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

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Abstract The NEMO High Performance Computing Cluster at the University of Freiburg has been made available to researchers of the ATLAS and CMS experiments. Users access the cluster from external machines connected to the World-wide LHC Computing Grid (WLCG). This paper describes how 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 clusters is coordinated through the ROCED service. A cloud computing 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 \cdot Particle Physics \cdot Grid Computing \cdot Benchmarks

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1 Introduction

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Particle physics experiments at the Large Hadron Col- 68 lider (LHC) need a great quantity of computing re- 69 sources for data processing, simulation, and analysis. 70 This demand will be growing with the upcoming High- 71 Luminosity upgrade of the LHC [1]. To help fulfill this 72 need, High Performance Computing (HPC) resources 73 provided by research institutions can be useful supple- 74 ments to the existing World-wide LHC Computing Grid 75 (WLCG) resources allocated by the collaborations.

This paper presents the concepts and implementa-77 tion of providing a HPC resource, the shared research 78 cluster NEMO at the University of Freiburg, to ATLAS 79 and CMS users accessing external clusters connected to 80 the WLCG with the purpose of running data production as well as data analysis on the HPC host system. The HPC cluster NEMO at the University of Freiburg is 81 deploying an OpenStack [2] instance to handle the virtual machines. The challenge is in provisioning, setup, 82 scheduling, and decommissioning the virtual research 83 environments (VRE) dynamically and according to de-84 mand. For this purpose, the schedulers on NEMO and 85 on the external resources are connected through the 86 ROCED service [3].

A VRE in the context of this paper is a complete $_{88}$ software stack as it would be installed on a compute $_{89}$ cluster fitted to the demands of ATLAS or CMS work- $_{90}$ loads.

2 Virtualization infrastructure

Hardware virtualization has become mainstream tech-₉₃ nology over the last decade as it allows both to host ₉₄ more than one operating system on a single server and ₉₅ to strictly separate users of software environments. Hard₅₆ ware and software stacks are decoupled and therefore ₉₇ complete software environment can be migrated eas-₉₈ ily. While widespread in computer center operation this ₉₉ technique is rarely applied in HPC.

2.1 Computing at the University of Freiburg

The computer center at the University of Freiburg pro-105 vides medium scaled research infrastructures like cloud,106 storage, and especially HPC services adapted to the107 needs of various scientific communities. Significant stan-108 dardization in hardware and software is necessary for 109 the operation of compute systems comprised of more 110 than 1000 individual nodes with a small group of ad-111 ministrators.

The level of granularity of the software stack provided is not fine enough to directly support the requirements of world-wide efforts like the ATLAS or CMS experiments. Therefore, novel approaches are necessary to ensure optimal use of the system and to open the cluster to as many different use-cases as possible without increasing the operational effort. Transferring expertise from the operation of the established local private cloud, the use of <code>OpenStack</code> as a cloud platform has been identified as a suitable solution for NEMO. This approach provides a more flexible software deployment in addition to the existing software module system. The resulting challenges range from the automated creation of suitable virtual machines to their on-demand deployment and scheduling.

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 and consists currently of 900 nodes with 20 physical cores and 128 GiB of RAM each. Omni-Path [4] spans a high speed low latency network of 100 Gbit/s between nodes. The parallel storage is based on BeeGFS [5] with 768 TB capacity.

2.3 Separation of software environments

The file system of a virtual machine or VRE is a disk image presented as a single file. From the computer center's perspective this image is 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 researcher's perspective the VRE is an individual virtual node whose operating system, applications and configurations as well as certain hardware-level parameters, e.g. CPU and RAM, can be configured fully autonomously by the researcher.

To increase the flexibility in hosted software environments, the standard bare metal operation of NEMO is extended with a parallel installation of OpenStack components [6]. The NEMO cluster uses Adaptive's Workload Manager Moab [7] as a scheduler of compute jobs. OpenStack as well can schedule virtual machines on the same nodes and resources. To avoid overlap, it is necessary to define the master scheduler which decides the job assignment to the worker nodes. Both Moab and OpenStack are unaware that another scheduler exists within the cluster and there is no API which enables

them to communicate with each other. Since the major-160 ity of users still use the bare metal HPC cluster, Moab ish61 deployed as the primary scheduler. It allows for detailedh62 job description and offers sophisticated scheduling fea-163 tures like fair-share, priority-based scheduling, detailedh64 limits, etc. OpenStack's task is to schedule the virtualh65 machines, but Moab will initially start the VRE jobsh66 and the VRE job will instruct OpenStack to start the167 virtual machine on the reserved resources with the required flavor, i.e. the resource definition in OpenStack.

