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The Meisner Minute

Editorial by Bob Meisner

Between 2008 and 2009, ASC embarked on estimating the minimum program manpower needed to sustain its core mission. This challenge was in response to steadily declining ASC budgets that did not accompany a change in the scope of our mission. The activity was termed right-sizing.

Domain experts from each laboratory (Lawrence Livermore, Los Alamos, and Sandia National Laboratories) were assigned to determine the steady-state staffing to accomplish our core simulation mission. The team concluded, and independent assessments validated, that the minimum necessary size was approximately **930 FTEs—550** of these for the program elements: *Integrated Codes (IC), Physics and Engineering Models (PEM)* and *Verification & Validation (V&V)*; **380** for program elements *Computational Systems and Software Environment (CSSE)* and *Facility Operations and user Support (FOUS).*

I have discussed the right-size results with congressional staffers as they review our budget for a sizable plus-up going into FY11. They have expressed concern about how we can execute an ambitious hiring plan on such short order. I believe we can add high-quality scientists, engineers, and technicians to the team next year and that laboratory leaders are preparing the staffing plans to demonstrate that. We have done our homework and now await the appropriation committee’s decisions as they balance our needs in yet another challenging budget year. Many thanks to all who had a hand in building our case. Suffice it to say that the FY11 plus-up by the Administration, provided at a time when the nation is freezing budget increases, is a welcome acknowledgement of the importance of the ASC Program’s contributions to nuclear deterrence.

Even as we enlighten stakeholders on our FY11 needs, we are preparing for FY12. During the second week of March, senior leaders from across the nuclear security enterprise met to discuss the FY12 budget needs. We are still in the early formative stages of the budget cycle and there is little substantive information to report at this time.

In addition to progress on the budget front, we continue to advance capabilities across the computing complex. Dimitri Kusnezov and Joan Woodard, the director for National Security Technologies and Systems at Sandia, presided over the dedication of the National Security Computing Center (NSCC) on February 25, 2010, making Red Storm and its supercomputing capabilities available to national security mission applications beyond stockpile stewardship. Furthermore, Roadrunner was successfully accredited for use in the classified computing environment as of February 19, not a minute too soon to contribute to the Level-1 Energy Balance milestone. Also, the Critical Decision 2 and 3 milestones for Cielo were approved by Brigadier General Harencak on March 17, giving the ACES team authority to sign a contract to deliver a petaflops class system for the national user facility at Los Alamos.

As always, your achievements reflect well on the program and establish a credibility that allows us to garner the resources needed to continue to provide for a credible nuclear deterrent under the test moratorium.

Dawn Opens Door for Uncertainty Quantification Calculations

The Lawrence Livermore National Laboratory's (LLNL's) ASC Verification and Validation (V&V) program successfully executed a full run of the Primary Metrics Project (PMP) on the classified Sequoia Initial Delivery System (Dawn) supercomputer. The PMP tool is used to assess the global accuracy of nuclear testing models used in LLNL's ASC computer codes. PMP Project Leader Tom McAbee indicated that the run duplicated the accuracy achieved on current LLNL supercomputers used for stockpile stewardship computations.

"This success opens the door for use of Dawn and Sequoia as an uncertainty quantification engine for solving the vexing problems encountered in the stockpile stewardship effort," said ASC V&V Program Leader Joe Sefcik.

Building on the high-performance computing success of Blue Gene/L, Dawn (a Blue Gene/P system, pictured above) will serve primarily as a bridge to accelerate the scaling and tuning of key petascale applications on Sequoia (a third-generation Blue Gene system). Dawn will also be used for weapon science and uncertainty quantification studies.

