

THE COMPUTERWORLD HONORS PROGRAM

CASE STUDY



LOCATION:
*Livermore, California,
United States*

YEAR:
2006

STATUS:
Laureate

CATEGORY:
Science

NOMINATING COMPANY:
IBM Corporation

ORGANIZATION:

Lawrence Livermore National Labs

PROJECT NAME:

Advanced Simulation and Computation

Summary

Computer simulation is becoming an indispensable tool for advancing science in virtually every scientific domain from genomics, medicine and the development of new materials to climatology, inertial confinement fusion and astrophysics. The Advanced Simulation and Computing (ASC) Program is a coordinated effort led by the U.S. Department of Energy's National Nuclear Security Administration (DOE/NNSA) and carried out by the three defense program laboratories: Lawrence Livermore, Los Alamos and Sandia. ASC's mission to develop high performance computing capabilities needed to ensure the safety, security and reliability of the nation's nuclear deterrent without nuclear testing has resulted in a transformation in the role of supercomputers in scientific discovery. Lawrence Livermore National Laboratory (LLNL), in partnership with IBM, has played a leading role in this transformation.

Introductory Overview

The drive to increase computer power that is transforming scientific discovery was launched as the Accelerated Strategic Computing Initiative (ASCI) in late 1995 and is today known as the Advanced Simulation and Computing (ASC) Program. The goal was to deliver the massive increase in computing power required to ensure the safety, security and reliability of the nation's nuclear weapons without conducting nuclear tests. The program also was focused on developing three-dimensional (3D) computer simulation codes to enable the Science-Based Stockpile Stewardship (SBSS) program. Under stockpile stewardship, nuclear testing would be replaced with integral weapons simulations and data from historic nuclear tests and surrogate scientific experiments, integrated through computer simulation.

Since the beginnings of ASCI in 1995, DOE/NNSA supercomputers at Livermore, Los Alamos and Sandia have dominated the Top500 list. The federal investment in high performance computing has helped fuel a renaissance in the supercomputing industry. Competition has led to the development of systems and applications that have had a broad impact on the larger scientific community. Supercomputers are vital to research in almost every scientific domain including genomics, drug development, materials science, climate change, inertial confinement fusion and astrophysics.



THE COMPUTERWORLD HONORS PROGRAM

CASE STUDY

ORGANIZATION:

*Lawrence Livermore
National Labs*

PROJECT NAME:

*Advanced Simulation
and Computation*

LOCATION:

*Livermore, California,
United States*

YEAR:

2006

STATUS:

Laureate

CATEGORY:

Science

NOMINATING COMPANY:

IBM Corporation

At the time the initiative was launched, scientists and engineers at the three labs estimated that a million-fold increase in computing power would be required to generate the most basic, or “entry level,” 3D simulations of nuclear weapons safety and performance. ASC aimed to achieve this in 10 years, before the expected retirement of nuclear test-experienced scientists from the active workforce. This increase was to come from advances in computer technology, augmented by improvements in numerical simulation methods.

The hardware platform strategy adopted by DOE/NNSA and the national labs was to establish a series of partnerships with U.S. computer companies to leverage their business models to accelerate high-end computing power. LLNL followed procurement processes that led to a series of partnerships with IBM, which resulted in the development of a series of increasingly powerful computer systems, culminating in 2005 with the deployment of the Purple and Blue Gene/L computer systems. ASC’s largest computing systems are managed as shared resources for use by code developers, designers and analysts at all three labs. Academic partners also are given access to comparable unclassified systems through the ASC Academic Strategic Alliance Program. The five alliance universities are helping define simulation methodology as they focus on nonweapons research in areas including gas turbine engines, fires and accidental explosions, rocket motors, astrophysical explosions, and dynamic material properties.

The realization of scientific discovery through advanced simulation has progressed with each new ASC platform. These high-end platforms now routinely enable weapons simulations aimed at ensuring the viability of the stockpile as nuclear weapons age well beyond their intended design lifetimes, in integrated nonweapons simulations by laboratory and ASC alliance researchers, and in pioneering component physics simulations investigating fundamental physical phenomena. The simulations follow scientific processes in 3D over length scales ranging from the nanoscale (10-15 meters) up to meters, and over time scales ranging from a nanosecond (10⁻⁹ seconds) up to days. This realization is possible only through the acceleration of computer power achieved under the ASC Program.

