User Managed Virtual Clusters in Comet

Rick Wagner, Philip Papadopoulos,
Dmitry Mishin, Trevor Cooper,
Mahidhar Tatineti
San Diego Supercomputer Center UCSD
9500 Gilman Drive #0505
La Jolla, CA 92093-0505 USA
rpwagner@sdsc.edu, phil@sdsc.edu,
dmishin@sdsc.edu, tcooper@sdsc.edu

Gregor von Laszewski, Fugang Wang, Geoffrey C. Fox Indiana University 919 E. 10th Street Bloomington, IN 47408 Iaszewski@gmail.com, kevinwangfg@gmail.com

ABSTRACT

Hardware virtualization has been gaining a significant share of computing time in the last years. Using virtual machines (VMs) for parallel computing is an attractive option for many users. A VM gives users a freedom of choosing an operating system, software stack and security policies, leaving the physical hardware, OS management, and billing to physical cluster administrators. The well-known solutions for cloud computing, both commercial (Amazon Cloud, Google Cloud, Yahoo Cloud, etc.) and open-source (OpenStack, Eucalyptus) provide platforms for running a single VM or a group of VMs. With all the benefits, there are also some drawbacks, which include reduced performance when running code inside of a VM, increased complexity of cluster management, as well as the need to learn new tools and protocols to manage the clusters.

At SDSC, we have created a novel framework and infrastructure by providing virtual HPC clusters to projects using the NSF sponsored *Comet* supercomputer. Managing virtual clusters on *Comet* is similar to managing a baremetal cluster in terms of processes and tools that are employed. This is beneficial because such processes and tools are familiar to cluster administrators. Unlike platforms like AWS, *Comet*'s virtualization capability supports installing VMs from ISOs (i.e., a CD-ROM or DVD image) or via an isolated management VLAN (PXE). At the same time, we're helping projects take advantage of VMs by providing an enhanced client tool for interaction with our management system called Cloudmesh client. Cloudmesh client can also be used to manage virtual machines on OpenStack, AWS, and Azure.

The article describes our design and approach to running virtual clusters, the tools we developed, and initial user experience.

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than ACM must be honored. Abstracting with credit is permitted. To copy otherwise, or republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee. Request permissions from permissions@acm.org.

**XSEDE16, July 17-21, 2016, ,

© 2016 ACM. ISBN 978-1-4503-4755-6/16/07...\$15.00 DOI: http://dx.doi.org/10.1145/2949550.2949555

CCS Concepts

•Computer systems organization \rightarrow Parallel architectures; •Software and its engineering \rightarrow Virtual machines;

Keywords

Virtual machine; Supercomputer;

1. INTRODUCTION

The national cyberinfrastructure trends supported by the National Science Foundation includes two important classes. The first is the tradition support of large scale parallel computing needs by sophisticated scientific applications and tightly coupled high-performance computing clusters and supercomputers. The other is the emerging long tail of computational science, driven by new scientific domains (e.g., bioinformatics, computational sociology, etc.) adopting the computer as a key tool for research and with rapidly changing software environments and workflows suited to loosely coupled systems, referred to as the "long tail of science" [10]. How to support these two classes of research in an efficient manner is a challenge being faced at all scales: departmental; campus; and nationally.

One approach to tackle this is to provide complete separate machines and environments in support of both. However it is a valid research question to ask whether the requirements for both classes could be provided by a joint operational and hardware infrastructure. This is where *Comet* [10] benefits the overall community by integrating some of the requirements from both and providing a prototype which combines these approaches. *Comet's* goal is to primarily target the long tail of science but its operation and use could be a model for possible future systems.

In contrast to other systems providing virtualization capabilities, *Comet* does not deploy an IaaS framework such as OpenStack [11]. Instead, it is operated as a standard Linux cluster, using a well known cluster management framework (Rocks [1]) and scheduler (Slurm [15]) and integrates virtualization concepts into them. As a result *Comet* uses the batch system to schedule, start, stop and manage VMs. This obviously is of great advantage as on the same machine can provide a traditional batch computing environment for established HPC users while leveraging the benefits of a queuing system to dynamically allocate physical resources for VMs. Moreover, the VMs have access to the InfiniBand

network using SR-IOV [9] and can perform RDMA operation between define groups of VMs. This makes *Comet* ideally targeted towards hosting virtual clusters instead of just loosely coupled VMs.

We have ensured that the management of the virtual clusters (VC) allows the use of common cluster tools such as Rocks, xCAT [20], or Warewulf [7] using semantics based off the experience of operating bare metal. This helps existing cluster administrators quickly build and manage their VC by targeting their current skills and tools. Once the VC is provisioned the administrator can deploy a custom software environment supporting their research group's unique needs. This is particularly valuable for groups with rapidly evolving software stacks from an emerging computational science field. Obviously such a model with integration into the queuing system has the advantage of better resource utilization in a resource starved environment but at the same time provides the necessary performance benefits that advances scientific applications need.