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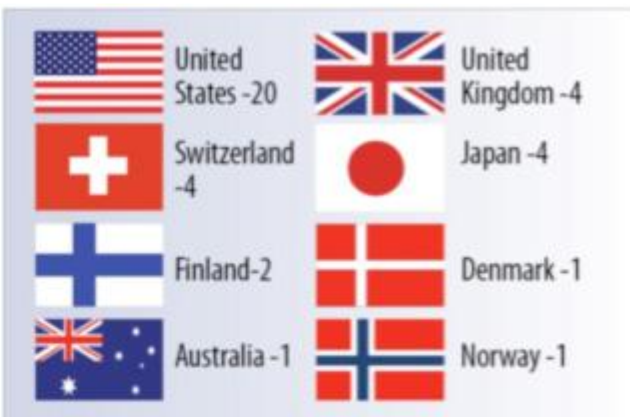
Red Storm Architecture Wins Technology Transfer Award

The Red Storm massively parallel processor (MPP) supercomputer architecture team has been selected as a winner of a 2010 award for excellence in technology transfer. These awards are presented annually by the Federal Laboratory Consortium for Technology Transfer and recognize laboratory employees who have accomplished outstanding work in the process of transferring technology to the commercial marketplace.

When reflecting on the partnership, Cray's president, Pete Ungaro, said, "Without a doubt, Cray's partnership with Sandia has been one of the most significant partnerships in the company's history. Not only did our collaboration on Red Storm result in significant scientific advancements and accomplishments in support of the Department of Energy's NNSA mission, it also spawned a very successful, proven line of Cray XT supercomputers starting with our XT3 system launched in 2005. What is even more significant is that the benefits of our relationship have extended beyond just Cray, Sandia, and the NNSA. Numerous high performance computing centers around the world have turned to the XT's MPP supercomputing architecture to help solve some of the world's most pressing scientific challenges, from systems of a single cabinet to the largest supercomputer in the world."



This illustration depicts the 37 derivative systems around the world, 20 of which are in the US. Red Storm revitalized a US industry, increasing HPC market share. With the commercialization of Re

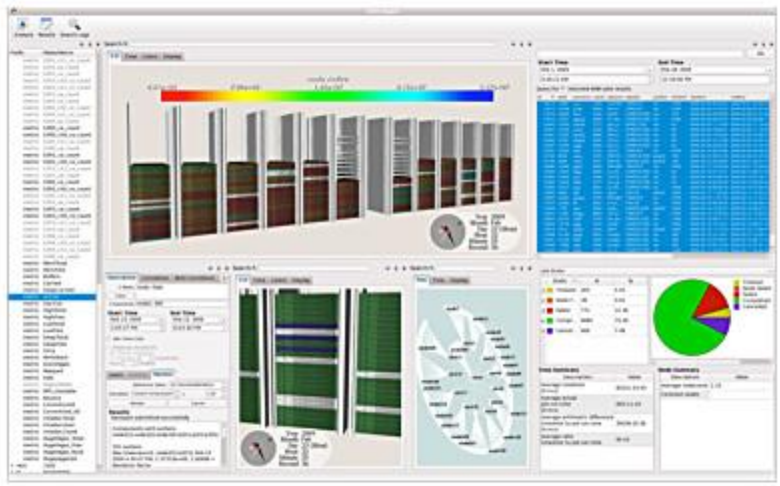
Collaboration with University Explores HPC Resilience

Sandia's OVIS project researchers have begun a collaboration with Louisiana Tech University's Extreme Computing Research Group (XCR). See http://xcr.cenit.latech.edu/blog.

OVIS is a tool for scalable data collection, analysis, visualization, and response invocation. See http://ovis.ca.sandia.gov. OVIS has been primarily targeted to resource analysis and failure prediction and mitigation for large-scale High Performance Computing (HPC) systems.

The collaboration will enable high reliability for extreme-scale HPC platforms by developing advanced capabilities for run-time failure prediction based on large-scale data fusion and new analytical approaches for quantifying the effectiveness of such predictions.

Sandia's OVIS software has been installed at LaTech.



This screenshot depicts the OVIS software monitoring Sandia's TLCC Glory cluster.OVIS and XCR Researchers at Louisiana Tech.

Energy Saving Facility Achieves Gold Level LEED Certification

The Terascale Simulation Facility (TSF) at Lawrence Livermore National Laboratory (LLNL) has received a Leadership in Energy and Environmental Design (LEED) gold level certification under the U.S. Green Building Council rating system.

LEED is an internationally recognized green building certification system. It provides third-party verification that a building or community was designed and built using strategies aimed at improving performance in energy savings, water efficiency, carbon dioxide emissions reduction, and other factors.

