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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 of the WLCG 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 · Particle Physics · Grid Computing · Benchmarks · Opportunistic Usage

1 Introduction

Particle physics experiments at the Large Hadron Collider (LHC) need a great quantity of computing re-

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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 requirement, High Performance Computing (HPC) re- 73 sources provided by research institutions can be useful 74 supplements to the existing World-wide LHC Comput- 75 ing Grid (WLCG) [2] resources allocated by the collab- 76 orations.

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This paper presents the concepts and implementa-78 tion of providing a HPC resource, the shared research 79 cluster NEMO [3] at the University of Freiburg, to AT-80 LAS and CMS users accessing external clusters connected to the WLCG with the purpose of accommodating data production as well as data analysis on the HPC 11 host system. The HPC cluster NEMO at the University of Freiburg is deploying an OpenStack [4] instance to 182 handle the virtual machines. The challenge is in pro-183 visioning, setup, scheduling, and decommissioning the 184 virtual research environments (VRE) dynamically and 185 according to demand. For this purpose, the schedulers 186 on NEMO and on the external resources are connected 187 through the Roced service [5].

A VRE in the context of this paper is a complete ⁸⁹ software stack as it would be installed on a compute ⁹⁰ cluster fitted to the demands of ATLAS or CMS workloads.

2 Virtualization infrastructure

Hardware virtualization has become mainstream tech-⁹⁴ nology over the last decade as it allows both to host ⁹⁵ more than one operating system on a single server and ⁹⁶ to strictly separate users of software environments. Hard⁹⁷ ware and software stacks are decoupled and therefore ⁹⁸ complete software environment can be migrated across ⁹⁹ hardware boundaries. While widespread in computer¹⁰⁰ center operation this technique is rarely applied in HPC.¹⁰¹

2.1 Computing at the University of Freiburg

The computer center at the University of Freiburg pro-106 vides medium scaled research infrastructures like cloud,107 storage, and especially HPC services adapted to the108 needs of various scientific communities. Significant stan-109 dardization in hardware and software is necessary for 110 the operation of compute systems comprised of more 111 than 1000 individual nodes combined with a small group 12 of administrators.

The level of granularity of the software stack pro-114 vided is not fine enough to directly support the require-115 ments of world-wide efforts like the ATLAS or CMS ex-116 periments. Therefore, novel approaches are necessary to 117

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 user defined 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 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 [6] spans a high speed low latency network of 100 Gbit/s between nodes. The parallel storage is based on BEEGFS [7] 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 within agreed upon limits.

To increase the flexibility in hosted software environments, the standard bare metal operation of NEMO is extended with an installation of OpenStack components [8]. The NEMO cluster uses Adaptive's Workload Manager Moab [10] as a scheduler of compute jobs. OpenStack as well can schedule virtual machines on the same nodes and resources. To avoid conflicts, 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 majority of users still use the bare metal HPC cluster, Moab is deployed as the primary scheduler. It allows for detailed job description and offers sophisticated schedul-

ing features like fair-share, priority-based scheduling,165 detailed time limits, etc. OpenStack's task is to deploy166 the virtual machines, but Moab will initially start the167 VRE jobs and the VRE job will instruct OpenStack168 to start the virtual machine on the reserved resources169 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-170 ter, Moab will first calculate the priority and the needed resources of the job and then inserts it into its queue.¹⁷¹ When the job is in line for execution and the requested¹⁷² resources are available, the job will start a script which¹⁷³ then starts the VRE on the selected node within the re-174 source boundaries. During the run-time of the VRE a¹⁷⁵ monitoring script regularly checks if the VRE is $still^{176}$ running and terminates the job when the VRE has¹⁷⁷ ended. When the job ends, OpenStack gets a signal to¹⁷⁸ terminate the virtual machine and the VRE job ends¹⁷⁹ as well. Neither Moab nor OpenStack have access inside 180 the VRE, so they cannot assess if the VRE is actually¹⁸¹ busy or idle. The software package Roced (described¹⁸² in further detail in Section 4) has been introduced to 183 solve this issue. It is used as a broker between different¹⁸⁴ HPC schedulers, translating resources and monitoring¹⁸⁵ usage inside the virtual machine, as well as starting and stopping VRE images on demand.