The paper is structured as follows. Next we provide some important terminology that we use throughout the paper (Section 1.1) and a more in depth look at the motivation (Section 1.2). We outline the architecture (Section 2) and report on our client interface (Section 3). We present some preliminary results (Section 4) and conclude our paper (Section 5).

1.1 Terminology

As the concept of using standard HPC infrastructure to manage virtual clusters is new and introduces abstractions that may not be available by standard virtualization frameworks such as OpenStack, AWS, and Azure, we provide the necessary terminology that we will use throughout this paper. The biggest difference we have is in the introduction of computesets. The definitions include:

Node: The term node is used to refer to individual computers in a virtual cluster. The term node is synonymous with Virtual Machine (VM).

Compute: A node with substantial computational resources used to perform work in a virtual cluster. Compute Nodes (CN) are started and stopped on request by the cluster administrator.

Frontend: A node with limited computational resources used to manage a virtual cluster. Frontend Nodes (FN) typically remain running 24 hours a day and can be started and stopped on request by the cluster administrator

Virtual cluster: A virtual cluster (VC) is a loosely or tightly connected network of FN and CNs managed together by a virtual cluster administrator.

Computeset: A group of CNs started together and being in some state (submitted, started, finished, failed). Each CN can only belong to 1 computeset in submitted or active state. Compute sets can be merged to build a larger virtual cluster on demand.

Image: A file containing the contents and structure (ISO9660) of a disk volume which can be attached as a cdrom to a node.

Image attach: Attach is an action applied to a node and image pair whereby the contents of the image are made available to a node on the next power on.

Image detach: Detach is an action applied to a node and image pair whereby the contents of the image are made

unavailable to the node on the next power on.

Console: An interactive representation of the screen of a node (text or graphical) provided to assist with node installation and management.

1.2 Motivation

The reasons for creating the novel *Comet* virtual environment are to define an efficient system architecture for virtual HPC clusters, provide VC performance comparable to the underlying physical system, and to deliver an HPC platfrom to the VC users and administrators in a familiar fashion. VMs that are started on *Comet* are running on the same servers as regular HPC jobs and VMs consequently have access to the same high-performance hardware, including the InfiniBand interconnect via SR-IOV, local flash drives, significant amounts of RAM and multicore CPUs with vector instruction sets. Combined with the semantics and management features we emphasize through our client interfaces we deliver near bare-metal experience to the users and administrators of the VCs. Hence the abstraction of a virtual cluster mimics that of a physical one.

Two of the features that enable this bare-metal approach for management are the private management VLAN and installation from an ISO image. Each VC has its own VLAN, enabling the PXE-boot from a frontend server and full control of an associated local network. Via this abstraction clusters can be management using existing tools mentioned earlier, in addition to Cobbler [5] which also handles bare-metal provisioning over a local network. Furthermore we can leverage other commercial cluster management software as well, like Bright Cluster Manager [3].

For installation and troubleshooting, a VM can be booted up from a regular ISO image uploaded to *Comet's* image server and mounted on the desired server on request. Using an ISO is for many the easiest way to install a frontend of a cluster—a machine running 24/7 and providing access and management for other nodes. Users can also start a compute nodes using a regular ISO, or PXE-boot from the frontend if an appropriate cluster management tool has been set up. Hence compute nodes can be installed with minimum effort while providing access to the desired OS supported by the KVM hypervisor. There is no need to conduct complex manipulations of images or limit use to a handful of sanctioned images. Users can control the installation process by opening the *Comet* VM console in a browser with the cloudmesh client tool (see Section 3).

HPC admins have extensive experience working with baremetal clusters and the existing tools. Switching to new paradigms could require significant resources in time, hardware and money spent to adopt such new approaches. This also includes finding or writing new tools to adapt to new system frameworks. *Comet's* virtual environment makes running virtual clusters straightforward by leveraging existing expertise of the users. Using such well known tools will avoid the significant learning curve associated for example with OpenStack as obvious from [12].

The disk image management on *Comet* is a unique feature that reduces the necessary storage and network infrastructure required while also providing VMs with fast local storage. In short, the KVM disk images for the VMs in a cluster are stored on a central server, but migrated to the container while the VM is running and flushed back when the VM is shut down. This lowers the effort needed for the

centralized storage server and limits the network bandwidth utilized to transferring the image. This design also provides VMs with disk performance based on the SSDs within the physical compute nodes.

