ASC eNews Quarterly Newsletter

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Springtime in Washington

Editorial by Bob Meisner

Ret. General Smolen has introduced some organizational changes in Defense Programs at NNSA HQ. A major change that affects the ASC Program is that Dimitri Kusnezov has been asked to lead NA-11, I have assumed the role of acting ASC Division leader, and Njema Frazier is the acting deputy ASC Division Leader.

Our budget continues to be a challenge. The Future-Years Nuclear Security Program (FYNSP) budget continues to drop until 2011 when it finally begins to see some small increases. In this falling budget environment, we are making decisions on the future of the program with certain principles in mind:

PRESERVE a simulation and modeling capability sufficient to certify and assess current weapons systems with a high degree of confidence.

INVEST in the weapons science base to increase our ability to predict behaviors beyond our current experience derived from nuclear tests.

USE CAPABILITIES in simulating nuclear device performance to analyze threats and develop responses to scenarios that span the space of possible hostile actions.

SUPPORT TRANSFORMATION by ensuring that only those activities necessary for DP and NNSA missions are funded.

My objective is to ensure that we can deliver essential capabilities and services for the nation even in the face of substantial budget cuts. This may require that we make some difficult decisions that may affect how the laboratories contribute to defense issues, and we are informing the NNSA management of the budget levels where such decisions may need to be made.

My intention at this point is to press forward on the primary activities of the program. We have made significant progress over the years in moving toward a more predictive capability, in establishing national computing priorities, and in standardizing our capacity computing. We have succeeded in applying the largest computing systems to enhancing the reliability and safety of our stockpile. I plan to work with you all to increase our string of accomplishments, to encourage imaginative approaches to problems, and to continue our collaborative tri-lab approach.

Five Research Institutions Selected to Become Part of ASC's New Academic Alliance Program

On March 7, 2008, the National Nuclear Security Administration (NNSA) announced the selection of its five new centers of excellence whose primary focus will be on the emerging field of predictive science. Five universities will receive $17 million each over a five-year period under NNSA's Predictive Science Academic Alliance Program (PSAAP) agreement:

- The Center for the Predictive Modeling and Simulation of High-Energy Density Dynamic Response of Materials at **California Institute of Technology**. (http://mr.caltech.edu/media/Press_Releases/PR13118.html)
- The Center for Prediction of Reliability, Integrity and Survivability of Microsystems (PRISM) at **Purdue University**. (http://news.uns.purdue.edu/x/2008a/080307MurthyMems.html)

- The Center for Predictive Simulations of Multi-Physics Flow Phenomena with Application to Integrated Hypersonic Systems at **Stanford University**. (http://news-service.stanford.edu/news/2008/march12/airplane-031208.html)
- The Center for Radiative Shock Hydrodynamics (CRASH) at **University of Michigan**. (http://www.ns.umich.edu/htdocs/releases/story.php?id=6397)
- The Center for Predictive Engineering and Computational Sciences (PECOS) at **University of Texas, Austin**. (http://www.utexas.edu/news/2008/03/07/ices/)

"Since the cessation of underground nuclear testing, NNSA has used simulation and modeling tools and capabilities developed by the Advanced Simulation and Computing (ASC) Program to support assessment and certification of our nuclear weapons stockpile," said NNSA Deputy Administrator for Defense Programs, Robert Smolen. "ASC's academic alliances have been the training ground where graduate students and post-doctoral researchers gain and hone skills necessary to carry out large-scale simulations."

Predictive science is the application of verified and validated computational simulations to predict the behavior of complex systems for which routine experiments are not feasible. The selected PSAAP centers will focus on unclassified applications of interest to NNSA and its three national laboratories: Lawrence Livermore National Laboratory, Los Alamos National Laboratory and Sandia National Laboratories.

The PSAAP centers will develop not only the science and engineering models and software for their large-scale simulations, but also methods associated with the emerging disciplines of verification and validation and uncertainty quantification. The goal of these emerging disciplines is to enable scientists to make precise statements about the degree of confidence they have in their simulation-based predictions.

"We expect the PSAAP alliances will continue to help develop the predictive science field and the workforce of the future, wherein simulations will be pervasive and instrumental in important, high-impact decision-making processes," said Robert Meisner, director of the NNSA ASC Program.

For further details on PSAAP, visit http://www.sandia.gov/NNSA/ASC/univ/psaap.html.

