

ASCI UPDATE

February 2001



Sandia Signs Cooperative Agreement with Celera

In January it was announced that Sandia National Laboratories and Celera Genomics will develop the next-generation software and computer hardware designs that will specifically answer the demand for computational biology and a full range of life science applications. Celera, the world's top human genetics research company, and Sandia signed a Cooperative Research and Development Agreement (CRADA) to write new computer software and the algorithms that will be used to analyze the dense maze of genetic code. The Accelerated Strategic Computing Initiative (ASCI) benefits from the synergism of Sandia's Defense Programs efforts with those defined in the CRADA. Compaq, who is not a CRADA signee but who is a partner in the effort, will provide engineering capability.

The level of cooperation demonstrated by this CRADA is necessary to provide the performance required for emerging genomics and proteomics applications at affordable prices, and the partnership with Compaq brings together the capabilities of three leaders in the fields of bioinformatics, high performance computing, and massively parallel systems. The National Nuclear Security Administration (NNSA) benefits from the CRADA because the Celera investments will provide the engineering foundation necessary for the next generation of supercomputers in the 100 teraOPS to 1 petaOPS range. Compaq is committing its engineering capability and will develop a machine that Celera, ASCI sites, or others could buy.

The goal of this partnership is to design an architecture that can be implemented in 10- or 100-teraOPS installments and that could result in Celera and Compaq reaching the petaflop (1000 teraOPS) level around 2010. Celera's current resource is a massively parallel Compaq Alpha processor farm of approximately 1000 processors that was heavily used for assembling the human genome. However, annotating these genomes is expected to require even greater resources, and the post-genomic problem of proteomics is anticipated to be up to 1000-fold more computationally demanding. Celera's computational needs are somewhat different than ASCI's, especially in terms of parallel data input/output, and addressing this issue will be the focus of the funds-in part of the CRADA as it pertains to the hardware architecture.

Bill Camp, Sandia's director of Computation, Computers and Mathematics stated that "Delivering affordable and scalable computer architectures is the foundation of modern supercomputing and has been the focus of Sandia research for more than a decade. Our knowledge will be useful because understanding the complexity of the human genome requires manipulating ever vaster amounts of information, using more advanced computing technologies than was required even for the assembly of the human genome itself. So we view this relationship as strategic for our continuing missions as an NNSA national security laboratory, look forward to providing world-class expertise in parallel algorithms and systems software in the cause of human health, and welcome the opportunity to play a role in developing what may be some of the most exciting science in recent human history."

Former Secretary of Energy Bill Richardson stated during the signing of the CRADA, "The next stage of the biotechnology revolution that was started by the

In the News...

Livermore's "Science Day" will be held March 21. They will showcase recent accomplishments in high-performance modeling and simulation. The agenda includes presentations and poster sessions of a broad range of science and technologies.

Construction has been completed on the newest addition to the Data Visualization Center Corridor at Sandia. More to come on this story.

Who's Who in ASCI Integrated Computing Systems...

PLATFORMS

Mark Seager
Livermore National Laboratory,
seager@llnl.gov

James Tomkins
Sandia National Laboratories,
jltomki@sandia.gov

Joe Thompson
Los Alamos National Laboratory,
rjt@lanl.gov

Human Genome Program will be fueled by the successful marriage of molecular biology with high performance computing science. As DOE helped develop the technology that made the human genome project possible, once again, it is forging ahead to provide the tools to bring the genome to life.”

According to Bill Blake, Vice President of High Performance Technical Computing at Compaq, “The key aspect of this R&D relationship is the simultaneous provision of algorithmic support, design of actual application software, and development of the system platform by three organizations with world-class competence in their respective areas. Our intent with this alliance is to apply the same full-system modeling approach to bioscience that has been so successfully applied to physical sciences in the Stockpile Stewardship Program.”

J. Craig Venter, Celera’s president and chief scientific officer, said, “As Compaq and [NNSA] move toward creation of the next generation of supercomputers for defense purposes, we look forward to helping both groups develop the new machines, software and algorithms to advance life sciences.”

Los Alamos Hosts Annual ASCI PI Meeting

The 2001 ASCI Principal Investigators (PI) Meeting was hosted by Los Alamos National Laboratory from January 22nd through the 25th. This annual event allows the NNSA, laboratory, and university alliance project managers to review project accomplishments and chart progress toward future goals. Dr. William H. Reed, Acting Director of the Office of Advanced Simulation and Computing Defense Programs, NNSA, provided the ASCI Program update. He reviewed the overall success of ASCI—planning and implementation, budget, reviews, and customer satisfaction. He stated that, with these successes, “We are beginning to make vital contributions to the Stockpile Stewardship Program.” He praised the staff who support ASCI, the management and leadership within the initiative, and the diversity of systems and software solutions that are vital to achieving project milestones.

ASCI Grid Will Be Operational Soon

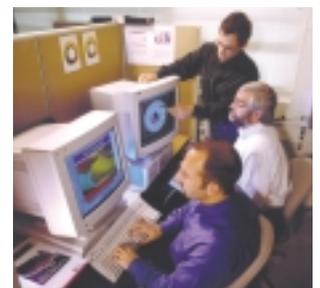
In the past, each of the NNSA laboratories had their own major computing system. While one laboratory could use the computing resources at another, it was difficult to do and resulted in little actual sharing of resources. The ASCI Grid will make it easy for a user at any laboratory

to use any of the computing resources within the Nuclear Weapons Complex. Now, after a two-year-long development effort, the ASCI Grid is nearly operational across the Nuclear Weapons Complex. Developed by the tri-lab Distributed Resource Management project for ASCI, the grid connects White, Red, Blue Mountain, and CPlant computing systems. It will enable both local and remote users to effectively access ASCI computers, storage, network, and visualization resources using a common set of desktop interfaces. The ASCI Grid services include work management, resource brokering, resource discovery, and monitoring.

The three-layered grid includes at the first layer the operating systems and local resource managers. The second layer is the Globus Toolkit, first developed at Argonne National Laboratory and modified by the tri-lab effort to meet NNSA security requirements. The third layer, developed by ASCI’s tri-lab effort, contains distributed resource management.

After accreditation at all three labs, the ASCI Grid will be the largest computational grid in the world with more processors (24,548) and a higher compute capability (~19 teraOPS) than any other grid existing. Sandia National Laboratories has received accreditation from NNSA for its set of services, and Los Alamos and Lawrence Livermore National Laboratories are expected to receive accreditation for the same set of services in the near future. Accreditation allows the national defense laboratories to run their grid services on secure networks.

Platforms



Scientists

The ASCI Grid will provide to the weapons designers, engineers and scientists the world class computing and visualization infrastructure required for the Stockpile Stewardship Program simulations.