In addition to production use of *Comet* VCs, the near bare-metal approach makes *Comet* them an excellent platform for training. Groups can learn how to use tools that work on their real systems in a controlled VM environment. With our solutions, we demonstrate that VCs are easy to set up, replicate, reinstall, and destroy. A new cluster can be booted up for a class and quickly torn down after its intended use [4]. Hence, we provide an efficient platform for trainees that need to get experience with software and services supported by access which is very close to the real hardware. Consequently, the huge benefit of our *Comet virtual clusters* is the combination of near bare-metal and VM features while utilizing existing HPC batch systems.

2. ARCHITECTURE

We provide a brief overview of the system architecture and summarize the components which support user managed virtual HPC clusters in Comet.

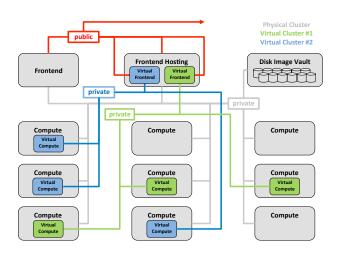


Figure 1: Physical system architecture

Summary The virtual cluster (VC) environment for *Comet* is implemented largely on top of production HPC resources. *Comet* standard compute nodes are used to host VC compute nodes (VCN) with resource allocation managed by the production scheduler. The allocation of standard compute nodes to the pool of nodes available for running VCNs can be adjusted on demand.

Once a VC is defined on *Comet* a VC administrator is able to install the VC frontend node (FN) with a system software management stack of their choice. With the virtual FN installed and configured the VC administrator is able to start and complete the installation and configuration of their VCNs. Installation of VCNs can be interactive and manual or fully automated as all nodes can be PXE installed inside the VC private network.

The resource usage of all VCNs is tracked as standard HPC jobs linked to specific XSEDE allocations and usage is reported to XSEDE via the standard mechanisms.

Nucleus. The management platform we developed for this coordination is called Nucleus and consists of a web service providing a REST API, a database for maintaining state of managed resources, and a message queueing system (based on RabbitMQ) providing connectivity and load balancing between system components. Nucleus handles authentication and authorization of VC administrators, tracks and orchestrates VCN state changes and resource utilization, provides console access to the VC nodes using Guacamole service. The state of VCNs is periodically pushed to the Nucleus management database. The Nucleus database provides all needed information to VC administrators requests for a state. The Nucleus database is "eventually consistent" with the state of the physical cluster. This approach minimizes the effect of VC administrator state requests on the production scheduler.

Rocks. Rocks KVM roll provides the mechanism for running and managing VMs on *Comet* physical hardware. Nucleus uses standard Rocks commands to periodically query the state of all physical and virtual resources and to execute commands on behalf of VC administrators to manage the resources belonging to their VC.

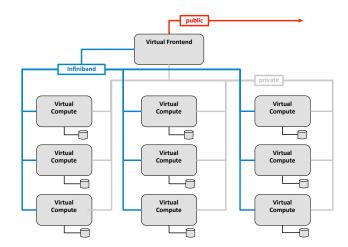


Figure 2: Virtual cluster network topology

Networking. Frontend and compute nodes are hosted on physical hosts with two (private and public) or one (private) 10Gbps Ethernet interfaces, respectively. The private network interfaces of all VMs in a VC are connected to a logical VLAN device. Logical VLAN devices are raw, tagged packet interfaces, using the Macvtap driver. Frontend public interfaces are bridged either directly to a 10GbE interface or to a virtual VLAN device on the physical host. Physical hosts also provide one FDR InfiniBand interface with one or more Single Root IO Virtualization (SR-IOV) virtual functions enabled. All VMs of a single VC are configured to use InfiniBand SR-IOV virtual functions with a single common pkey.

Scheduling. Frontend nodes run constantly at no charge and provide access to the compute nodes of their associated virtual cluster. VC administrators can start compute nodes on any physical compute node assigned by the *Comet* scheduler.

Image Storage. The implementation of VCs in *Comet* also requires a Network Attached Storage (NAS) (Disk Image

Table 1: REST interface of the Comet virtual cluster service.