It also is important to recognize the time urgency surrounding the ASC mission. Scientists and engineers responsible for the nuclear stockpile faced two significant time-critical challenges. On one level, the challenge was that the nuclear weapons were aging beyond their intended design lifetimes. It was anticipated that aging would cause changes, which simulation-based insight would be needed to determine if those changes impacted the performance, safety and reliability of the weapons. In addition, there was an issue with the aging of the scientists and engineers who had underground nuclear testing experience. These experts were necessary to judge whether the simulations were properly replicating underground test results. In 1995, a deadline of 2005 was set to develop an initial full-scale 3D capability to provide scientific insight via simulation. This target was deemed extremely ambitious but necessary to provide the degree of confidence needed for ongoing certification of the nation’s nuclear stockpile.

The program’s goals were so ambitious that some members of the scientific community doubted they could be achieved in the aggressive one-decade time frame. Not only was it a matter of an unprecedented scaling up of machines and codes to run the applications, but of building an infrastructure to support these massive systems; floor space, cooling, storage, and networks, which, combined with the system itself, would require enough electricity to power a small city. Despite the skepticism, LLNL scientists enthusiastically picked up the gauntlet and began working with IBM to meet these challenging goals. Along the way, scientists realized that to move beyond the entry level systems to petaflop computing (100,000 trillion operations per second), new ap-



THE COMPUTERWORLD HONORS PROGRAM

CASE STUDY

ORGANIZATION:

*Lawrence Livermore
National Labs*

PROJECT NAME:

*Advanced Simulation
and Computation*

LOCATION:

*Livermore, California,
United States*

YEAR:

2006

STATUS:

Laureate

CATEGORY:

Science

NOMINATING COMPANY:

IBM Corporation

proaches to system design would be required. Technological advances in industry allowed IBM, in partnership with LLNL scientists, to develop BlueGene/L (BGL), a radical departure from traditional system design. BGL currently holds the top ranking in the Top500 list of the world's fastest supercomputers (based on an industry benchmark), with a performance of 280 trillion operations per second. Because of its unique design, BGL lends itself to tackling materials science calculations -- such as what happens to nuclear materials when they age -- that complement and support the massive numerical simulations of nuclear weapons performance conducted on ASC Purple. The systems are suited to perform distinctly different but complementary scientific tasks.

IBM Blue Gene systems currently hold five of the top 10 rankings on the Top500 list (accepted as the industry measure) and these systems are now found in research centers around the world - the Netherlands, United Kingdom and Spain. Researchers have compared the advent of the new generation of supercomputers to the invention of the electron microscope, which allowed scientists to see things previously invisible, and the Hubble telescope, which has allowed astronomers to peer deeper into space than ever before. Supercomputers allow scientists to simulate scientific phenomena to a level of detail and accuracy never before possible, providing the insight and understanding that lead to scientific discovery. Computer simulation is now a peer to theory and experiment, the pillars of the scientific method defined by Sir Isaac Newton some 300 years ago.

Benefits

The technologies developed for ASC Purple and BGL are providing researchers in a wide variety of domains with unprecedented simulation capabilities that have transformed the role of computing in scientific discovery. High-fidelity 3D simulation, which allows researchers to replicate phenomena in great detail, offers a new tool for scientific investigation when experiments are impractical, either because they are too expensive, time-consuming or dangerous. Simulation also can be used to calibrate physical experiments, improving safety and data retrieval. For example, a physical global climate change experiment might require a laboratory the size of the planet with controlled initial conditions. Simulation complemented with manageable physical experiments offers the best alternative. Today's high performance computing capabilities are helping to advance national defense, medicine, bioscience, materials science, our understanding of the universe and climatology while the commercial success of ASC-funded computing technology has helped advance the nation's economic competitiveness.

ASC has over the last 10 years raised the bar for high-performance computing through its accelerated effort to reach the threshold of 100 teraflops computing, the capability to reliably conduct simulations of nuclear weapons safety and performance, as well as the predictive supporting materials science. ASC Alliance academic partners from five universities have helped to develop new codes allowing applications in a variety of fields such as astrophysics, rocket design, and simulations of accidents and fire environments, such as forest fires. The ASC Alliance partners are Stanford University, California Institute of Technology, University of Chicago, University of Illinois at Urbana-Champaign and the University of Utah, as well as other universities pursuing more focused research projects. These academic partnerships help create and validate simulation methodologies. This symbiosis is an important element of the ASC program intended to advance the entire scientific computing community.