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When a VRE job is submitted to the NEMO clus-168 ter, Moab will first calculate the priority and the needed resources of the job and then inserts it into its queue.¹⁶⁹ When the job is in line for execution and the requested 170 resources are available, the job will start a script which¹⁷¹ then starts the VRE on the selected node within the re- 172 source boundaries. During the run-time of the VRE a¹⁷³ monitoring script regularly checks if the VRE is still¹⁷⁴ running and terminates the job when the VRE has¹⁷⁵ ended. When the job ends, OpenStack gets a signal to 176 terminate the virtual machine and the VRE job ends¹⁷⁷ as well. Neither Moab nor OpenStack have access inside178 the VRE, so they cannot assess if the VRE is actually 179 active or idle. The software package ROCED (described¹⁸⁰ in further detail in Section 4) has been introduced to¹⁸¹ solve this issue. It is used as a broker between different¹⁸² HPC schedulers, translating resources and monitoring¹⁸³ usage inside the virtual machine, as well as starting and stopping VRE images on demand.

3 Generation of the image

The VREs for ATLAS and CMS software environments 1887 consist in OpenStack containers in the format of compatible VM images. These images are provided in an automatized way allowing versioning and archiving of the environments captured in the images.

3.1 Packer combined with Puppet

One approach to generate the image is the open-source₁₉₇ tool Packer [8], interfaced to the system configuration₁₉₈ framework Puppet [10]. Packer allows to configure an₁₉₉ image based on an ISO image file using a kickstart [9] file and flexible script-based configuration. It also provides an interface to Puppet making it particularly con-200 venient if an existing Puppet role is to be used for the images. If the roles are defined according to the host-201 name of the machine as is conventional in Puppet with₂₀₂ Hieradata, the hostname needs to be set in the scripts₂₀₃ supplied to Packer. Propagation of certificates requires₂₀₄

an initial manual start of a machine with the same hostname to allow handshake signing of the certificate from the Puppet server.

Packer's interface to Puppet allows a fully automated image generation with up-to-date and version-controlled configuration. At the end of the generation run, the image is automatically transferred to the OpenStack image server.

3.2 Image generation using the Oz toolkit

Another option to employ a fully-automated procedure is to use the OZ toolkit [11]. All requirements and configuration options of an image can be specified through a XML template file. 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 created, it is automatically compressed and uploaded to a remote cloud site. 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 HPC systems with support for virtualized research environments and commercial cloud providers offer 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 capable of maintaining thousands of batch jobs. Some cloud providers, for example Amazon with AWS Batch [12], provide a service for workflow management, however 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

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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

Integration Adapters Requirement Adapters **ROCED Core** .. integrates booted compute nodes ... supplies information about needed into existing batch server **Broker** compute nodes, e.g. queue size **HTCondor HTCondor** decides which machines to boot or shutdown Torque Torque **Grid Engine Grid Engine SLURM SLURM** Site Adapters .. boot machines on various Cloud Computing sites Hybrid HPC Cluster **Commercial Providers** OpenStack

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.

KIT since 2010 [3]. ROCED is written in a modular fash-233 ion in python and the interfaces to batch systems and234 cloud sites are implemented as so-called *Adapters*. This₂₃₅ makes ROCED independent of specific user groups or₂₃₆ workflows. It provides a scheduling core which collects₂₃₇ the current requirement of computing resources and de-238 cides if virtual machines need to be started or can be239 stopped. One or more Requirement Adapters report the 240 current queue status of batch systems to the central241 scheduling core. Currently, Requirement Adapters are 242 implemented for the Slurm, Torque/Moab, HTCondor₂₄₃ and GridEngine batch systems. The Site Adapters allow₂₄₄ ROCED to start, stop, and monitor virtual machines on₂₄₅ multiple cloud sites. Implementations exist for Amazon₂₄₆ EC2, OpenStack, OpenNebula and Moab-based virtu-247 alization at HPC centers. Special care has been put into₂₄₈ the resilience of ROCED: it can automatically terminate249 non-responsive machines and restart virtual machines₂₅₀ in case some machines have dropped out. This allows₂₅₁ VM setups orchestrated by ROCED with thousands of 252 virtual machines and many tens of thousands of jobs to253 run in production environments. The modular design₂₅₄ of ROCED is shown in Fig. 1.