	REST URL	Description
GET	/v1/cluster/	gets the list of all clusters
GET	/v1/cluster/{cluster.name}	Obtain details about the named cluster
DELETE	/v1/cluster/{cluster.name}	Destroy the named cluster
GET	/v1/cluster/{cluster.name}/compute/{compute.name}	Obtain the details of a named compute resource in
		a named cluster
DELETE	/v1/cluster/{cluster.name}/compute/{compute.name}	Destroy the named compute resource in a named
		cluster
PUT	$/v1/cluster/{cluster.name}/compute/{compute.name}/attach$	iso Attach an ISO to the named compute resource
		in a named cluster
PUT	/v1/cluster/{cluster.name}/compute/{compute.name}/poweroff	Power off the named compute resource in a named
		cluster
PUT	$/v1/cluster/\{cluster.name\}/compute/\{compute.name\}/poweron$	Power on the named compute resource in a named
		cluster
PUT	$/v1/cluster/\{cluster.name\}/compute/\{compute.name\}/reboot$	Reboot the named compute resource in a named
		cluster
POST	$/v1/cluster/\{cluster.name\}/compute/\{compute.name\}/rename$	Rename the named compute resource in a named
DITT		cluster
PUT	$/v1/cluster/\{cluster.name\}/compute/\{compute.name\}/reset$	Reset the named compute resource in a named
DITT		cluster
PUT	$/v1/cluster/\{cluster.name\}/compute/\{compute.name\}/shutdown$	Shutdown the named compute resource in a named
CET	/ 1 / 1 / 1 / 1 / 1 / 1 / 1 /	cluster
GET	/v1/cluster/{cluster.name}/frontend/	Obtain the details of a frontend resource in a named cluster
PUT	/v1/cluster/{cluster.name}/frontend/attach iso	Attach an ISO to the frontendresource in a named
PUI	/V1/Cluster/{Cluster.name}/frontend/attach iso	Attach an ISO to the frontendresource in a named cluster
PUT	/v1/cluster/{cluster.name}/frontend/poweroff	Power off the frontend of a named cluster
PUT	/v1/cluster/{cluster.name}/frontend/poweron	Power on the frontend of a named cluster
PUT	/v1/cluster/{cluster.name}/frontend/reboot	Reboot the frontend of a named cluster
PUT	/v1/cluster/{cluster.name}/frontend/reset	Reset the frontend of a named cluster
PUT	/v1/cluster/{cluster.name}/frontend/shutdown	Shutdown the frontend of a named cluster
GET	/v1/cluster/{cluster.name}/compute/{compute.name}/console/	Open VNC console to named compute resource
GET	/v1/cluster/{cluster.name}/frontend/console/	Open VNC console to name frontend resource
POST	/v1/computeset/	Power on a set of computes creating a ComputeSet
GET	/v1/computeset/	list the compute set
GET	/v1/computeset/ /v1/computeset/{computeset.id}	Obtain the details of the identified ComputeSet
PUT	/v1/computeset/{computeset.id}/poweroff	Power off the identified ComputeSet
PUT	/v1/computeset/{computeset.id}/poweron /v1/computeset/{computeset.id}/reboot	Reboot the nodes in the identified ComputeSet
PUT	/v1/computeset/{computeset.id}/reset	Reset the nodes in the identified ComputeSet
PUT	/v1/computeset/{computeset.id}/reset/ /v1/computeset/{computeset.id}/shutdown	Shutdown the nodes in the identified ComputeSet
GET	/v1/user	Returns Users details in JSON format
PUT	/v1/user	Returns Users details in JSON format
PATCH	/v1/user	Returns Users details in JSON format
GET	/v1/project	Returns project details
GET	/v1/image	Gets the list of images
POST	/v1/image	Adds and image
1001	/ v 1/ 1111008c	ridds and mage

Vault, Figure 1) — a server with a large disk pool for VM images and ISO files. VM images are stored as ZFS datasets on the NAS with each VM owning a single image. The Image Storage system orchestrates the creation and destruction of iSCSI targets providing read-only access to VM images resident on the NAS. This allows VMs to start booting almost instantly. Image Storage also migrates a copy of the VM image to the physical node hosting the VM and creates a local temp-write volume to receive writes from the VM while the migration is underway. After migration is complete the VM is briefly paused, the migrated VM image and temp-write image are merged, the iSCSI target is disconnected and the VM is resumed with both reads and writes accessing the local copy of the VM image. At this point the VM is fully autonomous from the NAS providing great capabilities of scaling without putting load on the NAS or network. Periodic snapshots of the local, ZFS backed, VM images are automatically created and copied back to the NAS keeping

VM images backed up in case the physical node crashes. The final synchronization of changes to VM images after VM shutdown allows the VM image state to be persisted until the next VM boot.

Messaging. We implemented an asynchronous communication system between the components of the image management system, and also Nucleus components connections using the AMQP messaging system RabbitMQ. We have Celery workers running in several locations in the system, receiving AMQP messages with jobs and normally replying with AMQP messages as well. This ensures smooth operation under high loads by scheduling jobs in a queue rather than trying to perform those as they come, and ease of scaling by adding more resources with running daemons.

REST Interface In order to support the concept of virtual clusters on *Comet* we provide a secure REST service to access them. The basic REST signatures are listed in Table 1. However the client interface that uses these rest calls pro-

vide additional functionality and allow easy scripting which is demanded by VC administrators. We describe the client in Section 3.

