Analysis of Scientific Cloud Computing requirements

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Abstract. While the requirements of enterprise and web applications have driven the development of Cloud computing, some of its key features, such as customized environments and rapid elasticity, could also benefit scientific applications. However, neither virtualization techniques nor Cloud-like access to resources is common in scientific computing centers due to the negative perception of the impact that virtualization techniques introduce. In this paper we discuss the feasibility of the IaaS cloud model to satisfy some of the computational science requirements and the main drawbacks that need to be addressed by cloud resource providers so that the maximum benefit can be obtained from a given cloud infrastructure.

1 Introduction

Nowadays Cloud computing has achieved great success in the enterprise world but it is still not common in the scientific computing field. Virtualization —that is a key component on the Cloud computing—, and its associated performance degradation, has traditionally been considered as not compatible with the computational science requirements. However, nowadays it is accepted that virtualization introduces a low CPU overhead [12] and that the penalty introduced in I/O can be significantly reduced with techniques such as SR-IOV [3] and PCI-Passthrough [4] that provide near native performance [5] using modern hardware with specialized support for virtualization.

Moreover, virtualization also brings some benefits that overcome its performance drawback, namely isolation and encapsulation. The isolation of VMs prevents influences from misbehaving VMs to impact on other running VMs, while encapsulation of VMs gives the means to provide load balancing and high-availability techniques. Virtualization also enables the consolidation of services by providing support for a wider range of services with the same physical hardware, that leads to a more efficient usage of the infrastructure and a reduction of maintenance costs.

This work complements some previous studies, such as Blanquer et al. [6], Ramakrishnan et al. [7] and Juve et al. [8]. This paper is focused in the set of requirements —for a resource provider and the cloud middleware— that a IaaS

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Cloud should provide for scientific usage, therefore there are some higher level aspects (namely programming models, job-oriented execution models, etc.) that are not covered by this paper. Also, it is worth noting that we are not focusing on higher level Cloud service models (such as PaaS or SaaS).

In Section 2 we give an outlook of the main benefits of using a Cloud Computing model for scientific research. In Section 3 a set of pilot use cases is described. From this preliminary group of applications, in Section 4 we have identified and established some requirements for a Scientific Cloud Infrastructure.

2 Cloud Computing benefits for scientific applications

Cloud Computing can be defined as “a model for enabling ubiquitous, convenient, on-demand network access to a shared pool of configurable computing resources (e.g., networks, servers, storage, applications and services) that can be rapidly provisioned and released with minimal management effort or service provider interaction.” [9]. This model allows many enterprise applications to scale and adapt to the usage peaks without big investments in hardware with a pay-as-you-go model.

On the other hand, Scientific Computing can be defined as the efficient usage of computer processing in order to solve scientific problems. It can be considered as the “intersection of numeral mathematics, computer science and modelling” [10] and spans a broad spectrum of applications and systems, such as High Performance Computing (HPC), High Throughput Computing (HTC), Grid infrastructures, small and mid-sized computing clusters, volunteer computing and even local desktops.

Many of the features of the Cloud Computing model are already present in current scientific computing environments: academic researchers have used shared clusters and supercomputers since long, and they are being accounted for their usage in the same pay-per-use basis —i.e. without a fixed fee— based on their CPU-time and storage consumption. Moreover, Grid computing makes possible the seamless access to worldwide-distributed computing infrastructures composed by heterogeneous resources, spread across different sites and administrative domains. However, the Cloud computing model fills some gaps that are impossible or difficult to satisfy and address with any the current computing models in place at scientific datacenters. In the following sections we describe the major benefits that the cloud computing model can bring to a scientific computing infrastructure.

2.1 Customized environments

One of the biggest differences between the Cloud model and any of the other scientific computing models (HPC, HTC and Grids) is the execution environment flexibility. While in the later ones the execution environment is completely fixed by the infrastructure and/or resource providers (e.g. the European Grid Infrastructure [1], one of the major grid infrastructures with 300+ resource centers providing

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1 See [http://www.egi.eu](http://www.egi.eu) for details
320,000+ cores, supports only 3 Operating System flavors), in the Cloud model the execution environments are easily adaptable or even provided by the final users. This makes possible the deployment of completely customized environments that perfectly fit the requirements of the final scientist’s applications.

