

# *A Study of Cloud Computing Environments for High Performance Applications*

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## **Abstract**

High performance applications requires high processing power to compute highly intensive and complex applications for research, engineering, medical and academic projects. In the traditional way, an organization will have to pay very high costs to run an HPC (High Performance computing) application. The organization has to purchase highly expensive hardware for running an HPC application and maintaining it afterwards. The HPC resources on the company premises may not satisfy all the demands of scientific application where resources may not suitable for corresponding requirements. Considering the case of SMEs (small and medium enterprises), an increasing demand is always challenging. Cloud computing is an on-demand, pay-as-you-go model, that offers scalable computing resources, unlimited storage in an instantly available way. In this paper we included requirements of HPC applications in cloud, cluster based HPC applications, types of clusters, Google's HPC Cloud architecture, performance analysis of various HPC cloud vendors and four case studies of HPC applications in cloud.

**Keywords:** Cloud, HPC, SMEs, EC2, POD Cloud, R-HPC

## **I. INTRODUCTION**

High Performance Computing (HPC) plays an important role in both scientific advancement and economic competitiveness of a nation - making production of scientific and industrial solutions faster, less expensive, and of higher quality. HPC is a key component in many applications: designing vehicles and airplanes; designing high-rise buildings and bridges; discovery of drugs; discovery and extraction of new energy sources like oil and natural gas; weather forecasting; and many more. HPC requires very high processing power to compute largely complex scientific applications. The advantage of pay-as-you-go computing has been an industry goal for many years starting from main frame, cluster and grid computing. Cloud computing takes grid computing to a whole new level by using virtualization to encapsulate an operating system instance and run it in a cloud whenever they need computational resources. In addition cloud storage can also be used independently with operating system instances. Cloud computing also offers unlimited storage and instantly available and scalable computing resources, all at a

reasonable metered cost. Cloud also having large data centres which is suitable for data-intensive applications.

## **II. HPC APPLICATIONS IN CLOUD**

With increasing demand for high performance, efficiency, productivity, agility and lower cost, since several years, information communication technology are dramatically changing from static silos with manually managing resources and applications, towards dynamic virtual environments with automated and shared services, i.e. from silo-oriented to service oriented architectures[15]. A "traditional" cloud offers features that are attractive to the general public. These services comprise single, loosely coupled instances (an instance of an OS running in a virtual environment) and storage systems backed by service level agreements (SLAs) that provide the end user guaranteed levels of service. These clouds offer the following features:

- Instant availability – Cloud offers almost instant availability of resources.
- Large capacity – Users can instantly scale the number of applications within the cloud.
- Software choice – Users can design instances to suit their needs from the OS up.
- Virtualized – Instances can be easily moved to and from similar clouds.
- Service-level performance – Users are guaranteed a certain *minimal* level of performance.

Although these features serve much of the market, HPC users generally have a different set of requirements:

- Close to the "metal" – Many man-years have been invested in optimizing HPC libraries and applications to work closely with the hardware, thus requiring specific OS drivers and hardware support.
- User space communication – HPC user applications often need to bypass the OS kernel and communicate directly with remote user processes.

- Tuned hardware – HPC hardware is often selected on the basis of communication, memory, and processor speed for a given application set.
- Tuned storage – HPC storage is often *designed* for a specific application set and user base.
- Batch scheduling – All HPC systems use a batch scheduler to share limited resources.

Depending on the user's application domain, these two feature sets can make a big difference in performance. For example, applications that require a single node (or threaded applications) can work in a cloud. In this case, the user might have a single program that must be run with a wide range of input parameters (often called parametric processing), or they might have dataflow jobs, such as the Galaxy suite used in biomedical research. These types of applications can benefit from most cloud computing resources.

Some applications can utilize highly parallel systems but do not require a high-performance interconnect or fast storage. One often cited example is digital rendering, in which many non-interacting jobs can be spawned across a large number of nodes with almost perfect scalability. These applications often work well with standard Ethernet and do not require a specialized interconnect for high performance.