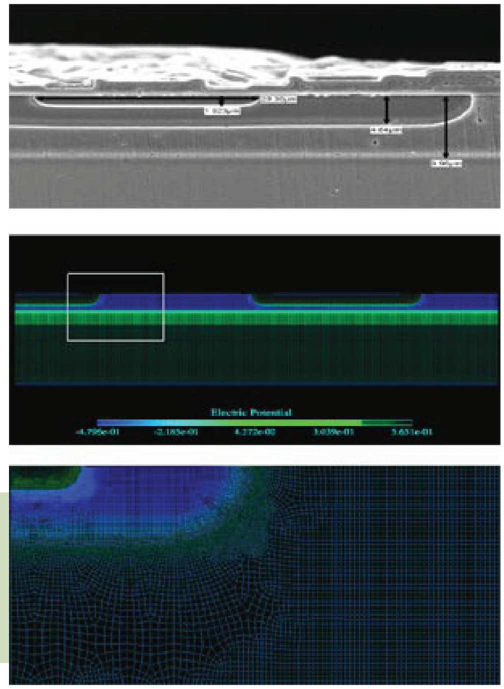
ASC Principal Investigators' Meeting Puts it all Together in Monterey, CA

The 2008 ASC Principal Investigators' Meeting was held February 25-27 in Monterey, California. The theme of this year's meeting was "Putting It All Together," highlighting the many ways that the ASC program is accomplishing its core mission and broadening its role for the future. Featured were three "end-to-end" sessions—one from each NNSA laboratory—that told a story of how a mission critical grand challenge is being met using the various program elements and "putting them all together." This theme was apparent through the many other programmatic, technical, and strategic presentations given by NNSA headquarters and laboratory staff during the two-day meeting.

Addressing the broadening mission of ASC, the meeting featured several presentations by experts from outside the program. These speakers discussed new applications of ASC tools, new challenges, and new opportunities for "putting it all together." A particular highlight of the meeting was the exciting work presented by the dinner banquet guest speaker, Dr. Vijay S. Pande, of Stanford University, on his project called Folding@home. The 2008 Principal Investigators' Meeting put it all together in presenting some outstanding technical accomplishments and broad programmatic activities of ASC, while providing some glimpses of a broader mission for the program in the future.

QASPR's Successful "Blind" Best Estimate Plus Uncertainty Predictions vs. Experimental Data for Radiation Effects Study

The Sandia Qualification Alternative to the Sandia Pulsed Reactor (QASPR) project team has successfully made "blind" predictions, with associated uncertainty quantification, of short-pulse neutron effects test data that were taken at the Sandia Pulsed Reactor (SPR) before shutdown of that facility in FY06. This short-pulse neutron environment is a key component of the hostile radiation environment suite to which nuclear weapon reentry systems must be qualified. The QASPR project, which is developing a combined test- and simulation-based alternative to the previous test-only weapon qualification process, has relied heavily on ASC-funded software tools and computational infrastructure. Specifically, this project has employed Sandia's ASC-funded RAMSES code for simulating the effects of short-pulse neutrons on electronic devices. RAMSES is built upon Sandia's ASC-funded Trilinos mathematical software library, and has employed Sandia's ASC-funded DAKOTA optimization/uncertainty quantification software toolkit. Sandia's Verification and Validation program provided the methodology to develop confidence in the predictive capability of RAMSES via software verification testing, along with validation studies involving comparisons to experimental test data. In addition, many of the RAMSES calculations were performed on the ASC Purple computer, with RAMSES accounting for 99% of the ASC tri-laboratory C1 class ("full machine") resources during the most recent Purple campaign. Current QASPR activities are focusing on additional "blind" comparisons of simulation data versus test data for more complex tests that also were conducted in the SPR facility before its shutdown at the end of FY06.



Electronic device micrograph (top), computational model of the device (center), and a detailed view of computational mesh used to model the device (bottom).