3. CLOUDMESH CLIENT

The Cloudmesh Client toolkit [16] is a lightweight client interface for accessing heterogeneous clouds, clusters, and workstations right from the user's computer. The client has its origin in [6, 19, 17]. With the client a user can manage their own set of resources enabling management of a personalized cyber infrastructure. It includes an API, a commandline client, and a commandline shell. Extensibility is provided via convenient abstractions. A local database allows caching of information from remote resources. This is an essential feature of Cloudmesh as it allows users to preserve a view of the infrastructure even in cases where it may not be reachable. Obviously, such a cache is especially useful for large scientific workflows and services that require the management of many tasks. Administrators naturally need such a cached view in order to identify faults and to effectively preserve the view of resources that need to be accessed or have been created in the past.

Furthermore, users can, via the provided abstractions, switch easily between or utilize together virtual machines from OpenStack, Amazon, Azure Clouds, and Comet virtual clusters [10]. Hence a greater ability to deal with faults or system failures can be achieved. Cloudmesh Client can be installed on Linux, OSX, and Windows. Currently we support backends to SLURM, SSH, OpenStack, Azure, and AWS. A Docker interface is planned. Next we provide a short overview of the main features of the Cloudmesh Client. Client based. Cloudmesh Client as the name indicates is a client based toolkit that installs and runs on the users or administrators computers. An optional prototype portal is also available as an add on.

Layered Architecture. Cloudmesh Client has a layered architecture (Figure 3) that allows easy development of new features. This also allows contribution by the community while developing integrated and smaller sub components. A resource abstraction layer allows the integration of a multitude of resources spanning HPC, Containers, and Cloud resources. This layered architecture is augmented with a number of components (Figure 4) that together build the overall and expandable Cloudmesh Client architecture providing a rich feature set.

State Caching. Cloudmesh contains necessary state about the resource and environment that a user may want to use. The information is managed in a database abstraction that would allow storing the data in a variety of databases such as SQL and MongoDB. At this time we have chosen SQLite to be the default database as it does not require any additional setup and is universally available on all operating systems without change. Previously we also provided a MongoDB based backend system, but for the *Comet* client it is beneficial to interact with the system without the need of additional services.

Security Management. For *Comet* users, it is beneficial that access to the backend services are enabled with

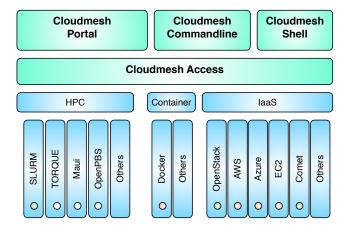


Figure 3: Cloudmesh layered architecture.

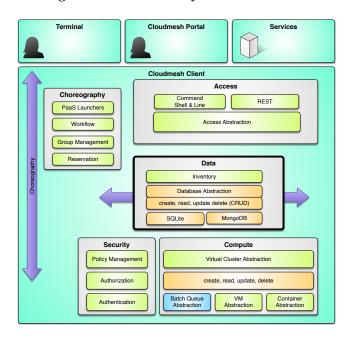


Figure 4: Cloudmesh component overview

cm comet cluster ID

- Show the cluster details
cm comet start ID vm-ID-[0-3] -walltime=6h

- Boot 3 nodes for 6 hours
cm comet iso attach image.iso ID vm-ID-3

- Attach an iso image
cm comet power on ID vm-ID-0

- Power on node 0
cm comet console ID vm-ID-0

- open the console for the node

Figure 5: Example Comet client commands

secure credentials managed on the user's machine as well as with token based service access. This reflects best practice by many supercomputing centers. Through abstractions integration with hosted security services [2] would also be possible. However our integration in clouds is naturally done outside such frameworks and allows user to individu-

¹In the past we supported AWS and Azure which we are integrating back into the client and will be available at time of publication. Our main focus so far was the ability to add OpenStack in support of upcoming systems such as Jetstream and virtual clusters such as used in *Comet*

ally add their credentials for services such as Azure, AWS, and other public clouds into the client easily. We have an exploratory project in place that looks at the use of Yubikeys for Cloudmesh Client and Cloudmesh Portal [21]. This will allow an additional 2 factor authentication as part of accessing services used by the users. Hence, the Cloudmesh Client deals with the secured connection and interaction by considering the appropriate interactions with the different backends. For the *Comet* virtualized cluster, it handles the initial apikey retrieval, once a user is authenticated to the nucleus service. It also handles all the subsequent calls in a secured fashion by dealing with the messages signing, encryption and decryption via utilizing proper libraries.

Command Shell and Command Line. Cloudmesh contains a command shell allowing scripts and interactive use. However we designed the command shell in such a way that each command can also be called from the command line reducing development and maintenance efforts. Through the Cloudmesh database abstraction the state is synchronized between different components.

