Parallel Computing and the Grid - Experiences and Applications
(Extended Abstract)

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1 Introduction

In recent years, grid computing developed from its first implementations as prototype grid environments to large-scale production grid infrastructures utilized during everyday work by scientists around the world. This demonstrates that the concept of the grid is more than merely a marketing phrase, but instead an enabler for new application domains in parallel and distributed computing. Among others, the EU EGEE Project [1] ("Enabling Grids for E-Science") is probably the worlds largest initiative for establishing a permanent grid infrastructure on a 24x7 basis. Such a grid that is always on and there to serve the community just like the ubiquitous networking infrastructures today is on the horizon, waiting for users to utilize it in their applications.

This paper explores the different possibilities for utilizing grids in applications, focusing on different parallel computing aspects as provided by grid environments. Basic concepts such as using the grid as a large data storage and management basis or as a collection of distributed supercomputers represents a new approach to computational science, where users are able to utilize unprecedented amounts of performance for tackling their scientific problems.

2 Parallel Computing on the Grid

In principle, we may distinguish two different aspects of parallel computing on the grid, the provision of different parallel computing techniques in general and their practical availability in existing grid computing infrastructures.

Starting with an overview of different existing grid infrastructures, such as the national Austrian Grid [3] project and the EU projects CrossGrid [2] and EGEE [1], we explore the provision of parallel computing technology in today's grid environments. This provides the basis for an overview of existing and future grid technologies for the parallel computing community, and answers to example questions, such as the following:

(a) Is it really feasible to execute a MPI program over distributed computing resources?

(b) Can the grid be used as a method to accessing different parallel computing resources more easily?

(c) Does the grid only permit message passing programs or are shared memory techniques applicable?

Each of these questions addresses different characteristics and options of parallel computing on the grid, where in fact different solutions may exist or have been attempted until today. By studying these characteristics, the problems in using grid infrastructures for parallel computing or rather the differences between traditional parallel computing systems and the grid become obvious.

3 Examples

The aspects described above are demonstrated with three different applications, which utilize the grid for tackling their particular scientific problems: Flooding crisis support, biomedical bloodflow simulation, and astrophysics visualization.

The flooding crisis support example [4] developed in cooperation with the Slovak Academy of Sciences focuses on a cascade of parameter studies, where meteorological, hydrological, and hydraulic simulations are performed to predict the behavior of water masses during flooding scenarios. With up to 1000 different executions, most of today's supercomputer systems would be overloaded. The grid seems to be the only viable solution for performing these simulations in time, especially with time being the critical factor in reacting to crisis scenarios.

The biomedical simulation [5] developed in cooperation with the University of Amsterdam, The Netherlands, utilizes MPI within their simulation codes to evaluate the blood flow in human arteries. This example is part of a training tool for surgeons, using real-life data from actual patients as the basis for placing bypasses. Clearly, the simulation should be as fast as possible to enable interactive positioning of the bypass, if possible within a sophisticated visualization environment.

Finally, the problem of visualizing large-scale data is addressed in the astrophysics visualization example [6], where an appropriate transfer function is needed for displaying available simulation data. Choosing the correct transfer function is important to gain insight in the behavior of the astrophysical objects, and is unfortunately far from being trivial, nor can it be performed automatically. This example demonstrates a semi-automatic approach, where parameter studies are combined using a genetic computing approach. In order to keep the human user in the loop, the usage of parallel computing techniques for real-time interaction is mandatory.

4 Acknowledments

The work described in this paper has been supported by a series of colleagues from the Joh. Kepler University Linz, the University of Innsbruck, the Slovak Academy of Sciences and the University of Amsterdam. Project funding has been received from the EU Commission through the CrossGrid project (IST-2001-32243), the EGEE project (INFSO-508833), and the Austrian Grid project funded by the Austrian bm:bwk, Federal Ministry for Education, Science and Culture under contract GZ 4003/2-VI/4c/2004.

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