Scientific Computing for National Security

The Advanced Simulation and Computing (ASC) Program is a national program that enables the Department of Energy and National Nuclear Security Administration Stockpile Stewardship mission. ASC creates simulation tools to be used in concert with expert scientific judgment to certify that the stockpile is safe, reliable, and secure.

Cover:
Detail from 2-billion-atom simulation of a Kelvin-Helmholtz instability developing at the sheared interface between two molten metals modeled using Lawrence Livermore's ddcMD code on BlueGene/L. ASC's capability computing enables researchers to study such fluid instabilities with unprecedented atomic resolution to validate continuum approximations.

As a program, ASC's main goal is to enable Stockpile Stewardship by:

- Improving the confidence in prediction through simulations
- Integrating the ASC Program with certification methodologies
- Developing the ability to quantify confidence bounds on the uncertainty of our results
- Increasing predictive capability through the development of more accurate physics and engineering models and tighter integration of simulation and experimental activities
- Providing the necessary computing capability to code users, in collaboration with industrial partners, academia, and government agencies

For more information, visit http://www.sandia.gov/NNSA/ASC/

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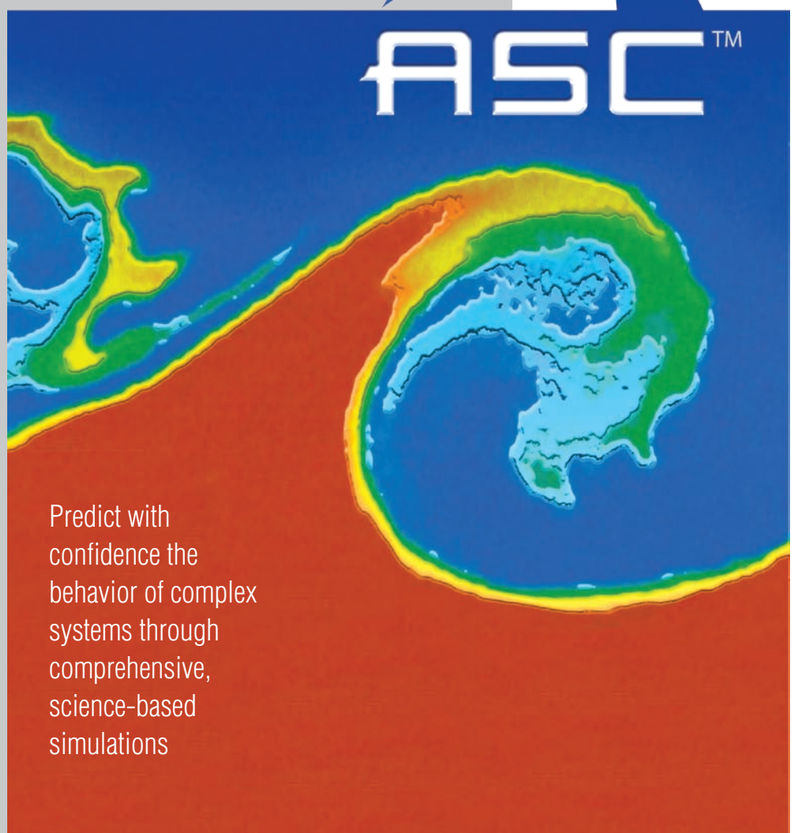
Advanced Simulation & Computing™

Scientific Computing for National Security



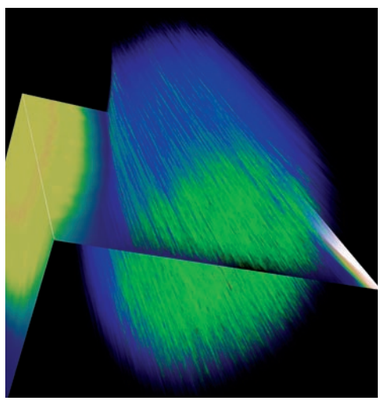
Predict with confidence the behavior of complex systems through comprehensive, science-based simulations

Platforms Tailored to Mission Goals

Capacity Computing

Capacity computing is accomplished through the use of smaller and less expensive high-performance systems to run parallel problems with more modest computational requirements. Capitalizing on the commodity Linux clusters in use throughout the scientific community, ASC has developed a procurement strategy that builds a common hardware environment across the three defense laboratories—Lawrence Livermore, Los Alamos, and Sandia National Laboratories. The objective is to build, field, and integrate many Linux clusters of various sizes into service through a concept of scalable units. A consistent user environment and common operating system for the capacity computers across the laboratories will facilitate inter-site collaboration. Currently, the life cycle of a capacity system is about four years.

Prototype of a new tri-lab Linux capacity cluster. Scalable units (SUs) will be aggregated into multi-SU clusters of two, four, six, or eight SUs. The multi-SU clusters represent 20, 40, 80, 120, and 160 teraFLOPS of capacity computing.