3 Generation of the VRE image

The VREs for ATLAS and CMS software environments 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

A reasonable approach to generate the image is the 199 open-source tool Packer [11], interfaced to the system 200 configuration framework Puppet [13]. Packer allows to 201 configure an image based on an ISO image file using a kickstart [12] file and flexible script-based configuration. It also provides an interface to Puppet making it 202 particularly convenient if an existing Puppet role is to be used for the images. If the roles are defined accord-203 ing to the hostname of the machine as is conventional in 204 Puppet with Hieradata, the hostname needs to be set205 in the scripts supplied to Packer. Propagation of cer-206 tificates requires an initial manual start of a machine 207 with the same hostname to allow handshake signing of 208 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 Open-Stack image server.

3.2 Image generation using the Oz toolkit

Another option to employ a fully-automated procedure is to use the Oz toolkit [14]. 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 [15], 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.

$4.1~{\tt Roced}$

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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 KIT since 2010 [5]. 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

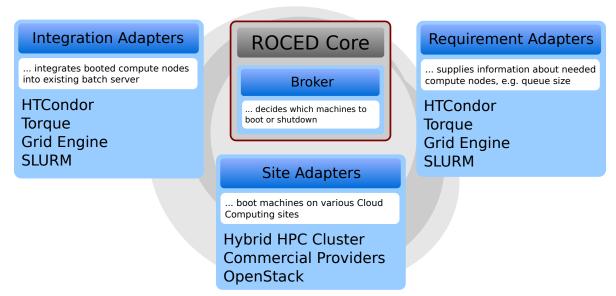


Fig. 1 Overview of the Roced modular design. The Roced Core contains the Broker which decides when and on which sites new virtual machines are booted. The Requirement Adapters report about the utilization and resource requirements of the attached batch systems. The Site Adapter is responsible to manage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

makes Roced independent of specific user groups or₂₃₈ workflows. It provides a scheduling core which collects239 the current requirement of computing resources and de-240 cides if virtual machines need to be started or can be241 stopped. One or more Requirement Adapters report the242 current queue status of batch systems to the central243 scheduling core. Currently, Requirement Adapters are244 implemented for the Slurm, Torque/Moab, HTCondor₂₄₅ and GridEngine batch systems. The Site Adapters allow₂₄₆ Roced to start, stop, and monitor virtual machines on₂₄₇ multiple cloud sites. Implementations exist for Amazon₂₄₈ EC2, OpenStack, OpenNebula and Moab-based virtu-249 alization at HPC centers. Special care has been put into250 the resilience of Roced: it can automatically terminate₂₅₁ non-responsive machines and restart virtual machines₂₅₂ in case some machines have dropped out. This allows₂₅₃ VM setups orchestrated by Roced with thousands of 54 virtual machines and many tens of thousands of jobs to₂₅₅ run in production environments. The modular design₂₅₆ of Roced is shown in Fig. 1.

4.2 Using HTCondor as front-end scheduler

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The open-source project HTCondor provides a workload₂₅₉ management system which is highly configurable and₂₆₀ modular [16]. Batch processing workflows can be sub-₂₆₁ mitted and are then forwarded by HTCondor to idle₂₆₂ resources. HTCondor maintains a resource pool, which₂₆₃ worker nodes in a local or remote cluster can join. Once₂₆₄ HTCondor has verified the authenticity and features of₂₆₅

