ASC™ ASCeNews QUARTERLY NEWSLETTER

NA-ASC-500-06-Vol.1 Issue 1

October 2006

The View from HQ

by Dimitri Kusnezov

As I write this, we don't know the result of the upcoming elections, but whichever direction the elections go, we can expect the strong support of both sides of Congress to continue for the ASC program. We have a critical leadership role in national security and have demonstrated success in managing the program and delivering high-quality products.

Looking back over our accomplishments from last year there are several that demonstrate the reach of our program. Our influence on the computing industry is profound. We delivered on our long-term goal this year of making available to users a 100 TF computer system—the Purple computer at Livermore. Also, because of ASC leadership there were two new commercially successful product lines introduced last year by our industry partners: the Blue Gene/L computer at Lawrence Livermore and Red Storm at Sandia. We also completed the initial phases of another potentially ground-breaking computer, the Roadrunner computer at Los Alamos.

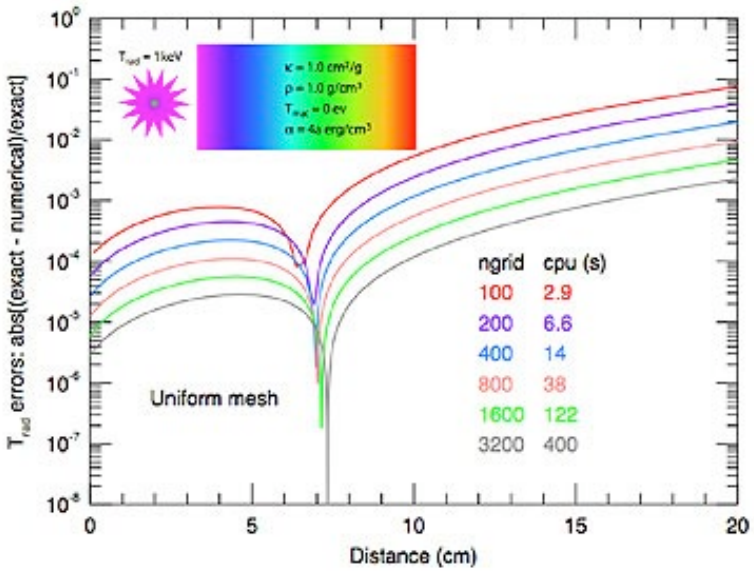
But we are primarily measured on what we deliver using these advanced computer systems. The most visible product over the past year was the RRW feasibility study. This study involved all three national weapons laboratories. It was completed in a remarkably short time—a few months rather than the historical time of years—because of the dedication of our people at the labs and because of tools that ASC has made available to stockpile stewards over the past decade.

As the codes are the repository of our nuclear weapons expertise, we recognize the broad national needs we must meet, such as forensics, attribution, accident scenarios and emerging threats. This is an important role that is especially timely because of the recent Democratic Peoples Republic of Korea incident and the growing concern in the international community regarding proliferation of nuclear devices.

We as a program are in a time of transition that reflects the changing world. But we have an important job to do for the nation, and I'm proud to be part of this team.

Tri-Lab Test Suite Probes ASC Code Capability

LANL scientists achieved a new landmark with the first complete coverage of the Tri-Lab Verification Test Suite on 1-D, 2-D, and 3-D grids. The Tri-Lab Test Suite probes three aspects of an ASC code's capability. The first inquiry examines the ability of the code to generate the correct answers to test problems with known solutions. The second probe scrutinizes the quality of those answers on uniform and nonuniform grids. The third probe quantitatively assesses how quickly the ASC code converges to the correct answer as the number of grid points is increased, and if that convergence rate is compatible with the expected theoretical maximum rate. Daily runs of the suite on a development code contribute to new releases of an ASC code being "born verified." This work was part of the basis for two Defense Programs Awards of Excellence for the ASC Program in October 2006.