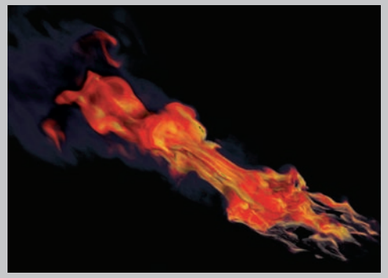


Experiments at the National Ignition Facility (NIF) will use the world's most powerful laser to implode capsules containing deuterium and tritium to the high temperatures and densities at which nuclear fusion occurs. The PF3D code simulates the propagation of the laser beam through the ionized gas surrounding the capsule. Simulations provide crucial input to the design of NIF experiments and will greatly reduce the number of laser shots required to achieve ignition.

Capability Computing

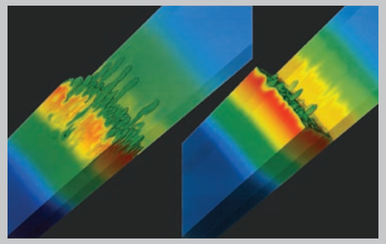
Capability computing refers to the use of the most powerful supercomputers to solve the largest and most demanding problems with the intent to minimize time to solution. A capability computer is dedicated to running one problem, or at most a few problems, at a time. The capability computers ASC Purple at Lawrence Livermore and ASC Red Storm at Sandia are used to solve multiscale, multiphysics problems for the nation's Stockpile Stewardship Program—a program for maintaining the safety and reliability of the nation's nuclear weapons. These capability systems are managed as tri-lab resources similar in value and uniqueness to large experimental facilities. Major programmatic computing efforts for capability systems are organized as computing work packages and are reviewed and prioritized for relevance, importance, and technical merit. The life cycle for capability systems is about five years. Capability computing systems, while designed to run the largest jobs, can also be operated with capacity-computing workloads. In this way, they serve as bridges to the next generations of capacity systems.

The 124-teraFLOPS Red Storm computer represents a highly balanced and integrated hybrid (capacity/capability) machine well-suited to running a mix of weapons performance, stockpile science, and engineering applications.



A visualization created on Red Storm of how a specific fire event might affect a weapon.

Between its 94 teraFLOPS classified and its 6 teraFLOPS unclassified environment, ASC Purple achieved the major milestone set in 1996 for a 100-teraFLOPS-class computer dedicated to a few, very demanding problems from Los Alamos, Sandia, and Lawrence Livermore.

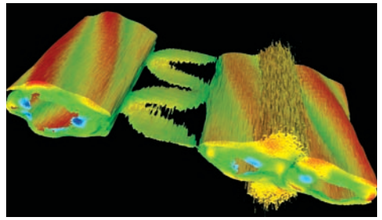


Three-dimensional high-resolution "Grand Challenge" simulations on ASC Purple, in support of the National Ignition Campaign, are being performed to select capsule designs that minimize instability growth. The figure shows simulations before (l.) and after optimization (r.) of the design to minimize penetration of beryllium into the fusion fuel (a deuterium-tritium mixture).

Advanced Systems

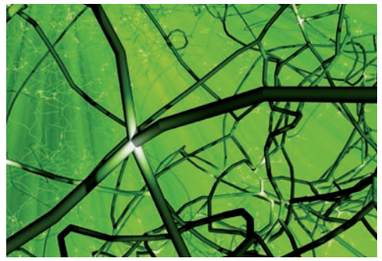
Advanced systems extend the limits of technology by exploring promising architectural approaches. A major element of ASC's advanced systems strategy is to understand future systems that will likely be quite different in nature from current capability and capacity systems. Acquisition and use of these systems enable ASC to examine new directions for future general-purpose weapons system computing, while at the same time applying new technology to current problems. The pay-off is the promise of moving past "Moore's law" restrictions that are threatening to curtail the speed increases seen over the past decades, and that there will be follow-on systems that can use code modifications that address future stockpile simulation obligations. This advanced systems strategy helps lead ASC into the future, limits vulnerability, and helps both the Nuclear Weapons Complex and U.S. industry maintain a differentiating competitive advantage. It also attracts qualified people with the promise of being able to make new contributions at the frontiers of supercomputing.

The Roadrunner Phase I base system provides 71 peak teraFLOPS of capacity computing resources for weapons simulations. It uses Opteron X64 Advanced Micro Devices (AMD) processors with a high-speed InfiniBand 4X interconnect. The final Roadrunner system, pending assessments, is planned for 2008 and is based on an advanced hybrid architecture containing both Opteron and IBM enhanced double-precision Cell processing elements.



Magnetic reconnection in electron-positron plasma in large-scale, 3D systems has been examined using the VPIC code developed at Los Alamos to run a 16-billion particle problem on Roadrunner Phase 1. Such codes are being prepared to run multi-scale, multi-physics problems that are well-suited to the Roadrunner hybrid cell architecture planned for 2008.

BlueGene/L, an advanced system machine, is well-suited to run molecular dynamics applications at extreme speeds to address materials aging issues confronting the Stockpile Stewardship Program. BlueGene/L is also demonstrating its effectiveness in running multi-scale, multi-physics codes at unprecedented scale on a compact, low-power platform.



ParaDiS dislocation dynamics simulation of molybdenum. Simulations run on BlueGene/L revealed the formation of previously undiscovered multi-junctions that were subsequently verified experimentally. The evolution and interaction of dislocations in the crystal structure contribute to strain hardening of the material.