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 [17] 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 VRE for CMS contains the HTCondor client startd. This client is started after the machine has fully booted and connects to the central HTCondor pool at 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 above, the open-source workload managing system Slurm [18] has been interfaced into Roced by the ATLAS group at University of Freiburg. Slurm provides a built-in functionality for the dynamic startup of resources in the Slurm Elastic Computing module [19]. However, this module is based on the assumption of a fixed maximum startup time of the machines. In the considered case, due to the

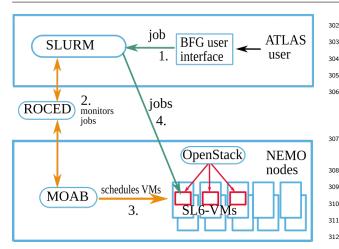


Fig. 2 Implementation of Roced with Slurm on the BFG clus- 313 ter used by ATLAS researchers.

queue in the host system, the start of a resource can be delayed by a significant, varying time period. In addi-316 tion the transfer of information, such as error states, from one scheduler to the other, and therefore to the 317 user, is very limited. Therefore, Roced has been chosen 318 as the interface between the Moab scheduler on the host 319 system and the Slurm scheduler on the submission side.320

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The scheduling system is illustrated in Fig. 2. For₃₂₁ Slurm, it is necessary that each potential virtual ma-₃₂₂ chine is registered in the configuration at the time of₃₂₃ start of the Slurm server as well as the client. Slurm con-₃₂₄ figurations also need to be in agreement between server₃₂₅ and client. Therefore, a range of hostnames is registered₃₂₆ in the configuration in a way that is mapped to po-₃₂₇ tential IP addresses of virtual machines. These virtual₃₂₈ machines have a fixed number of CPUs and memory₃₂₉ assigned and are registered under a certain Slurm par-₃₃₀ tition. When a job is submitted to this partition and no₃₃₁ other resource is available, information from the Slurm₃₃₂ squeue and sinfo commands is requested and parsed₃₃₃ for the required information.

Since the ATLAS Freiburg group comprises three₃₃₅ sub-groups, each mapped to a different production ac-₃₃₆ count on NEMO, special care is taken to avoid interfer-₃₃₇ ence of resources used by another account to ensure fair₃₃₈ share on NEMO, while allowing jobs from one group to₃₃₉ occupy otherwise idle resources of another group.

Roced determines the amount of virtual machines341 to be started and sends the corresponding VRE job342 submission commands to Moab. After the virtual ma-343 chine has booted, the hostname is set to the IP de-344 pendent name which is known to the Slurm configura-345 tion. A cron job executes several sanity checks on the346 system. Upon successful execution of these tests, the347 Slurm client running in the VM starts accepting the348 queued jobs. After completion of the jobs and a cer-349

tain 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

The ROCED-based solution described above 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). To prove the usefulness of this approach statistical analyses of the performance of the virtualized setup both in terms of CPU benchmarks and usage statistics have been conducted.

5.1 Benchmarks

Benchmark tests are performed with the primary goal to measure the performance of the CPU for High Energy Physics applications. Alongside the legacy HEP-SPEC06 (HS06) benchmark [20], the performance of the compute resources is furthermore evaluated with the ATLAS Kit Validation KV [23], a fast benchmark developed to provide real-time information of the WLCG performance and available in the CERN benchmark suite [21]. The primary target is to measure the performance of the CPU for High Energy Physics applications. The KV benchmark is making use of the simulation toolkit GEANT4 [24] to simulate the interactions of single muon events in the detector of the ATLAS experiment and provides as outut the number of events produced per second. It constitutes a realistic workload for High Energy Physics jobs.