IBM's Blue Gene system, first developed through the ASC program, is now being used for



THE COMPUTERWORLD HONORS PROGRAM

CASE STUDY

ORGANIZATION:
*Lawrence Livermore
National Labs*

PROJECT NAME:
*Advanced Simulation
and Computation*

LOCATION:
*Livermore, California,
United States*

YEAR:
2006

STATUS:
Laureate

CATEGORY:
Science

NOMINATING COMPANY:
IBM Corporation

scientific research at centers throughout the United States, Europe and other parts of the world. Some examples include the following. The Netherlands' Low Frequency Array radio telescope uses a six-rack Blue Gene machine based at the University of Groningen to analyze data from 15,000 antennas spanning an area of 350 km in diameter. Researchers at the University of Edinburgh, UK, are using a single-rack Blue Gene machine to simulate protein folding and fluid mixing. Japan's National Institute of Advanced Industrial Science and Technology is using its four-rack system to boost drug development. IBM and Ecole Polytechnique Federale de Lausanne have entered into a joint research agreement that leverages the unique computational capabilities of the Blue Gene/L system. The first project under this agreement, codenamed Blue Brain, will allow EPFL and Watson Research scientists to develop a detailed model of the Neo Cortical Column (NCC) - a set of 10,000 neurons that represents the fundamental building block of the human brain.

In the United States a single-rack Blue Gene is being shared by the National Center for Atmospheric Research and the University of Colorado, which runs simulations of ocean, weather and climate behavior. A team at the San Diego Supercomputing Center is using a single-rack Blue Gene to run Enzo, the center's software that simulates how galaxies evolved from the Big Bang. The Iowa Board of Regents approved the funding for one Blue Gene rack for Iowa State University (ISU). ISU's system will be used by Principal Investigator Srinivas Aluru for genome classification. MIT will use its Blue Gene machine initially for quantum chromodynamics (QCD) optimization. Princeton will use its system for multiple science applications in the astrophysical sciences, molecular dynamics and plasma physics areas. Boston University professors will use Blue Gene to explore QCD, the theory of the mysterious force that holds quarks inside nuclear particles, which is key to describing what goes on at high-energy accelerators.

The Importance of Technology

Rapidly advancing computing technology on multiple fronts was the key to changing the role of modeling and simulation in the weapons program from one in support of underground nuclear testing to one enabling a regimen of no nuclear testing. Computer simulation is the cornerstone of science-based stockpile stewardship, which replaces underground nuclear testing with a combination of full-system nuclear weapons calculations, as well as data from past nuclear tests and surrogate experiments, tied together by simulation.

ASC not only had to deliver bigger and faster computer systems, but also deploy an entire supporting infrastructure: new applications, networks, visualization capabilities, archiving and storage and the physical environment allowing all of these to work in concert.

Originality

The technological leap required to achieve the ambitious goals laid out by ASC in 1995, required a revolution in the way DOE/NNSA, the national labs and their industrial partners did business. The effort required each partner to take greater risks. Technologies had to be advanced simultaneously on a number of fronts: applications, computer systems, networks, visualization, archives and other infrastructure support. Failure on any front could have jeopardized the entire enterprise.

The classic business model of scientists and engineers providing the computer vendor with a



THE COMPUTERWORLD HONORS PROGRAM

CASE STUDY

ORGANIZATION:

*Lawrence Livermore
National Labs*

PROJECT NAME:

*Advanced Simulation
and Computation*

LOCATION:

*Livermore, California,
United States*

YEAR:

2006

STATUS:

Laureate

CATEGORY:

Science

NOMINATING COMPANY:

IBM Corporation

list of requirements and then waiting for the machine to be designed and built would not have worked. Accelerating scientific computing technology required the researchers who would use the systems to work in close collaboration with computer designers and system builders from conception through deployment.

The ASC Program is original in its approach to the ambitious enterprise it undertook. ASC engaged the broader scientific computing community through the ASC Alliance program and established intimate collaborative arrangements with computer companies via the PathForward program, which supported progress from conception through deployment and operation.

Success

Blue Gene/L is helping scientists at Los Alamos, Sandia and Lawrence Livermore national labs address vital materials aging issues in the nuclear stockpile.

