Chapter 9
Opportunities and Challenges in Porting a Parallel Code from a Tightly-Coupled System to the Distributed EU Grid, Enabling Grids for E-sciencE

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ABSTRACT

Any large scale computation, either in the science or arts, requires high performance computing (HPC) facilities. This computational environment may change over time. Thus the source code of a computation needs to be ported. The change in the computational architecture or system can make the porting of code between various HPC facilities challenging. This chapter introduces an example of an engineering application which runs on a HPC facility and the porting from a local computing facility to Enabling Grids for E-sciencE (EGEE) is described in detail.

The computational architecture of Enabling Grids for E-sciencE is introduced as it made our code porting very challenging, and the discussion presented is directly applicable to EGEE users. The final solution to the code poring problem is proposed, and its performance is examined. The solution to this problem be generally faced in the other large scale computation and so is applicable to users of other HPC facilities. This chapter gives a hint to those who have difficulties in applications with heavy data Input/Output (I/O) under the computational environment whose weak point is the data I/O.

INTRODUCTION

Research on distributed and parallel systems is one of the most important areas in computer science. This area is based on the exploitation of large computational and data storing capabilities. While the main components *i.e.*, processors and hard drives in a single computer are becoming smaller but with larger storage capacity and higher processing performance, distributed systems can integrate these individual resources into one large, heterogeneous, dynamic system that allows users to benefit from the possible improved performance. These systems are called grid.

The main goal of a well-maintained grid is to provide large scale resources connected via the Internet to researchers in the natural sciences and engineering who have applications with high demands for compute resources, or storing more data than a single machine can accommodate. Certainly, these applications must be parallelised to fully exploit the resource capabilities, and make them run faster in grid systems.

Researchers are nowadays surrounded with a variety of grid computing facilities. Some are more suitable to one's application than others but the cost and the performance of each HPC facility is also different. Furthermore, the cost, the performance and the suitability are always changing over time. Therefore researchers have to be prepared for the change in the computational facility and have to be able to adjust to the new computational environment.

This chapter shares the authors' experience of a significant change to the computational environment used in the daily research activities and provides some hints to those who may face the similar situation.

The authors' experience is based on the Enabling Grids for E-sciencE (EGEE) project.

The EGEE project-family, founded by the European Commission, started on April 2004. It has provided academic and industrial researchers the means to have access to large computing resources. It is focused on developing and maintaining a robust and powerful grid network and components, and to attract new users from industry by standardized training and dissemination events.

A new grid-middleware, called gLite was developed during this project. Its aim was to organize and connect the components of the large and international grid system. The last project of this family (EGEE-III) was ended on April 30th 2010. The new project was created to continue the development of distributed systems internationally in Europe and is called European Grid Initiative(EGI). In this project all of the old organizational-ideas have been reformed. EGI manages the collaborative work of NGIs (National Grid Initiatives) that are created to support the national grid-community and maintain the related grid-services.

Another but no less important project, founded by the European Commission is EMI (European Middleware Initiative). This project aims at integrating the three major European grid middleware systems (ARC, gLite, Unicore) into a unified middleware distribution (UMD) in order to support the co-operation of researchers in the same research field but with different grid-middlewares.

The section on Computation in Electromagnetics discusses the motivation of our research and introduces the core part of the equations necessary to understand the nature of our computation. Furthermore the section talks about the computational environment we used before we faced a significant change. The section on EGEE computational facility introduces the computational architecture of Enabling Grids for E-sciencE(EGEE), which is significantly different from our initial architectures. The section on the Adaptation of our code to EGEE describes the problems which we faced and presents the solutions. The section on Future research direction gives some insight and suggestion for the improvement of the computational algorithms as well as the algorithms which could be applied to the data I/O problems.

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