Moving up the HPC tree, you'll find interconnect-sensitive applications that require low latency and high throughput interconnects not found in the traditional cloud. Indeed, most of these interconnects (e.g., InfiniBand and High-Performance Ethernet) require "userspace" communication pathways that do not involve the OS kernel. This method makes the use of cloud virtualization very difficult because most virtualization schemes cannot manage "kernel bypass" applications (i.e., these are "on the wire" data transfers that are hard to virtualize). If high-performance networks are not available, many HPC applications run slowly and suffer from poor scalability (i.e., they see no performance gain when adding nodes).

Also in the tree are many I/O-sensitive applications that, without a very fast I/O subsystem, will run slowly because of storage bottlenecks. To open up these bottlenecks, most HPC systems employ parallel file systems that drastically increase the I/O bandwidth of computing nodes.

Another growing branch includes performance accelerators or SIMD units (parallel computing Single-Instruction Multiple Data processors) from NVidia and AMD/ATI. This type of hardware is very specific to HPC systems and therefore is not found on typical cloud hardware.

At the top of the tree are applications that push on all levels of performance (compute, interconnect, and storage). These applications require fast computation (possible a SIMD unit), fast interconnects, and high-performance storage.

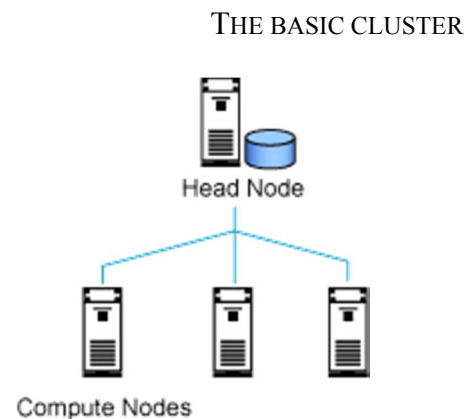
Clearly, this computing environment is not found in a typical cloud and is unique to the HPC market. Attempting to run this level of application on a typical cloud will provide sub-par performance.

Finally, any remote computation scheme needs to address the "moving big data problem." Many HPC applications require large amounts of data. Many clouds, even those that offer HPC features, cannot solve the problem easily. In particular, if the time to move large datasets to the cloud outweighs the computation time, then the cloud solution is now the slow solution. Interestingly, the fastest way to move data in these cases is with a hard disk and an overnight courier. (It seems the station wagon full of tapes is still the fastest way to transport data.)

With all the differences between the traditional cloud and HPC applications, users will be interested to know that HPC clouds and cloud-like resources are available. A number of companies, including Penguin, R-HPC, Amazon, Univa, SGI, Sabalcore, and Gompute offer specialized HPC clouds. Notably absent is IBM who, at this time, does not offer public HPC clouds. The company, however, does provide many options for constructing internal or private.

### III. HPC IN CLUSTERS

A high performance computer appropriate for most small and medium-sized businesses today is built from what are basically many ordinary computers connected together with a network and centrally coordinated by some special software. Because the computers are usually physically very close together, the common term for a high performance computer today is a *cluster*[5]. The basic structure of a cluster based computing is shown in the figure



High-Performance Computing (HPC) clusters are characterized by many cores and processors, lots of memory, high-speed networking, and large data stores – all shared across many rack-mounted servers. User programs

that run on a cluster are called jobs, and they are typically managed through a queuing system for optimal utilization of all available resources. An HPC cluster is made of many separate servers, called nodes, possibly filling an entire data center with dozens of power-hungry racks. HPC typically involves simulation of numerical models or analysis of data from scientific instrumentation. At the core of HPC is manageable hardware and systems software wrangled by systems programmers, which allow researchers to devote their energies to their code.

A successful HPC cluster is a powerful asset for an organization. At the same time, these powerful racks present a multifaceted resource to manage. If not properly managed, software complexity, cluster growth, scalability, and system heterogeneity can introduce project delays and reduce the overall productivity of an organization.

