Change Is in the Air

Editorial by Bob Meisner

Change is in the air in Washington, as it is across the nation...

It is risky to speculate on the next Administration’s expectations for NNSA and to what level the new team will support our efforts in the service of stockpile stewardship, but the early indications are certainly positive. Secretary Gates, who has agreed to remain a part of the President-elect Obama’s cabinet for at least a year, said at a speech in Minot Air Force Base in North Dakota that America’s security depends on a reliable and credible nuclear deterrent. “As long as others have nuclear weapons, we must maintain some level of these weapons ourselves to deter potential adversaries and to reassure over two dozen allies and partners who rely on our nuclear umbrella for their own security, making it unnecessary for them to develop their own.” Clearly, the Secretary of Defense understands our mission, and all indications are that he will support it energetically. For the position of Secretary of Energy, President-elect Obama has nominated a world-renowned physicist, the Director of Lawrence Berkeley labs, Stephen Chu. We know from public statements that a major priority for him will be alternate forms of energy production, and we believe that he will be an effective spokesperson for the scientific underpinnings and the necessity for a deep understanding of the performance of nuclear weapons as well as the avoidance of technological surprise from our potential adversaries. Who better to serve as a champion for science than a Nobel Prize winner in Physics who has been director of a premier science lab in the Department.

Although we look forward to strong support from the next Administration, resources will most certainly be tight. NNSA has put together a proposed 2010 budget for the transition team so that this next budget cycle can be developed on an accelerated time scale. I can tell you that this proposed budget does not reverse the negative trajectory that the ASC program has experienced over the past couple of years, and it can only be made to work by making some hard choices. We are currently being challenged to determine the appropriate level of funding needed to sustain a viable computing and simulation capability for the nuclear weapons program.

To that end, we have initiated an effort, with full involvement and support of the three Defense Program laboratories to understand in detail the specific capabilities that must be preserved in computing and simulation to ensure that the Administration and legislators can make informed decisions about what is required to maintain our nuclear deterrent. I recognize that an essential ingredient of our program is to enable our scientific and engineering staff to think deeply and creatively about the problems that may affect our understanding of the issues facing the stockpile and also about the wider spectrum of threats to our national security and I am committed to ensuring that this component is supported into the future.

I will need all of your help in making the case for the long-term viability of the ASC program. We will need to mount a concerted effort to tell our compelling story to the new team that will take office on January 20th, 2009 about the importance of maintaining a viable capability in support of our nation’s security. We will have a new slate of people who we must inform and educate about what we do and our level of accomplishment in national defense. We have a record to be proud of in our service to the nuclear security of our country, which has enabled the continuance of the testing moratorium. It is the proud achievement of the Defense Program laboratories to have maintained the essential capabilities for 18 years beyond testing, recruiting the best and motivating them to contribute to this national challenge. I am counting on our working together with the Labs to get out our message regarding the crucial nature of our mission and to be sure that it is heard.
Impact Simulations on Red Storm Address National Security Problem

At the request of the Missile Defense Agency, Sandia researchers used ASC's Red Storm supercomputer to address a complex, unprecedented mission. The objective was to protect against potential loss of life due to the uncontrolled reentry of a 2270 kg satellite and destroy its 450 kg hydrazine propellant tank. Preparation required countless hours of collaborative analysis to determine the feasibility of the SM3 interceptor to achieve this goal. Sandia was responsible for defining hit point requirements to achieve this objective using advanced modeling and simulation tools. In addition, Sandia assisted in predicting post-intercept satellite debris, and assessing kill/no-kill based on pre-event modeling. For more details, please go to http://www.sandia.gov/LabNews/081010.html

A handout describing the exhibit panels can be accessed on the following link: http://www.sandia.gov/LabNews/081010.html

ASC Simulation Capabilities Used to Address Aircraft Bomb Issues

Application of ASC’s high-performance computing capabilities to support areas other than the nation’s nuclear weapons complex is becoming more common. The latest beneficiary of DOE’s/NNSA’s investment is the Transportation Security Administration, which has received numerous briefings from an ASC tri-lab team on how computational modeling can help identify aircraft vulnerabilities. For more on this story, please go to: http://www.sandia.gov/LabNews/081010.html

Lawrence Livermore Teams with Computing Industry Leaders to Develop an Advanced Technology Cluster Testbed

Lawrence Livermore National Laboratory (LLNL) has teamed with 10 computing industry leaders to accelerate the development of powerful next-generation Linux clusters in a project dubbed Hyperion.