Reconstruction Method Developed

A Sandia team (Stewart J. Mosso,Christopher J. Garasi, Richard R. Drake, and Allen C. Robinson) has developed and implemented a second-order accurate material interface reconstruction method in the ALEGRA High Energy Density Physics (HEDP) code. This method provides a higher fidelity approach for the simulation of material motion. The higher-order interface reconstruction algorithm is being applied to Rayleigh-Taylor unstable interfaces between conductive materials under rapid acceleration from very strong magnetic forces induced by large electrical currents. These interfaces are commonly encountered within simulations of experiments completed on Sandia's Z machine. The simulation of material motion is particularly sensitive to the accuracy of the reconstruction method. Lower order methods produce more ejecta, which has a large effect on the material state, especially the compression/stagnation of the materials by magnetic forces.

The new method, called Patterned Interface Reconstruction (PIR), evolved from the Young's Method (AWE) and the Stability Point ideas of Blair Swartz (LANL). This algorithm is a computationally efficient yet accurate method. A simple demonstration [375 KB] is the motion of a slab through a mesh, in which the PIR method reproduces the analytic result. A second demonstration 1.2 MB] is of a sphere moving through a mesh. In both demonstrations, as the material interface exits the mesh boundary, little or no distortion of the interface occurs. This is in contrast to the unsmoothed method in which mesh boundary effects show large distortions of the interfaces for both slab [366 KB] and sphere. [1.2 MB]

Winner of an R&D 100 Award, Sapphire Helps Find Useful Data

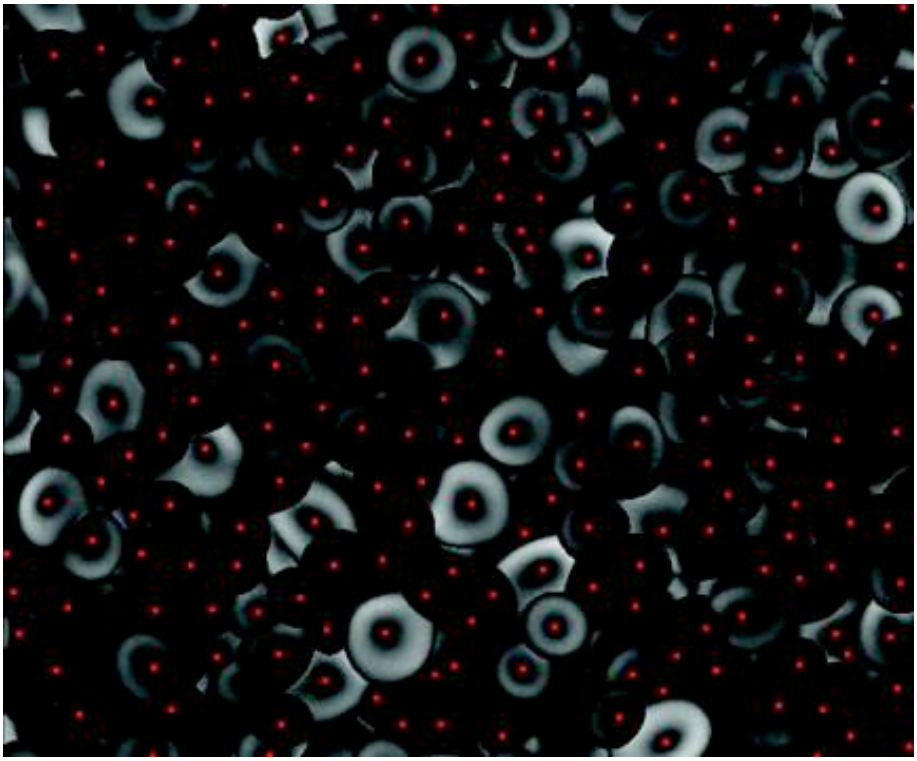
One of the great challenges researchers face today is extracting the information they need from enormous data sets. A Lawrence Livermore team, partly funded through ASC's Pre- and Post-Processing Environment (PPPE) effort, has developed analysis algorithms allowing the exploration of large, complex, and multidimensional data sets. The technology has been dubbed Sapphire and recently captured one of seven R&D 100 Awards received by Lawrence Livermore from the trade journal *R&D Magazine* for being among the top 100 industrial innovations worldwide for 2006.

