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

Felix Bührer1 · Frank Fischer4 · Georg Fleig4 · Anton Gamel1,3 · Manuel Giffels4 · Thomas Hauth4 · Michael Janczyk3 · Konrad Meier3 · Günter Quast4 · Benoît Roland1 · Ulrike Schnoor1,2 · Markus Schumacher1 · Dirk von Suchodoletz3 · Bernd Wiebelt3

Received: 8 November 2018 / Accepted: 19 April 2019 / Published online: 24 May 2019
© Springer Nature Switzerland AG 2019

Abstract
A setup for dynamically providing resources of an external, non-dedicated cluster to researchers of the ATLAS and CMS experiments in the WLCG environment is described as it has been realized at the NEMO High Performance Computing cluster at the University of Freiburg. Techniques to provide the full WLCG software environment in a virtual machine image are described. The interplay between the schedulers for NEMO and for the external clusters is coordinated through the R0C0ED 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

Introduction
Particle physics experiments at the Large Hadron Collider (LHC) need a great quantity of computing resources for data processing, simulation, and analysis. This demand will be growing with the upcoming High-Luminosity upgrade of the LHC [1]. To help fulfill this requirement, High Performance Computing (HPC) resources provided by research institutions can be useful supplements to the existing World-wide LHC Computing Grid (WLCG) [2] resources allocated by the collaborations.

This paper presents the concepts and their implementation for providing a HPC resource, the shared research cluster NEMO [3] at the University of Freiburg, to ATLAS 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 host system. The NEMO cluster deploys an OpenStack [4] instance to handle the virtual machines. The challenge is in dynamically provisioning, setting up, scheduling, and decommissioning the virtual research environments (VRE) according to demand. For this purpose, the schedulers on NEMO and on the external resources are connected through the R0C0ED service [5].

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.

Virtualization Infrastructure
Hardware virtualization has become mainstream technology over the last decade as it allows to host more than one operating system on a single server and to strictly separate users of different software environments. Hardware and software stacks are decoupled, such that complete software environments can be migrated across hardware boundaries. While widespread in computer center operation this technique is rarely applied in HPC.

* Ulrike Schnoor
ulrike.schnoor@cern.ch
1 Universität Freiburg, Physikalisches Institut, Hermann-Herder-Str. 3, 79104 Freiburg, Germany
2 Present Address: CERN, CH-1211 Geneva 23, Switzerland
3 Universität Freiburg, Rechenzentrum, Hermann-Herder-Str.10, 79104 Freiburg, Germany
4 Karlsruher Institut für Technologie, Institut für Experimentelle Teilchenphysik, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany
Computing at the University of Freiburg

The computer center at the University of Freiburg provides medium scale research infrastructures such as cloud, storage, and especially HPC services adapted 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 by a small group of administrators.

To support complete research environments which are required by world-wide efforts such as the ATLAS or CMS experiments, 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 OpenStack as a cloud platform has been identified as a suitable solution for NEMO. This approach makes possible the deployment of a user-defined software stack in addition to the environment modules [6] solution, which allows, on a per-user basis, to choose specific versions of given software packages. The resulting challenges range from the automated creation of suitable virtual machines to their on-demand deployment and scheduling.

Research Cluster NEMO

The research cluster NEMO is a cluster for research in the federal state of Baden-Württemberg in the scientific fields of Elementary Particle Physics, Neuroscience and Microsystems Engineering. Operation started on August 1, 2016. It currently consists of 900 nodes with 20 physical cores and 128 GiB of RAM each. Omni-Path [7] provides a high-speed, low-latency network of 100 Gbit/s between nodes. The parallel storage has 768 TB of usable capacity and is based on BeeGFS [8].

A pre-requisite to execute a VRE is the efficient provisioning of data which has to cross institutional boundaries in the CMS use-case. A significant bandwidth is needed to transfer the input data into the VRE from the storage system at the Karlsruhe Institute of Technology (KIT) and to store back the results. The NEMO cluster is connected with two 40 Gbit/s links to the main router of the University of Freiburg which itself is linked to the network of scientific institutions in Baden-Württemberg, BelWü, at 100 Gbit/s.

Separation of Software Environments

The file system of a 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 [9]. The NEMO cluster uses Adaptive’s Workload Manager Moab [11] 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 scheduling features such as fair-share, priority-based scheduling, and detailed time limits. OpenStack’s task is to deploy 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 with the required flavor, i.e. according to the resource definition in OpenStack.

A VRE job is like any other bare-metal job. When a VRE job is submitted to the NEMO cluster, Moab first calculates the priority and the needed resources of the job and then inserts it into its queue. If the VRE job is in line for execution and the requested resources are available, the job runs a script which starts the VRE (a virtual machine in our case) on the selected node within the resource boundaries. This can be compared to a bare-metal job script starting a scientific software. By means of a monitoring script, the VRE job is aware of the running state of the virtual machine and can therefore terminate itself when the virtual machine has shut down. If on the contrary the VRE job ends while the virtual machine is still running, e.g. because it has hit its wall time limit, OpenStack is notified and terminates the virtual machine. Neither Moab nor OpenStack have access inside the VRE, so they cannot assess if the VRE is actually busy or idle. The software package RUCED (described in further detail in “Interfacing Batch Systems and Virtual Resources Using RUCED”) has been introduced to solve this issue. It is used as a broker between different HPC schedulers, translating resources and monitoring usage inside the virtual machine, as well as starting and stopping VRE images on demand.
**Generation of the VRE Image**

The VREs for ATLAS and CMS software environments consist in OpenStack compatible VM images. These virtual machines are provided in an automated way allowing versioning and archiving of the environments captured in the images.