Hyperion brings together Dell, Intel, Supermicro, QLogic, Cisco, Mellanox, DDN, Sun, LSI and RedHat to create a large-scale testbed for high-performance computing technologies critical to NNSA’s work to maintain the aging U.S. nuclear weapons stockpile without underground nuclear testing, and industry’s ability to make petaFLOPS (quadrillion floating operations per second) computing and storage more accessible for commerce, industry, and research and development.

The goal of the project is to provide a development, testing, and scaling environment for new cluster technologies and infrastructure critical to the mission requirements of ASC. This includes testing new hardware and software technologies and forming long-term relationships to ensure continuity in the development of new technologies for ever-larger systems over the long haul.

Important technologies for scaling up computing clusters include Open Fabrics Enterprise Edition (OFED) InfiniBand™ Open Source software; Lustre Open Source Parallel File System; and Open Source Operating System Software and cluster tools used by the Tri-Lab Linux Capacity Clusters, which serve researchers at LLNL, Los Alamos, and Sandia. In addition, Hyperion will help lay the foundation for future
petascale ASC computing platforms by facilitating the development of processors, memory, networks, storage and visualization.

For more information, view the press release.


**The Power of Interactive Simulation: SC08 Roadrunner Demo**

The Los Alamos exhibit booth at SC08 featured a rack of 48 Cell processors of ASC’s Roadrunner hardware to run demonstrations. A demonstration code was run using a new version of the PPM gas dynamics code with a special treatment of the multifluid flow using the Piecewise-Parabolic Boltzmann scheme (PPB). The small interactive runs performed in the demonstrations at SC08 ran to completion in just 7 minutes.

The computational power of the Roadrunner hardware is so great that the flow can be seen to evolve literally as one watches the display screen. The demo showed a real-time display of the computation, not a saved animation! Even on this single rack of Roadrunner hardware, multifluid the PPM code runs fast enough to allow user-driven interaction.

This simple flow problem provides an example of the power of interactive simulation. In the demo, the Roadrunner hardware, together with the very accurate PPM code with PPB multifluid volume fraction advection, enables detailed experiments to be performed while you wait. The PPM code scales linearly up to the full size of the Roadrunner peta-FLOPS machine.

Once one has decided on the most interesting parameters for a problem like this one through an exploratory, interactive session, the grid can be increased to hundreds of billions of cells. Phenomenal accuracy and detail can then be achieved for guiding the design, testing, validation, and ultimately, application of subgrid-scale models of such turbulent mixing within larger and much more complex flows.

For more information contact Guy Dimonte, William Dai, or Matt Sheats at LLNL, and Paul Woodward at University of Minnesota, Laboratory for Computational Science and Engineering.

**Kansas City Plant Moves to TLCC Platforms to Support W76 AF&F Production**

The Kansas City Plant (KCP) has leveraged the work done by the three NNSA defense labs in an effort to bring forward the next generation of capacity platforms to the Nuclear Weapons Complex. One of the latest Tri-Lab Capacity Cluster (TLCC) platforms is now positioned at KCP for weapons manufacturing support. KCP’s mission is to produce many of the non-nuclear components for systems and is constantly challenged with maintaining high quality output with small production runs. Simulation technologies only enhance this mission, with the TLCC platform now enabling more coupled-physics and parametric studies.

