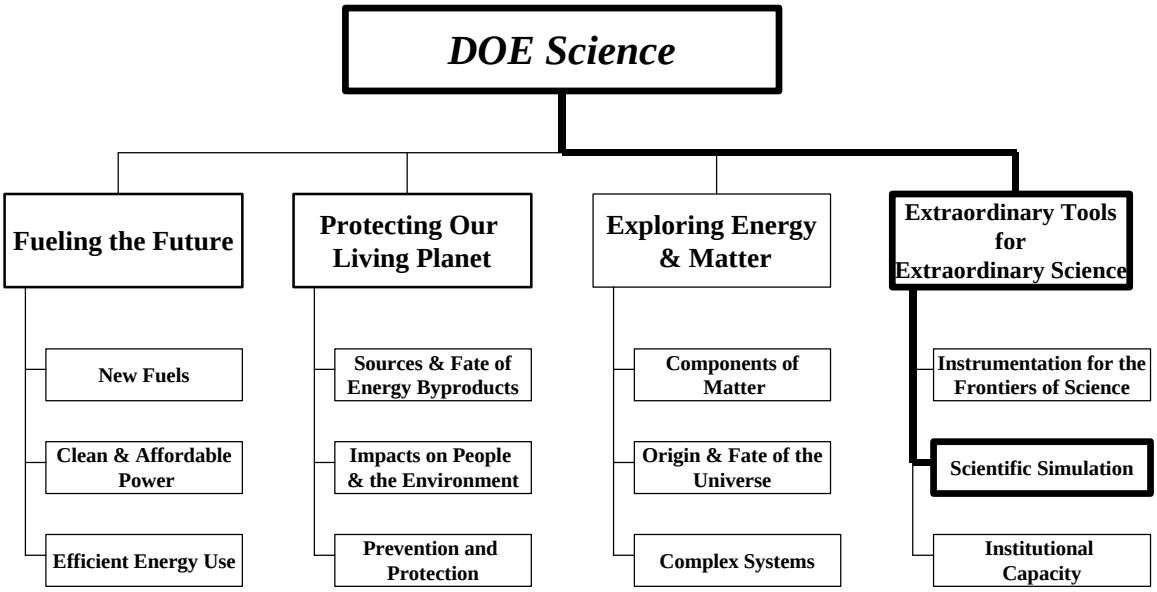
Chapter 12
Scientific Simulation

Scientific Challenge: ***To achieve computation and simulation as a critical tool in future scientific discovery.***



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Today computing is an integral part of virtually all scientific research. The World Wide Web was first developed by high-energy physicists to improve the scientific effectiveness of large, geographically distributed detector projects. As the price of microprocessors has fallen, computers have become an integral part of most advanced scientific instruments. In fact in many cases it would be impossible to accurately determine where the "instrument" ended and the "computer" began. Finally, high performance computers will be major instruments for scientific discovery in the coming years because they provide us with unique ways in which to view and analyze the world.

Simulation of physical systems on computers has been a critical component of DOE's (and its predecessor agencies') programs for 50 years. Driven initially by requirements for nuclear weapons design, computing is now critical to all of the missions of the Department. This has led the department to adopt a three-element approach to scientific simulation: (1) development of the advanced computer representations of physical systems of interest, (2) ultra high performance computational and communications facilities, and (3) development of the computational and software tools that enable scientists in the disciplines to make effective use of the computational and communications facilities. This approach is integral to the strategy for planning the future of scientific simulation in the Department. DOE's effective coupling of these elements has led to its leadership in the field.

Applications Software

Description, Objectives, and Research Performers

These activities focus on developing, testing, and using advanced computer software that realistically models physical processes. Significant portions of this activity are integrated into the management of all of the science programs of the Department. Examples of the types of applications software developed include global climate and ocean models, relativistic quantum chemistry software to understand the behavior of plutonium and uranium compounds in soil, and software to model fluid flow in combustion devices. These efforts have two common objectives: first, to increase the fidelity of the mathematical models of the physical phenomena under study; and, second, to find and implement ways of translating these models into computer code in ways that achieve very high efficiency and performance. This research is primarily conducted at national laboratories and universities.

Research Challenges and Opportunities

The rapid increase in computer speeds over the past decade has made possible applications with unprecedented fidelity to the natural world. It is now possible, for example, to create coupled atmosphere-land-ocean climate models with sufficient resolution to describe regional processes accurately. This change is opening up whole new fields of predictive computational inquiry. However, the applications developers must overcome significant challenges to take advantage of these resources. Both the range of physical phenomena that need to be included and the increased complexity of the next generations of computers will require large, interdisciplinary teams to develop and analyze the results of the next generation of scientific applications. In addition, the rate of change of the underlying computer systems implies that scientific software will have to be developed that is capable of being moved from one generation of hardware to the

next many times during its life. Finally, implementing the appropriate scientific models on the next generation of hardware with perhaps 10,000 processors will require discovering new ways to represent physical models on computers.

