HPC in the Cloud Environment: Challenges, and Theoretical Analysis

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Abstract - The vision of omnipresent information was only a fantasy in the mid 1990’s. Constant improvements in pervasive computing have enabled technologies like Cloud Computing a potential to cater for technology users from all walks of life. HPC user community, who mostly require mid to extensive computational capabilities with less latency possible stand to reap through the benefits conceived.

This paper provides a view into how Cloud Computing can support the HPC and describes the technologies and functions that can help them improve efficiency, reduce costs and enable new capabilities. The analysis carried out help users determine which applications, services and technologies should be considered for development and deployment “in the Cloud” to meet their goals.

Keywords High Performance Computing, Cloud Computing, HPC Cloud

1 Introduction

High-performance computing (HPC) is one of the contexts in which the adoption of Cloud Computing paradigm is discussed. HPC users are traditionally, accustomed to directly managing very complex parallel systems and performing a very fine-tuning of their applications on existing hardware. Deploying such applications on a Cloud where users voluntarily place almost all control on the execution environment, leaving the management of datacentres to the Cloud owner calls for a conscientious and deliberate technique [4]. It is necessary to take a step back and systematically study the Cloud paradigm to see how best organisation/users who accustomed to core traditional HPC notion can take advantage of HPC Cloud [1].

The three typical service models widely in use today for Cloud Computing are Software as a service (SaaS), Infrastructure as a Service (IaaS), and Platform as a Service (PaaS). With so much progression happening in the Cloud world, there now exist service models like Data Analytics as a Service (DAaaS). HPC/Grid as a Service are emerging as useful models to enable HPC on the Cloud [13][10][32]. Selecting the appropriate service model depends on certain factors, such as availability of suitable application software, need for development and test environment need for effective computing infrastructure control and management required distribution of data, services, and infrastructure, existence and complexity of enterprise IT infrastructure and datacenter/warehouse [10][24][30].

The most common solution is the adoption of the IaaS paradigm as far as HPC is concerned. IaaS typically provide pre-configured hardware resources to users through a virtual interface. Unlike PaaS and SaaS, IaaS does not include applications or even an operating system, implementing, all of that is left up to the customer, it simply enables access to the infrastructure needed to power or support that software. IaaS can provide extra storage for corporate data backups, network bandwidth for a company website server, or it can even enable access to high power computing which was previously only accessible to those with supercomputers. Amazon EC2, IBM SoftLayer, and Google’s Compute Engine (GCE) are popular IaaS offerings which implicitly power a huge portion of the backbone of the internet, whether users realise it or not. An IaaS cloud environment is based on a virtualisation engine. Virtualisation provides illusion of multiple independent replicas of every physical machine in the Cloud by means of a hypervisor [2][5][6]. Each replica has its own address space, devices, and network connections and is capable of running any software, including operating system that could be run on a stand-alone machine. Currently, a number of different Virtual Machine (VM) environments are readily available and can be used to provide server virtualisation, namely VMWare [11], Xen [12], Virtual Box [8].

The virtual engines differ in the approach used to run the host operating systems depending on the exploitation of hardware CPU virtualisation technologies (e.g. Intel VT and AMD-V) and on the type of licensing, either open-source or closed-source. The virtual engine can run the host in an unmodified fully virtualised approach or para-virtualised approach which is aware of the presence of the hypervisor [14]. On top of virtualisation engines, which physically manage the hardware, cloud environments offer a service-oriented interface for managing the virtual machines (create, destroy, suspend, migrate from a physical system to another, change the amount of available memory or the number of virtual CPUs assigned). There also exist a large set of
secondary services for managing the secure access to resources and for auditing and billing. At the state of the art, there exist many solutions for building up a cloud environment. It is therefore suitable to make use of all the Cloud service offerings to have a comprehensive HPC Cloud model. For an organisation that has in-house HPC equipment and only need specific services from the Cloud, selecting addible cloud services is of benefit [9].