The timing could not be better for KCP in support of the current production builds for the W76 Arming, Firing and Fusing (AF&F) system upgrades. The current challenges include both early manufacturing variance issues and rate production methods.
Computer simulations allow for an understanding into process variables and margins, and allow for confidence in the generation of products. Applications being processed on the new hardware include braze operations on interconnect headers, welding of sub-assemblies for safining devices, forging operations in support of vendor-procured reservoir parts and cavity blown encapsulations. Typical solution applications using the SNL Sierra suite of tools are 64-256 cores in size.

A New Warm-Dense-Matter Computational Modeling Development Announced

Sandia ASC-funded researchers are developing novel kinetic algorithms to study the equilibration, stopping power, and fusion reactivity of dense, radiating, burning multi-component, multi-species plasmas.

Fully relativistic, electromagnetic simulation of moderately-to-strongly coupled plasmas and warm-dense-matter makes use of non-linear inter-particle potentials calculated by a scalable implicit field solver. Validation of the simulations, within the LSP particle-in-cell code framework, against two-component hypernetted chain models enable the study of fundamental physical properties of coupled plasmas, including electron-ion temperature equilibration, and slowing-down of energetic charged particles in dense plasmas. Other applications include the study of the impact of impurities on various thermodynamic properties in warm-dense-matter, thermonuclear burn, and mix.

These algorithms are being used to study Thermonuclear Burn Initiative physics at the microscopic level, with the goal of developing accurate sub-grid models of the relevant processes for use in continuum codes.

Latest version of DAKOTA Released

Version 4.2 of the DAKOTA software toolkit was released and deployed in November 2008, and offers substantial advancements that enable efficient, robust analysis and design of critical systems in the presence of uncertainty (illustrated in the attached plot).

DAKOTA, which is currently in use at Sandia, Los Alamos, and Lawrence Livermore National Laboratories to support the nuclear weapon stockpile stewardship program and other national security programs, is also used broadly by academic, government, and corporate institutions for sensitivity analysis, uncertainty quantification, parameter estimation, and design optimization studies. (see: http://www.cs.sandia.gov/dakota)

Specific algorithmic improvements include:

- Uncertainty quantification: new stochastic collocation method based on Lagrange polynomial interpolation and more scalable generalized polynomial chaos methods, extended Latin hypercube sampling distributions and incremental random sampling;
• Optimization: new bi-level, sequential, and multi-fidelity optimization under uncertainty algorithms based on stochastic collocation and polynomial chaos, generalization of efficient global optimization technique;

• Calibration: new capability for surrogate-based model calibration, improved support for model calibration under uncertainty and weighted nonlinear least squares;

• Framework: new radial basis function and moving least squares surrogates, more efficient evaluation cache, and model recursion refinements.

DAKOTA 4.2 provides significant usability improvements, including a newly designed input parser, additional method tutorials, and examples demonstrating coupling DAKOTA to parallel simulation codes for analysis. These examples will be used in upcoming training classes at several sites. There is also improved platform support for Macintosh and Windows.

Finally, Version 4.2 allows more convenient and robust integration into other software libraries, such as Trilinos and Xyce, with special emphasis on efficiency for large-scale applications.

**New 3-D Ion Beam Simulation Capabilities Explored via Sensitivity Analysis**

Funded by the ASC Program, initial sensitivity studies of ion beam performance have been completed, using the new three-dimensional modeling capabilities of Sandia’s Aleph physics simulation code.

This study has characterized the effects on Aleph’s predictions of current density, due to variations in physics model parameters and numerical algorithm parameters. This is a key step in understanding: (a) the domain of applicability of the physics models in Aleph, and (b) the best values for the numerical parameters.
algorithm parameters that produce fast, correct results. The latter is particularly important, since Aleph’s run time can vary by an order of magnitude (10 hrs vs. 100 hrs) depending on the numerical parameter settings. This study also employed Sandia’s DAKOTA software toolkit to establish the Aleph run matrix for the sensitivity study, and to execute the Aleph runs on Sandia’s Thunderbird Institutional/ Nuclear Weapons Capacity Computing Cluster. Follow-on studies will perform a validation of the Aleph physics model via quantitative comparisons to experimental data.

