PROCEEDINGS OF SCIENCE

From Large Scale to Cloud Computing

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The interest for cloud computing is increasing due to scalable and dynamic resource it provides. Also it eliminates the initial infrastructure cost and effort from client side. Both concepts are interesting for companies giving computational services. This was the motivation to develop a cloud version of our mould filing analysing tool for cloud resources.

In migration of the complete pipeline of the simulation we found out several similarities with large scale computing. Our perspective of cloud computing was for many small to medium calculations, however we found out that many developments are similar to the ones for large scale computing. In this presentation we describe such similarities and point out how they affect in our development in both lines.

The first similarity comes from the heterogeneous nature of both disciplines which affect in the same way to the solvers. Other connection is the data transfer which affects the pre-post processing in general while the objectives are different. In cloud reducing the data transfer results in reduction of the service cost and in large computing the objective is reducing it to be practical. Finally some solutions to the mentioned problems will be purposed and their effectiveness in each discipline will be discussed.

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1. Introduction

The use of cloud storage for share working and document transfer has grown very fast in the recent years and matured to be used by mass of users. This technology leads to cloud computing which becomes more and more interesting due to the dynamic nature of the resource it provides.

The cloud shares some similarities to HPC facilities with some advantages and disadvantages. The similarity comes from the fact that the paradigms used for development of the applications (MPI, openMP, etc.) are the same. Cloud comes with advantage of more control over OS which is very important in time of maintenance and support of industrial applications. One disadvantage is the less control over the hardware and the possible heterogeneity found in the given underline machine. Another drawback is the communication speed between nodes and also with the local machine.

In this work we mark out the similarities we found between this two fields of work and the reusable part of large scale development in cloud computing.

2. Experiences

This study of the cloud computing for industrial applications and comparing it with HPC computing is based on experiences described in this section.

2.1 High Performance Computing

The authors have created and actively develop the Kratos Multiphysics framework which is an open source framework for parallel multi-physics programs development. It is written in C++ and combines the efficiency with the modularity comes from object oriented design [1]. The framework and some of its applications has been migrated to high performance computing platforms where shows appropriate performance and scalability up to thousands of processes [2]. All these developments provide essential experience in HPC computing and highlight the difficulties to be addressed in this work.

2.2 Industrial Application

With its origin in academy, CIMNE tries to carry the state of the art methods into the industry via its spin offs. One of the examples of this technology transfer can be found via Quantech ATZ which is a spinoff of the CIMNE commercializing software for metal forming processes (Stampack) and also mould filling process (Click2Cast). The latter is the subject of the current work. Click2Cast is a mould filling simulation software which is a very automatic and simple program from user point of view. On the other side it solves a complex thermal and fluid coupled problem which requires large calculation demand. The ease of use, robustness and HPC are all came together in this software and provide important experience for this study. The interface is based on GiD pre-post processor which reveals the problems in post processing addressed in this work.

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2.3 Cloud Computing

The Click2Cast has been ported to the amazon cloud service. The solver is based on Kratos Multiphysics which is migrated to the cloud services. The linux version of the solver has been ported. This migration made known the problems addressed in this work.

3. Common Problems

The high performance computing and cloud computing has several common problems to deal with. We divide them into two different categories:

- calculation technology and implementation
- Visualization and data mining

In this section the difficulties in each category will be described.

3.1 Calculation

One of the important benefits of the cloud computing is accessing to large computer resources. Usually the hardware provided is not comparable with the ones in HPC facilities in performance. Taking into account the effect of virtualization and other latencies, a serial calculation may become less efficient than a dedicated workstation. So the parallelization of the code is a must. On the other side the amount of shared memory cores are in order of 16 to 64 (though increasing) so MPI parallelization becomes another key point. Another goal for cloud computing would be the use of very large computing resources. Considering the less performance of the network in these facilities in comparison with HPCs, scaling becomes more difficult.

