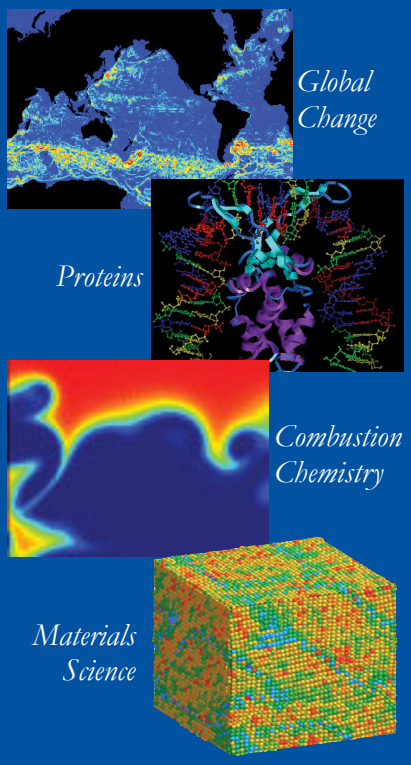
Office of Science

U.S. Department of Energy

Advanced Scientific Computing Research

The Office of Science's Advanced Scientific Computing Research (ASCR) program supports fundamental research in applied mathematics, computer science, and networking—and provides world-class, high-performance computational networking tools that enable the Department of Energy (DOE) to succeed in its science, energy, environmental remediation, and national security missions. The program annually funds research at about 65 academic institutions and 10 DOE laboratories. More than 2400 scientists in universities, Federal agencies, and U.S. companies use ASCR-funded high-performance computers each year. Research communities that benefit from these resources include structural biology; superconductor technology; medical research and technology development; materials, chemical, and plasma sciences; high energy and nuclear physics; and environmental and atmospheric research.

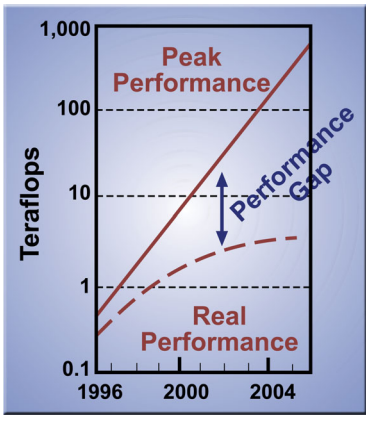


The Opportunity

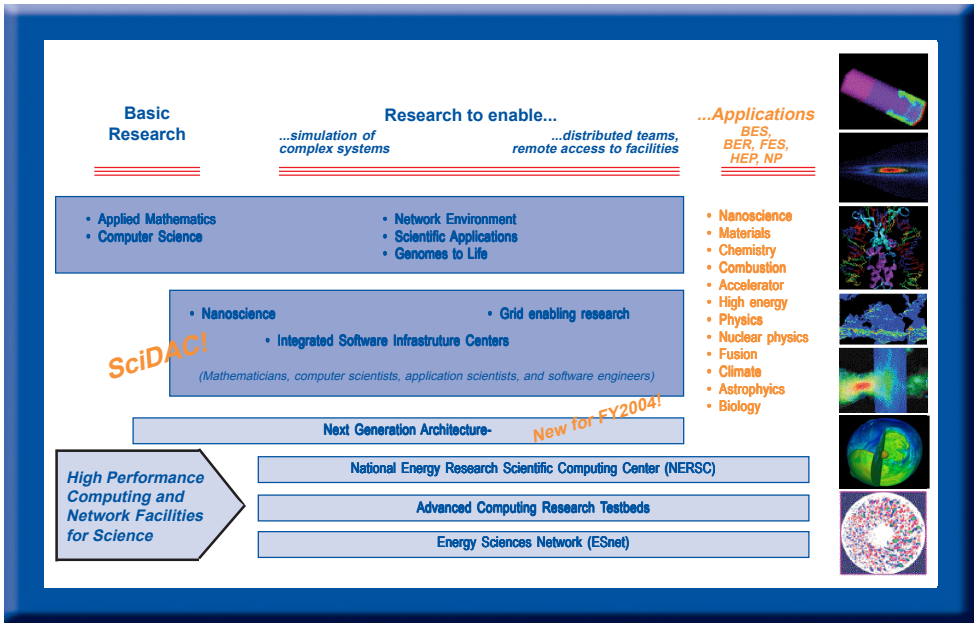
Computational modeling and simulation made dramatic contributions to the advancement of science in the 20th Century. Driven by rapid technological advances within the past two decades, computing and high-speed networking have emerged as powerful tools for science. However, unless software keeps pace with the terascale computers being developed, scientists will not be able to take full advantage of these powerful new research tools. A focus for ASCR is to bring software advances up to the same level as these hardware advances. These computational tools are essential to the development of new energy technologies and the discovery of new scientific knowledge. The Office of Science has numerous scientific questions that can only be addressed through advances in scientific computing, such as predicting climate change or understanding complex biological systems.

The Challenge

ASCR plays a major role in the Scientific Discovery through Advanced Computing (SciDAC) program. This is a set of coordinated investments across all Office of Science mission areas with the goal of achieving breakthrough scientific advances through computer simulation that were impossible using theoretical or laboratory studies alone. By exploiting advances in computing and information technologies as tools for discovery, SciDAC encourages and



enables a new model for multi-disciplinary collaboration among research scientists, computer scientists, computational scientists, and mathematicians. The product of this collaborative approach is a new generation of scientific simulation codes that can fully exploit terascale computing and networking resources and close the gap between theoretical performance and what can typically be achieved in practice on current-generation supercomputers. The SciDAC program will bring simulation to a parity level with experiment and theory in the scientific research enterprise as demonstrated by major advances in climate prediction, plasma physics, particle physics, astrophysics, and computational chemistry.



Computing systems hardware and software infrastructure

ASCR is developing software tools that enable scientists to remotely access and control facilities and share data effectively with colleagues on a routine basis. Advanced networking and distributed computing techniques must become ubiquitous. Existing barriers associated with remote resource access and the integration of geographically distributed resources must be overcome through the development of innovative software tools and protocols.

Investment Plan

Research on Next Generation Computer Architectures expands the ASCR research portfolio to identify and address major computer architecture bottlenecks to the performance and capability of critical DOE science applications. In this context, solutions will be developed to enable scientific simulations on high-end computers that include computer hardware technology, architecture, and design trends motivated from a scientific user perspective. Research investments will be made to couple computational scientists and computer scientists with U.S. computer vendors to orient future computer architectures towards the needs of science. Further research will improve the performance of simulations on high-end computers, remove constraints on the human-computer interface, and discover the specialized information management and analysis techniques that scientists need to manage, analyze, and visualize extremely large data files.

The Benefits

High-performance computing provides a new window for researchers to observe the natural world at a fidelity that could only be imagined a few years ago. Research investments in advanced scientific computing equip researchers with premier computational tools to advance knowledge and to solve the most challenging scientific problems facing the Nation.

Contact

Dr. C. Edward Oliver, Associate Director
Office of Advanced Scientific
Computing Research
Office of Science
U.S. Department of Energy, Headquarters
19901 Germantown Road
Germantown, MD 20874-1290
Phone: 301-903-7486 Fax: 301-903-4846
E-mail: Ed.Oliver@science.doe.gov
Website: www.science.doe.gov/ascr

July 2003