As mentioned above, the most common solution to exploit cloud power in the context of HPC is to get a pay-per-use infrastructure. Unlike other cloud users, most HPC users usually exploit parallel hardware, and so they would like to get parallel hardware to execute their explicitly-parallel applications. They want to receive from the Cloud a possibly high number of powerful machines with fast interconnect that could resemble a high-performance computing cluster, (that is, they exploit the Cloud as a provider of Cluster on-Demand (CoD) systems). Cloud users request and obtain from the Cloud clusters that they can configure according to their software requirements. This is possible since these are in fact virtual clusters, whose management, even in terms of the number of nodes and their configurations, is completely delegated to the Cloud user [7].

The profitability is all the key difference between a real cluster system and the virtual cluster received from the Cloud. On one hand, a virtual cluster may be economically convenient, is fully configurable, and requires no long-term investment. On the other hand, it is not as fast as a physical cluster. Furthermore, understanding the limits of the Cloud interconnect is essentially impossible. After all, that is the idea of a Cloud, you cannot put your hands on its components. This is great for the end user, but is frustrating for the advanced HPC user who needs to identify the real hardware the application is running on. Cloud environments, from the HPC point of view, are a centralised resource of computational power with an objective of offering computational power to final users [7].

The above-discussed issues focus on the technological state of the art of Cloud and HPC, describing the architectural solutions offered. In most Clouds the performance of clusters is lost due to virtualisation, relatively slow networks and Cloud overheads which are the main reasons for the very slow diffusion of virtualisation and Cloud techniques into HPC environments. However, there are very good motivations for the adoption of VMs in this context. As everyone involved in HPC knows, during recent years there has been a continuous proliferation of different operating system versions. Many applications have strict requirements for their execution environments. Often the applications’ environment requirements are mutually incompatible and it is not reasonable to modify or to re-install system software on-the-fly to make applications work. Moreover, partitioning the computing hardware into closed environments with different characteristics is not an efficient solution. With that being said, it is reasonable to think that, apart from the inevitable performance loss, Cloud techniques will progressively spread into HPC environments [15].

The expansions of HPC Cloud providers are fairly evident and even the large public Cloud providers such as Microsoft are introducing authentic HPC technology to the Cloud as the Cloud market has matured. This change opens up the possibility for new users that wish to either expand their current computing capabilities or take the initial drive and try HPC technology without investing huge sums of money on an internal HPC infrastructure.

This explains the deliberation to integrate HPC with Cloud Computing [16][33] [17][18][34].

2 Cloud Computing Taxonomy

A rigorous Cloud Computing definition based on current literature is presented in this section. Based on the presented definition, taxonomy of current Cloud and HPC solutions is presented. Problems are identified based on what properties from the supplied definition of HPC Cloud in Section 4.1 are not satisfied by existing Clouds. If the means by which a property has been exposed is deemed inadequate, the poorly exhibited property is also considered a problem [20][22].

2.1 HPC Cloud Definitions

Neither Cloud Computing nor HPC Cloud have a concrete and commonly accepted definition. According to Gartner [22], Clouds are characterised by five properties:

1. Service-based - all resources within the Cloud system are to be made available via services that have well defined interfaces.

2. Scalable and Elastic - clients only use resources and amounts they need.

3. Shared - all resources are used at their full utilisation and not dedicated to any client.

4. Metered by Use - clients make use of Clouds on a pay-as-you-go basis.

5. Uses Internet Technology - Cloud services are built and accessed using Internet technologies, often the World Wide Web.

The NIST definition of Cloud Computing broadens Gartner’s definition in that clients have broad network access. This means that the Cloud is accessible via any network enabled device and requires Clouds to monitor and reconfigure resources based on service usage.
In another study, 21 experts were asked for their definitions of Cloud Computing [23].