As described before one of the disadvantages of the cloud is the lack of control over the hardware they offer at each instant. Many of the providers only provide you virtual cores with different categories of performance without revealing the underlying real hardware. So hardware optimization becomes less effective in cloud computing. While most of the time the underlying hardware for a parallel instant is the same but there are even no guarantee about that. All of these increase the importance of heterogeneous hardware support from algorithm level to the implementation of the code.

The dynamic nature of the cloud service implies the lack of control over machine load in time of execution. This means that some cores are in machines dedicated only to this job and some others may have also share the memory and other cores of the underlying hardware with other jobs submitted. Sharing the machine can change the performance of the code drastically, especially for memory intensive calculations (like FEM simulations). In these types of calculations all processes are synchronized and delay in execution of one them (due to the share load) results in delay in whole execution. This may also happened in HPC facilities but is easier to be avoided.

It can be seen that the parallelization in the cloud has to deal with the similar problems of large scale parallelization: more network overhead, complex load balancing and hardware heterogeneity.

3.2 Visualization and data mining

The connection to cloud facilities is via internet. The internet velocity is increasing and is suitable even for streaming or other data intensive applications. But the amount of data produced in a simulation can be much larger than to be handled effectively by internet connection. An example is running one night simulation which produces hundreds of gigabytes of results and takes one day to be downloaded from the server.

Many cloud services may charge for the data transfer from the server. So downloading the results from the server to the local even for smaller results can have cost drawback.

The local resources may cause a limitation in visualization. One of the targets of the cloud computing is to enable running simulations from a laptop or even a tablet. While the calculation is perform in the server side, the limited resources of these local resources prevent them from managing and visualization of the large results.

Large scale computing has to deal with very large results. In another scale cloud computing is dealing with the same problems: less results, but over slower network and local machine. Again we have a common problem to solve.

4.Common Solutions

The solutions for the problems described in the previous section can be divided in following categories: adapting the working process, innovative algorithms and improved implementation. The calculation problems can be solve with new algorithms and better implementation considering the heterogeneity while the visualization needs the adaption of the working process.

4.1 Calculation Solutions

Innovative algorithms are necessary for effective use of the cloud facilities. These algorithms logically have to reduce the amount of data passes through the network. But a more important aspect to be considered is the reduction of synchronization points (or times). Less synchronization lets better non-uniform load balancing over heterogeneous machines. It also reduces the network traffic and even more important, decreases the effect of communication latencies.

While in some cases the innovative algorithms are necessary, in other cases the existing algorithms can be already suitable. Grid computing and multi-scale simulation can be considered as existing solutions which are easily portable to the cloud computing.

From the implementation point of view the codes must be optimized considering the heterogeneity and less knowledge of the hardware. This can be achieved by adapting different programing paradigm and implement hybrid approaches. In this way the code can be adapted more effectively to the hardware provided.

Another solution to be considered is the HPC specific cloud services giving more hardware transparency and load control. Although some cloud services provide such a service, but the service can be improved.

4.2 Visualization Solutions

Dealing with the visualization problems requires a change in the working process. Everything has to be done in the server side with remote visualization. This affects drastically the implementation of the pre and post processors as described in following part.

The first adaption is data mining in server side. This leads to handle distributed data over the cloud in parallel. In this aspect it came close to big data paradigms. Data mining in server highly reduces the amount of data to be transferred over internet to the local machine. It also fulfils the objective of simulation using small local resources like laptops and tablets.

Simplification of the model can be used to reduce the transfer data size and make the local simplified model more manageable in local resources. In this case the goal is to provide offline result visualization over simplified model.

Finally remote visualization is the approach coherent with cloud service. However this implies graphical resources in the server side for optimum results.

5. Conclusions

The problems arise in cloud computing are similar to the ones in large scale computing. The calculation over cloud has to deal with less network performance, non-uniform load balance, heterogeneous machines and hybrid paradigms. The visualization and data mining has to be changed in the same way for cloud and large scale computing: data mining in server, simplification and remote visualization are the key solutions.

On the service side, the cloud services has to provide better HPC services with more hardware transparency and less virtualization. Better control of affinity is also important for memory intensive applications. A better HPC service helps the migration of the existing codes to the cloud services.

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