Simulation for Predictive Science: The Promises and the Challenges of Exascale Computing

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Summary: Large-scale simulation is a key tool, together with experimentation, used to gain understanding of and model materials and their behavior under extreme physical conditions, and to incorporate that understanding into a broader framework that allows one to explore and predict how complex, engineered systems behave, particularly under conditions which cannot be directly tested through experiments. These are difficult tasks, and it is anticipated that exascale (10^18 FLOPs, or floating point arithmetic operations per second) computing will be needed to solve many of the key challenges. However, the evolution of computing technology has reached one of those junctures where continued performance growth can only be achieved with a significant shift in the computing architecture, presenting many challenges to systems and applications. The experience gained within the U.S. Department of Energy (DOE) National Nuclear Security Administration (NNSA) Advanced Simulation and Computing (ASC) Program to date performing simulations on petascale (10^15 FLOPs) computers using advanced architectures, such as IBM’s cell or Blue Gene technology, gives us some insight into what are both the opportunities and the challenges we are likely to face as we move on to the exascale level of scientific computing. Planning for a broad-based effort, jointly sponsored by NNSA and the DOE Office of Science, has been initiated through seven U.S. National Laboratories. Co-design of algorithms, software and hardware will be a critical means to achieve success, and three national co-design centers have been funded.

Abstract

Users of high-performance computing, and indeed all information technology related sectors including manufacturing, financial and other services, science and engineering, defense and government, entertainment, etc., have for several decades grown to be dependent upon continuous performance improvement characterized by Moore’s Law, which states that processor speeds will double every eighteen months. However, due to the physical limitations of silicon, the rate of increase of single-processor performance has slowed, and is expected at best to level out. Parallelism is currently deemed to be the only solution for meeting the demand for continued performance growth [1]. However, limitations imposed by power consumption and the increasing costs of energy will constrain even the performance of parallel computing systems unless the computer designers take fundamentally different approaches [2]. This is largely driven by the need to minimize data movement, the cost of which threatens to overwhelm the cost of performing the mathematical operations (Figure 1) unless radical new approaches to the computer architectures and the means of programming applications to run on them are devised [3].

The refactoring of application approaches is a burden, but also presents opportunities to achieve new levels of scientific discovery not previously accessible, both features glimpsed in early experiences and results using the pioneer Roadrunner system, a petascale hybrid architecture built by IBM using PowerXCell 8i processors and run at Los Alamos since 2009 (Figure 2). Top level technology challenges for exascale systems initially defined in a DARPA study in 2008 are still seen as our greatest challenges: energy and power, memory and storage, concurrency and locality, and resiliency [4].

Reaping the performance benefits of the technology changes will only be realized through a co-design approach that considers the algorithms, software stack, hardware system, and applications together, and
the technology “sea change” presents us with the perfect opportunity to do so. The Exascale effort in the U.S. has evolved as a broad-based effort sponsored by the DOE, jointly through NNSA and the Office of Science, and planned primarily by seven National Laboratories (collectively referred to as the E7), including Lawrence Livermore, Oak Ridge, Los Alamos, Argonne, Sandia, Lawrence Berkeley, and Pacific Northwest, and actively engaging all relevant potential industrial partners. The effort is structured to promote both industrial competition and community cooperation in developing the elements that must span and integrate across diverse hardware systems. Three national co-design centers have been initiated by the Office of Science Advanced Scientific Computing Research (ASCR) to tackle the co-design concept in the context of three distinct application arenas: combustion, advanced reactors, and materials, with the objective of jointly enabling exascale-ready applications and systems.

Within this partnership, the intent of NNSA is to develop its computational tools as part of a predictive science capability in support of national security interests. Basic scientific understanding of material properties, scale bridging, and materials behavior under extreme physical conditions are key components and strong drivers of both large-scale scientific computing and experiments. Exascale computing will likely be needed to address materials modeling challenges. The predictive capability aims to incorporate the understanding gained and models developed using experiments and calculations into a broader simulation framework that will allow one to explore and predict how complex, engineered systems behave, particularly under conditions which cannot be directly tested through experimentation. Exascale computing, in the broader sense that incorporates co-design, is considered to be a requirement of that capability.

References


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