Chapter 5
Using High Performance Scientific Computing to Accelerate the Discovery and Design of Nuclear Power Applications

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ABSTRACT

Present High Performance Scientific Computing (HPSC) systems are facing strong limitations when full integration from nano-materials to operational system is desired. The HPSC have to be upgraded from the actual designed exa-scale machines probably available after 2015 to even higher computer power and storage capability to yotta-scale in order to simulate systems from nano-scale up to macro scale as a way to greatly improve the safety and performances of the future advanced nuclear power structures. The road from the actual peta-scale systems to yotta-scale computers, which would barely be sufficient for current calculation needs, is difficult and requires new revolutionary ideas in HPSC, and probably the large-scale use of Quantum Supercomputers (QSC) that are now in the development stage.

INTRODUCTION

The present chapter briefly describes the evolution of supercomputers and the performances of the present computers from the point of view of the processing speed and memory size (Proffitt, 2012).

There are several architectural developments briefly described together with related issues such as: calculation quality assurance, failure tolerant architectures and power consumption.

The discussion is made from the point of view of needed resources for a complex quantum molecular dynamics application on each material structure. The magnitude of the calculation is carefully analyzed in order to include the smallest aspects and integrate them in a system that grows until it reaches the minimum practical limits. Here

DOI: 10.4018/978-1-4666-7461-5.ch005

from practical limits is understood the limit in time and space of the propagation of meaningful interaction, which considered explicitly may increase the quality of the approach.

The development of the new supercomputers as seen from the point of view of the need to simulate more completely the nano-materials presented before for being used in nuclear power structures.

The concept of harmony (Popa-Simil, 2012) is used in a various complex manner (Kuznetsova, 2005). On one side it represents the complex matching between the quantum reactions we aim to control and the material structure we aim to put in place that is rewarding the effort by high efficiency and high safety of the overall process. On the other hand it is referred as matching inside the supercomputer structure, matching the processors with memory and connection devices, driving to a harmonious calculation process development and the capability to know instantly when the process is right or wrong, allowing eliminating errors in early stages.

The chapter ends with a brief description of the quantum computing (Cho, 2012) approaches and the successes obtained in quantum communication using entangled particles and performing quantum cryptography, as a mean to assure fast, reliable information exchange inside and outside computing structures (Love, 2013).

The chapter highlights the aspect that the need triggers inventivity and future computer development will be closely bound to the new invention in hardware and software, driven by various computing needs.

AVAILABLE ARCHITECTURES AND SOLUTION APPROACHES

In this chapter we will discuss and compare current supercomputers' architecture and resource distribution solutions in order to classify them with respect to different performance evaluation parameters. We will also study the potential and suitability of existing approaches to co-exist with the classical infrastructure and use more the future distributed computing resources; more specifically, social networks on the cloud and cloud over social networks.

The development in the quantum computing and information teleportation will bring a new generation of supercomputers by two orders of magnitude faster and more compact, using complex quantum processors, that will open new horizons and will require changes in operation systems.

The 20-petaflops Titan supercomputer (olcf 2013) at Oak Ridge National Laboratory (Anthony, 2012), was world's fastest supercomputer during 2012. Cray's XC30 architecture, is supposed to allow the creation of supercomputers faster than 100 petaflops—100 quadrillion floating-point operations per second.

China is preparing the 100-petaflops, Tianhe-2 (Anthony, 2013) to be deployed by 2015, which in November 2013 become No.1 with only 33Pflops, and it was the successor to Tianhe-1A—a supercomputer that briefly held the title of World's Fastest back in 2010 (a first for China).

Cray's XC30 blade, with a bunch of Intel Xeon compute nodes marks an interesting shift away from AMD Opteron CPUs to the Intel Xeon (Murray, 2012)—the E5-2600 (Sandy Bridge) family of chips, because, Intel's latest Sandy Bridge- and Ivy Bridge-based chips are superior to AMD's offerings, and because, Intel acquired Cray's interconnect technology earlier this year. The XC30 debuts the new Aries interconnect—and Intel now owns Aries.Each XC30 blade (server rack) will contain four compute nodes, each of which contains two Xeon CPUs. There are 16 blades in an XC30 chassis, and three chassis per cabinet, totaling 384 CPUs per cabinet. Each cabinet will initially be capable of around 66 teraflops. Using 1,500 cabinets will scale up to 100 petaflops. At 1,500 cabinets, will host 575,000 CPUs and over 4.5 million individual cores (9 million, including Hyper-Threading). Each node can have up to