"Our ability to generate data far outstrips our ability to explore, analyze, and understand it," said Chandrika Kamath, of the Center for Applied Scientific Computing and leader of the Sapphire project. "Data that were measured in gigabytes (billions of bits of information) until recently, now are being measured in terabytes (trillions of bytes) and will soon approach the petabyte (100,000 trillion bytes) range.

"Often, the data are complex, available either as time-series data, or as images. In order to achieve our scientific goals, we need to fully exploit this data by extracting all the useful information from them. This is the idea behind Sapphire," Kamath added.

By applying ideas from data mining, video processing, statistics, and pattern recognition, lab researchers are developing new computational tools and techniques to extract useful information from huge data sets.

Sapphire technology is being applied in a variety of disciplines, including plasma physics experiments and simulations, remote sensing imagery, video surveillance, climate simulations, astronomy, and fluid mix experiments and simulations. The lab team has six patents on Sapphire technology.



Sapphire software is being used to characterize and track bubbles and spikes in an 80 terabyte data set from a 3-D, high-fidelity simulation of the Rayleigh-Taylor instability. This image shows the bubble counts using the magnitude of the X-Y velocity at the bubble boundary. Only 1/36 of the 2-D data is displayed.

ASC Roadrunner Era Begins at LANL: Near-term capacity with a future hybrid accelerated option

The first components of the Roadrunner supercomputer arrived in Los Alamos on September 25, just two weeks after the contract with IBM was signed. The primary goals for the Roadrunner system are as follows:

- Providing a large-capacity computing resource for LANL weapons simulations
- Implementing optional upgrade to petascale hybrid accelerated architectures capable of supporting future LANL workload.
- Becoming a lead participant in the industry-wide path toward hybrid accelerated computing devices for HPC.

Milestone-Supported Study Shows Promising Results

A Sandia FY06 ASC Algorithms Level 2 milestone, "Algorithms for error-corrected reliability analysis in risk-informed design" was recently completed. It combines error estimation and adaptivity, uncertainty quantification, and probabilistic design capabilities for application to the analysis and design of bistable microelectromechanical (MEMS). The report reveals that through the use of error estimation and adaptive mesh refinement, solution verification can be performed in an automated and parameter-adaptive manner. The resulting uncertainty analysis and probabilistic design studies are shown to be more accurate, efficient, reliable, and convenient.

2006 Milestones [PDF 2.4 MB]

Sandia Achieves Turnkey Distance Visualization of Large Data ParaView

In September 2005, Sandia National Laboratories achieved a turnkey distance visualization milestone with the latest release of ParaView, an open source visualization tool. High energy density physics (HEDP) analysts in New Mexico visualized terabyte-sized data from ASC Purple in California. Though Purple has no specialized graphics hardware such as accelerated graphics cards, and the link itself is encrypted, the out-of-the-box solution of ParaView's client/server architecture delivered results that delighted analysts.

"Wow," was one customer's reaction, in comparing ParaView's performance to other tools. ParaView delivered a 2x increase in performance for modest sized data (27 million unstructured cells), and was the only usable tool for an HEDP dataset consisting of 274 million unstructured cells.

This achievement is remarkable in part because it used the current release version of ParaView (2.4.4), which includes important Sandia contributions. We expect this work to have impact on a wide range of problems at other institutions, through the code available for download at http://www.paraview.org.

Release of New Tools Improves Streamlining

On October 3, Sandia's DART (Design Through Analysis Realization Team) group released an integrated suite of tools to benefit their customers within the analysis and nuclear weapons groups. This release, driven by past ASC milestones, provides analysts and designers a carefully integrated suite of tools that use a metadata layer to provide flexibility and agility. The tools are provided within a project management framework that also provides artifact tracking, pedigree, and archiving. The tools within the suite include modeling, geometric editing, decomposition, meshing, model management, material property management, workflow management, job submission, and post-processing.