Protection Against Erroneous Monte Carlo Calculations

Note that Monte Carlo calculations are statistical by nature. Every time a Monte Carlo calculation of a problem is done, a different answer (estimated mean) for the problem results. Without knowledge of a confidence interval, “the” answer from a Monte Carlo calculation is almost meaningless. It is like a political poll, the answer depends on the random choice of the particular people polled. The average result of the poll is meaningful only if there is an estimate of the error in the poll numbers. Just as no sophisticated political campaign would base actions on a poll with a huge margin of error, no scientist or engineer wants to base the analysis of nuclear systems on calculations with unknown margins of error.

Monte Carlo calculations rely on the central limit theorem of statistics to produce valid confidence intervals for the estimates. The central limit theorem, in turn, requires the estimates to have finite variances. Current Monte Carlo codes (e.g., MCNP) are not protected against attempting calculations having infinite variance, so current practice is simply to assume that the variance is finite, unless there is some obvious empirical evidence to the contrary. The necessity of this assumption means that the stated confidence intervals may not be valid in some cases.

In a paper available online in Mathematics and Computers in Simulation, Los Alamos staff R. R. Picard and T. E. Booth report mathematical proofs that a small, but extremely general, sampling modification, converts many infinite variance samplings seen in practice to finite variance samplings. Furthermore, empirical evidence suggests that this small modification, in fact, will convert all infinite variance samplings to finite variance samplings. To see the paper, go to http://dx.doi.org/10.1016/j.matcom.2008.11.014.

The figure shows how the error behaves in a slab penetration problem both with and without the sampling modification.
Roadrunner Maintains Top Supercomputing Spot

Roadrunner, the world’s first petaFLOPS system, ushers in a new era of computing for all applications of national interest. A revolutionary change, Roadrunner puts the nation on a different path to discovery. Though the revolution is not necessarily about speed, Roadrunner maintained its lead on the TOP500 list of supercomputers. The 32nd edition of the world’s top supercomputers was released on November 14, 2008, showing Roadrunner in the number one position with 1.105 petaFLOPS. Also cited for extraordinary energy efficiency, Roadrunner is number seven on the November 2008 Green500 list. The full Roadrunner system is now installed at Los Alamos.

Like other ASC supercomputers, Roadrunner will continue to challenge the state of art for computer scientists and manufacturers. Commended for its government and industry HPC collaboration, Los Alamos and its Roadrunner partners IBM, Panasas, and Voltaire received prestigious annual awards from the HPCwire online news and information web site that focuses on high-productivity computing. They received both the Readers’ Choice Award and Editors’ Choice Award for Top supercomputing achievement, and Editors’ Choice Award for Best HPC collaboration between government and industry.

Like a large experimental facility, Roadrunner is a tool for scientific insight to unknown physics in weapons systems as well as investigations in materials science, bioenergy, cosmology, plasma physics, epidemiology, and nanomaterials. Plans are to begin 4-month open-science runs in January 2009 to help with system stabilization efforts. For more information on Roadrunner open-science projects, go to http://www.lanl.gov/asc/docs/rr_open_science_final.pdf.

Red Storm Regains Position in Top 10 Fastest Computers


It described the architectural design that has allowed this machine to evolve and remain viable as hardware technology advances. Since last quarter, a new Top 500 list was published in November. In its new configuration, Red Storm achieved 204.2 teraFLOPS when running the HPL (High Performance Linpack) benchmark. This result moved it from the 12th position to the 9th position in the ranking.

Red Storm is now a mixture of dual and quad core nodes, from two different generations of AMD processors. Extensive testing has shown that for a number of ASC applications, the core performance is interchangeable. As a result, applications can run on a mixture of nodes without introducing a load imbalance. The additional contention for network and memory access in the quad-core processors is mostly offset by enhancements in the quad core processor (increased TLB entries, faster memory subsystem, and increased concurrent floating point operations.)