Each expert used at least two of Gartner’s properties and some consider that Cloud Computing offerings fall under one of three broad categories:

- **Infrastructure as a Service (IaaS)** - virtual servers are provided where clients are able to create their required platforms from the (virtual) hardware upwards.

- **Platform as a Service (PaaS)** - complete hardware and software configurations (platforms) are offered to clients and maintained by Cloud providers.

- **Software as a Service (SaaS)** - clients are offered software applications/services and only have to focus on their use.

This analysis shows that Cloud Computing based on the description by Gartner and current Cloud offerings is made possible through the combination of virtualisation, Web services, and scalable data centers. With the recent emergence of HPC in Cloud Computing which give rise to the idea of HPC Clouds and/or HPC as a service once again there is the question of what the term HPC Cloud stands for and what properties need to be exhibited. Thus HPC Clouds are viewed as having the following properties:

1. **Web Service-Based** - all resources from data storage to cluster job management are done via self-describing Web services with Web APIs for software processes and Web forms for human operators.

2. **Use the Pay as You Go Model** - all HPC clients are billed for the resources they use and amounts thereof.

3. **Elastic** - if a client has a task that consists of multiple jobs in a required sequence (workflow) HPC Clouds are expected to allocate and release required services/resources in response to changes in the workflow.

4. **Clusters Are Provided On-Demand** - clients should be able to specify requirements and then (i) discover an existing cluster for immediate use or (ii) have an existing cluster reconfigured to satisfy client requirements.

5. **Guaranteed Performance** - typically, if cluster nodes are allocated to clients, all nodes are expected to be within close proximity to each other.

6. **Virtualisation** - for flexibility, Cloud Computing will require the use of virtualisation. However, virtualisation should be made an optional feature to HPC clients: they may have applications that do not work in virtual environments due to high latency sensitivity.

7. **Easy to Use** - clusters (physical or virtual) can be complex thus need to be simplified. First, unintuitive user interfaces (such as command lines) can frustrate human users into finding work around.

Second, some researchers, even experts may wish to spend more time conducting research rather than on HPC application and application configuration/modification.

These properties of the provided HPC Cloud definition are used to propose a simple HPC Cloud taxonomy that considered both major types of HPC Cloud solutions: virtualised HPC Clouds and physical HPC Clouds.

Figure 1 presents a typical HPC Cloud architecture with modules that require further development to fully meet the needs of HPC users. HPC users have different resource requirements and work, meaning a general purpose HPC Cloud architecture is not always good enough. General purpose Clouds have limited options when it comes to computational accelerators. Part of their problem is their virtualised nature, making it difficult to orchestrate and expose high-end resources such GPUs and FPGAs. High-end accelerators are not “plug and play”, and thus require purpose built, vertically integrated platforms with optimised turnkey workflows to really exploit their potential. On most Cloud platforms you get the least common denominator of compute, storage, and network, with some deviations toward higher end resources, but well within the confines of the overall general purpose infrastructure. Specialised Cloud providers such as Nimbix deliver optimised, vertically integrated platforms to cater to these specific high end use cases. Specialised Cloud platforms do two things differently. First service providers in this space focus exclusively on these types of workflows, simulation, analytics and machine learning amongst others. Second, specialised Cloud providers focus on solution cost rather than unit economics. While unit prices may be higher on specialised Clouds, overall solution costs are significantly lower. In short specialised Clouds allow users to focus exclusively on their domain expertise not on how to configure and operate Cloud platforms themselves. This democratisation without compromise is the key to unlocking long term innovation.

There is plenty of room for both general purpose and specialised Clouds in our world. Most people, businesses and organisations leverage multiple Clouds on a daily basis already, and choosing specialised platforms for high-end workloads versus compromising with lesser resources should be no exception. Our hunger for computing capabilities of all sorts is outpacing its supply, which means we will continue to see a very diverse ecosystem of Cloud Computing companies catering to all walks of life.
One of the most effective means of understanding Cloud Computing in the HPC context is to look to multiple use cases that have been springing up with particular velocity over the years.