"This is truly a noteworthy achievement for NNSA and LLNL that symbolizes our commitment to transforming the Cold War-era nuclear weapons complex into a modern, efficient nuclear security enterprise," said Brig. Gen. Garrett Harencak, NNSA principal assistant deputy administrator for military application, in a congratulatory communication.

Completed in late 2004, the TSF is a 253,000-square-foot building that houses some of the world's fastest supercomputers, including the Sequoia Initial Delivery System (Dawn), BlueGene/L, and Purple—ASC systems largely dedicated to stockpile stewardship. TSF represents an innovative design that emphasizes function over form.

Examples of factors, or "points," contributing to LEED certification include air flow management in each of the 24,000-square-foot computer rooms, raising the air temperature in the computer rooms, raising cooling system water temperature, and using an automated electrical usage system to reduce off-hours power consumption in the office tower.

"This achievement demonstrates LLNL's and NNSA's commitment to energy efficiency and reducing our carbon footprint," said Dona Crawford, associate director for Computation." Gold level LEED certification was the result of the kind of team effort that is a hallmark of this Laboratory."

Successful ASC PI Meeting Brings Together Scientists, Researchers, and Sponsors

The Advanced Simulation and Computing (ASC) Program's Principal Investigators (PI) meeting was held in Las Vegas Feb. 8–11, 2010, to share research, scientific discoveries, computing status, and future computing goals in support of NNSA's Stockpile Stewardship Program. More than 150 people attended this year's meeting and listened to 27 technical presentations.

The PI meeting, held every two years, is the primary forum for face-to-face communication within the ASC Program elements. It provides a venue in which technical staff from the nation's three defense laboratories (Los Alamos, Lawrence Livermore, and Sandia), from ASC's Alliance partners at eight universities across the country, and from the Federal ASC Program office can share ideas, insight, and technical progress.

"It's essential to hold the PI meeting, as our program is becoming more integrated across the tri-lab each year," said Dan Nikkel, technical advisor to the Office of Advanced Simulation and Computing in Washington, D.C., and LLNL scientist. "This meeting provided a good overview of the ASC Alliances, from both the outgoing and incoming Alliance Centers. The team at Headquarters greatly appreciated this year's meeting."

The goals for the PI meeting included:

- Document program progress.
- Showcase progress to DOE/NNSA.
- Showcase the ASC Program to other organizations.
- Inform other ASC Program elements of progress and activities in specific areas.
- Identify/communicate future program directions.
- Build the tri-lab team within a social dimension.
- Set levels for activities across the tri-lab.
- Identify areas needing additional focus and energy.
- Provide opportunities for specialized meetings within the larger meeting.
- Establish cross-site collaborations.

"The ASC PI meeting was very successful in realizing our goals," said Brian Carnes, LLNL's ASC deputy program director. "Thank you to all who participated, including the speakers, the tri-lab organizing committee, and the LLNL support staff. It's hard for people not directly involved to understand the amount of effort and emotional energy that gets put into running one of these meetings," Brian continued. "Everyone involved should feel justifiably proud of the result of their efforts."

Sandia Hosts Workshop on Upcoming ASC Machines

Sandia held a workshop to explore the impact of upcoming ASC machines to application development on February 3, 2010 at its Computer Science Research Institute. Workshop speakers presented the hardware and software architectures of current and upcoming HPC systems available to Sandia ASC application developers. Armed with that information, attendees then convened to discuss the key features in the upcoming systems that will facilitate application development, those that might introduce new challenges to development and lastly, to identify what additional information was needed by developers. Commonality; batch queues for regression and scalability testing; and efficient support for dynamic libraries were seen as important features. One area of concern was the huge degree of parallelism coupled with flat, if not decreasing, amounts of memory per processor core. More information was needed on tools for code development. In particular, the developers requested a way to assess the performance of threaded algorithms without major rewrites of their MPI-everywhere code. There was also concern that threaded algorithms might need to be implemented differently, or may behave differently, on each system.

Members of the tri-labs are planning a workshop on HPC code development tools on March 24 and 25 at Sandia and Los Alamos, respectively. The workshop at Lawrence Livermore is tentatively planned for later in the Spring. Sandia is exploring the possibility of a third workshop on studying advanced architectures using the Structured Simulator Toolkit. Threading would be an important area of study in that workshop.