Cloudmesh Client Portal. Previously, we distributed Cloudmesh with client, server, and a portal in one package. This however turned out to be too complex to be installed for some of our less technically skilled user communities. Thus we split up the original Cloudmesh into multiple independent packages, such as the Cloudmesh Client and the Cloudmesh Portal. The portal provides currently a minimal feature set to manage virtual machines and HPC jobs. It showcases how to integrate the client and the rest services in more elaborated portal frameworks. We will expand upon the existing features and make the portal more feature complete. Due to our focus on the Comet community, the commandline client has an increased development priority as it allows users to automatize advanced DevOps workflows through scripting.

Cloudmesh Comet. We are actively developing the client interface for SDSC's Comet [14] supercomputer allowing near bare metal provisioning. The interface reuses Cloudmesh components and technologies while interfacing with the Comet Nucleus REST interface. Through this interplay the virtual cluster administrators are enabled to utilize tools and services that the they typically use to manage an on-premise bare metal cluster. As part of this development we have developed an easy to use high level command line interface specifically targeted to Comet's features. This includes the following functionality:

- Configuring the nucleus service endpoint and the authentication tokens or keys.
- Getting information and status of the users cluster(s), nodes, computesets, and other entities.
- Power management of the cluster frontend node.
- Request resource allocation to boot the users node(s); and release the resource upon completion.
- Power management to shutoff, power on, reboot compute node(s) during the lifetime of the requested resource allocation.
- Getting console access to the frontend node or a running compute node
- System ISO image management. This includes listing available ISO images, upload new images, and attach/detach an ISO to/from one or more compute nodes.
- Convenient management commands to, for example, renaming compute nodes either individually or in batch.

Some example commands are depicted in Figure 5. The manual page is shown in Figure 6.

```
comet init
comet 11 [CLUSTERID] [--format=FORMAT]
comet cluster [CLUSTERID] [--format=FORMAT]
comet computeset [COMPUTESETID]
                 [--allocation=ALLOCATION]
                 [--cluster=CLUSTERID]
                 [--state=COMPUTESESTATE]
comet start CLUSTERID
            [--count=NUMNODES]
            [COMPUTENODEIDS]
            [--allocation=ALLOCATION]
            [--walltime=WALLTIME]
comet terminate COMPUTESETID
comet power (on|off|reboot|reset|shutdown)
            CLUSTERID [NODESPARAM]
comet console CLUSTERID [COMPUTENODEID]
comet iso list
comet iso upload [--isoname=ISONAME] PATHISOFILE
comet iso attach ISONAME CLUSTERID [COMPUTENODEIDS]
comet iso detach CLUSTERID [COMPUTENODEIDS]
comet node rename CLUSTERID OLDNAME NEWNAME
Options:
  --format=FORMAT
                          Format is either table, ison,
                          yaml, csv, rest [default: table]
  --count=NUMNODES
                          Number of nodes to be powered on.
                          When this option is used, the
                          Comet system will find a NUMNODES
                          number of arbitrary nodes that
                          are available to boot as a
```

computeset --allocation=ALLOCATION Alocation to charge

--walltime=WALLTIME Walltime requested for node(s).

An integer followed by a unit (m,h,d,w, for minute, hour, day)

E.g., 3h, 2d --isoname=ISONAME Name of iso image

--state=COMPUTESESTATE List computeset with the given

state. The state could be submitted, running, completed

CLUSTERID The assigned name of a cluster, e.g. vc1
COMPUTESETID An integer identifier assigned to a

computeset

computeset

Arguments:

COMPUTENODEID A compute node name, e.g., vm-vc1-0

If not provided, the requested action

will be taken on the frontend node of the specified cluster

COMPUTENODEIDS A set of compute node names in hostlist

format, e.g., vm-vc1-[0-3]

If not provided, the requested action will be taken on the frontend node of the gracified cluster.

node of the specified cluster

NODESPARAM Specifying the node/nodes/computeset to

act on. In case of integer, will be intepreted as a computesetid; in case

of a hostlist format,

e.g., vm-vc1-[0-3], a group of nodes; or a single host is also acceptable,

e.g., vm-vc1-0

ISONAME Name of an iso image at remote server PATHISOFILE The full path to the iso image file to

be uploaded

Figure 6: Cloudmesh Comet CLI Manual Page

As previously mentioned, the Cloudmesh Comet Client deals with the authentication to CometNucleus and handles the subsequent request in a secured fashion. It also processes

the returned result from the requests and is able to present feedback in various formats. This is essential as it enables the user either for read in the terminal in a human readable format such as tables or for easy scripting while being able to access the information in YAML, JSON, or CSV. Furthermore, the client creates data mashups from multiple information requests via the REST interfaces in order to generate combined information views. A good example is the Cloudmesh Client cluster view as it combines the data from the cluster call and computeset call to generate a view with node information, comuputeset association and status, account and allocation data, all included in one view for easy consumption.