This lack of flexibility in the current computing infrastructures —where a specific (or a very limited group) operating system flavor with a specific set of software and libraries is deployed across all the available computing nodes— forces most applications to go through a preparatory phase before being executed to adapt them to the execution environment idiosyncrasies, such as library and compiler versions. Moreover, some scientific applications use legacy libraries that are not compatible with the available environments, rendering this preparation step quite time-consuming or even impossible in some cases. The users could get rid of this procedure to an extent if they were able to provide its own computing environment, that will be the one used for its computations.

The requirement of a fixed operating system and the absence of customization has been identified \cite{11} as one of the main show-stoppers for many scientific communities to adopt Grid computing technologies. Only large communities are able to tackle this issue, thanks to dedicated manpower to manage and adapt their software development and deployment to the available scenarios.

Providing custom execution environments independently of the underlying physical infrastructure also allows long-term preservation of the application environment and opens the possibility of running legacy software with current and future hardware, which may help in the long-term preservation of data (and analysis methods for those data) of scientific experiments.

\subsection*{2.2 On-demand access with rapid elasticity}

The Cloud model is based on on-demand and pay-as-you-go access that gives the illusion of infinite resource capacity that can rapidly adapt to the needs of the user. Although providing an infinite resource capacity is not feasible in scientific datacenters, on-demand access to resources is useful for interactive tasks.

Resources in the cloud model are elastically provisioned and released, opening the door to using disposable environments without the overhead of a physical deployment would imply (hardware preparation, re-installation, configuration). These kind of disposable environments can be used for large-scale scalability tests of parallel applications, or for testing new code or library versions without disrupting production services already in place.

\subsection*{2.3 Non-conventional application models}

Most scientific computing resources (supercomputers, shared clusters and grids) are focused on processing and execution of atomic tasks, where each of these tasks may be parallel or sequential and they may have interdependencies between them or be executed concurrently. All the tasks have a common life-cycle: they are started, they process some data and eventually return a result.
However, in an Infrastructure as a Service (IaaS) Cloud, this traditional task concept does not exist: instead of tasks, users manage instances of virtual machines, which are started, stopped, paused and terminated according to the needs of the users. This different life-cycle makes possible to create creation of complex and dynamical long-running systems. For example this feature is used in the simulation of dynamic software agents, as in [12,13]; the decision making process in urban management [14] or behavioral simulations using shared-nothing MapReduce techniques [15].

3 Application use cases

In this section we present some preliminary use cases deployed in our private Cloud testbed. Although the applications are executed successfully in the current infrastructure, we have identified some drawbacks that should be addressed so that the scientific users could get even a better experience. These topics will be further discussed and described on Section 4.

3.1 PROOF

The Parallel Root Facility (PROOF) [16] is a commonly used tool by the High Energy Physics (HEP) community to perform interactive analysis of large datasets produced by the current HEP experiments. PROOF performs a parallel execution of the analysis code by distributing the workload (input data to process) to a set of execution hosts in a single program, multiple data (SPMD) fashion.

PROOF is used in the last phases of the physics analysis to produce the final plots and numbers, where the possibility of interactively change the analysis parameters to steer the intermediate results facilitates the researchers work and allows them to reach faster to better results. Data analyzed in this phase contains the relevant physics objects in set of files —produced by several previous processing and filtering steps of the original raw data collected from the detector— that may range from several GBytes to a few TBytes.

These analysis tasks are usually I/O bounded [17] due to the big volume of data to process and their relatively low CPU requirements: most codes perform filtering of the data according to the relevant physics to be measured.

Running PROOF requires the pre-deployment and configuration of a master, that acts as entry point and distributes the workload, and a set of workers where the user’s analysis code is executed. There are tools that automatize the creation of such deployments, which is not trivial for most users, in batch-system environments [17,18], but the machines are shared with other jobs, which may cause a degradation of the performance.