While Cloud Computing has much to offer HPC (such as low cost, availability and on demand service provision), few Cloud based HPC solutions exist. There are even vendors that claim to provide HPC Cloud solutions but are simply resellers for other Cloud Computing vendors. CloudCycle [3] is such a vendor that sits on top of Amazon and sells HPC products to clients. In this section we show what HPC product offerings currently exist from Cloud Computing providers and examines what properties they exhibit from the HPC Cloud definition presented in the section above.

3.1 Amazon Cluster Compute Instances

An IaaS Cloud, Amazon’s Elastic Compute Cloud (EC2) offers virtual machines (instances) to clients who then install and execute all required software. EC2 offers a catalogue of instance types that detail the (virtual) hardware specifications and range from small 32 bit systems to large multicore 64 bit systems. There have been successful attempts to create clusters within EC2 manually yet others have deemed EC2 unviable solely on the network communication performance [35][34]

Recently, Amazon has offered the Cluster Compute Instance for HPC [24] which offers a (combined) 23 gigabytes of RAM, 16 Terabytes of storage and use 10 Gigabit Ethernet. In terms of the HPC Cloud definition, Cluster Compute Instances only exhibit the properties of being service based, clients paying for what they use, and the use of Gigabit Ethernet for performance. However, Cluster Compute Instances are still not adequate, as the property of ease of use is not exhibited. Clients are required to install cluster management software.

3.2 Microsoft AZURE

A PaaS Cloud, Microsoft Azure [25] provides complete hardware and software configurations on-demand. Thus, clients focus on the development and management of their own services and can make the services discoverable via the .NET Service Bus [21]. However, nothing more than a unique URI of each service is publishable.

In terms of support for HPC, Azure only acts as “supporting” to clusters running Microsoft’s HPC Server 2008 [26]. On site clusters lacking available resources can connect and off load tasks to Azure. Overall, the only property (through the use of clusters extending to Azure) is elasticity.

3.3 Adaptive Systems’ Moab

Adaptive Systems is a provider of HPC cluster management software and a provider who helped in the creation of Amazon’s Cluster Compute Instances. While Adaptive does not provide a Cloud per se, it is worth describing, as clusters are comprised of hardware and software. Of interest to this section are the Moab Adaptive HPC Suite and the Cluster Management Suite which contains a Cluster Manager, Workload Manager and Access Portal [27].

The Moab Adaptive HPC Suite allows each cluster node to automatically change its installed operating systems on-demand. For example, a cluster comprised of Linux nodes is able to change a required number of nodes to Windows, thus allowing the job to run. This feature, based on the definition in Section 2.1, exhibits the properties of clusters on-demand and ease of use.

The Cluster Manager offers the ability to partition clusters into virtual clusters, thus giving clients the illusion they are operating whole clusters dedicated to them. While Quality of Service functionality is offered, it is limited to functional aspects of cluster jobs such as the maximum amount of time the client will tolerate the job being in a queue. In general, this offering exhibits the cluster on demand property (as with the Adaptive HPC Suite).

In terms of workflows, orchestration of multiple services/executables, there is the Moab Workload Manager. It is a scheduler with a few extra features: it is possible for jobs to change their resource allocations during execution (for example, the first five minutes use a single node, the next five use two nodes, etc.) and integration with existing grids.
Finally, Access Portal provides job submission, monitoring and control to clients with a graphical view of the cluster job load based on the individual nodes. The problem with the portal is that getting jobs on the cluster is user unfriendly; the web page is mostly a wrapper for a command line. While Adaptive Systems does make reference to HPC on Cloud Computing, they do not provide a tangible solution. All they offer is architecture for resource consolidation.

4 Physical HPC Offerings in the Cloud

With Cloud Computing’s use of virtualisation, performance overheads are often exaggerated by some experts. Irrespective, there are clients that simply prefer to use physical servers over virtual servers.