For more information, please go to: http://www.sandia.gov/ASC/rs-news.html

Los Alamos Hosts Predictive Science Panel

On November 12 through November 14, 2008, the Predictive Science Panel (PSP) met at Los Alamos. The PSP meets twice annually alternating between Lawrence Livermore (LLNL) and Los Alamos national laboratories to evaluate progress toward the goal of a credible predictive capability, answering the question: How do you know it’s right?
From the outbriefing on the last day of the meeting, the PSP noted “impressive progress on Roadrunner, and codes are being ported and used successfully on Roadrunner.” The PSP advocated for and laid out potential strategies for gaining fuller acceptance and support of the ASC Program with the new administration. The message is that ASC is a critical tool needed for the nation to help make decisions regarding nuclear strategies independent of the diversity and size of the stockpile. The PSP also noted good progress on W76-1 alternate materials studies.

The PSP requested that a 3-lab white paper be written on Quantification of Margins and Uncertainty (QMU) and Advanced Certification.

The PSP had a favorable response on the technical presentations delivered at the meeting. The presentations were organized into these technical categories:

- High-fidelity Simulations Enabled by ASC Tools
- ASC Tools Supporting Stockpile Decisions
- Non-Stockpile National Security Applications & ASC

**ASC Hosts Risk Management Workshop for High-Performance Computing Centers**

At the request of the DOE Office of Science, ASC at Lawrence Livermore National Laboratory (LLNL) hosted a two-day Risk Management, Theory and Practice (RMTAP) workshop Sept. 18–19 in San Francisco.

The purpose of the workshop, which was sponsored by the Office of Science/Advanced Scientific Computing Research and the NNSA/ASC program, was to assess current and emerging techniques, practices, and lessons learned for effectively identifying, understanding, managing, and mitigating the risks associated with acquiring leading-edge computing systems at high-performance computing centers (HPCCs).

“The findings of the workshop have been tallied and analyzed, said Mary Zosel, workshop organizer. “The overall impression was that formal risk management models apply to HPCC, with minimal special tailoring. All organizations are using some form of the risk analysis procedures, but there’s room for improvement. There was strong consensus that the top risk categories relate to scaling and that communications—especially with the platform partner—are an important part of best practices.” A formal report is now being prepared, and follow-on activities are being proposed.

Representatives from 15 high-performance computing (HPC) organizations, four HPC platform partners, and four government agencies attended the workshop, which was chaired by LLNL Deputy Department Head Terri Quinn. Each day of the workshop was organized as a plenary session followed by a track of four breakout sessions.

More information about the workshop is available at the RMTAP Web site, https://rmtap.LLNL.gov/.

**ASC Booth Showcases Numerous Achievements at SC08 in Austin, TX**

With a theme of “Leading HPC—Past, Present and Future,” the ASC Program once again demonstrated the numerous tri-lab advances in high performance computing at the International Conference on High-Performance Computing, Networking, Data Storage, and Analysis. Sponsored by the Association for Computing Machinery (ACM) and the Institute of Electrical and Electronics Engineers (IEEE) Computer Society, this year’s conference was held in Austin, TX, from November 15th to the 21st.

Led by Sandia National Laboratories this year, the booth was once again visited by U.S. and international experts and students in the field of high performance computing. ASC participants from the each laboratory served on conference committees, presented at technical conference sessions, gave demonstrations at the booth, and set up the booth. Booth participants had a full schedule of presentations and demonstrations.
ASC (formerly ASCI) has been exhibiting its lab-developed technologies at Supercomputing since 1996. The first tri-lab booth was set up at the conference in Pittsburgh.

**Visualization Team Upgrades ASC PowerWalls**

Lawrence Livermore National Lab (LLNL) recently completed upgrades to the ASC visualization theaters to improve overall picture quality and reliability or add the ability to project native PowerPoint files. Built and maintained by the ASC Program, the Lab's PowerWalls are extremely large multiprojector displays used for demonstrations, press conferences, visits, scientific collaborations, and other events that require high-resolution display capabilities.