Early work on Blue Gene/L included a simulation of the solidification of the metal tantalum under extreme pressure and temperatures by a team of Livermore scientists. The simulation not only demonstrated BGL's capabilities, it provided valuable insight into the nature of the material at a level of detail never before possible. Scientists were able to simulate what happens to tantalum atom by atom in increasingly larger arrays of atoms, ranging from 64,000 atoms to 524 million atoms. The work earned the Livermore team the 2005 Gordon Bell Prize, widely regarded as the Oscar of supercomputing, at the annual Supercomputing conference held in November 2005 in Seattle.

"These simulations allow us for the first time to examine the process of solid formation at high temperature and pressure from the atomistic level. We can actually watch, atom by atom, as macroscopic grains grow out of the liquid and form structures," said Fred Streitz, a physicist at LLNL and leader of the tantalum team. "This allows us to better understand the properties of these metals and has important implications for the development of stronger metals, such as those that might be used for aircraft or automobile components as well as other applications."

ASC scientists and engineers have benefited from previous ASC platforms located in the three weapons labs including: ASC Blue Pacific, White, Purple and Blue Gene/L at LLNL; ASC Blue Mountain and Q at Los Alamos; and ASC Red and Red Storm at Sandia.

When ASC began and the first supercomputing systems were brought on line there were plenty of skeptics. There were those who didn't believe ASC would come close to meeting its ambitious goals and there were those who questioned the value of placing so much emphasis on simulation as a tool for doing "predictive" science.

"There have always been tensions in the scientific community between experiment and simulation. Among some veteran researchers there was an interpolative science mind set and resistance to relying so much on simulation," said Mark Seager, the computer scientist who has played a key role in the development of ASC platforms at Livermore. "This is a good tension to have because it has helped refine the role of simulation in science."

The ASC program has worked hard to make these systems progressively more accessible and easier to use thanks to organizations such as the Livermore Computing Center. While researchers may have taken a while to warm to early platforms like ASC Blue Pacific, subsequent systems proved increasingly popular. High-performance computing resources at the defense program



THE COMPUTERWORLD HONORS PROGRAM

CASE STUDY

ORGANIZATION:
*Lawrence Livermore
National Labs*

PROJECT NAME:
*Advanced Simulation
and Computation*

LOCATION:
*Livermore, California,
United States*

YEAR:
2006

STATUS:
Laureate

CATEGORY:
Science

NOMINATING COMPANY:
IBM Corporation

labs are currently heavily subscribed and the Labs can't bring new systems on line fast enough to satiate scientists' thirst for more number crunching power.

Difficulty

The obstacles the ASC program faced at the outset were formidable. ASC represented a technological acceleration with few precedents and one that would require a new way of doing business for DOE/NNSA, the national labs, industry and academia. A prerequisite was forging partnerships with members committed to the program's goals and willing to take the risks inherent in this enterprise.

Increasing computing power one million fold in less than 10 years also would require an unwavering financial commitment from Congress.

ASCI required some cultural changes within the tri-lab defense program community. As in delivering insight, building an initiative proved to be as complicated as the required technologies themselves. The problem was that to deliver insight, a wide variety of technologies had to be developed simultaneously. This required a fundamentally multi-disciplinary approach that in many ways ran counter to the traditional ways that defense programs and the national laboratories have been organized and managed.

The delivery of insight via simulation requires a system approach to the technologies. It is not enough to have the world's most powerful computers to run the simulations unless the applications also exist. Likewise, having powerful computers and applications is worthless if the means to understand the resulting data does not exist. This meant that ASCI had to engage a wide variety of specialists, including nuclear weapon scientists and engineers, mathematicians, material scientists, computer architects, programmers, networking engineers, security specialists, system administrators, procurement specialists, and others. As the program progressed and the size and power requirements of the computers became known, this group would even include building architects and electrical engineers.

Up until the beginning of the ASCI program, the national laboratories tended to run programs that were technically very deep, but did not cross many disciplines. In the scientific world this was not terribly unusual because science at the national laboratory and university level required "world class" understanding of specific topics. That requirement dictated that the scientists involved stay focused on their particular topic areas. Starting with the founding of Los Alamos during the Manhattan Project, this approach served the national laboratories very well, allowing them to focus on understanding a particular area before building on that understanding to gain more insight.