New Development Tool Enables Automatic Data Collection

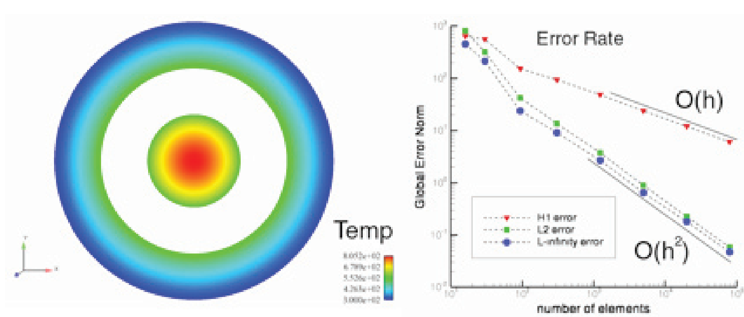
The ALE3D Code Team has completed a migration of its software development processes to the SourceForge Enterprise Edition (SFEE) collaborative development tool. SFEE, a commercial tool from CollabNet, is installed locally on Lawrence Livermore's yellow-net and is a secure, centralized, enterprise solution for optimizing and managing distributed software development.

SFEE's implementation will improve quality and productivity of software and software development processes by providing centralized tools within a common framework. The SFEE tools being used by ALE3D include Task Manager, Trackers, Wiki, Discussion Forums, Document Manager, interface to Source Code Repositories, File Release, Notification, Monitoring, and Reports. SFEE is being used to track tasks, milestones, project planning and management, software issues, requirements, specifications, design decisions, weekly group meeting notes, peer review notes, walkthrough notes, viewgraphs, emails, individual progress reports, process improvement planning, and implementation. The File Release tool is used to archive and distribute source code and builds. SFEE interfaces to Subversion (an open-source version control system) for source code management.

SFEE has enabled important contractually required artifacts to be collected automatically as part of the workflow, thus relieving developers of onerous documentation tasks. Better communication is achieved by centralizing information and automated collaboration between team members, which improves developer productivity and quality.

Encore Error Estimation Toolkit with Method of Manufactured Solutions

Encore is a component of SIERRA Mechanics that provides quantitative error estimates for simulation results or adaptive grid refinement. This information can be used to quantify or reduce the solution error. The Encore software toolkit has been extended to enable the Method of Manufactured Solutions (MMS). Using the Encore/MMS capability, developers and users of engineering and physics simulation software can perform code verification that is mathematically rigorous. Given a manufactured solution, Encore



A verification problem for coupled conduction and thermal radiation using the Encore/MMS capability in SIERRA Mechanics. Temperature contours are shown on the left, and convergence rates are shown on the right. Encore has quantified that the simulation has the expected accuracy, providing evidence that the numerical algorithms have been implemented correctly.

provides the necessary code input and then quantifies the difference between the code output and the manufactured solution. Recently, the Encore/MMS capability has been used in multiphysics thermal/fluid simulations and in fire environment simulations using SIERRA Mechanics, under the auspices of the ASC Verification and Validation Program. Under the ASC National Code strategy, the SIERRA Mechanics package will provide engineering code capabilities required for related weapons analysis across the three NNSA laboratories.

New Scalable Solver for SIERRA Mechanics

Linear solvers are the central building block of many applications. These solvers must be robust, accurate, scalable, and fast. The complexity arising from the growing number of constraint equations is of particular concern in this regard. These constraints make model building easier, but have been extremely challenging to iterative solvers.

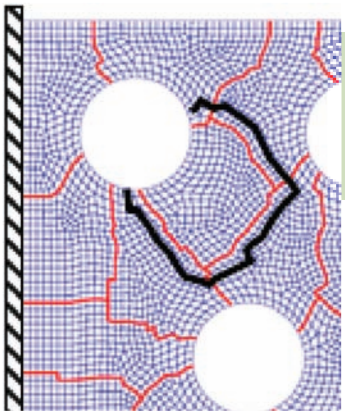


Figure 1. Overlapping grids used in the Schwarz preconditioner

Working with the ASC structural dynamics application team, a new solver has been developed that will address growing problem size and complexity of applications. The new solver is based on an overlapping Schwarz preconditioner (Figure 1), and its computer implementation was facilitated in large part by the parallel linear algebra services available in Trilinos.

On performance test suite problems, such as the one shown in Figure 2, this solver is often faster than previous ones, with speedups in excess of five times on some problems. The solver is more robust than its predecessor CLOP and handles large numbers of constraints quite efficiently, which has been an issue with other solvers. This new solver has been run on a wide suite of test problems with up to 3.5 M degrees of freedom.