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4.2 Using HTCondor as front-end scheduler

The open-source project HTCondor provides a workload₂₅₇ management system which is highly configurable and₂₅₈ modular [13]. Batch processing workflows can be sub-₂₅₉ mitted and are then forwarded by HTCondor to idle₂₆₀

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 are available to connect from within isolated network zones, e.g. via a Network Address Translation Portal, to the central HTCondor pool. The Connection Brokering (CCB) service [14] 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 startd the HTCondor client pre-installed. 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.

4.3 Using SLURM as front-end scheduler

Alternatively to the approach described in the previous section, the open-source workload managing system Slurm [15] has been interfaced into ROCED by the ATLAS group at University of Freiburg. While Slurm

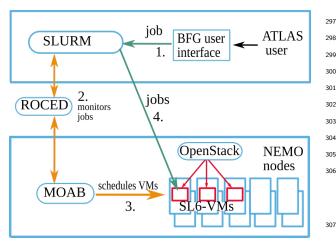


Fig. 2 Implementation of ROCED with Slurm on the BFG clus- $_{\rm 308}$ ter used by ATLAS researchers.

provides a built-in functionality for dynamic startup of presources in the *Slurm Elastic Computing* module [16], size this has been found to be unsuitable for resources which are not expected to be available within a fixed time pe-314 riod, 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 to the other, and therefore to the user, is very limited to the other, and therefore to the user, is very limited the Moab scheduler on the host system and the Slurm scheduler on the submission side.

The scheduling system is illustrated in Fig. 2. For₃₂₀ Slurm, it is necessary that each potential virtual ma-₃₂₁ chine is registered in the configuration at the time of₃₂₂ start of the Slurm server as well as the client. Slurm con-₃₂₃ figurations also need to be in agreement between server₃₂₄ and client. Therefore, a range of hostnames is registered₃₂₅ in the configuration in a way that is mapped to po-₃₂₆ tential IP addresses of virtual machines. These virtual₃₂₇ machines have a fixed number of CPUs and memory₃₂₈ assigned and are registered under a certain Slurm par-₃₂₉ tition. When a job is submitted to this partition and no₃₃₀ other resource is available, information from the Slurm₃₃₁ squeue and sinfo commands is requested and parsed₃₃₂ for the required information.

Since the ATLAS Freiburg group comprises three₃₃₄ sub-groups, each mapped to a different production ac-₃₃₅ count on NEMO, special care is taken to avoid interfer-₃₃₆ ence of resources used by another account to ensure fair₃₃₇ share on NEMO, while allowing jobs from one group to₃₃₈ occupy otherwise idle resources of another group.

ROCED determines the amount of virtual machines $_{340}$ to be started and sends the corresponding VRE job $_{341}$ submission commands to Moab. After the virtual ma- $_{342}$ chine has booted, the hostname is set to the IP de- $_{343}$

pendent 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 released and can be reused by future VREs.

5 Analysis of performance and usage

This approach has been implemented and put into production by the research groups at the University of Freiburg (Institute of Physics) and the Karlsruhe Institute of Technology (Institute of Experimental Particle Physics). The following section presents the statistical analysis of the performance of the virtualized setup both in terms of CPU benchmarks and usage statistics.

5.1 Benchmarks

Alongside the legacy HEP-SPEC06 (HS06) benchmark [17], the performance of the compute resources is furthermore evaluated with the ATLAS Kit Validation KV [20], a fast benchmark developed to provide real-time information of the WLCG performance and available in the CERN benchmark suite [18]. The KV benchmark is making use of the simulation toolkit GEANT4 [21] to simulate the interactions of single muon events in the detector of the ATLAS experiment and provides as ouput the number of events produced per second. As our primary target is to measure performances of CPUs in the context of High Energy Physics applications, the KV benchmark constitutes a realistic workload.

To assess the impact of the virtualization, the performance of the same hardware configuration (20 cores Intel Xeon E5-2630 CPUs) has been determined either deployed via the standard bare metal operation on the NEMO cluster (NEMO bare metal) and on the ATLAS Tier-3 center in Freiburg (ATLAS Tier-3 bare metal), or as virtual machines on the NEMO cluster (NEMO VM). On the ATLAS Tier-3 bare metal and on the virtual machines running on the NEMO cluster, hyperthreading (HT) technology is activated. Both are using Scientific Linux 6 [22] as operating system. The NEMO bare metal has no HT activated due to the more general use case of the system, and uses CentOS7 as operating system [23]. The scores of the HEP-SPEC06 and KV

benchmarks have been determined for these three configurations as a function of the number of cores actually used by the benchmarking processes. This number ranges from 2 to 40 for the ATLAS Tier-3 bare metal and for the NEMO VM, for which HT is enabled, and from 2 to 20 for the NEMO bare metal, for which HT is not implemented. The benchmarks have been run 20 times for each core multiplicity value, and the means and standard deviations of the corresponding distributions have been extracted.