**Packer Combined with Puppet**

One approach to generate the image is the open-source tool Packer [12], interfaced to the system configuration framework Puppet [14]. Packer allows to configure an image based on an ISO image file using a kickstart [13] file and flexible script-based configuration. It also provides an interface to Puppet making it particularly convenient 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 Hiera, the hostname needs to be set in the scripts supplied to Packer. Propagation of certificates requires 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 transferred to the OpenStack image server.

**Image Generation Using the Oz Toolkit**

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

**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 [16], provide a service for workflow management, however, these offers 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-scalable batch system and a virtual machine scheduler is desirable.

**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 [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 makes ROCED independent of specific user groups or workflows. 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/Moab, 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 have 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. The modular design of ROCED is shown in Fig. 1.

**Using HTCondor as Front-End Scheduler**

The open-source project HTCondor provides a workload management system which is highly configurable and modular [17]. 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 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 [18] 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 CMS group at the KIT is using HTCondor for scheduling the jobs to be submitted to NEMO. 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.

**Using Slurm as Front-End Scheduler**

Alternatively to the approach described above, the open-source workload managing system Slurm [19] has been interfaced into ROCED by the ATLAS group at the University of Freiburg. Slurm provides a built-in functionality for the dynamic startup of resources in the Slurm Elastic Computing module [20]. However, this module is based on the assumption of a fixed maximum startup time of the machines. In the considered case, due to the queue in the host system, the start of a resource can be delayed by a significant, varying time period. In addition the transfer of information, such as error states, from one scheduler to the other, and therefore to the user, is 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.

The scheduling system is illustrated in Fig. 2. 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 assigned 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 subgroups, each mapped to a different production account on NEMO, special care is taken to avoid interference of resources used by another account to ensure fair share on NEMO, while nevertheless allowing jobs from one group to occupy otherwise idle resources of another group.

ROCED determines the amount of virtual machines 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 released and can be reused by future VREs.

Analysis of Performance and Usage

The RUCED-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 KIT (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.

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 [21], 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 [22]. 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 output 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 NEMO cluster, bare-metal jobs are restricted to 20 cores, which was chosen to accommodate all use cases. The operating system is CentOS7 [26]. 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.

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

**Usage Statistics**

Figure 4 shows the utilization of virtual machines which were orchestrated by RöCED 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 16,000 NEMO cores. Due to the wall-time limitation at NEMO, RöCED is going to drain virtual machines before hitting the limit. Draining job slots do not accept new jobs, while already started ones potentially still occupy parts of the nodes in draining mode, which can lead to an overall efficiency degradation. One counter measure is to utilize those nodes in a so called backfilling mode by taking into account the remaining wall-time and to assign short running jobs to the concerned nodes.

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 set of worker nodes running virtualized jobs changes dynamically from job to job, since the VREs are started by a standard bare-metal job.

Initially almost the whole NEMO cluster was available to the CMS users, since they could already profit from their VRE being deployed while other users had to wait for the installation of specific scientific software. This explains the high usage by VREs in the first months of operation. As more and more software became available for bare-metal usage the fraction of bare-metal jobs started to increase and correspondingly the fraction of VRE jobs decreased. At the same time, the CMS group at KIT also gained access to other opportunistic resources which were handled by the KIT RöCED instance as well. Due to the longer queue on NEMO, the other resources were preferred by RöCED, and therefore the total number of VRE jobs from the CMS group on NEMO decreased.

![Fig. 4](image-url) 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.

![Fig. 5](image-url) Estimated usage of the NEMO cluster in the time from September 2016 to September 2018. The orange bars indicate the usage by jobs running directly in the hosts’ operating system, while the blue bars are jobs running in virtual machines. The decrease of VRE jobs is partially explained by an increasing number of bare metal jobs submitted.
Conclusions and Outlook

A novel 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 the University of Freiburg has been implemented. An interface between the schedulers of the host system and the external systems from which requests are sent is needed to monitor and steer jobs in a scalable way. This interface has been provided by the deployment of the cloud meta-scheduler ROCED. The approach can be adapted to work with other platforms and could be extended to container technologies like Singularity [10].

The CPU performance and usage of the setup have been analyzed for the job execution environment. The expected performance loss due to the virtualization has been found to be sufficiently small to be compensated by the added flexibility and other benefits of this setup.

A possible extension of such a virtualized setup is the provisioning of functionalities for snapshots and migration of jobs. This would facilitate the efficient integration of long-running monolithic jobs into HPC clusters.

