Chapter 13
The Sicilian Grid
Infrastructure for High Performance Computing

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ABSTRACT
The conjugation of High Performance Computing (HPC) and Grid paradigm with applications based on commercial software is one among the major challenges of today e-Infrastructures. Several research communities from either industry or academia need to run high parallel applications based on licensed

DOI: 10.4018/978-1-4666-0906-8.ch013
software over hundreds of CPU cores; a satisfactory fulfillment of such requests is one of the keys for the penetration of this computing paradigm into the industry world and sustainability of Grid infrastructures. This problem has been tackled in the context of the PI2S2 project that created a regional e-Infrastructure in Sicily, the first in Italy over a regional area. Present chapter will describe the features added in order to integrate an HPC facility into the PI2S2 Grid infrastructure, the adoption of the InfiniBand low-latency net connection, the gLite middleware extended to support MPI/MPI2 jobs, the newly developed license server and the specific scheduling policy adopted. Moreover, it will show the results of some relevant use cases belonging to Computer Fluid-Dynamics (Fluent, OpenFOAM), Chemistry (GAMESS), Astro-Physics (Flash) and Bio-Informatics (ClustalW)).

INTRODUCTION

The growing demand for parallel programming and High Performance Computing (HPC) poses a question: Grids (Foster & al., 2001) try to maximize the overall infrastructure exploitation instead of the performance of each single application running on them; in fact, the quality policies address the performance of the whole infrastructure over long periods, instead of the performance of each single run. For instance, a typical quality parameter for Grids is the total number of jobs run over a month. Grid users usually have a different point of view and they decide among the various computing solutions (proprietary cluster, buying time on a supercomputer, etc.) having in mind the time performance of their own applications as the most relevant parameter to be evaluated and traded-off with the expensiveness of the candidate solution. Bridging the gap between Grid and HPC may result in a great advantage for Grids as the business of massive parallel applications can bring novel resources and foster infrastructures’ sustainability. Some technical aspects of running HPC programs on Grids have been described in a recent paper (Orlando & al., 2008). Obviously the hardware equipment is the basic factor driving the application performance. The usual choice during the building of a Grid infrastructure is to have more processors instead of the fastest ones, in order to run more jobs simultaneously. This is one of the differences (probably the most important one) between an HPC cluster dedicated (often tailed) on a single application and a general-purpose Grid infrastructure. Nevertheless, as it happens for many technologies, adaptability and procedure standardization can largely compensate for the use of commercial components and architectures instead of customized ones. For instance, sharing resources allows more processors compared to the average dedicated clusters and this feature may be exploited to enhance the performances for well-scalable applications.

Having in mind the above considerations, the strategic importance of such HPC applications comes from the growing demand about this specific computing paradigm arising from both academic institutions and private enterprises. Small/medium size companies may take advantage of the Grid infrastructures to run HPC programs otherwise too much expensive for either hardware costs or lack of human expertise. Acting as a reliable, standardized and reasonably fast HPC facility, a Grid infrastructure can sensitively enlarge the range of its users. This is easier to happen for a regional Grid whose Virtual Organization (VO) usually gathers all the institutions acting on the same area, resulting in a more versatile and multi-disciplinary community compared to the international VOs that are often devoted to a single discipline. The following sections describe the efforts that the Sicilian Grid infrastructure is...
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