Introducing Extreme Scale Science

The Department of Energy (DOE) has critical scientific problems which will require computing resources significantly greater than our current state of the art. The current designs do not extend to the capabilities and significant challenges such as those addressed in the following articles.

The issues discussed include, but are not limited to:

- Physical limits are being approached which will significantly affect future large-scale computing system architectures, and there is only limited experience at this time to gain needed insight into new architectural features, especially at scale.
- Key platform technology innovations have to occur, including system power, reliability, availability and serviceability, memory and communications improvements, and scalable system software infrastructure.
- New models, new science and algorithm development, and programming models are needed to handle new levels of parallelism. For example, the next-generation National Nuclear Security Administration (NNSA) Sequoia system will have more than one million processors and support about 6.5 million threads. Exascale systems will be significantly larger.

The goal of the extreme scale computing initiative is to undertake a 10-year campaign to provide up to 1,000 times more powerful computing resources to meet critical DOE mission needs. The research would include the entire spectrum from simulation of new ideas through development of prototype hardware and transfer of the underlying knowledge to U.S. industry. The Office of Science (SC) and NNSA are expected to partner on this initiative. Extreme scale computing is critical to DOE mission needs in energy, the environment, and national security. Computational Partnerships with SC and NNSA application scientists, computer scientists, and applied mathematicians are expected to develop the new scientific applications codes that will be required. As part of this initiative, ASCR and NNSA will identify long-term research into the development of a robust, open-source computational environment for peta- to exascale systems, including system software, tools, and mathematical libraries that will be common to both systems. A major intermediate goal of this initiative is the development of a 200–300 petaflop/s prototype with common software stack by the end of five years and designed to meet DOE mission needs based on the input from each of the Center's application partners.

Investments in applied mathematics and computer science-based research programs will continue to advance understanding of the complexities of extreme-scale computing and can breed breakthroughs in key areas, such as uncertainty quantification, verification and validation.

The following articles on energy, climate, biology, security, hardware, and software address some of these issues and are intended to begin a dialogue within the science and technology communities on the scope and timing for proceeding to the exascale.

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