A IaaS Cloud testbed provides support to these kind of interactive analysis (i.e short lived sessions initiated on-demand by the users and with high performance access to data) with customized environments where the PROOF daemons run isolated from other workloads and are disposed as the analysis finishes.
3.2 Particle Physics Phenomenology

As many other communities, the particle physics phenomenology groups develop their own software for producing their scientific results. Software packages developed by the community have evolved independently for several years, each of them with particular compiler and library dependencies. These software packages are usually combined into complex workflows, where each step requires input from previous codes execution, thus the installation and configuration of several software packages are mandatory to produce the scientific results. Moreover, each scientific scenario to be analyzed may require different versions of the software packages, therefore the researchers need to take into account the different package versions characteristics for installing and using them. Some of these packages also require access to proprietary software (e.g. Mathematica) that is license-restricted. Although institutional licenses may be available, these are difficult to control in shared resources (like grids or clusters) due to the lack of fine grained access control to resources.

Setting up a proper computing environment becomes a overhead for the everyday work of researchers: they must solve the potential conflicts that appear when installing them on the same machine; and the fixed execution supported by the resource providers forces them to deploy the tools in ad-hoc clusters or even their own desktops.

A cloud computing testbed allows these researchers to deploy a stable infrastructure built with the exact requirements for their analysis where each machine is adapted to the different scientific scenarios to be evaluated, i.e. with the specific software versions needed for the analysis. The cloud infrastructure should be able to enforce any usage or license restrictions for proprietary software.

The possibility of creating snapshots of the machines also allows the recovery of previous experiments easily without recreating the whole software setup. These users would benefit from contextualization tools that automatically sets up and handles any dependencies of the software packages needed for the analysis upon machine creation \[19\].

3.3 Pattern Recognition from GIS

The Vegetation Indexes (NDVI\(^2\) and EVI\(^3\)) estimate the quantity, quality and development of the vegetation in a given area \[20\] by means of remote sensor data, such as satellite images. Using pattern recognition techniques it is possible to analyze the behavior of this index, so as to make a non-supervised vegetation classification. The analysis of such data also opens the door to other applications such as fire detection, deforestation and vegetation regeneration. For these data to be analyzed several specialized tools need to be deployed, such as Modis (satellite data analysis tools), GRASS and GDAL (geospatial libraries and tools), PROJ4 (cartographic data management) and R statistical programming environment (along with a large set of additional R modules for interacting with the other pieces of software).

\(^2\) Normalized Difference Vegetation Index
\(^3\) Enhanced Vegetation Index
These analysis were carried out in advance in the Grid so all the required software had to be installed beforehand. This required from the intervention of a local support team, so as to ensure the correct deployment of the tools and applications. During this process, incompatibilities were found between the dependencies of the required software and the operating system libraries installed. This process delayed the start-up of the actual data process several weeks. Moreover, the users faced a new computing environment and had to be instructed on how to interact with the installed software in order to use the correct versions that had to be installed in non-standard locations. Finally, the data produced were stored in an external database —that had also to be deployed— so that they could be finally accessed and analyzed by the scientists.

This use-case could profit from the Cloud computing testbed in two ways. Firstly, they could deploy a ready to compute self-contained image, bundling all the required software into it; and secondly, they could deploy their own infrastructure to store and retrieve their data. By doing so, they would reduce the time needed to start with the analysis (as the software is ready to be executed), the usage entry barrier (as they are deploying its own environment and they are familiar with it) and leverage the management of the external database service to the Cloud middleware (so they do not need to host a physical server for it).

4 Requirements for a Scientific Cloud Infrastructure

From our experience supporting the execution of the applications described on Section 3 we have gathered some requirements that a scientific cloud infrastructure should provide to its scientific users (however, this is not an exhaustive list and they are not formal requirements). We have classified these requirements in three groups: application level requirements, for requirements relevant for easing the usage of cloud resources; specialized hardware, for requirements related to high-performance access to specialized facilities; and enhanced scheduling policies, for those policies that the cloud provider should adopt to provide an adequate service for scientific users.

