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Supercomputers in Grids

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ABSTRACT

This article describes the state of the art in using supercomputers in Grids. It focuses on various approaches in Grid computing that either aim to replace supercomputing or integrate supercomputers in existing Grid environments. We further point out the limitations to Grid approaches when it comes to supercomputing. We also point out the potential of supercomputers in Grids for economic usage. For this, we describe a public-private partnership in which this approach has been employed for more than 10 years. By giving such an overview we aim at better understanding the role of supercomputers and Grids and their interaction.

Keywords: *grids; simulation in industry; supercomputers*

INTRODUCTION

Supercomputers have become widely used in academic research (Nagel, Kröner and Resch, 2007) and industrial development over the past years. Architectures of these systems have varied over time. For a long time special purpose systems have dominated the market. This has changed recently. Supercomputing today is dominated by standard components.

A quick look at the list of fastest computers worldwide (TOP500, 2008) shows that clusters built from such standard components have become the architecture of choice. This is highlighted by the fact that the fraction of clusters in the list has increased from about 2 % in 2000 to about 73 % in 2006. The key driving factor is the availability of competitive processor technology in the mass market on the one hand and a growing awareness of this potential in the user community on the other hand.

These trends have allowed using the same technology from the level of desktop systems to departmental systems and up to high end supercomputers. Simulation has hence been brought deep into the development process of academia and industrial companies.

The introduction of standard hardware components was accompanied by a similar trend in software. With Linux there is a standard operating system available today. It is also able to span the wide range from desktop systems to supercomputers. Although we still see different architectural approaches using standard hardware components, and although Linux has to be adapted to these various architectural variations, supercomputing today is dominated by an unprecedented standardization process.

Standardization of supercomputer components is mainly a side effect of an accelerated standardization process in information technology. As a consequence of this standardization process we have seen a closer integration of IT components over the last years at every level. In supercomputing, the Grid concept (Foster and Kesselman, 1998) best reflects this trend. First experiments coupling supercomputers were introduced by Smarr and Catlett (1992) fairly early – at that time still being called metacomputing. DeFanti et al. (1996) showed further impressive metacomputing results in the I-WAY project. Excellent results were achieved by experiments of the Japan Atomic Energy Agency (Imamura et al., 2000). Resch et al. (1999) carried out the first transatlantic metacomputing experiments. After initial efforts to standardize the Grid concept, it was finally formalized by Foster et al. (2001).

The promise of the Grid was twofold. Grids allow the coupling of computational and other IT resources to make any resource and any level of performance available to any user worldwide at anytime. On the other hand, the Grid allows easy access and use of supercomputers and thus reduces the costs for supercomputing simulations.

DEFINITIONS

When we talk about supercomputing we typically consider it as defined by the TOP500 list (TOP500, 2008). This list, however, mainly summarizes the fastest systems in terms of some predefined benchmarks. A clear definition of supercomputers is not given. For this article we define the purpose of supercomputing as follows:

- We want to use the fastest system available to get insight that we could not get with slower systems. The emphasis is on getting insight rather than on achieving a certain level of speed.

Any system (hardware and software combined) that helps to achieve this goal and fulfils the criteria given is considered to be a supercomputer. The definition itself implies that supercomputing and simulations are a third pillar of scientific research and development, complementing empirical and theoretical approaches.

Often, simulation complements experiments. To a growing extent, however, supercomputing has reached a point where it can provide insight that cannot even be achieved using experimental facilities. Some of the fields where this happens are climate research, particle physics or astrophysics. Supercomputing in these fields becomes a key technology if not the only possible one to achieve further breakthroughs.

There is also no official scientific definition for the Grid as the focus of the concept has changed over the years. Initially, supercomputing was the main target of the concept. Foster & Kesselman (1998) write:

A computational grid is a hardware and software infrastructure that provides dependable, consistent, pervasive, and inexpensive access to high-end computational capabilities.

This definition is very close to the concept of metacomputing coupling supercomputers to increase the level of performance. The Grid was intended to replace the local supercomputer. Soon, however it became clear that the Grid concept could and should be extended and Foster, Kesselman & Tuecke (2001) describe the Grid as

… flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources.

This is a much wider definition of the concept which goes way beyond the narrow problem of supercomputing. For the purpose of this article we use this second definition. We keep in mind though that the Grid started

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