Overcoming these challenges will dramatically improve our ability to predict the behavior of physical systems through simulation. Prediction of mechanical properties of materials from microscopic structure; predictive design of low-emission diesel engines; and predictive models for complex systems such as fusion plasmas, pollutant flow through geological structures, and biological molecules are only a few of the advanced applications that will become possible. This type of computing will also enable the integration of optimization with predictive simulation and result in faster, more cost-effective design of processes ranging from particle accelerators for basic science to chemical processes in refineries.

Research Activities

The development of high performance applications software for scientific simulation is embedded in all of the scientific programs of the department. Current applications that use the National Energy Research Scientific Computing Center (NERSC) come from all of the areas supported by the Office of Science. In addition to the efforts which are embedded in the individual programs, DOE has conducted DOE-wide competitions such as the "Grand Challenge" component of DOE's High Performance Computing and Communications (HPCC) program. These projects represent partnerships between computer, computational, and other scientists to develop new techniques and make significant advances in the scientific state-of-the-art. The breadth of effort is demonstrated by the list of the current projects: global ocean and climate modeling; first principle micromechanical and continuum modeling of concentrated materials, methods, microstructure and magnetism; numerical tokamak turbulence project; particle physics phenomenology from lattice quantum chromodynamics; computational chemistry of nuclear waste characterization and processing, relativistic quantum chemistry of actinides; advanced modeling for next generation accelerator applications; grand challenge applications of high energy and nuclear physics data; high performance computational engine for the analysis of genomes; and supercomputer solution of massive crystallographic and microtomographic structural problems.

DOE's Defense Programs' Accelerated Strategic Computing Initiative (ASCI) also supports significant efforts in the development of software for weapons applications. Finally, detailed planning for future efforts in development of applications has occurred to understand, model, and predict the effects on the earth's global environment of atmospheric greenhouse gas emissions, with an emphasis on carbon dioxide; understand, model, and predict the behavior and properties of combustion processes and devices; and revolutionize basic scientific research by the application of teraflop computational resources in areas including materials sciences, structural genomics, high energy and nuclear physics, subsurface flow, and fusion energy research.

Accomplishments

- Software to model magnetism in metal alloys recently exceeded 1 teraflop in sustained performance.

- High resolution models for global ocean flow now accurately predict the path of the Gulf Stream as well as important large-scale ocean eddies, which transport energy from Africa across the Atlantic.

- State-of-the-art software, called NWChem, accurately models the chemistry of plutonium and uranium compounds.

Ultra High Performance Computational and Communications Facilities

Description, Objectives, and Research Performers

In addition to supporting the development of applications software, DOE supports many of the highest performance computing and communications facilities in the world. These facilities, just as other leading-edge facilities supported by the Department, have always had two roles: production of scientific results which are critical for the Department's missions and development of the hardware and software technologies that are required for the next generation of computational and communications facilities. These activities are supported at national laboratories, often in close partnership with U.S. firms that manufacture the computers and operate the underlying communications infrastructure.

Research Challenges and Opportunities

Operating computational and communications facilities at this scale presents significant challenges. Often technologies from a number of manufacturers need to be coordinated and made to interoperate to provide the end-to-end service that scientists require. Meeting these challenges requires a mix of skills from computer science, mathematics, data storage, computer hardware, and advanced software. In addition, because most of these facilities operate the most advanced technology currently available, they must develop much of the supporting software themselves because it is not available from commercial vendors. These facilities will enable scientific simulation to help solve pressing scientific questions related to the nuclear arsenal, climate prediction, combustion, and basic science in general.

Meeting these challenges will enable DOE to provide its researchers with the facilities they need to change science through simulation. In addition, DOE's facilities will become a model for facilities operated by universities and the commercial sector in much the same way that NERSC was the model for the NSF supercomputer centers.

Research Activities

Current examples of such computing research takes place at facilities such as NERSC, the computing facilities operated by the weapons laboratories, the advanced computing research facilities operated by the Office of Science at Argonne National Laboratory, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, and Oak Ridge National Laboratory, and more specialized computing resources such as the molecular sciences computing resource at Pacific Northwest National Laboratory's EMSL. In addition to computing facilities the Office of Science operates ESNet, a high performance network which links computational

and experimental facilities to users and is a critical component of the research infrastructure for the nation.

Detailed planning is currently underway for the next generation of computer and communications facilities that build on the experience of ASCI and move scientific simulation to the next frontier of multi-teraflop computing for future applications.

Accomplishments

- NERSC is the most powerful unclassified computer facility in the nation. At the recent Supercomputing Conference in Orlando, FL, the Gordon Bell Prize for highest performance computer application was awarded to a team that included NERSC. In addition, the three other finalists were from DOE computing facilities.

- NERSC's predecessor, the Magnetic Fusion Energy Computer Center, in partnership with other DOE facilities, pioneered interactive access to supercomputers. This approach, which allows users to observe their computer code while it is running, revolutionized the way in which supercomputers were used.