A successful HPC cluster requires administrators to provision, manage, and monitor an array of hardware and software components

Clusters are the predominant type of HPC hardware these days; a *cluster* is a set of MPPs (In clusters, also known as *massively parallel processors (MPPs)*, they don't share the same memory;). A processor in a cluster is commonly referred to as a *node* and has its own CPU, memory, operating system, and I/O subsystem and is capable of communicating with other nodes.

## Clustering-Definitions

The term "cluster" can take different meanings in different contexts. There are three types of clusters:

- Fail-over clusters
- Load-balancing clusters
- High-performance clusters

### Fail-over clusters

- The simplest fail-over cluster has two nodes: one stays active and the other stays on stand-by but constantly monitors the active one. In case the active node goes down, the stand-by node takes over, allowing a mission-critical system to continue functioning.

### Load-balancing clusters

- Load-balancing clusters are commonly used for busy Web sites where several nodes host the same site, and each new request for a Web page is dynamically routed to a node with a lower load.

## High-performance clusters

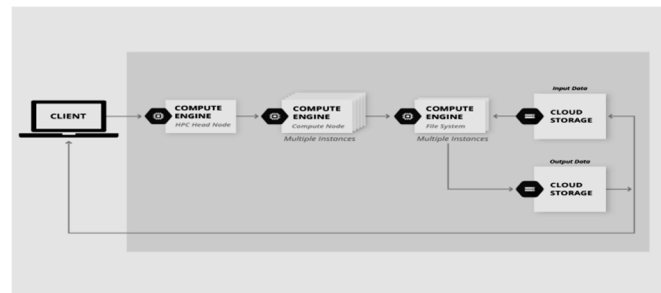
- These clusters are used to run parallel programs for time-intensive computations and are of special interest to the scientific community. They commonly run simulations and other CPU-intensive programs that would take an inordinate amount of time to run on regular hardware.

Some features of clusters are as follows:

- Clusters are built using commodity hardware and cost a fraction of the vector processors. In many cases, the price is lower by more than an order of magnitude.
- Clusters use a message-passing paradigm for communication, and programs have to be explicitly coded to make use of distributed hardware.
- With clusters, you can add more nodes to the cluster based on need.
- Open source software components and Linux lead to lower software costs.
- Clusters have a much lower maintenance cost (they take up less space, take less power, and need less cooling).

## IV. HIGH PERFORMANCE COMPUTING CLUSTER IN A CLOUD ENVIRONMENT

High Performance Computing clusters can be created on the Google Cloud Platform by utilizing Google Compute Engine VMs and Google Cloud Storage[3]. By running HPC workloads in Google's Cloud, customers can augment on-premise HPC clusters or run all their jobs in the cloud



The compute portion of the HPC cluster consists of a Head Node running scheduling and management software on a Google Compute Engine VM. The compute/worker nodes are also running on Google Compute Engine VMs. Instances sizes can be selected to match the workload. Choices include Standard, High Memory or High CPU instances in 1, 2, 4, 8 or 16 core sizes. Instances can also be added or deleted depending on the resources needed. The

user has a choice of various commercial packages or open source software components to create the cluster.

Compute Engine VMs can also be used to create a file system for the cluster. Two popular options are NFS and Gluster. This is an optional component as the Compute Nodes can also access Google Cloud Storage directly.

Google Cloud Storage provides the backend storage for the cluster. This is a durable, highly available storage option making it an excellent choice for HPC work. Google Cloud SQL is also available for structured input or output data. The input data can be uploaded by the client directly into Cloud Storage or uploaded with the job. The resulting data can be downloaded to the client or left in the cloud for storage or further processing.

## V. PERFORMANCE ANALYSIS OF VARIOUS HPC CLOUD VENDORS

### V.1 PENGUIN COMPUTING

One the first vendors to introduce a true HPC cloud was Penguin Computing[8]. The Penguin On Demand, or POD cloud, was one of the first remote HPC services. From the beginning, POD has been a bare-metal compute model similar to an in-house cluster. Each user is given a virtualized login node that does not play a role in code execution. The standard compute node has a range of options, including dual four-core Xeon, dual six-core Xeon, or quad 12-core AMD processors ranging in speed from 2.2 to 2.9GHz with 24 to 128GB of RAM per server and up to 1TB of scratch local storage per node.