Bare-Metal Cloud Services:

Many Cloud providers provide a virtualisation layer of software on the servers available for use. While virtualisation software makes it easier to manage a range of Cloud services, some customers require the faster performance, control and flexibility afforded by installing software directly onto the system. Virtualisation is not a requirement for Cloud-based Computing as some may believe. A bare-metal environment that is an exact copy of the operating environment that may exist within an internal data center can be created (Penguin Computing) [31]. The purpose of this section is to examine HPC Cloud offerings that use physical servers instead of virtual servers.

4.1 Silicon Graphics Cyclone

Cyclone is a Cloud that does not use virtualisation and offers itself to clients as both a SaaS and an IaaS Cloud. As a SaaS Cloud, Cyclone provides a wide array of applications for numerous scientific fields [29] from BLAST for biology experiments to Semantic Miner for Web ontologies. In terms of an IaaS Cloud, all that can be learned is that clients are able to install their own applications as in EC2, clients are provided with a server with an installed operating system as a starting point. However, the hardware specifications are extremely vague with the only detail published that the machines use Intel Xeon processors. As with previous Cloud offerings, the pay-as-you-go billing model is exhibited. However, that is the only property exhibited.

4.2 Penguin Computing on Demand (POD)

A similar solution to Cyclone, Penguin Computing’s POD offers physical cluster nodes to clients as utilities. Physical servers are used to carry out application execution while clients access POD via allocated (virtual) login servers. While Penguin Computing claims security on its POD offering, an examination of the documentation shows that the security relies on best practices (trust). Furthermore, when a client submits a job to a compute node in POD, the nodes performing the execution become dedicated to the client. While advertised as a Cloud, no HPC Cloud property is exhibited by POD. In general, POD is a remotely accessible cluster, not a Cloud by definition [28].

5 Expert Views on the Integration of Cloud Computing with HPC

Interesting observations of experts who are against the idea of Cloud Computing for HPC include views [3] by “Dr. Iordache, Dr. Kranzmuller, and Dr. Yelick who oppose the possibility of Cloud for HPC by claiming and stating that:

- HPC is about performance while virtualisation in Clouds is about adding more latency (overhead).
- There are only very limited uses for the public Cloud in HPC. For applications with larger storage requirements or closely coupled parallel processes with high I/O requirements, Clouds are often useless.
- There is a part of the workload in scientific computing that is well-suited to the Cloud, but it is not the HPC end, it is really the bulk aggregate serial workload that often comes up in scientific computing, but that is not really the traditional arena of HPC.”

Not all experts are against the idea, there are studies showing the effectiveness and opportunity of Clouds for HPC but the delivery of HPC performance with commercial Cloud Computing is not yet mature. However, the computational environments used in the study (Amazon’s EC2 and NCSA cluster) have inconsistent hardware and software specifications, and the experiment details are not specified precisely.

Professor Ian Foster, Microsoft’s Dan Reed, and Ms. Hemsoth stated:

- When HPC Clouds are to be assessed, optimisation for response time should be considered rather than the utilisation maximisation used on supercomputers. Based on that, EC2 is one Cloud for HPC offering that is promising.
- In response to the increasing costs of IT infrastructure, use and maintenance, the emergence of Cloud Computing, coupled with powerful software on clients offers a solution to this mystery. The net effect will be the accessibility of research capabilities that are only just available to the most elite scientists.

An analysis of HPC and Clouds shows that:

(i) The concept of HPC clouds has been rejected by some researchers because Clouds use virtualisation;
(ii) Not all problems require powerful and expensive clusters;
(iii) Organisations, although they depend on storing and processing large data, they are not prepared to invest in private HPC infrastructures;
(iv) HPC on Clouds offers cost and scalability advantages to clients.

