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Next-generation Technology Impacts on the ASC Program

Guest editorial by Bill Archer, LANL ASC Program Director (acting)

Recently I've had reasons to review the goals of ASCI from 1995. There were two related goals: develop a 100-TFlop/s computer and develop 3D weapon codes to run on it. The program succeeded at both of these goals by 2007. What we then found was that there was a long way to go for a practical 3D capability, in both hardware and software. Even with Cielo, a 1.3-PFlop/s system, certain high-resolution 3D simulations are still beyond our reach.

The 3D simulations on Cielo have taught us that the 100-TBytes of memory available on half the system is not enough, and that I/O and archiving of 25-TB files is a problem. We also learned that node failures during a run must be managed to ensure throughput. These lessons have been incorporated into the mission needs of the next ASC system, Trinity, which is currently being procured by the Alliance for Computing at Extreme Scale (ACES) LANL-SNL partnership.

At this time all we know for sure about Trinity is that it will <u>not</u> be a conventional cluster like Cielo.

The ASC program has two next-generation technology machines, Roadrunner, the world's first 1-PetaFlop/s system and Sequoia, the first 20-PetaFlop/s system. Trinity is likely to incorporate features similar to both machines. The weapon codes will feel the full impact of these technology changes.

As we move forward to Trinity the weapon codes and supporting models will require a significant amount of re-work to be able to efficiently use the next generation of hardware. At the same time we have to continue supporting the Stockpile Stewardship Program, especially the on going and planned Lifetime Extension Programs (LEP). This will require shifting the program from supporting assessments to supporting primary reuse, design and certification. And, we have to continue developing an improved understanding of both primary and secondary physics to improve our predictive capability. Obviously, doing all of this at once will challenge the program.

Don't think that getting onto the next-generation systems is just an effort for the code teams, or even just the IC program element; it will require the combined effort of the entire program to successfully execute this. Both physics models and data access routines will need to be modified by PEM. The reworked codes will have to be evaluated by V&V. A new programming model will have to be provided by CSSE, as well as resiliency solutions. FOUS will have to provide the machines, but also the supporting infrastructure for cooling and power, and new ways to handle large data sets for visualization, storage, and archiving. Moving our focus beyond stockpile assessment to design and certification will be equally challenging for the entire program.

The next few years are going to be both exciting and challenging for the ASC program. They will be very similar to 1995-2005 when both computing technology and stockpile stewardship were changing direction. We are at a time when new ideas must be tried, and everyone in the ASC program has to work together to build the future.

DRAFT

[everything from here on has not reviewed for classification yet]

LDRD Funds Early Career Research Projects

LANL's Laboratory Directed Research & Development (LDRD) organization awarded twelve Fiscal Year 2013 Early Career Research projects of which three awards were for ASC Program researchers. Proposals from Abigail Hunter, Chengkun Huang, and Christopher Ticknor were selected from a total of 27 proposals that were submitted to the competition by researchers across Los Alamos. They will receive up to $225,000 per year for 2 years. "Early career research is one of the most important mechanisms for retaining top-notch scientific talent and aiding in the transition to a staff position," said Deputy LDRD Program Director Jeanne Robinson.

Abigail Hunter's proposal "Novel Mesoscale Modeling Approach for Investigating Energetically Driven Nanoscale Defect/Interface Interactions," was accepted. Abigail is in the Lagrangian Codes Group in LANL's Computational Physics Division.

Chengkun Huang, in the Applied Mathematics and Plasma Physics Group in the Theoretical Division, will be funded for his proposal "First Principle Study of Relativistic Beam and Plasma Physics Enabled by Enhanced Particle-in-Cell Capability."

Christopher Ticknor, who first came to the Los Alamos as a Metropolis postdoctoral fellow, works in the Physical and Chemistry of Materials Group in the Theoretical Division. His proposal title is “Stochastic Modeling of Phase Transitions in Strongly Interacting Quantum Systems.”

Photo credit: Sandra Valdez, Los Alamos National Laboratory

Cielo Working at Full Tilt for Stockpile Stewardship

The ASC Program's capability-class workhorse, Cielo, concluded its third capability computing campaign (CCC) on January 27, 2013. Cielo performed at approximately 80% overall utilization of the machine for CCC-3, which began on May 22, 2012. These campaigns support simulations for Los Alamos, Lawrence Livermore, and Sandia national laboratories.