Getting applications running POD HPC clouds can be quite simple, because Penguin has more than 150 commercial and open source applications installed and ready to run on the system. Installing other applications is straightforward and available to users. Nodes with two NVidia Tesla C2075 computing processors are available.

In terms of network, POD nodes are connected via nonvirtualized, low-latency 10Gb Ethernet (GigE) or QDR IB networks. The network topology is local to ensure maximum bandwidth and minimum latency between nodes. Storage systems are made available via 10GigE to the local compute cluster. Additionally, POD has redundant high-speed Internet with remote connectivity ranging from 50Mbps to 1Gbps.

Several storage options are also available, starting with high-speed NFS using 10GigE attached storage. Beyond NFS, there are parallel filesystem options attached via multiple 10GigE links and InfiniBand. Lustre and Panasas

high-performance storage systems also can be provided. Finally, dedicated storage servers are available. These systems can isolate data and facilitate encryption/decryption of high volumes of data by using physical shipping rather than Internet transfer.

POD offers a suite of tools to help manage your computation. Aptly called PODTools, Penguin offers a collection of command-line utilities for interacting with their HPC cloud. Beyond the standard SSH login, POD Tools provide the ability to submit jobs, transfer data, and generate reports. Additionally, Penguin POD can be seamlessly integrated into existing on-site clusters to outsource excess workloads – often known as “cloud bursting.” All these capabilities are encrypted and offer a high level of security.

Perhaps Penguin’s biggest asset is a long history of delivering on-site HPC solutions. This experience has allowed them to develop a staff of industry domain experts. They also have long list of additional services that supplement their POD offering. These include on-premises provision of cloud bursting to the POD cloud, remote management of on-premises HPC services, cloud migration services, private remote HPC as service environments, and private internal clouds.

### V.2 R-HPC

R-HPC[9] offers R-Cloud, wherein clients can “rent” HPC resources. R-Cloud offers two distinct computing environments. The first is a Shared Cluster, which offers a login to shared nodes and a work queue. This environment offers a classic cluster environment and is essentially a “shared cluster in the sky.” Users are billed by the job, creating a pay-as-you go HPC service. No support or administration services are provided. The second environment comprises virtual private clusters that are carved out of a shared configuration. Use can be on-demand with VLAN access. These systems are billed on a 24/7 basis.

R-HPC can provide new 3.4GHz quad core Sandy Bridge-based systems with 16GB of RAM/node (4GB/core), DDR 2:1 blocking InfiniBand, and 1TB of local disk. Additionally, they have dual-socket 2.6GHz eight-core Sandy Bridge with 128GB of RAM/node (8GB/core), QDR non-blocking InfiniBand, 1TB of local storage, and 1TB global storage. These offerings are rounded out by Magny-Cours, Nehalem, and Harpertown systems. GPU-based systems in beta test are provided for dedicated users.

Most applications can be set up and running within one day (although R-HPC notes that licensing issues can delay the process for some users). Similar to Penguin’s products, all

the interconnects, which include DDR, QDR, FDR, and GigE, are run on the wire with no OS virtualization layer. Storage options include 10 GigE attached NFS/SMB with Lustre over IB as a possible upgrade. If ultimate storage performance is needed, R-HPC also offers the Kove RAM disk storage array. All dedicated systems have block storage for security, whereas the shared clusters use shared NFS (no private mounts).

R-HPC will make service level agreements on a case-by-case basis depending on the customers needs. In terms of workflow management, Torque/OpenPBS is the most common scheduler; however, Maui and Grid Engine (and derivatives) can be provided as needed. Interestingly, cloud bursting, although possible with R-HPC systems, is almost never requested by customers. Another interesting aspect of R-HPC offerings includes Windows HPC environments.

R-HPC offers performance tuning and remote administration services as well. They have extensive experience in HPC and can provide “tuned” application-specific private clusters for clients.