An interesting discussion and analysis established on the above views are:

- Vendors such as SGI and Penguin do not offer virtualisation in their HPC offerings; they provide customised servers.
- There are very many bioinformatics, engineering, social sciences problems that could be successfully solved on less powerful clusters and on demand (without a need for waiting in a queue for execution). Furthermore, many clients do not wish to purchase, deploy, run and maintain even smaller clusters.
- Organisations prefer to concentrate on their mission statement activities, and clients prefer to concentrate on their problems, research, and development. Clouds allow on demand resource usage: the allocation and release is proportional to current client consumption, thus clients only pay for what they use. This implies the availability of Cloud resources is more important than performance. However, there is no guarantee that paying for (renting) extra nodes on a Cloud will guarantee significant performance improvement.

Even when purchase, installation and deployment of a cluster is complete, the cluster still incurs ongoing costs (mostly electrical power for cooling) long after research projects are finished. Besides the low cost and simplified access to specialised, high(151,257),(249,279)(322,257),(420,279)(493,257),(591,279) throughput systems, there is also the opportunity to improve collaboration between research projects. Instead of only making large datasets available to various research teams, it is now possible to expose whole research environments as on-demand services. Thus, it is clear that HPC Clouds have a bright future [3].

6 Transparent Cost Model

For companies and organisations considering moving from an in-house data center to an external one (the Cloud), financial factors may drive the decision. There are a number of factors to consider when comparing an on-site data center with a Cloud-based provider.

- **Capital expenditure (CAPEX):** As new hardware is developed and released by systems vendors, the cost to purchase servers must be considered. Many data centers have thousands of systems that are accessed continually, so careful planning is needed to ensure that only portions of the computing or storage infrastructure are replaced at a given time. As users demand more interaction with larger and larger data, new computer servers must be acquired. As newer and faster processors are released frequently by CPU providers at similar costs, IT purchasers must refresh systems on a regular basis, just to satisfy their end-user demands. This can lead to significant amounts of CAPEX on a regular, repeating basis.

- **Operational expenditure (OPEX):** As data centers have become more complex, significant effort is required to plan, maintain and manage the resources. With every new system acquired, it must be provisioned and integrated into the existing environment. Storage systems must be monitored for failure, and backup services implemented. In addition to managing the systems, software and storage, other costs such as power for the hardware and for the cooling and air circulation must be planned for. Each new compute or storage system requires a certain amount of power and cooling. Expert personnel are a significant cost as well. Knowledgeable staff in the specifics of complex applications (tuning for certain inputs) are required for an efficient implementation for the desired workloads. Over time, the operational expenses will be more than the original cost of the hardware.

Customers using a Cloud provider for HPC applications acknowledge that a cost is involved. It is important to make transparent to the users the entire cost of running their applications in the Cloud, in order to make valid and detailed comparisons to a comparison of on-premises versus the Cloud.

- **CPU granularity billing:** Since a physical server contains a number of sockets, each of which contains multiple cores and an HPC application that will run for some time, the actual cost to the user is important. Billing based on actual cores used rather than the entire server will be more reflective of the actual use of the computer system.

- **Prices are public:** A number of charges by the provider to the customer would comprise the final bill. It is important that when using a Cloud provider for HPC applications that all costs are made public so that the customer can make their own decision as to the benefits of using the Cloud versus in-house options.

- **No transport costs:** Since the data upload and download for an HPC application may be significant, some providers may charge for this service. The value of using the Cloud for running HPC applications is the application itself, so transport costs and billing should be avoided.

- **Storage costs:** As with any significant computing application, the amount of data produced can be large. It is reasonable to expect that there will be some sort of storage cost associated with HPC applications. Even if the transport costs are low to zero such that data could be moved back and forth to the customer site from the Cloud provider, this would delay the start-up of future...
runs on the same data as that data would have to be then transferred back up to the provider. Understanding the storage costs in terms of capacity and time frame is very important.

7 References