Computer Science and Enabling Technologies

Description, Objectives, and Research Performers

This program provides applications developers with the tools they need to make effective use of ultra-scale computer and communications facilities. These efforts provide mathematical algorithms and software, debugging and performance tuning tools, data management and visualization software, and tools to support collaboration over networks. These activities are carried out at national laboratories and universities with industrial partners in some cases.

Research Challenges and Opportunities

The complexity of the next generation of computer hardware as well as the massive amounts of data (millions of gigabytes) that they will generate pose significant challenges. A further challenge is coupling mathematicians and computer scientists into the next-generation applications teams effectively while maintaining strong, focused research programs in these disciplines.

These challenges must be met to enable scientists to take advantage of large-scale computation. Success here will make scientists across DOE more effective and productive. In addition, the computer science and enabling technology base that is produced will be critical for industrial acceptance of this scale of computing and promises to dramatically improve the productivity of U.S. industry and the viability of the U.S. high performance computing industry.

Research Activities

Activities include applied mathematics and areas of computer science that are relevant for high performance computing and remote access to facilities. Researchers in computer science and

enabling technology are working to overcome significant challenges and to enable important scientific applications. Software must be designed to support machines not only for the near future but for the next decade. Complex applications must be managed to incorporate more sophisticated physical models, using advanced numerical techniques, and begin to be combined into large-scale "simulation systems" that include the linkage of two or more previously stand-alone models (e.g., ocean-atmosphere- biosphere or fluid-structures-chemistry). Development and user environments must enable ubiquitous collaboration and distributed computing capabilities to support large interdisciplinary teams. Researchers must extract insight from, manage, and visualize petabyte scale data archives. Applications scientists and computer scientists and mathematicians must form more effective long-term collaborations.

All of these efforts must be balanced research, development, and deployment activities carried out in partnership with universities and commercial software and hardware vendors.

Accomplishments

- The DOE applied mathematics program, which was started by John von Neumann in the 1950s, has produced most of the high performance numerical linear algebra routines in the world.

- DOE pioneered remote access to supercomputers in the early 1970s and developed much of the underlying message-passing software that makes today's massively parallel computers useful.

- Phillip Colella, a mathematician at Lawrence Berkeley National Laboratory, received the 1998 Sidney Fernback Award from the Institute of Electrical and Electronics Engineers (IEEE) Computer Society, for his "outstanding contribution in the application of high performance computers using innovative approaches."

Portfolio Summary

This portfolio area, "Scientific Simulation," encompasses research from many research programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific programs that strongly support, support, or provide facilities for applications software, ultra high performance computational and communications facilities, and computer science and enabling technologies. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these programs are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive RSPs (Combined Budget: $815.45 Million)
Advanced Computing and Communications Facility Operations
Advanced Computing Software and Collaboratory Tools
Applied Mathematics
Chemical Physics Research

Climate Change Prediction Program
Environmental and Molecular Sciences Laboratory (EMSL)
Facility Operations: AGS
Facility Operations: Fermilab
Facility Operations: SLAC
General Technology: Accelerator R&D
Geosciences
High Energy Physics Theory
High Performance Computer Networks
High Throughput DNA Sequencing
Mechanical Behavior and Radiation Effects
Plasma Theory and Computation
Production DNA Sequencing Facility
Science Education Support
Scientific Computing Application Testbeds
Theory & Simulations of Matter, Engineering Physics
Understanding and Predicting Protein Structure

Moderately Supportive RSPs (Combined Budget: $1,175.13 Million)
Adv. Particle Accelerator Concepts
Atmospheric Radiation Measurement (ARM) Program Infrastructure
Atmospheric Radiation Measurement (ARM) Program Research
Atomic, Molecular, and Optical Science"
Carbon Cycle Research
Computer Science to Enable Scientific Computing
CP Violation - B-Meson System
CP Violation - K-Meson System
Electroweak Interactions
Energy Biosciences
Engineering Behavior
Experimental Condensed Matter Physics
General Purpose Plant & Equipment (GPP/GPE)
General Technology: Detector R&D
Hadron Spectroscopy
Heavy Element Chemistry
Laboratory Technology Research and Advanced Energy Projects
Materials Chemistry
Mechanical Systems, Systems Science, and Engineering Analysis
Multiprogram Energy Lab Facilities Support (MELFS)
Neutrino Mass and Mixing
Neutron and Light Sources Facilities
Neutron and X-Ray Scattering
Particle Astrophysics & Cosmology
Physical Behavior of Materials
Search for Higgs & Supersymmetry
Small Business Innovation Research (SBIR) Program
Small Business Technology Transfer (STTR) Program
Spin Structure of Nucleons
Strong Interactions, Supersymmetry & Particles
Structure of Materials

Theoretical Nuclear Physics
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Research Summary.