Reasserting U.S. Leadership in Scientific Computation

Summary

The U.S. faces a major challenge in scientific computation, the foundation of scientific discovery in the 21st Century. A clear path, however, is available for the U.S. to regain leadership in this critical field.

The U.S. has lost the lead in climate science research. Other areas of computational science critical to the Department of Energy's (DOE's) mission are at risk. The Earth Simulator, a supercomputer in Japan (NEC-GS40) dedicated to climate science, became operational in April 2002. The first results from the Earth Simulator are stunning. We currently estimate that climate codes implemented on the GS40 outperform ours by one to two orders of magnitude. In the face of this development, and given the science and policy imperatives associated with climate research, U.S. climate scientists have no recourse other than to travel to Japan and form partnerships with Japanese scientists to use the GS40. Furthermore, certain classes of science can only be investigated on the Earth Simulator.

The Earth Simulator is on the Moore's Law[1] trajectory of rapid innovation. It is distinguished by a design that is optimized to meet the needs of scientific computing rather than those of the commercial market.

The Earth Simulator is a general-purpose computer. We expect the Japanese will build on this success and expand their assault on U.S. computational science leadership. Their strategy is clear: provide a focused ultra-high-end computing resource, recruit the best and brightest scientists to collaborate on its use, acquire the knowledge to dominate a computational science discipline and develop the codes to harness that knowledge.

[1] Gordon E. Moore's simple observation more than three decades ago that circuit densities of semiconductors had and would continue to double on a regular basis.

We understand this strategy very well because we developed it and used it to attain world leadership in the areas of computational science important to DOE's mission. If we allow the Japanese to deploy our strategy uncontested, we will surely lose the lead in other computational science disciplines.

Since computational science contributes to DOE's energy and national security missions, the implications of falling behind other nations in advanced scientific computing are widespread and potentially grave.

The Office of Science's Role

The Office of Science has been the world leader in using advanced computers as tools for scientific discovery for the past 50 years. We have worked closely with U.S. computer vendors to bring their high-end machines into productive use.

The Office of Science invented the concept of concentrating unprecedented computing power to advance science and to achieve breakthroughs in targeted applications disciplines. We used this model to establish the Magnetic Fusion Energy Computing Center over 25 years ago, which has grown and diversified to become the National Energy Research Scientific Computing Center (NERSC). The National Science Foundation adopted this successful model for their supercomputer centers. The Office of Science has made a series of investments in computational science—through focused computing capability resources at the William R. Wiley Environ-

mental Molecular Sciences Laboratory (EMSL), the Center for Computational Sciences, and at NERSC.

The Office of Science still has outstanding interdisciplinary teams of application scientists, mathematicians, and computer scientists ready to take on great challenges.

The Scientific Discovery through Advanced Computing (SciDAC) program and the computational science collaborations under way between the Advanced Scientific Computing Research program and programs in Biological and Environmental Research, Basic Energy Sciences, and Fusion Energy Sciences are preparing scientists across the Nation to take advantage of Earth Simulator-scale computing resources. But even before the SciDAC program, the Office of Science was only able to satisfy a third of its requirements for high-performance computing. The Earth Simulator will put U.S. scientists at a 10 to 100-fold disadvantage vis-à-vis their colleagues in Japan.

The Approach

The Office of Science has an opportunity to restore U.S. pre-eminence in the computational sciences. A successful response might include the following steps:

- Domestic vendors could provide systems that match or exceed the GS40. Building such a system is not constrained by the technology. However, a strong partnership between the DOE and the vendors will be needed to evaluate and to drive the development of promising computing architectures for science simulations.

- In the short term, the science gap in the U.S. created by the Earth Simulator can be reduced by significantly enhancing the existing high-end computing capability as well as networking and incorporating the best available U.S. technology.

- In the mid and long term, the threat from the Earth Simulator to U.S. science can be eliminated and substantially surpassed in a 5-year time period through an aggressive, integrated portfolio of investments. Program elements and activities may include advanced architecture development, computational science and enabling technology research, and focused technology deployment in support of its mission applications.

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