Ecological Impact of Green Computing Using Graphical Processing Units in Molecular Dynamics Simulations

Izabele Marquetti, North Carolina A&T State University, USA
Jhonatam Rodrigues, North Carolina A&T State University, USA
Salil S. Desai, North Carolina A&T State University, USA

ABSTRACT

Molecular dynamics (MD) models require comprehensive computational power to simulate nanoscale phenomena. Traditionally, central processing unit (CPU) clusters have been the standard method of performing these numerically intensive computations. This article investigates the use of graphical processing units (GPUs) to implement large-scale MD models for exploring nanofluidic-substrate interactions. MD models of water nanodroplets over flat silicon substrate are tracked wherein the simulation attains a steady state computational performance. Different classes of GPU units from NVIDIA (C2050, K20, and K40) are evaluated for energy efficiency performance with respect to three green computing measures: simulation completion time, power consumption, and CO₂ emissions. The CPU+K40 configuration displayed the lowest energy consumption profile for all the measures. This research demonstrates the use of energy efficient graphical computing versus traditional CPU computing for high-performance molecular dynamics simulations.

KEYWORDS

Graphical Processing Units, Green Computing, High Performance Computation, Hybrid 3D Printing, Industry 4.0, Molecular Dynamics, Nanomanufacturing

INTRODUCTION

Green Computing

Computing technologies are usually associated with high energy consumption. Thus, the energy efficiency of hardware and operating systems has become a financial and environmental concern (Zhu, Sun, & Hu, 2012). In the United States, desktop computers can represent around 10% of the consumption of the commercial electricity. Also, high-performance computers require a powerful cooling system for heat dissipation, thereby exacerbating the energy consumption. Consequently, computers can produce carbon dioxide equivalent to millions of cars (Li, 2012). The choice of software also influences the energy consumption profile and needs to be evaluated for power optimization purposes. Therefore, green practices are necessary to be incorporated into the design and operation.

DOI: 10.4018/IJGC.2018010103

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of systems. Green computing is a recent approach which allows computer systems to be energy efficient by implementing newer technologies to reduce power consumption without compromising their performance (Binder & Suri, 2009; Singh, 2015; Zhou, Xiao, Yang, & Gong, 2016; Zhu et al., 2012). In addition, to improve the efficiency and economy of computer systems, green computing also considers the reduction of computer systems impact on the environment and people. These include the achievement of energy savings and environmental protection, which can impact the life cycle of computer systems (Zhang, Gong, & Li, 2011). Harmon and Auseklis (2009) define green computing as improving the efficiency of computing resources while minimizing the environmental impact, considering the entire life cycle of a product. This can be achieved by reducing the consumption of water, energy, limited resources and avoiding the use of hazardous materials, thereby minimizing all waste in the entire supply chain.

The practice of green computing involves the design, manufacture, use and proper disposal of computers and all subsystems, such as printers, monitors, and storage devices, in an efficient and effective way that causes minimal impact to the environment (Velte, Velte, & Elsenpeter, 2008). These can be achieved in our daily routine with simple actions, such as switching off the computer when not being used, choosing computer monitors that are more energy efficient (LED backlighting), keeping the computer well-maintained and optimized, disabling unnecessary programs that start automatically, recycling computer parts, batteries and printer cartridge (Appasami & Suresh Joseph, 2011; Chakraborty, Bhattacharyya, Nargiza, & Bedajna, 2009).

Green computing can be considered in terms of both software and hardware. In software, its objective is to obtain methods that increase the efficiency of programs, decreasing storage space and saving energy. Some examples include Cloud Computing, Distributed Computing, and High-Performance Computing. For hardware, green computing includes certain technologies that enable a significant reduction in the energy consumption and the emissions footprint, while increasing economic efficiency and facilitating recycling (Zhang et al., 2011).

**Graphical Processing Units**

Graphics processing units (GPUs) have emerged in the past few years as an alternative to Central Processor Units (CPUs) due to their powerful capacity for applications that demand high computational resources. GPUs have advanced from a fixed-function processor with great three-dimensional (3D) graphics to a powerful programmable processor with application programming interface (API), resulting in processors with high arithmetic capacity. These processor units are now designed for large and parallel computation requirements with a focus on throughput instead of latency, having different applications than a CPU architecture (Owens et al., 2008). Owens et al. (2008) emphasize the importance of GPUs for scientific computing applications to solve large and complex computational problems, including protein simulations, scalable molecular dynamics simulations, and calculations of electrostatic potential maps.

In high-performance computing, energy consumption (Jan et al., 2012) is an important factor because significant computing power is required to solve intensive calculations and execute simulations. In addition to that, it is possible to reduce the amount of time to perform an operation and increase the productivity (Vijayaraghavan, Garg, Vijayaraghavan, & Gao, 2015). Studies in the green computing field show that a large amount of energy can be saved by focusing on environmental protection and conservation of energy (NRC, 2010). Zhang et al. (2011) used three computing systems to evaluate parameters such as green-related indexes to improve the green computing systems. Singh, Naik, and Mahinthan (2015) demonstrated that the choice of energy-efficient API with optimal parameters have a significant impact on energy savings for different servers. As an example, it was possible to save up to 76% energy during a file reading routine. Cecilia (2013) presented GPU implementations of two different nature-inspired optimization methods to validate hardware enhancements using Nvidia’s Fermi architecture. Picariello, Rapuano, and Villano (2013) have developed a measurement system and test-bench architecture to measure the instantaneous power consumption from the power line of
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