The solver has been integrated into the ASC software development cycle and will be included in the SIERRA Mechanics Structural Dynamics module software release planned for April 2008. The Sierra Mechanics capabilities are widely used at Sandia for thermal and mechanical response predictions on weapon component design and qualification programs, as well as for analyses to assist with SFI closures. The SIERRA Mechanics package is also the Engineering Code cornerstone of the ASC National Code strategy for consolidating and focusing code development efforts within the three NNSA laboratories.

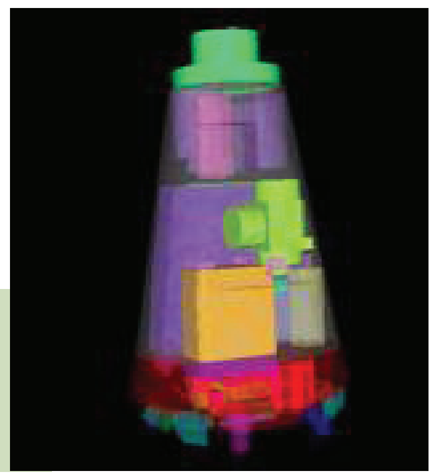


Figure 2. The new solver achieves over 5x improvement for some test problems.

MOU Signed on High Performance Computing Collaboration

A Memorandum of Understanding was signed on March 7, 2008, by Sandia National Laboratories (Sandia) and Los Alamos National Laboratory (LANL) to formalize the New Mexico Alliance for Computing at the Extreme Scale (ACES), which will provide High Performance Computing (HPC) capability computing for NNSA's stockpile stewardship mission. The ACES will create the strongest possible HPC team in the US to meet NNSA's most challenging computing needs and also support the decision to reduce capability computing sites across the NNSA Complex. Independently, LANL and Sandia have been world leaders in HPC for several decades. By bringing these two organizations together in the ACES partnership, stronger, more tightly integrated technical teams will emerge, efficiencies will be realized, and facilities at the two institutions will be optimized. The partnership is built on the strengths of both national laboratories. Joint teams have been formed to design, architect, deploy, and operate future NNSA production capability platforms. These platforms will support weapons physics and engineering calculations that require running across an entire platform.

W78 Drop Impact Sensitivity Analysis with SIERRA Mechanics Software

InIn a project jointly funded by the Sandia's ASC Verification and Validation Program and by Sandia's weapons engineering program, a full-system finite element structural model of the W78 has been built and is being employed to simulate accidental drop impact events. This study is an important component of the safety technical basis assessment for the W78 and will identify possible damage mechanisms that could lead to the loss of assured safety of the weapon. These simulations employ Sandia's SIERRA Mechanics software to capture the complex internal component and subsystem deformations that occur during the impact event. These simulations were enabled by new and robust material contact algorithms developed for SIERRA.

To date, 50 different drop impacts have been simulated to assess the sensitivity of the warhead's structural response to variations in impact velocity and angle. This sensitivity analysis will identify the worst-case set of impact conditions. Subsequent uncertainty quantification (UQ) studies will be performed using Sandia's DAKOTA optimization/UQ software, coupled with SIERRA, to assess the effect of material property uncertainties on the structural response of the W78. This structural response information will be used by the W78 system designers to quantify margins and uncertainties for the safety-critical components in the W78.

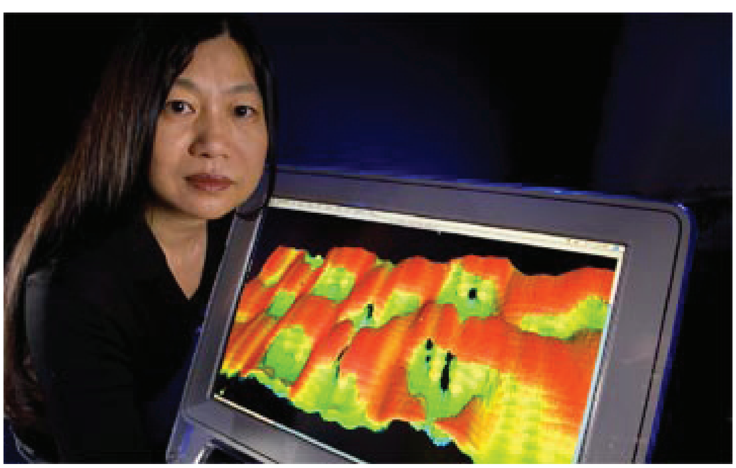
Red Storm Supports High-Priority Simulations for National Security Needs

During 12 weeks beginning December 8, 2007, Red Storm was configured as completely classified, applying the entire resource to support two high-priority calculations involving separate Sandia missions. The initial work was interrupted to make room for a time-urgent set of calculations, which were accomplished on time and consumed over 6 million node hours. The original project reclaimed the system and continued processing to completion, utilizing over 12 million node hours executing jobs using 12,900 dual processor nodes. Both of these programs were classified, and information is being tightly controlled; but the service provided by the Red Storm system and visualization and data management clusters, as well as the support provided by operations teams, were essential in the successful execution of these nationally important runs.