Cloudmesh Client Comet Python API. Cloudmesh Client is written in Python and provides in addition to the commandline and command shell a Python API. This API provides high level functionality such as data mashups that are not available in the REST interface and provides therefor additional convenient abstractions [18].

Easy Installation. The Cloudmesh Client is easy to install. It is available via pip and the source code is publicly hosted on Github [18]. Python 2.7 and Python 3.5 is supported.

4. RESULTS AND USECASES

We report on some of our use cases while focusing in particular on the use of virtual machines and virtual clusters, as well as giving an outlook of selected planned improvements based on lessons learned.

4.1 Heterogeneous VM Management

Over the last 2 years we have used Cloudmesh in a number of classes and research projects to access clouds from a variety of sources. This includes the management of classes with more than 70 users, but also the support of individual researchers with the need to conduct infrastructure experiments. Cloudmesh has been shown to be able to access Chameleon Cloud, CloudLab, Cybera in Canada, HP cloud, Amazon WS, Azure. Most recently we also showcased potential access to Jetstream. One of the interesting benefits of this rich diversity is that educational efforts can be targeted for a particular platform while the interface to them for managing virtual machines is the same. In our experience with classes and potential user this is an advantage, as when the switch of a single variable (e.g., the name of the cloud) a VM or VC can be created on a different infrastructure reducing the load on the original system. Hence, reliability can be increased without introducing additional complex and divergent interfaces for the diverse set of clouds. Future use cases will include class use of Comet VC for a planned graduate course that can serve up to 140 new applicants to the newly created data science program at Indiana University. As we demonstrated with Cloudmesh Client we would also be able to access other XSEDE resources such as Jetstream and Bridges once they become available to us and offer programable interfaces that we can integrate in Cloudmesh.

4.2 OnDemand Hackathon Support

In February 2016 SDSC hosted a hackathon [4] related to the activities of CAIDA the Center for Applied Internet Data Analysis. "CAIDA provides macroscopic insights into Internet infrastructure, behavior, usage, and evolution, fosters a collaborative environment in which data can be acquired, analyzed, and (as appropriate) shared, improves the integrity of the field of Internet science, and informs science, technology, and communications public policies." The hackathons theme was live measurements and monitoring of the global Internet routing system (BGP). A total of 90 attendees participated in the event representing a mix of Academia, Industry and Institutions. Comet provided compute resources to participants, including several virtualized nodes, that were essential for the success of the event. Over 15,000 SUs were used during 24 hours of activities. The virtualized nodes were especially important as they allowed CAIDA administrators to install a different OS and application software stack than that which exists on Comet.

4.3 Open Science Grid

The Open Science Grid (OSG) [13] provides an integrated facility to access compute resources through distributed high throughput computing for researchers in the US. The resources are contributed by the community and organized by OSG. Many projects are executed on OSG, one of which is the Laser Interferometer Gravitational-Wave Observatory (LIGO). LIGO is "designed to open the field of gravitational-wave astrophysics through the direct detection of gravitational waves predicted by Einstein's General Theory of Relativity" [8].

Comet has delivered 700,000 SUs to LIGO via OSG since its inception. Thus Comet contributed considerably to both efforts, OSG and LIGO. In November 2015 OSG began operating a VC on Comet and immediately began running calculations related to LIGO. The integration within OSG has been conducted in two modes to demonstrate its wide usability (see Figure 7).

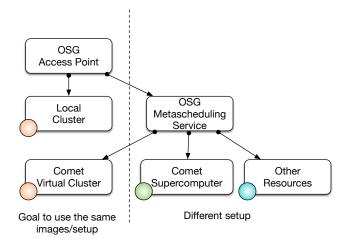


Figure 7: Open Science Grid use cases

The first mode is the traditional integration of a supercomputing allocation while utilizing the batch system and existing specialized integration of batch job capabilities accessed by the OSG metascheduler. This mode requires additional layers of abstraction between the OSG metascheduler and the batch system on the compute resource. The second one is the integration of a VC that is based on software used for the operation of the local OSG cluster and thus shares the same infrastructure requirements in regards to operating system and other services. Hence no abstraction layer is needed as a standard OSG system definition and software

stack can be used and run on the VC. In contrast to other virtualization infrastructures and efforts we are currently exploring the utilization of MPI jobs within the VC to make use of the underlying high performance networking infrastructure accessible from within the OSG VMs. These VMs already utilize the virtualized InfiniBand HCAs to access storage.

5. CONCLUSIONS

We have proven that it is possible to integrate virtual machine management leveraging an existing HPC batch queuing systems as part of the operation of a major national scale compute infrastructure. This novel technology solution and operational model provides the ability to integrate best practices from both approaches, traditional supercomputing and utilizing virtual machines to further the long tail of science. Overall management of such a system is reduced as it is well integrated in to HPC administrators familiar toolset. This applies both to the operation of *Comet* and the virtual clusters it hosts.