As these campaigns go forward, there is a large and growing demand for large-scale, up to full-system jobs. Cielo is operated by the New Mexico Alliance for Computing at Extreme Scale (ACES), a partnership between Sandia and Los Alamos national laboratories. It is the petascale resource for conducting NNSA weapons simulations in the 2011–2015 timeframe. Built by Cray, Inc., it is installed at Los Alamos National Laboratory.

After a system outage for upgrading the Cray Linux Environment, CCC-4 started on February 4. CCC-4 has initiated an impressive workload for stockpile stewardship and weapons science. Initial requests oversubscribed the time available by a factor of more than five.

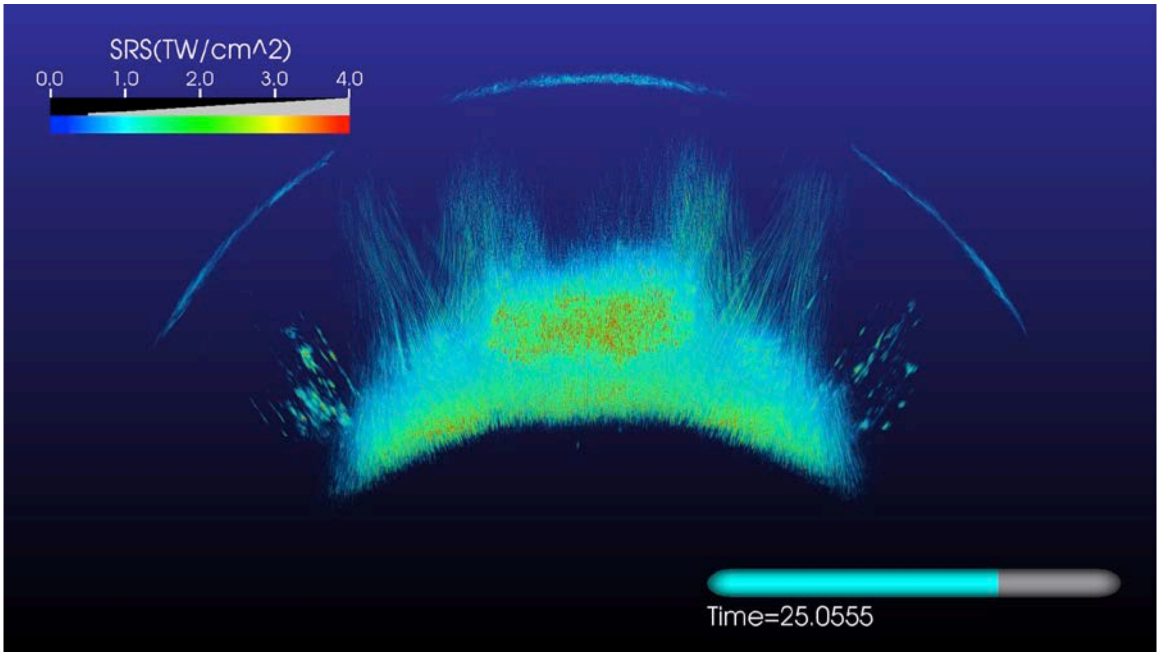
Numerous campaigns are increasing the job size to utilize the full-system, or near full-system, capability. Three users will use 102 thousand cores for their jobs: 3D weapons studies, a safety study, and 3D particle transport. Co-design scaling studies by Sandia National Laboratories will use the full system.