4.1 Application level requirements

The deployment of customized environments is one of the biggest advantages of the Cloud Computing model against any other traditional paradigms, but it may also represent a drawback for users that are not familiar with systems administration. In this context, scientific application catalogs and contextualization mechanisms are needed.

Scientific Application Catalogs The Cloud Computing flexibility to deploy customized virtual machines has associated the responsibility of create and manage them. Most scientific users are not prone to create, manage and maintain their own system images, nor have the skills or knowledge to perform those tasks in a secure and efficient way. These users may profit from a Cloud infrastructure where a
predefined set of supported images is already deployed, containing a wide range of the software they need. This ready to use Scientific Application Catalog can lower the entry curve for this new infrastructure.

Another aspect of this application catalogs is the access to licensed and institutional software — that is, software specially designed and/or tuned to be executed and integrated within an institution. In this cases, only restricted access to the images will be provided to the users, so that only the allowed ones are able to run the requested software. For example, access to shared and clustering filesystems — such as IBM GPFS, Lustre, etc. — can only be provided to machines that are trusted and properly configured. Offering these images in the catalog with restricted access, will give access to these resources easily.

**Image contextualization** The contextualization of images can be defined as the process of installing, configuring and preparing software upon boot time on a predefined virtual machine image. This way, the pre-defined images can be stored as generic and small as possible, since all the customizations will take place on boot time.

The image contextualization is tightly coupled with the Scientific Application Catalogs described in Section 4.1. The catalogs are useful for bundling self-contained and ready to use images, but sometimes this is something not feasible, because the required software evolves and changes frequently its version, because the software is under a development and debugging process and it is not practical to bundle it inside a self-contained image or simply because it needs some user-defined data so that it can be properly customized.

In those cases, instead of creating and uploading a new image for each application version and/or modification (a tedious process that is a time consuming task for the image creator), the installation and/or customization can be delayed until the machine boot time. By means of this mechanism the newest version can be automatically fetched and configured, or the defined and variable user-data provided to the image. This is done by means of ready to use and compatible image that contains all the necessary dependencies and requisites for the scientific applications to be installed. This contextualization-aware images will then be launched with some metadata associated, indicating which the software to install and configure.

Nowadays powerful configuration management tools exist that can help with the implementation of the described contextualization mechanisms. Tools such as *Puppet* [21], *CFengine* [22], *Chef* [23], etc. make possible to define a machine profile that will be then applied to a machine, so that an given machine will fit into that profile after applying it. However, these languages and tools introduce a steep learning curve, so that the cloud middleware should provide a method to expose the defined profiles to the users easily.

### 4.2 Specialized hardware

Scientific Computing sometimes requires access to specialized hardware that is not often present at a commercial provider, that is not focused towards scientific computing.
High performance communications Most parallel applications need low-latency, high speed network interconnects (such as Infiniband or 10GbE) in order to be efficiently executed. These interconnects are common in HPC environments, but they are not so common in cloud providers. Moreover, this hardware normally does not have the support for being virtualized or shared between several virtual machines. In order to give access to these devices two solutions exist: PCI passthrough with IOMMU or Single Root I/O Virtualization (SR-IOV).

High performance data access It is common that data oriented workloads demand high speed access towards the data to be analyzed. In a cloud framework, the data is normally decoupled from the instance that is running, meaning that it is being stored elsewhere not known a priori by the user. For example, block devices can be attached from a central storage location over the network (by means of Ata over Ethernet or iSCSI) to a running instance. If access to the data is not efficient enough, the computation will be executed on the node will suffer from a performance penalty that will make it unusable.

4.3 Enhanced scheduling policies

Scientific applications need of enhanced scheduling policies that take into account not only the requested and available resources, but also the kind of execution that is going to be done and any special requirement that the scientific user may have.

Instance co-allocation Some workloads require of the parallel execution of tasks across several nodes. In this context, large requests have to be discriminated between non-dependent and tightly-coupled or parallel nodes. Although the former can be provided in a first-come, first-server basis; the later ones need of some advances scheduling features, so that the collocation of instances makes possible that the user’s tasks can be properly orchestrated. This way, not only the resources should be reserved in advance, but also the overheads and delays introduced by the cloud management software should be taken into account so that the instances have the same boot time.