Additionally, we developed a powerful client interface to *Comet's* virtualization system. The Cloudmesh client was developed with the goal to interface easily and to enable its users to have access programmatically to *Comet* via a Python API, a command shell, a commandline tool and a prototype portal. Furthermore as new features become available the client provides an easy mechanism to be updated.

We have utilized the tools and capabilities provided in this paper in a variety of different scenarios and shown that they are beneficial for the particular effort. As part of our efforts new use cases, namely training and development, have emerged.

We will expand upon our current already operational prototypes and integrate them into a production system that will be available soon (during Q2 2016). Users that are interested today to explore the virtual modality of *Comet* or Cloudmesh client for comet should contact the authors of the paper.

6. ACKNOWLEDGMENTS

Comet is supported by NSF grant: ACI #1341698 Gateways to Discovery: Cyberinfrastructure for the Long Tail of Science.

7. REFERENCES

- [1] Rocks cluster. URL: http://www.rocksclusters.org/.
- [2] J. Basney, M. Humphrey, and V. Welch. The myproxy online credential repository. Softw., Pract. Exper., 35(9):801–816, 2005. URL: http://dblp.uni-trier.de/ db/journals/spe/spe35.html#BasneyHW05.
- [3] Bright cluster manager. URL: http://www.brightcomputing.com/.
- [4] Caida hackaton. URL: https://www.caida.org/workshops/bgp-hackathon/1602/.
- [5] Cobbler. URL: http://cobbler.github.io/.
- [6] G. Laszewski, M. Hategan, and D. Kodeboyina. Workflows for e-Science: Scientific Workflows for Grids, chapter Java CoG Kit Workflow, pages 340–356. Springer London, London, 2007. URL: http://dx.doi.org/10.1007/978-1-84628-757-2_21, doi:10.1007/978-1-84628-757-2_21.

- [7] LBNL. Warewolf. URL: http://warewulf.lbl.gov/.
- [8] URL: https://www.ligo.caltech.edu/.
- [9] G. K. Lockwood, M. Tatineni, and R. Wagner. Sr-iov: Performance benefits for virtualized interconnects. In Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment, XSEDE '14, pages 47:1–47:7, New York, NY, USA, 2014. ACM. URL: http://doi.acm.org/10.1145/2616498.2616537, doi:10.1145/2616498.2616537.
- [10] R. L. Moore, C. Baru, D. Baxter, G. C. Fox, A. Majumdar, P. Papadopoulos, W. Pfeiffer, R. S. Sinkovits, S. Strande, M. Tatineni, R. P. Wagner, N. Wilkins-Diehr, and M. L. Norman. Gateways to discovery: Cyberinfrastructure for the long tail of science. In Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment, XSEDE '14, pages 39:1–39:8, New York, NY, USA, 2014. ACM. URL: http://doi.acm.org/10.1145/2616498.2616540, doi:10.1145/2616498.2616540.
- [11] Openstack. URL: http://www.openstack.org/.
- [12] openstack.org. Openstack user survey. URL: http://www.openstack.org/assets/survey/ April-2016-User-Survey-Report.pdf.
- [13] Open science grid. URL: http://www.opensciencegrid.org/.
- [14] SDSC. Comet user guide. URL: http://www.sdsc.edu/support/user_guides/comet.html.
- [15] Slurm. URL: http://slurm.schedmd.com/.
- [16] G. von Laszewski. Cloudmesh web page. Web Page. URL: http://cloudmesh.github.io/client/.
- [17] G. von Laszewski, G. C. Fox, F. Wang, A. J. Younge, A. Kulshrestha, G. G. Pike, W. Smith, J. Vöckler, R. J. Figueiredo, J. Fortes, and K. Keahey. Design of the futuregrid experiment management framework. In Gateway Computing Environments Workshop (GCE), 2010, pages 1–10, Nov 2010. doi:10.1109/GCE.2010.5676126.
- [18] G. von Laszewski and F. Wang. Cloudmesh client source code. URL: https://github.com/cloudmesh/client.git.
- [19] G. von Laszewski, A. Younge, X. He, K. Mahinthakumar, and L. Wang. Experiment and workflow management using cyberaide shell. In Cluster Computing and the Grid, 2009. CCGRID '09. 9th IEEE/ACM International Symposium on, pages 568–573, May 2009. doi:10.1109/CCGRID.2009.66.
- [20] Extreme cluster/cloud administration toolkit. URL: https://xcat.org/.
- [21] Yubico.com. Yubico keys. Web Page. URL: https://www.yubico.com/products/yubikey-hardware/.