"Each theater has its own advantages," said Becky Springmeyer, visualization project leader. "Some have conference room settings, one has auditorium seating, and another is a sizeable room that hosts large review panels and events. Our theaters include hardware and software designed not only for presentation use, but also for scientists to analyze data, share results, and visualize the massive amounts of data generated on our HPC platforms."

One PowerWall received a projector upgrade that substantially improves the image quality and allows 3D stereographic images to be displayed, which give scientists an innovative way to display their research. Specially formatted movies are required for stereo, and viewers must wear 3D glasses to get the proper effect. Also, the number of projectors driving the PowerWall was reduced from eight to six, and the new projectors are a higher resolution than previous models. This change improved the overall image quality of the PowerWall and reduced the number of interfaces between the projected images.

Modem upgrades were performed on two PowerWalls. The new modems allow the PowerWalls to receive clearer, brighter, and more reliable video signals from the Linux clusters, thus improving the...
image quality of both systems. The fiber infrastructure between two buildings was also updated and provides a major improvement for the one of the theaters.

In one of the PowerWall conference rooms, a Macintosh computer that uses a single lower-resolution projector was installed. “Talks projected on the PowerWalls are converted to a special ‘streaming movie’ format with greatly enhanced resolution that plays efficiently from our clusters,” said Spring-meyer. “The Mac system was installed so that presentations can be projected in their native Powerpoint format on a single projector, rather than the PowerWall. The Mac can more easily accommodate users’ last-minute updates to presentations, and users can incorporate special effects and animations in their slides.”

The ASC theater facilities are important visualization resources available to all employees working on ASC programs.

**ASC Salutes Paul Henning**

If you can imagine how it would be to be faced with demonstrating performance on a radically new computer architecture and to write code without having the real processors, memory, or interconnect, then you can understand how exciting Paul Henning’s life has been while working on the new Roadrunner supercomputer. A technical staff member in the Computing, Computation, and Statistical Sciences Division at Los Alamos National Laboratory (LANL), Paul has been involved with the ASC Program since January 1999.

As part of LANL’s Advanced Algorithms and Applications Team, Paul is a key contributor to the Roadrunner project. His implementation of a hybrid radiation transport application was one in a suite of performance demonstrations that changed the course of the Roadrunner project to gain full support for execution of the third phase of the petascale machine last December. He also led the design of a hybrid computing communications API (application program interface) specification.

Paul recalls that designing the communications API was risky, because the hardware design had not yet been finalized. “We drew on the experience that we had with the Cell processors and parallel communications to design a flexible API.” That flexibility was tested almost immediately when LANL and IBM devised a new, more power-efficient architecture. “Although the library implementation had to change, the API accommodated the radical design change.”

Paul is working with NNSA and ASC university alliances to be part of the solution to technical problems surrounding this shift in complexity and technology. According to Paul, “The new computers shift complexity from the hardware to the software, making our codes even more intricate. In order to put these new machines to work for us on scientific computing problems, we will have to develop new programming models and prepare developers to work in new environments.” Paul is enthusiastic about the opportunities that are present with the challenges that must be met to keep one leap ahead of technology. “It is very exciting,” he says, “to be involved in computing at this time of rapid innovation.”

Paul has a Ph.D. in Computer Science from the University of Iowa. Before coming to Los Alamos, Paul worked as a student at NASA Ames Research Center and Sandia National Laboratories. While at NASA Ames, Paul was part of a team that had an instrument on the Mars Pathfinder mission—the first rover on Mars. Recalling the excitement of being at mission control at the Jet Propulsion Laboratory for the touchdown of the rover, Paul expresses how fortunate he feels to be involved in cutting-edge projects. “Whether it’s rovers or supercomputers, the best part is the opportunity to work on great teams. I can’t wait to see what is next.”
To see Paul’s presentation Milagro II, a discussion of a different approach to put Milagro on Roadrunner, what results were obtained, what was learned, and what is next, go to the Roadrunner technical seminars at http://www.lanl.gov/orgs/hpc/roadrunner/rrseminars.shtml

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