DART's goal is to streamline the modeling and simulation, provide better traceability and thus to improve the responsiveness and quality of the analyses. Many of the tools have been released independently and continue to have significant impact, both at SNL and throughout the weapon complex. This integrated release now allows teams of users to coordinate their analysis efforts and provides a powerful mechanism for data to be passed effectively between these tools. Such data include assembly structures, material identifiers and properties, and Quality Assurance records. This unlimited release is available on the classified and unclassified systems.

Moab Software to Standardize Workload and Resources Across NNSA

The ASC Program has selected Cluster Resources, Inc.'s, Moab workload and resource management software as a standard for use across NNSA's high-performance computing systems. The contract is the largest cluster and grid management contract in history. "Cluster Resources is honored to be selected," said David Jackson, CEO of Cluster Resources, Inc. "There is no organization in the world which matches the technical expertise and scope of compute systems found at ASC in terms of scalability and architectural complexity."

Lawrence Livermore, Sandia, and Los Alamos national laboratories initiated the search for a common resource and workload management solution to improve usability and manageability of their diverse resources and to attain an improved return on their significant computing investment. In addition, the laboratories also sought to enhance reporting for managed resources and to optimize resource utilization while maintaining the flexibility required to meet the individual needs of each site and project. All three laboratories have highly heterogeneous environments with systems that range from large-scale Intel and AMD Opteron-based systems provided by IBM, HP, Dell, and others, to more exotic and powerful systems such as Cray's XT3 and IBM's BlueGene.

As part of its initial acceptance and deployment, Moab will first be installed on the new unclassified Atlas system at LLNL, obtained through the Peloton procurement. LLNL has started working with Cluster Resources on a migration and acceptance plan. LLNL will also develop a tri-lab support model to help leverage support across the ASC Program.

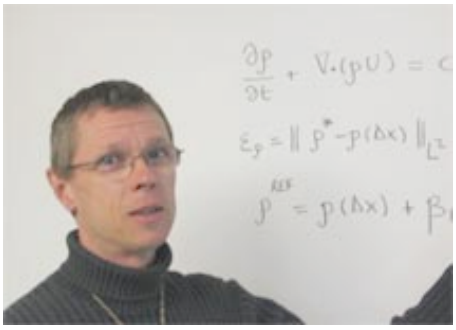
The Moab solution adds significant manageability and optimization to HPC resources, while providing deployment methods that effectively minimize the risk and cost of adoption. Unique Moab capabilities allow it to be transparently deployed with little or no impact on the end-user; these capabilities include system workload, resource, and policy simulation, batch language translation, capacity-planning diagnostics, nonintrusive test facilities, and infrastructure stress testing.

Contract Awarded for Tri-Lab Resource Management System

Cluster Resources, Inc. (CRI) is the winning bidder for a new tri-lab resource management system. This award marks the beginning of a multi-year collaboration between the tri-labs and CRI. Their resource management system, Moab, will first be deployed on the Atlas machine at Lawrence Livermore, which is a 44-teraFLOPS M&IC Peloton cluster. It will then be gradually migrated to other Lawrence Livermore systems. One of the key features of this solution is that users will continue to be able to use their familiar LCRM commands, through the implementation of wrappers and translators. For more information go to http://www.clusterresources.com

Los Alamos Develops V&V Course

During spring 2006, the ASC Verification and Validation (V&V) Program element at Los Alamos supported the development of a one-quarter graduate course on code verification, model validation, and the quantification of prediction uncertainty. The course was taught by François Hemez of the Applied Physics ("X") Division through the Engineering Institute, a joint, multidisciplinary research and educational program between Los Alamos and the University of California, San Diego (UCSD). Course content includes activities for verifying the convergence of calculations, quantifying experimental and numerical uncertainty, eliciting expert knowledge, and validating simulation predictions. Fourteen graduate students passed the course, which was presented by video-conferencing and a video-streaming-enabled website hosted by the UCSD Jacobs School of Engineering. Student evaluation of the course was quite positive, and there are plans to expand this activity. Beyond its programmatic relevance for developing a predictive capability for the DOE Complex, the course serves the ancillary function of training and recruiting the next generation.



