SciCloud: Cloud for high-performance scientific computing

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Thesis

High-performance scientific computing can be done over cloud infrastructure and can be guaranteed a performance that is comparable to bare metal machines currently used in supercomputers or dedicated commodity clusters.

Rationale

Since the digital computer was invented, it has been an important tool in doing science. In fact, without it, progress in science will be quite slow. Several scientific breakthroughs have been made possible because of digital computers. From the sequencing of the human genome to the discovery of the Higg's Boson particle, the digital computer has its very important role. From simple arithmetic to modeling biological and physical systems, the digital computer is able to deliver the result of experiments in an accurate and timely manner.

Scientific applications, such as equation solvers and simulations, are very CPU-intensive and Memory-intensive. These applications, because of their heavy computational and storage requirements, are usually run in high-performance computing (HPC) infrastructures using supercomputers or commodity clusters for distributed computations. Setting up such infrastructures requires a lot of initial capital and technical investments. Once the infrastructure has been set up, maintenance costs will also be required to update the hardware and software components. Although these infrastructures are indeed useful, studies have shown that they are underutilized[1]. Their usage depends on the computing demand pattern of scientists and researchers. Most HPC clusters in research centers cater to a mix of researchers from different study areas. For example, physicists and chemists may share the same HPC cluster running on Linux operating system. Differences in usage requirements of these researchers affect the overall operation of the cluster. Provisioning the hardware and software requirements needed for scientific computing is thus very challenging because of these factors.

Despite the recent advances in hardware (increased processing speed and memory) and their decreasing costs, typical users do not harness the full capacity of their machines, either because the software they are using does not support them or their computing needs do not require access to the full capacity of their machines. Web browsing and word processing, for example, usually do not require high-performance machines whereas gaming needs them for an enhanced user experience. Another example is the case of laboratory computers used for instruction in academic institutions. Despite having the latest processors and a good amount of memory, they are typically used just for simple programming exercises which do not require the full access to hardware performance. These underutilized machines can be used for scientific computing needs.

Machines used in clusters are usually dedicated, which means that they cannot be used for other general-purpose computing needs. When running tasks, the number of machines used from the clusters used are usually statically set often with the assistance of system administrators managing the cluster. A scientist who needs to perform a simulation need to contact the cluster administrator to schedule the job that must be run.

Nature of Scientific Applications

Cloud Computing

Objectives

The main objective of this research is to develop cloud computing solutions to improve high-performance scientific computing. Specifically, this work aims to

- 1. evaluate existing public cloud offerings (Amazon EC2, Microsoft Azure) for applicability in scientific computing tasks;
- 2. deploy a private cloud setup using OpenStack for testing;
- 3. identify and describte the characteristics of scientific applications that make it a challenge to execute them on the cloud; and
- 4. develop a novel framework and architecture to make it easy and efficient for scientists to perform scientific experiments on the cloud.

Methodology

References

[1] Simon Ostermann, Alexandria Iosup, Nezih Yigitbasi, Radu Prodan, Thomas Fahringer, and Dick Epema. A performance analysis of EC2 cloud computing services for scientific computing. In *Cloud Computing*, pages 115–131. Springer, 2010.