SciDAC-2
Scientific Discovery through Advanced Computing

Michael Strayer
Associate Director for Advanced Scientific Computing Research, Office of Science,
U.S. Department of Energy
Acting Director, MICS (Mathematical Information and Computational Sciences)
Director, SciDAC (Scientific Discovery through Advanced Computing)


Five years ago SciDAC was launched as an experiment in computational science. The goal was to form partnerships among science applications, computer scientists, and applied mathematicians to take advantage of the potential of emerging terascale computers.

This experiment has been a resounding success. SciDAC has emerged as a powerful concept for addressing some of the biggest challenges facing our world.

As significant as these successes were, I believe there is also significance in the teams that achieved them. In addition to their scientific aims these teams have advanced the overall field of computational science and set the stage for even larger accomplishments as we look ahead to SciDAC-2.

I am sure that many of you are expecting to hear about the results of our current solicitation for SciDAC-2. I’m afraid we are not quite ready to make that announcement. Decisions are still being made and we will announce the results later this summer. Nearly 250 unique proposals were received and evaluated, involving literally thousands of researchers, postdocs, and students. These collectively requested more than five times our expected budget. This response is a testament to the success of SciDAC in the community.

In SciDAC-2 our budget has been increased to about $70 million for FY 2007 and our partnerships have expanded to include the Environment and National Security missions of the Department. The National Science Foundation has also joined as a partner.

These new partnerships are expected to expand the application space of SciDAC, and broaden the impact and visibility of the program. We have, with our recent solicitation, expanded to turbulence, computational biology, and groundwater reactive modeling and simulation. We are currently talking with the Department’s applied energy programs about risk assessment, optimization of complex systems – such as the national and regional electricity grid, carbon sequestration, virtual engineering, and the nuclear fuel cycle.

The successes of the first five years of SciDAC have demonstrated the power of using advanced computing to enable scientific discovery. One measure of this success could be found in the President’s State of the Union address in which President Bush identified ‘supercomputing’ as a major focus area of the American Competitiveness Initiative.

Funds were provided in the FY 2007 President’s Budget request to increase the size of the NERSC-5
procurement to between 100–150 teraflops, to upgrade the LCF Cray XT3 at Oak Ridge to 250 teraflops and acquire a 100 teraflop IBM BlueGene/P to establish the Leadership computing facility at Argonne. We believe that we are on a path to establish a petascale computing resource for open science by 2009.

We must develop software tools, packages, and libraries as well as the scientific application software that will scale to hundreds of thousands of processors. Computer scientists from universities and the DOE’s national laboratories will be asked to collaborate on the development of the critical system software components such as compilers, light-weight operating systems and file systems.

Standing up these large machines will not be business as usual for ASCR. We intend to develop a series of interconnected projects that identify cost, schedule, risks, and scope for the upgrades at the LCF at Oak Ridge, the establishment of the LCF at Argonne, and the development of the software to support these high-end computers.

The critical first step in defining the scope of the project is to identify a set of early application codes for each leadership class computing facility. These codes will have access to the resources during the commissioning phase of the facility projects and will be part of the acceptance tests for the machines.

Applications will be selected, in part, by breakthrough science, scalability, and ability to exercise key hardware and software components. Possible early applications might include climate models; studies of the magnetic properties of nanoparticles as they relate to ultra-high density storage media; the rational design of chemical catalysts, the modeling of combustion processes that will lead to cleaner burning coal, and fusion and astrophysics research.

I have presented just a few of the challenges that we look forward to on the road to petascale computing. Our road to petascale science might be paraphrased by the quote from e e cummings, ‘somewhere I have never traveled, gladly beyond any experience . . .’