Ten-Year University Alliances Program Nears End

Annual site reviews were held during August and September 2006 of the five ASC Strategic Alliances Program (ASAP) centers of excellence: the California Institute of Technology, University of Chicago, University of Illinois at Urbana-Champaign, Stanford University, and University of Utah. The reviews were conducted by the associated Tri-lab Sponsoring Team (TST) for each Center and the Alliance Strategy Team (AST). The TST Leads led the reviews.

Started in 1997, ASAP ends in 2007. Each Center's review focused on its technical progress, its legacy (not only to its university but also to the scientific community), and its impact on the three defense laboratories. Ambitious full-system simulations for the tenth year have been planned, assuming access to the needed computational resources is available.

Each Center has made significant progress in the past year and reported on important legacies. The program's impact on the three laboratories was discussed in terms of research collaborations, laboratory hires from the five Centers, and some transfer of scientific results and code. Review reports are being prepared for each center. The AST will also publish a summary report documenting review findings for the ASC Execs.

For more information on each Center, go to:

http://www.sandia.gov/NNSA/ASC/univ/univ.html
http://csdrm.caltech.edu/
http://flash.uchicago.edu/website/home/
http://www.csar.uiuc.edu/
http://www.stanford.edu/group/cits/index.html
http://www.csafe.utah.edu/

Follow-On University Program, Predictive Science Academic Alliance Program (PSAAP) Initiated

Following in the footsteps of the soon-to-conclude ASAP, the newly authorized Predictive Science Academic Alliance Program (PSAAP) has been initiated. Authorized by the ASC Execs, the primary goal of the PSAAP is to establish validated, large-scale, multidisciplinary, simulation-based "Predictive Science" as a major academic and applied research program.

A bidders meeting was held at the Dallas-Fort Worth Airport on May 16 and 17, 2006, and a Request for Interest (RFI) was released on June 15, 2006. There were 34 responses to the RFI received on July 17, 2006. Responses covered broad areas of scientific domains. A review of the RFI responses was completed on August 10, 2006, by a panel of experts from the three defense laboratories, other DOE national laboratories, federal agencies, and academia. Eighteen respondents have been encouraged to submit full proposals. The current plan is to release a Request for Proposals (RFP) in November 2006. The goal is to place PSAAP subcontracts by October 1, 2007. For more information, visit
http://www.llnl.gov/asci/alliances/psaap/psaap.html

ASCI Red Retired

ASCI Red was the first computer system to achieve more than 1 teraFLOP on the LINPACK benchmark, claiming the number one spot on the TOP500 list of major supercomputer systems in the world in June 1997. It was declared excess property and retired in July, 2006.

The disk subsystem was sanitized via physical destruction of the recording media, and the components of the system were designated scrap and physically rendered unusable. A ceremony in June marked the retirement/decommissioning the ninth anniversary of the commissioning of the system.

ASCI Red remained number one on this list until being bested by ASCI White at Lawrence Livermore in November 2000. Along the way, its performance on the benchmarks increased from the initial 1.068 teraFLOPs measured in June 1997 to 1.338 teraFLOPs in November 1997, to 2.1213 teraFLOPs in June 1999, and finally to 2.3796 teraFLOPs in November 1999. This run of seven consecutive #1 positions was unprecedented and has not been duplicated. In addition to being the first system toattain 1 teraFLOP, it was the first measured above 2 teraFLOPs, and, quite unexpectedly, would still have placed on the TOP500 list in November 2005 and June 2006 had it remained in service.