The provided solution extends the available compute resources for HEP calculations and could be one possibility to cope with new data from the upcoming High-Luminosity upgrade of the LHC. Since HEP VREs are perfect for backfilling this could be used on various cluster resources.

Acknowledgements This research is supported by the Ministry of Science, Research and the Arts Baden-Württemberg through the bwHPC grant and by the German Research Foundation (DFG) through grant no INST 39/963-1 FUGG for the bwForCluster NEMO. The work of F.B. and T.H. was supported by the Virtual Open Science Collaboration Environment (ViCE) project MKW 34-7547.221 funded by the Ministry of Science, Research and the Arts Baden-Württemberg. The work of U.S. was supported by the Federal Ministry of Education and Research within the project 05H15VFCA1 “Untersuchung von Proton-Proton-Wechselwirkungen im ATLAS-Experiment am Large Hadron Collider” in the framework of “Verbundprojekt 05H2015 - Physik bei höchsten Energien mit dem ATLAS-Experiment am LHC (BMBF-FSP 103)”. The work of T.H. was supported by the Federal Ministry of Education and Research within the project 05H15VKCCA “Physik bei höchsten Energien mit dem CMS-Experiment am LHC”.

References

1. ATLAS Collaboration (2018) Estimation of ATLAS computing needs vs predictable increase on a flat budget. ATLAS Public results https://twiki.cern.ch/twiki/pub/AtlasPublic/ComputingAndSoftwarePublicResults/cpuHLLHC.pdf. Accessed 19 Sept 2018
2. Eck C et al (2005) LHC computing grid: technical design report. CERN-LHCC-2005-024
3. bwForCluster NEMO https://www.hpc.uni-freiburg.de/nemo. Accessed 20 Oct 2018
4. OpenStack: open source cloud computing software. https://www.openstack.org/. Accessed 03 July 2018
5. ROCED cloud meta-scheduler project website. https://github.com/roced-scheduler/ROCED. Accessed 03 July 2018
6. Environment modules open source project, environment modules. http://modules.sourceforge.net. Accessed 07 Feb 2019
7. Intel (2015) Omni-Path: intel architects high performance computing system designs to bring power of supercomputing mainstream. https://newsroom.intel.com/news-releases/intel-architects-high-performance-computing-system-designs-to-bring-power-of-super-computing-mainstream. Accessed 20 Sept 2018
8. BeeGFS parallel cluster file system. https://www.beevfs.io/content/. Accessed 20 Sept 2018
9. von Suchodoletz D, Wiebelt B, Meier K, Janczyk M (2016) Flexible HPC: bwForCluster NEMO, proceedings of the 3rd bwHPC-symposium
10. Janczyk M, Wiebelt B, von Suchodoletz D (2017) Virtualized research environments on the bwForCluster NEMO, proceedings of the 4th bwHPC symposium
11. Adaptive Computing Moab. http://www.adaptivecomputing.com/moab-hpc-basic-edition/. Accessed 03 July 2018
12. Packer: tool for creating machine and container images for multiple platforms from a single source configuration. https://www.packer.io/. Accessed 03 July 2018
13. Redhat: Kickstart. https://access.redhat.com/documentation/en-us/red_hat_enterprise_linux/5/html/installation_guide/ch-startkickstart2. Accessed 03 July 2018
14. Puppet Enterprise. IT automation for cloud, security, and DevOps. https://puppet.com/. Accessed 03 July 2018
15. Oz image generation toolkit. https://github.com/clalancette/oz. Accessed 03 July 2018
16. Amazon AWS Batch https://aws.amazon.com/batch/. Accessed 03 July 2018
17. HTCondor workload manager https://research.cs.wisc.edu/htcondor/. Accessed 03 July 2018
18. HTCondor Connection Brokering http://research.cs.wisc.edu/htcondor/manual/v8.6/3_9Networking_includes.html. Accessed 03 July 2018
19. Slurm workload manager https://slurm.schedmd.com. Accessed 03 July 2018
20. Slurm Elastic Computing https://slurm.schedmd.com/elastic_computing.html. Accessed 03 July 2018
21. HEPiX Benchmarking Working Group: https://twiki.cern.ch/twiki/bin/view/Physics/Atlas/PerformanceTesting and http://hepix.org/benchmarking.html. Accessed 29 Jan 2018
22. Alef M et al (2017) Benchmarking cloud resources for HEP. J Phys Conf Ser 898(9):092056. https://doi.org/10.1088/1742-6596/898/9/092056
23. De Salvo A, Brasolin F (2010) Benchmarking the ATLAS software through the kit validation engine. J Phys Conf Ser 219(2010):042037. https://doi.org/10.1088/1742-6596/219/4/042037
24. Agostinelli S et al (2003) GEANT4: a simulation toolkit. Nucl Instrum Meth A 506:250. https://doi.org/10.1016/S0168-9002(03)01368-8
25. Fermilab and CERN, Scientific Linux 6. http://www.scientificlinux.org/. Accessed 03 Nov 2018
26. The CentOS Project, CentOS Linux 7. https://www.centos.org/. Accessed 03 Nov 2018

Publisher’s Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.