### V.3 Amazon EC2 HPC

Perhaps the most well-known cloud provider is Amazon[1]. Inquiries to Amazon were not returned, so information was gleaned from their web page. Originally, the EC2 service was found not suitable for many HPC applications. Amazon has since created dedicated “cluster instances” that offer better performance to HPC users. Several virtualized HPC instances are available on the basis of users’ needs. Their first offering is two Cluster Compute instances that provide a very large amount of CPU coupled with increased network performance (10GigE). Instances come in two sizes, a Nehalem-based “Quadruple Extra Large Instance” (eight cores/node, 23GB of RAM, 1.7TB of local storage) and a Sandy Bridge-based “Eight Extra Large Instance” (16 cores/node, 60.5GB of RAM, 3.4TB of local storage).

Additionally, Amazon offers two other specialized instances. The first is a Cluster GPU instance that provides two NVidia Tesla Fermi M2050 GPUs with proportionally high CPU and 10GigE network performance. The second is a high-I/O instance that provides two SSD-based volumes, each with 1024GB of storage.

Thus, using the small usage case (80 cores, 4GB of RAM per core, and basic storage of 500GB) would cost US\$ 24.00/hour (10 Eight Extra Large Instances). The larger usage case (256 cores, 4GB of RAM per core, and 1TB of fast global storage) would cost US\$ 38.4/hour (16 Eight Extra Large Instances).

Amazon does not charge for data transferred into EC2 but has a varying rate schedule for transfer out of the cloud; additionally, there are EC2 storage costs. Therefore, the total cost depends on compute time, total data storage, and transfer. Once created, the instances must be provisioned and configured to work as a cluster by the user.

## VI. HPC CLOUD CASE STUDIES

### VI.1 HPC APPLICATIONS ON AMAZON

Amazon Web Services (AWS) is Amazon’s cloud computing platform, with Amazon Elastic Compute Cloud (EC2)[1] as its central part, first announced as beta in August 2006. Users can rent Virtual Machines (VMs) on which they run their applications. EC2 allows scalable deployment of applications by providing a web service through which a user can boot an Amazon Machine Image(AMI) to create a virtual machine, which Amazon calls an “instance”, containing any software desired. A user can create, launch, and terminate server instances as needed and paying by the hour for active servers. EC2 provides users with control over the geographical location of instances which allows for latency optimization and high levels of redundancy.

### VI.2 NAS Parallel Benchmark on Amazon EC2

In order to find out if and how clouds are suitable for HPC applications, Ed Walker (Walker 2008) run an HPC benchmark on Amazon EC2[1]. He used several macro and micro benchmarks to examine the “delta” between clusters composed of state-of-the-art CPUs from Amazon EC2 versus an HPC cluster at the National Center for Supercomputing Applications (NCSA). He used the NAS Parallel Benchmarks (NAS 2010) to measure the performance of these clusters for frequently occurring scientific calculations. Also, since the Message-Passing Interface (MPI) library is an important programming tool used widely unscientific computing, his results demonstrate the MPI performance in these clusters by using the mpptest micro benchmark. For his benchmark study on EC2 he use the high-CPU extra large instances provided by the EC2 service. The NAS Parallel Benchmarks (NPB 2010) comprise a widely used set of programs designed to evaluate the performance of HPC systems. The core benchmark consists of eight programs: five parallel kernels and three simulated applications. In aggregate, the benchmark suite mimics the critical computation and data movement involved in computational fluid dynamics and other “typical” scientific computation. Research from Ed Walker (2008) about the runtimes of each of the NPB programs in the benchmark shows a performance degradation of approximately 7%–21% for the programs running on the EC2 nodes compared to running them on the NCSA cluster

compute node. Further results and an in-depth analysis showed that message-passing latencies and bandwidth are an order of magnitude inferior between EC2 compute nodes compared to between compute nodes on the NCSA cluster. Walker (2008) concluded that substantial improvements could be provided to the HPC scientific community if a high-performance network provisioning solution can be devised for this problem.