The Computer Science Research Institute (CSRI) at Sandia in Albuquerque.

Roadrunner Open Science Featured in *Physics of Plasmas* Journal

A research paper about work that made heavy use of the Roadrunner supercomputer during its open-science phase is one of three articles featured as a "Research Highlight" in *Physics of Plasmas*, the premier journal in the plasma physics discipline. The abstract, an image, and a link to the article were featured prominently on the front page of the journal's Web site: http://pop.aip.org/pop/research_highlight_archive. In December 2009, the article was the seventh in the rank of most downloaded article for the month.

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Greg Bronevetsky Garners DOE Early Career Award

Greg Bronevetsky of Lawrence Livermore is dedicating his early scientific career to ensuring that the increasing power, size, and complexity of the supercomputers critical to national security research do not come at the expense of their reliability.

Greg's sponsors have recognized the importance of his work with a U.S. DOE Early Career Award. He will receive $500,000 a year for the next five years to conduct his research.

Today's terascale supercomputing systems, such as the Sequoia Initial Delivery System (Dawn), already have hundreds of thousands of compute cores, and the petascale systems such as Sequoia, which is to be delivered in 2011, will have more than 1 million compute cores, millions of memory chips, and hundreds of thousands of disk drives.

"At these scales supercomputers become unreliable simply because of the large numbers of components involved," said Greg. "The next generation exascale (1 million trillion operations per second) machines are expected to encounter continuous hardware failures."

The role of computational science is to ensure applications critical to research in national security and basic science continue to develop and progress "in spite of such faults," he said.

The focus of Greg's project is to understand the effects of hardware faults and failures on computer applications by developing an automated methodology that is more efficient and less costly than current methods.

"My goal is to make large-scale computing systems more usable, manageable, and reliable despite their growing complexity," he said. "To this end, I am focused on developing automated methods to analyze the behaviors of hardware and software systems. This will enable a new generation of systems that can deliver high performance and productivity even on increasingly complex and unreliable supercomputing systems."

The current state-of- the-art is to run an application of interest thousands of times, each time injecting it with a random fault. The result is a profile of the application errors most likely to result from hardware faults and the types of hardware faults most likely to cause each type of application error.

"However, since this procedure is extremely expensive, it can only be done for a few applications of great importance," Greg said. "I will conduct research on a novel modular fault analysis methodology where the application will be broken up into its constituent software components, such as linear solvers and physics models."

Fault injection will then be performed on each component to produce a statistical profile of how faults affect and travel through the component, he explained. "These component profiles will then be connected to produce a model of how hardware faults affect the entire application."

Greg received his doctorate in computer science from Cornell University in 2006 at which time he came to the Laboratory as a Lawrence Fellow postdoc. He became a employee in August 2009.

ASC-Relevant Research

Lawrence Livermore
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ASC Salutes Guy Dimonte

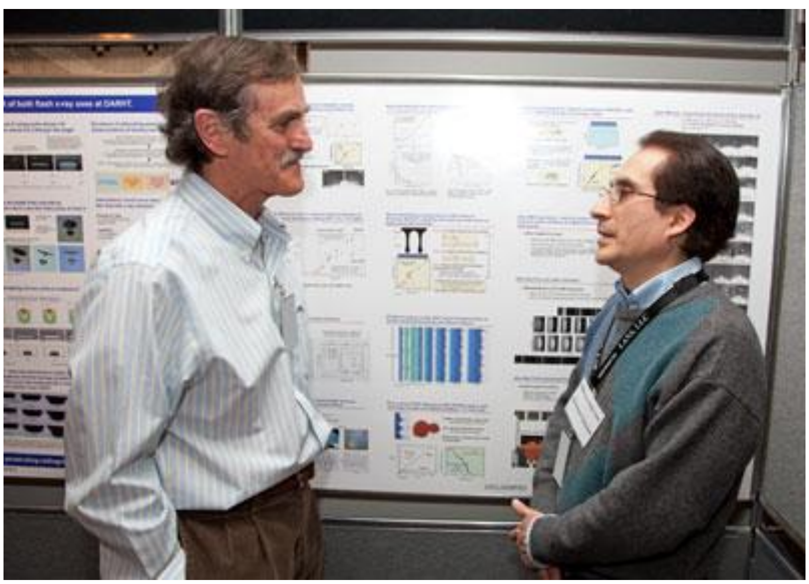
"For the first time it appears that there can be a picture of ejecta formation at the molecular level that will have parameters that represent rather faithfully the atomic-scale physics, although the interatomic potentials are empirical."