This traditional approach to developing scientific insight provided another challenge for organizing ASCI. This was the institutionalized competition among the national laboratories. A common method of checking the validity of the insights of the scientific method was "peer review." The idea behind peer review was that other scientists, who had an equally deep understanding of a particular area, would review the work of another. These reviews would involve much discussion and study, and often entailed replicating experiments to check the results. The challenge for peer reviewing nuclear weapons science was that the science was classified and not reviewable by the general scientific community.

For that reason, as well as the need to increase the pace of development of the hydrogen bomb



THE COMPUTERWORLD HONORS PROGRAM

CASE STUDY

ORGANIZATION:

*Lawrence Livermore
National Labs*

PROJECT NAME:

*Advanced Simulation
and Computation*

LOCATION:

*Livermore, California,
United States*

YEAR:

2006

STATUS:

Laureate

CATEGORY:

Science

NOMINATING COMPANY:

IBM Corporation

after World War II, Lawrence Livermore National Laboratory was founded. The idea was that a second laboratory would be able to provide the independent peer review of the others within the classified environment. Sandia National Laboratories was an offshoot of Los Alamos' Z Division. It focused on the engineering aspects of the weapons and operated independently. As a result, the three national laboratories were encouraged to be competitive with each other. When new weapons were being produced, competitions were held to see which laboratory would come up with the best design. ASCI had to overcome this legacy of independence and competition.

In the beginning ASCI was received with skepticism from many quarters because of the exceptionally challenging goals it set with its vision to "create leading-edge computational modeling and simulation capabilities critically needed to promptly shift from nuclear test-based methods to computational-based methods . . ." Resistance came from within the DOE, from the Department of Defense (DoD) "customers," and from within the weapons laboratories. In addition, there was skepticism in the computer industry that the enormous increases in computer performance could be achieved on a 10-year time scale.

Within DOE, ASCI was viewed with concern because it was new and required increased funding. This challenge was overcome by building a program that earned congressional support. Congress provided new funds to DOE in Fiscal Year 1996, and significantly increased the funding levels in subsequent years. Resistance within DOE also was overcome by managing the program as a cooperative effort among the three weapons labs and DOE, guided by a "one-program, three-labs" strategy.

DoD leadership and the military services responsible for nuclear weapons were skeptical that simulation could match the confidence achieved previously through nuclear tests ("Admiral's tests"). This challenge was overcome, in part, by demonstrating through high-level reviews by the JASONS, a DoD Blue Ribbon Panel, and the GAO, that the program was well planned and managed to achieve its objectives. DoD resistance also was met by adding a major "Verification and Validation" program element to focus on increasing the level of confidence in the simulations.

Within the laboratories, there was resistance from old-line weapons designers and analysts who wanted to stay with experiment-based methods. This resistance was overcome first by lab management, who recognized the need to build new simulation capabilities for an era without nuclear testing. Later, acceptance of the new simulation tools by designers and analysts grew rapidly as they exercised the enhanced capabilities on new, much more powerful computers to support the stockpile.

Resistance also came from the computer industry, since the program required large, rapid increases in computer power. In the 1990s, companies like Kendall Square and Thinking Machines went out of business after building large, but uneconomic parallel computers. Industry resistance was overcome through a computer acquisition strategy based on partnerships with computer companies to leverage their commercially viable product lines. This represented a major change for the production of large specialty machines to emphasizing the use of commercial, off-the-shelf technology. ASC also invested in critical technologies, such as high-speed interconnects, to enable future generation computers. As a result, resistance in the computer industry was overcome. ASC broke the one-teraflop barrier in 1997 with the Intel "Red" machine, deployed a series of powerful machines from several companies, and achieved its 10-year targets with the deployment of the IBM Purple and BlueGene/L computers. Laboratory personnel,



THE COMPUTERWORLD HONORS PROGRAM

CASE STUDY

ORGANIZATION:
*Lawrence Livermore
National Labs*

PROJECT NAME:
*Advanced Simulation
and Computation*

LOCATION:
*Livermore, California,
United States*

YEAR:
2006

STATUS:
Laureate

CATEGORY:
Science

NOMINATING COMPANY:
IBM Corporation

working with companies like IBM, created a robust computational infrastructure to support the effective use of these new computers.

Only by steadily overcoming these levels of resistance was ASC able to provide the combination of application software, advanced computing platforms and supporting infrastructure to enable the revolution in the use of simulation to transform scientific discovery.