The system was in production use by Sandia, Lawrence Livermore, Los Alamos, and University Alliance partners until it was removed from service in October 2005 in a cost-reduction move for the program. Performance of major programs on ASCI Red was to be used as a benchmark for the required performance of its replacement, the Red Storm system developed in partnership with Cray. The Red Storm system was required to perform at least seven times faster than the ASCI Red system, a measurement that required many sets of tests to be run on ASCI Red during its last few months in service.

The room-sized system was incredibly stable during the last few years of service, a testament to the robust aspect of the architecture and the skill and dedication of the personnel charged with designing, developing, and operating this unique system. Intel developed the system in cooperation with Sandia and used a Sandia-developed light weight kernel operating system for the "compute nodes," which contributed to the longevity of the system and its operating efficiency.

Following DOE/NNSA policy, the system was declared excess property in July 2006. The disk subsystem was sanitized via physical destruction of the recording media, and the components of the system were designated scrap and physically rendered unusable. A ceremony marking the retirement/decommissioning was held in June on the ninth anniversary of the commissioning of the system. Attendees at the ceremony signed a commemorative plaque containing a picture of the system. Arrangements have been made to send a cabinet to the Smithsonian Institution where it will join other significant computers on display. Additionally, Sandia is negotiating with the Computing History Museum in Mountain View, California, to have them add parts of ASCI Red to their collection.

ASCI White Retired

As reported in the October issue of the NNSA newsletter, ASCI White, the supercomputer at Lawrence Livermore, was shut down in July of this year.

Read the story on page 3 of the October NNSA Newsletter.
http://www.nnsa.doe.gov/docs/newsletters/2006/nl_2006Oct_NNSA_News.pdf [1.2 MB]

Recently Completed:

- The major Tri-lab runs required for the Q1FY07 Purple, 100-TF Environment L1 milestone, which is led by Terri Quinn (LLNL), Rand Rheinheimer (LANL), and Judy Sturtevant (SNL), have been completed.
- The first set of Capability Computing Campaign (CCC) runs on Purple began on schedule on October 16, 2006.
- The LANL Roadrunner system is the first ASC platform to go through the DOE Order 413.3A process for "Program and Project Management for the Acquisition of Capital Assets."
- 2006 Reviews for the ASC L1 Centers at Caltech, the University of Chicago, the University of Illinois, Stanford, and the University of Utah were completed in August and September. (See the article in the ASCeNews for more details.)

ASC Salutes

Editor's note: Each quarter, the ASC Program will feature the outstanding contributions of one of its numerous tri-lab scientists, engineers, and administrators. This month, we proudly present Dr. Anthony Giunta.

Tony Giunta giving a presentation on Verification, Validation, and Quantified Margins and Uncertainties at a recent joint US-Russian Federation workshop for scientists and engineers. (April 2006)

Dr. Anthony (Tony) Giunta is a technical staff member in the Validation and Uncertainty Quantification Department within Sandia National Laboratories' Engineering Sciences Center. For seven years, Dr. Giunta has been involved in a wide range of ASC-funded projects that span the research, development, and application spectrum. Early in his Sandia career, Dr. Giunta performed research on advanced optimization and uncertainty quantification (UQ) algorithms that were implemented in the DAKOTA software toolkit. Over the past three years, he has been focused on applying UQ methods to engineering and scientific problems of interest to DOE and DoD. Primarily, his UQ applications work has focused on the Qualification Alternatives to the Sandia Pulsed Reactor (QASPR) program, numerous stockpile performance assessment studies for NNSA's Defense Programs office, and several work-for-others projects involving DOD. In addition to his UQ applications, Dr. Giunta collaborates with staff from Sandia, LANL, and LLNL to create and apply methods for the quantification of margins and uncertainties (QMU) in assessing the surety of the stockpile. Dr.Giunta describes his UQ/QMU work as delivering a "best estimate plus uncertainty, not just a single 'point estimate' of system performance." Tony credits the ASC Program with creating the environment in which these important stockpile surety questions can be addressed. "The ASC Program has put tremendous capability and capacity computing into the hands of our technical staff. The challenge we now face is determining the best mix of high-fidelity (capability) computing and medium-fidelity (capacity) computing for each project, in order to deliver a 'best estimate plus uncertainty' that is on-time and on-budget for our customers."