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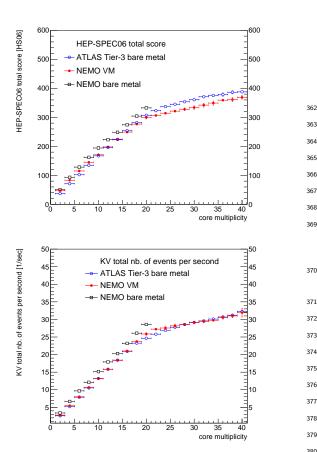


Fig. 3 Total score as a function of the core multiplicity for the HEP-SPEC06 (top) and KV (bottom) benchmarks for the ATLAS Tier-3 bare metal (blue open circles), the NEMO382 VMs (red full circles) and the NEMO bare metal (black open383 squares). The data points represent the average values of the benchmarks for each core multiplicity, and the vertical bars show the associated standard deviations.

The HEP-SPEC06 and KV results are presented in 1888 Figure 3 for the three configurations considered. The 389 total scores of the two benchmarks are increasing un-390 til the maximum number of physical cores has been 1991 reached, and are characterized by a flattening increase 2992 afterwards. The scores of the virtual machines running 393 on the NEMO cluster are only slightly lower than those 394

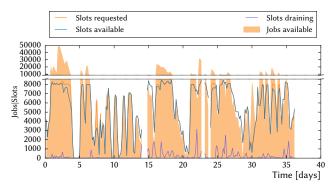


Fig. 4 Utilization of the shared HPC system by booted virtual machines. Up to 9000 virtual cores were in use at peak times. The fluctuations in the utilization reflects the patterns of the submission of jobs by our institute users. The number of draining slots displays the amount of job slots still processing jobs while the rest of the node's slot are already empty.

obtained for the NEMO bare metal, and the loss of performance due to the virtualization does not exceed 10%. For the VMs running on the NEMO cluster and the ATLAS Tier-3 bare metal, the interplay between the virtualization and the different operating systems leads to very similar scores for the two configurations, particularly for the KV benchmark, and the loss of performance is smaller than 10% as well.

5.2 Usage statistics

Fig. 4 shows the utilization of virtual machines which were orchestrated by ROCED depending on the resource demands of the users of the KIT group. At peak times, up to 9000 virtual cores were filled with user jobs, consuming more than a half of the initial 16000 NEMO cores.

The usage of the hybrid cluster model is presented in Fig. 5. 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 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 required scientific 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

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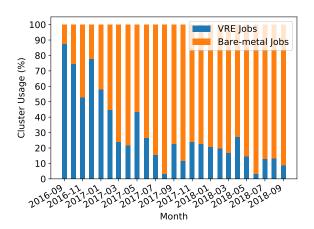


Fig. 5 Usage of the NEMO cluster in the time between 440 September 2016 to June 2018. The blue bars indicate the us- $^{1.3}_{441}$ age by jobs running directly in the hosts' operating system, $_{_{442}}$ while the orange bars are jobs running in virtual machines.

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446 are not forced to use VREs and therefore could $\operatorname{run}_{447}^{-1}$ bare-metal jobs as well.

6 Conclusions and Outlook

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A system for the dynamic, on-demand provisioning of 454 virtual machines to run jobs in a high energy physics455 context on an external, not dedicated resource as ${\rm re}^{\scriptscriptstyle -456}$ alized at the HPC cluster NEMO at the University of $_{458}^{--}$ Freiburg has been described. An interface between the 459 schedulers of the host system and the external system⁴⁶⁰ from which requests are sent is needed to monitor and $^{461}\,$ steer jobs in a scalable way. This is implemented in $_{\scriptscriptstyle 463}^{-}$ the ROCED package which is deployed for the described₄₆₄ use-cases. This approach can be generalized to other⁴⁶⁵ platforms and possibly also other forms of virtualized $^{466}\,$ environments (e.g. containers).

The CPU performance and usage of the setup have469 been analyzed. The expected performance loss due to $^{\!470}$ the virtualization has been found to be sufficiently small 471 to be compensated by the added flexibility and other $_{473}$ benefits of this setup.

A possible extension of such a virtualized setup is⁴⁷⁵ the provisioning of functionalities for snapshots and mi- $^{476}\,$ gration of jobs. This would facilitate the efficient inte-478 gration of long-running monolithic jobs into HPC clus-479

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