concentrating massively parallel jobs on the same or adjacent high performance network switches.

A system for the dynamic, on-demand provisioning of virtual machines to run jobs in a High-Energy Physics context on an external, not dedicated resource as realized at the HPC cluster "NEMO" at University of Freiburg has been described. Reasons for the need for an interface between the schedulers of the host system and the external system from which requests are sent have been explained. The performance and usage have been analyzed for selected cases.

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