Newly Designed Web Site for the Los Alamos ASC Program

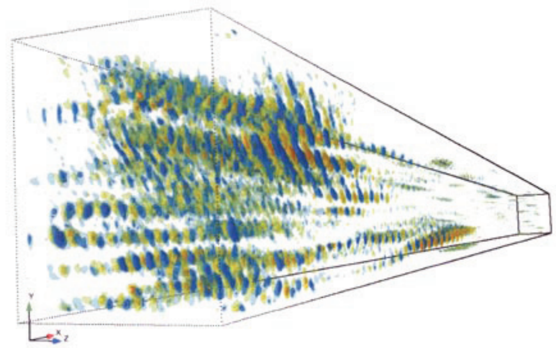
Los Alamos has published a newly designed ASC Web site available to the public at http://www.lanl.gov/asc. It features short articles about relevant research in a section called "A New Way to Understand." There are several links to information about the Roadrunner project, including its public Web site and a Roadrunner Fact Sheet.

ASC Salutes



Lin Yin is one of the more prolific and successful users of the VPIC [1] kinetic plasma modeling code. A technical staff member in Plasma Theory and Applications section of the Applied Science and Methods Development Group of the Applied Physics Division (X-Division) at Los Alamos National Laboratory (LANL), Lin has led the VPIC verification and validation effort. She has done high-impact PIC modeling in several settings, including electron sources in x-ray radiography, laser plasma interaction, laser-ion accelerators, magnetic reconnection, collisionless shocks, and kinetic Alfvén waves. She is the point of contact for laser-plasma interaction kinetic modeling at LANL, where she serves as liaison between the laser-plasma experimental and modeling teams.

Lin received her Ph.D. in Plasma Physics from the University of California, Los Angeles, in 1998. Lin came to LANL as a Director-Funded Postdoctoral Fellow in 1999 and became a technical staff member in 2001. She won DOE and NNSA Defense Programs Awards of Excellence in 2004 and 2006 for her work in kinetic plasma modeling in service of programmatic objectives. She is a highly accomplished scientist, having published over 50 peer-reviewed journal publications, and she is a Principal Investigator of numerous projects in kinetic plasma research.



New physics insight has been gained from recent large-scale 3-D VPIC simulations on the base system of Roadrunner by the VPIC team. These simulations use over 170 x 109 particles and 14 x 109 grids, 10 times larger than those possible before Roadrunner, and are the largest plasma particle-in-cell simulations to date.

VPIC simulation of backward Stimulated Raman Scattering (SRS) in the kinetic regime. Iso-surfaces of longitudinal electrostatic field show filament structures resulting from trapped particle modulational instability and self-focusing of electron plasma waves [2], the key physics underlying nonlinear SRS saturation. The laser is launched from the simulation geometry near face.

On the full Roadrunner machine, the VPIC team expects to be able to do PIC simulations with a trillion particles at a significant fraction of the theoretical 1 PFLOPS maximum. That would be 6 times larger than the current state of the art (and 100 times larger than what is typical) in the plasma physics community. Roadrunner will enable VPIC simulations at a size thought to be impossible only a few years ago, simulations of unprecedented fidelity that will drive discovery and push the boundaries of exploration in areas such as thermonuclear burn, laser-plasma interaction, ion source generation, and space and astrophysics applications.

[1] K.J. Bowers, B.J. Albright, L. Yin, B. Bergen, and T.J.T. Kwan, "Ultrahigh performance three-dimensional electromagnetic relativistic kinetic plasma simulation," *Phys. Plasmas* 15, 055703, (March 5, 2008).

[2] L. Yin, B. J. Albright, K. J. Bowers, W. Daughton, H. Rose, "Saturation of Backward Stimulated Scattering of a Laser Beam in the Kinetic Regime," *Phys. Rev. Lett.* 99, 265004 (2007).

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