### VI.3 LINPACK Benchmark on Amazon Cluster Compute Instances

In July 2010, Amazon announced its Cluster Compute Instances (CCI 2010) [1] specifically designed to combine high compute performance with high performance network capability to meet the needs of HPC applications. Unique to Cluster Compute instances is the ability to group them into clusters of instances for use with HPC applications. This is particularly valuable for those applications that rely on protocols like Message Passing Interface (MPI) for tightly coupled inter-node communication. Cluster Compute instances function just like other Amazon EC2 instances but also offer the following features for optimal performance with HPC applications:

- When run as a cluster of instances, they provide low latency, full bisection 10Gbps bandwidth between instances. Cluster sizes up through and above 128 instances are supported.
- Cluster Compute instances include the specific processor architecture in their definition to allow developers to tune their applications by compiling applications for that specific processor architecture in order to achieve optimal performance. The Cluster Compute instance family currently contains a single instance type, the Cluster Compute Quadruple Extra Large with the following specifications: 23 GB of memory, 33.5 EC2 Compute Units (2 x Intel Xeon X5570, quad-core “Nehalem” architecture), 1690 GB of instance storage, 64-bit platform, and I/O Performance: Very High (10 Gigabit Ethernet). As has been benchmarked by the Lawrence Berkeley Laboratory team (2010), some applications can expect 10x better performance than on standard EC2. For the Linpack benchmark, they saw 8.5x compared to similar clusters on standard EC2 instances. On an 880-instance CC1 cluster, Linpack achieved a performance of 41.82 Tflops, bringing EC2 at #146 in the June 2010 Top 500 rankings.

### VI.4 MATLAB on Amazon Cluster Compute Instances

Another recent example for HPC on EC2 CCI comes from the MATLAB team at MathWorks (MATLAB 2010) which tested performance scaling of the backslash (“\”) matrix division operator to solve for  $x$  in the equation  $A*x = b$ . In their testing, matrix  $A$  occupies far more memory (290 GB)

than is available in a single high-end desktop machine typically a quad core processor with 4-8 GB of RAM, supplying approximately 20 Gigaflops. Therefore, they spread the calculation across machines. In order to solve linear systems of equations they need to be able to access all of the elements of the array even when the array is spread across multiple machines. This problem requires significant amounts of network communication, memory access, and CPU power. They scaled up to a cluster in EC2, giving them the ability to work with larger arrays and to perform calculations at up to 1.3 Teraflops, a 60X improvement. They were able to do this without making any changes to the application code. Each Cluster Compute instance runs 8 workers (one per processor core on 8 cores per instance). Each doubling of the worker count corresponds to a doubling of the number of Cluster Computer instances used (scaling from 1 up to 32 instances). They saw near-linear overall throughput (measured in Gigaflops on the y axis) while increasing the matrix size (the x axis) as they successively doubled the number of instances.

## VII. CONCLUSION

In this paper, we have presented the advantage of running HPC applications in the cloud environment is that using on-demand cloud resources can reduce the cost of maintenance and save on purchase of the software and equipment. But existing HPC applications are not always expected to be able to be taken entirely into a cloud environment, due to current HPC Cluster’ dominant position. Therefore, we also present a combined HPC mode in which HPC applications can use cloud and on-premises resources together. We also conducted a study of performance of HPC applications in various HPC cloud vendors. We included case studies with Amazon EC2 for various benchmarks. Given the varied requirements for HPC clouds, it is understandable that the range of options can vary greatly. Solutions range from shared remote clusters to full virtualized systems in the cloud. Each method brings its own feature set that must be matched to the users’ needs. Finally, the above items are not intended to be an exhaustive list of HPC cloud providers. Others exist, and given that the market is new and growing, more vendors will be coming online in the near future. Many other factors should also be considered besides the brief analysis offered here. Your best results will come from doing due diligence and testing your assumptions. Perhaps the most important aspect of cloud HPC is the ability to work with your vendor, because having a good working safety net under your cloud might be the best strategy of all.

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