"The ejecta studies are models of how to combine experiment with advanced simulations. The ejecta simulations are connected not only to real-world experiments but also to virtual experiments. Virtual experiments could be defined as subscale simulations on petaflops-scale computers that can do a physically meaningful job of uncovering the transition from atomic scales to continuum scales."

—Comments from the *2009 Report of the ASC Predictive Science Panel at Los Alamos* by John M. Cornwall, Chair.

Guy Dimonte is part of a multi-disciplinary team that came together at LANL to develop a physics-based ejecta source and transport model to be implemented and validated in the ASC codes. The work, labeled as world-class science by the Predictive Science Panel, includes

- Experiments using proton radiography (pRad) at LANSCE and with probes at the Special Technology Laboratory (STL) in Santa Barbara, CA
- Modeling of Richtmyer-Meshkov instability (RMI)
- Numerical simulations using high-resolution 3D ASC science codes
- Model integration within the ASC Shavano Project



Guy Dimonte, on the left, shares some thoughts with fellow collaborator Guillermo Terrones.

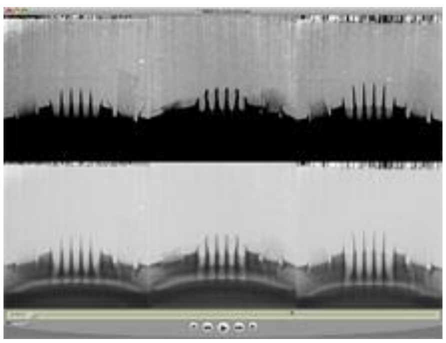
The ejecta problem has not yet been solved because it involves hydrodynamic instabilities in materials with complex equations of state and constitutive relations. As a result, only a multi-disciplinary effort involving different skill sets and numerical and experiments tools has any chance of succeeding. This multi-disciplinary approach is critical for solving complex problems, and few laboratories have the required skills sets and facilities like LANL.

The team is using all of LANL's ASC/HPC platforms including Roadrunner to inform the physics models in the area of hydrodynamic instabilities and thermonuclear burn. Such models are important for multi-physics codes, and they need validation with experiments and/or high-resolution, single-physics simulations. The latter are needed because experiments in the high-energy density regime are difficult and don't always give all of the required information for informing and validating the models. Physical and computer scientists have successfully converted a continuum hydrodynamics code, a particle-in-cell code and a molecular dynamics (MD) code onto Roadrunner to perform the single-physics simulations with unprecedented fidelity.

In order to cover the more than six orders of magnitude in scales, we perform multi-scale analysis by augmenting the microscopic MD simulations by Tim Germann (LANL) with large-scale hydrodynamic simulations by Guillermo Terrones (LANL) and P. Ramaprabhu (U North Carolina). They are complemented by experiments that are being performed at pRAD and STL by Billy Buttler (LANL) to help develop ejecta source and transport models. These models will then be implemented into the multi-physics codes for real-world calculations. During this process, the team has learned how ejecta is formed by the Richtmyer-Meshkov instability, and this has "explained" some existing experimental data. Going forward, the simulations are being used to design even better experiments on pRad and STL so that the team may rigorously test the new models.

The team is in the process of documenting their work for publication in peer-reviewed journals, but they have described preliminary results at the Nuclear Explosives Design Physics Conference, joint working groups (JOWOGs), program reviews, and workshops.

The vision for the future is to execute the multi-disciplinary strategy that has been organized and developed to solve an important problem for our programs. The team expects that their work will involve some technical breakthroughs, but they will also learn how to better plan and execute such difficult tasks allowing for better service to the nation in solving pressing technical problems related to security, energy, and climate.



Proton radiographs of Richtmyer Meshkov instability: into vacuum (left) and 4 Atm of Neon (center) and Xenon (right). The presence of gas causes the long spikes of Tin to break up into small particulates that stagnate due to the large drag force from the gas.

Click image to see entire movie.