Dr. Giunta is engaged in a broad array of research and applications involving engineering of complex systems. His research interests include multifidelity physics modeling techniques for engineering system uncertainty quantification and design optimization. This is a multidisciplinary field that combines engineering systems design, applied mathematics, statistics, and computer science. This research directly supports Dr. Giunta's engineering applications work, which involves high-consequence, computationally challenging national security problems of interest to the DOE and DoD.

Dr. Giunta is an expert in the field of multifidelity and multidisciplinary engineering design optimization, and in the use of high-performance computing resources for engineering design. He has participated in numerous invited technical panels and workshops covering these topics, and he is the author of over 50 technical publications including 11 peer-reviewed journal publications. Dr. Giunta is a member of the Multidisciplinary Design Optimization Technical Committee of the American Institute of Aeronautics and Astronautics, as well as the Activity Group on Optimization and the Activity Group on Computational Science and Engineering of the Society of Industrial and Applied Mathematics.

Prior to joining the technical staff at Sandia, Dr. Giunta was a National Research Council Postdoctoral Fellow in residence at the NASA Langley Research Center in Hampton, Virginia. His postdoctoral research focused on sensitivity analysis methods for high-fidelity, coupled-physics aero-structural aircraft models. He earned a Ph.D. in Aerospace Engineering in 1997 from the Department of Aerospace and Ocean Engineering at Virginia Tech in Blacksburg, Virginia. His dissertation research investigated the use of statistical modeling techniques in multidisciplinary aircraft design optimization.

Photo Album—ASC Execs Offsite Meeting, Vail, CO, October 11 and 12, 2006

Who's Who

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Joining ASC HQ

Ken Alvin, of Sandia National Laboratories, is at HQ working on the Code Capability Matrix, Code Strategy, the joint ASC/Science Predictive Capability Framework effort, and an L2 milestone coverage and gap anlaysis.

April Commodore has joined the ASC Office and is covering MRT data collection and entry, classified document inventory and access, ASC Seminars, and A300s.

Leaving the ASC Program

Des Pilkington will be starting a one-year temporary assignment at AWE in the UK in November where he will perform research as part of ASC's new Thermonuclear Burn Initiative (TBI). Des has been the tri-lab lead for the TBI since Dimitri Kusnezov kicked off the initiative in the spring. For the last four years, Des has been the Deputy Associate Program Leader for Computational Physics in LLNL's B-Program assisting Tom Adams in leading nuclear performance simulation code development.

Tom Adams, a central figure in the ASC Program since its inception, retired from LLNL in September. Most recently Tom was LLNL's ASC Integrated Codes co-leader and Associate Program Leader for Computational Physics in B-Program responsible for nuclear performance simulation code development. Prior to coming to LLNL in 1998, Tom had a long, distinguished career at Los Alamos National Laboratory where he was one of the founders of ASCI.

Upcoming Events

November 1, 2006

Annual NNSA HQ review of the ASC Program. Dimitri Kusnezov will present the review to Ambassador Brooks.

November 2, 2006

Q4 ASC QPR to NA-10

November 11-17, 2006

Supercomputing Conference SC06 (http://sc06.supercomputing.org/)

December 5, 2006

Deliver advanced ASC physics and engineering simulation capabilities to support the W76 and the W80 LEP/certification

December 14-15, 2006

Review for the Q1FY07 Purple, 100-TF Environment L1 milestone at LLNL

ASC Web site

http://www.sandia.gov/ASC/NNSA/

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SAND 2006-6930W

 Developed and maintained by Sandia National Laboratories for NA.114

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.