To assess the impact of the virtualization, the performance of the identical 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, hyper-threading (HT) technology is activated. Both are using Scientific Linux 6 [25] as the operating system. On the cluster NEMO bare metal jobs are restricted to 20 cores by cgroups, since the application mix is broader than on HEP clusters. The operating system is CentOS7 [26]. The scores of the HEP-SPEC06 and KV benchmarks have been determined for these three

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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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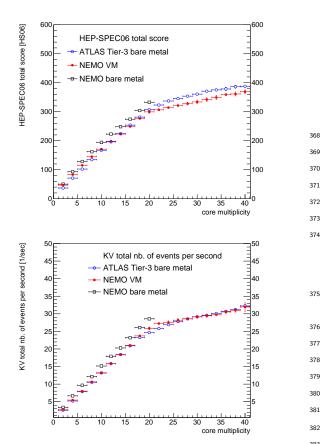


Fig. 3 Total score as a function of the core multiplicity for the HEP-SPEC06 (top) and KV (bottom) benchmarks for the ATLAS Tier-3 bare metal (blue open circles), the NEMO385 VMs (red full circles) and the NEMO bare metal (black openses squares). The data points represent the average values of the $_{387}$ benchmarks for each core multiplicity, and the vertical bars show the associated standard deviations.

The HEP-SPEC06 and KV results are presented in₃₉₁ Figure 3 for the three configurations considered. The₃₉₂ total scores of the two benchmarks are increasing un-393 til the maximum number of physical cores has been394 reached, and are characterized by a flattening increase₃₉₅ afterwards. The scores of the virtual machines running396 on the NEMO cluster are only slightly lower than those 397 obtained for the NEMO bare metal, and the loss of 398

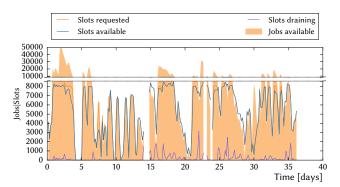


Fig. 4 Utilization of the shared HPC system by booted virtual machines. Up to 9000 virtual cores were in use at peak times. The fluctuations in the utilization reflects the patterns of the submission of jobs by the CMS users at the physics institute in Karlsruhe. The number of draining slots displays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

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 migrate from other ressources. 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.

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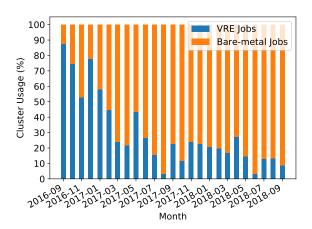


Fig. 5 Estimated usage of the NEMO cluster in the time 44 from September 2016 to September 2018. The blue bars indi-45 cate the usage by jobs running directly in the hosts' operating 45 system, while the orange bars are jobs running in virtual machines. The decrease of VRE jobs is partially explained by an 48 increasing number of bare metal jobs submitted.

6 Conclusions and Outlook

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A novel system for the dynamic, on-demand provision-455 ing of virtual machines to run jobs in a high energy₄₅₇ physics context on an external, not dedicated resource₄₅₈ as realized at the HPC cluster NEMO at the Univer-459 sity of Freiburg has been implemented. An interface⁴⁶⁰ between the schedulers of the host system and the ex-462 ternal system from which requests are sent is needed to₄₆₃ monitor and steer jobs in a scalable way. For this work-464 flow the cloud meta-scheduler Roced has been imple-465 mented and deployed for the described use-cases. The₄₆₇ approach can be adapted to work with other platforms₄₆₈ and could be extended to container technologies like⁴⁶⁹ Singularity [9].

The CPU performance and usage of the setup have₄₇₂ been analyzed for the job execution environment. The⁴⁷³ expected performance loss due to the virtualization has⁴⁷⁴ been found to be sufficiently small to be compensated⁴⁷⁵ by the added flexibility and other benefits of this setup.⁴⁷⁷

A possible extension of such a virtualized setup is 478 the provisioning of functionalities for snapshots and mi- 479 gration of jobs. This would facilitate the efficient inte- 481 gration of long-running monolithic jobs into HPC clus- 482 ters.

The provided solution extends the available com-455 pute ressources for HEP calculations and could be one486 possibilitly to cope with new data from the upcom-487 ing High-Luminosity upgrade of the LHC. Since HEP⁴⁸⁸ VREs are perfect for backfilling this could be used on₄₉₀ various cluster ressources.

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