Short startup overhead When a request is made, the virtual images have to be distributed from the catalog to the compute nodes that will host the virtual machines. If the catalog repository is not shared or the image is not already cached by the compute nodes, this distribution will introduce a penalty on the start time of the requested nodes. This distribution penalty can be quite significant in large systems, or when bigger requests are made by a user.

Large requests are common in scientific workbenches, so a mechanism should be provided to ensure that these request are not penalized by this transfer time. Some possible solutions could be to share the image catalog, to pre-schedule the image transfers in advance or to utilize some efficient and intelligent distribution methods for the requested images instead of downloading them from a central location.
Performance aware placement A virtual machine can potentially share the same physical host with other machines. This can introduce a performance degradation if the machines are competing for the utilization of the system resources. For example, two machines that are executing some I/O consuming task can interfere between them. This issue has to be handled by the scheduler so that two competing machines are not scheduled in the same node.

On the other hand, as we already explained in Section 4.2, the requested nodes may need access to specialized hardware such as low-latency interconnects (for example Infiniband), GPGPUS, etc. In these cases, not only the scheduler has to be aware of these available resources, but also the cloud middleware should be able to manage them. These resources are normally attached to the virtual machines without being virtualized (that is, attaching the PCI device directly to the node) so they deserve a different treatment.

Spot and preemptable instances Long-running tasks are common in computational science. Those kind of workloads do not require from interactivity and normally are not time-bounded. Such tasks can be used to fill the computing infrastructure usage gaps, thus a better utilization of the resources will be obtained. This is normally done in traditional scientific infrastructures by means of several techniques, such as backfilling, priority adjustments, task preemption and checkpointing.

However, a virtual machine can be transparently paused into a safe state that can be resumed later on. This allows to create new execution types at a lower cost for the users, such as the so called by some commercial providers spot-instances: machines that will run whenever there is enough room for them, but that can be preempted, paused or even destroyed by higher priority tasks. This is an interesting topic for the scheduling field of Computer Science: the usage of reverse-auction [24] and other economical models [25] opens the door to a better utilization of the resources, by making attractive for some users to utilize the infrastructure in the usage-valley periods whenever they can afford to pay the price for those resources.

Bare metal provisioning There may be some situations where the user needs to run a native operating system instead of a virtual system. Some use-cases for the bare-metal provisioning are the deployment of machines that need to access to a given hardware that cannot be virtualized and/or directly attached to the virtual machine, non-x86 architectures, databases, etc.

4.4 Absence of vendor lock-in

Interoperability is an important feature for many communities. The usage of open standards such as the Open Cloud Computing Interface (OCCI) [26], Cloud Infrastructure Management Interface (CIMI) [27] and Cloud Data Management Interface (CDMI) [28] is way to avoid the vendor lock-in that currently exists with many commercial cloud vendors.

At a lower level it is also important also the adoption of the standards so as to avoid the “hypervisor lock-in”. In this context, the adoption of the Open
Virtualization Format (OVF) should be considered for the distribution of virtual appliances.

5 Conclusions

Cloud computing has permeated into the IT industry in the last few years, and it is nowadays emerging in scientific computing environments. However, there are still some gaps that need to be filled so that the computational science could completely benefit from it. In this paper we have made a sort review of the advantages that a cloud computing model can offer to scientific users and how either the middlewares and the resource providers need to adapt to satisfy their new potential users.

Cloud middlewares are normally arising from the commercial providers—being Open Source or not—and they are normally focused to satisfy their needs, that are not the same as the scientific users requirements. From our experience, one of the main fields needing from improvement in these middlewares is the scheduling, as described in Section 4.3. There is also room for improvement in additional and higher level applications, such as image catalogs and machine contextualization systems as described in Section 4.1.

Scientific computing datacenters have to move towards a mixed and combined model, where a given user can still access their traditional computational power—that is, using a batch system or using the Grid—but also they should provide their users with some additional cloud power that will complement the former computing models. This way, either the users the users will benefit from a richer environment, and resource providers can get a better utilization of their resources, since they will allow for new execution models that are currently not available.

References

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