High Performance Computing in Engineering and Science

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Summary. High Performance Computing (HPC) has left the realm of large laboratories and centers and has become a central part in simulation in engineering and science. We summarize the basic problems and describe the state of the art. A concept for an integrated approach is presented. This covers hardware and software aspects. Examples are presented to show the potential of an HPC workbench for engineering and science.

1 Introduction

High Performance Computing (HPC) simulation has long become a tool for scientific discovery and engineering development. In scientific research simulation is a third way of getting insight – besides the classical methods of theoretical and experimental work. The advantages of simulation over these two traditional methods are manifold: simulations can easily be reproduced and repeated anytime and anywhere – given the necessary computational resources; simulation experiments can easily be modified with an infinite number of variations at the scientists hand; all kinds of dangerous experiments can be avoided by using computer simulations – the best example being the US Accelerated Strategic Computing Initiative (ASCI) project [1] which aims at replacing atomic bomb tests by advanced simulation on supercomputers. In engineering simulation has become a central part in the life cycle of commercial products. Simulation is introduced already in the design phase and lasts until the customer support phase [2]. The key issue in industry is a reduction of cost which can be achieved by avoiding lengthy, tedious and expensive experiments on the one hand. On the other hand parameter variations can help to focus on the most promising design alternatives very early in the product development process. The worst scenarios can be sorted out early on.

The growing importance and changing role of simulation both in science and in the industrial production process lead to increased requirements both in terms of performance and in terms of usability of HPC systems. These
issues are addressed in this paper. The structure of the paper is as follows: section 2 analyzes the key issues for HPC in science and engineering both with respect to hardware and software. From this we derive a concept for an integrated simulation workbench which is described in section 3. An example for an integrated simulation based on such a workbench is described in more detail in section 4.

2 Key Issues for HPC Simulation

There is no exact definition of a high performance computer. Commonly it is assumed that the most powerful – and expensive – systems at any point in time are high performance computers or supercomputers. In order to be ahead of the competition supercomputers have always made use of innovative concepts both in hardware and software. Many of these concepts were later integrated into standard products. Today there is an ongoing discussion about which way to go in hardware and software development.

2.1 Hardware Issues

When Seymour Cray founded his first company he did so in order to have the freedom of developing the fastest supercomputer without having to consider the general commercially driven market for computers. Until then a computer was by definition also a supercomputer - and only a few research and government institutions were able to afford such systems. With the reduction in prices in the 60s a much wider market was opened for manufacturers. Since then hardware development is mainly driven by the mass market.

Cray was able to build specially designed supercomputers because of the cold war thinking of the time. Supercomputers were needed to build better weapons. Research institutions and universities benefited from this by being able to acquire supercomputers for the price that was to some extent subsidized by governmental organizations concerned with weapon development and security.

With the fall of the iron curtain in 1990 and the end of the cold war this unique and somewhat pathological market situation changed dramatically. US governmental institutions changed their funding strategy and turned away from vector supercomputing. It became common wisdom that a thousand commodity parts would do better than one highly sophisticated processor - and besides that would be cheaper. This thinking has had a major impact on supercomputing for at least one decade.

Parallel Computing

In the early 90s parallel computing - a concept that was investigated as early as the 60s - finally achieved a breakthrough in the market. Increased speed