Results from Cielo's Capability Computing Campaigns

A few of the unclassified results from the CCC3 tri-labs are highlighted below. In addition, there were numerous stockpile projects done by weapons program scientists. The results from these projects help to understand and accurately calculate nuclear tests that had anomalous results. These results are important to validate our understanding of the physics relevant to nuclear weapons. Simulations such as these began with the inception of the ASC Program in 1995 (formerly the ASCI Program), but have needed larger machines than those available at the time. For example, LANL researcher Bob Weaver ran a particular weapon simulation on the Blue Mountain machine, which had to be run as a "cutoff," or truncated, problem because the calculation was too big to run on the machine. In addition, the level of resolution was below that desired, due to the limitations of the machine size. Since that time, he has run versions of the problem to utilize these ASC machines as much as possible: White, Roadrunner, and now Cielo. With Cielo, he is now able to run full-scale 3D simulations with remarkable fidelity, but he is still not able to run the complete simulation. It will have to wait until the next-generation supercomputer Trinity is deployed at LANL. The need for running full-scale 3D simulations with increased fidelity is the design basis for the Trinity platform.

Integrated Simulation of Laser Plasma Interaction (LPI) in NIF Experiments, Steve Langer, PI; Code pF3D

This project begins an investigation of how to account for backscattered light in a self-consistent manner in simulations of ignition experiments at NIF. The pF3D code is used on Cielo to simulate backscatter in overlapping beams, and interesting temporal and spatial structure is seen. The Cielo computer was recently used to simulate three interacting quads. The spatial variability of the backscattered light shows an enhancement from interacting quads. The runs on CCC-3 do a better job of simulating backscatter in regions where quads overlap.



This figure shows a volume visualization of the laser light backscattered by Stimulated Raman Scattering (SRS). The SRS occurs in bursts and is shown near the end of a burst when the scattered light comes mostly from the region where the quads overlap (the arc of light at the bottom).

Informing Predictive Models Using 3-D Simulations of Localization and Initiation in Polycrystals and HE, Nathan Barton, PI; ALE3D and mdef (crystal mechanics)

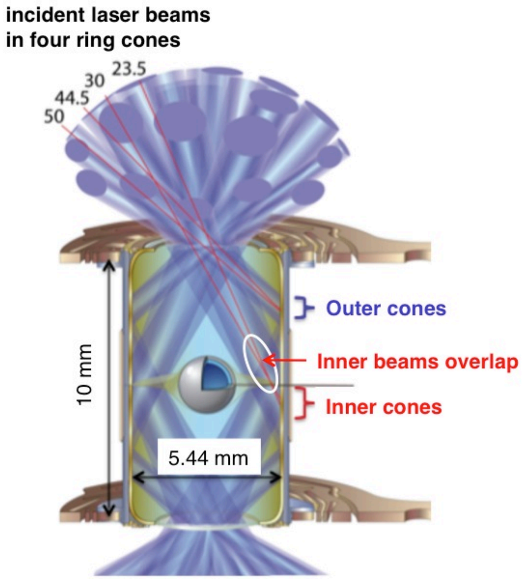
This project enabled exploration of phase transformation and plasticity kinetics. To better model strength and phase dynamics of materials, they ran simulations to provide details that are not experimentally accessible at the rates and pressures needed. The results illuminate interplay between nucleation and growth and among interacting mechanisms. The results contribute to ASC Physics and Engineering Models milestones.

The figures show progress of phase transformation in iron under high rate loading conditions. Dark regions have transformed from Alpha to Epsilon phase.

Direct Numerical Simulations of Thermonuclear Burn; Daniel Livescu, PI; CFDNS
This work complements ongoing work to develop and validate the Besnard-Harlow-Rauenzahn (BHR) mix model used in ASC simulations.

First Principles Diffusion Coefficients of DT-Pu; Christopher Ticknor, PI; ofmd.f90
This work explored first principles calculations of the diffusion coefficients for mass transport in a deuterium-tritium (DT) plutonium warm dense plasma.

Mitigating Stimulated Raman Scattering (SRS) in Inertial Confinement Fusion (ICF) Hohlraums; Lin Yin, PI; VPIC
This work studies SRS, a type of laser-plasma instability of concern for laser-driven fusion experiments such as those underway at NIF.



The figure shows a schematic of a NIF ignition target showing the inner and outer beam cones and the VPIC simulation region where inner beams overlap.

Towards Accurate Simulation of the Abnormal Thermal Fire Environment for Stockpile Stewardship; Paul Lin, PI; Sierra/Fuego
The goal for this project is safety and reliability of the stockpile for the abnormal thermal fire environment. It is a B61 LEP requirement to accurately predict the abnormal thermal fire environment.

Summary

Cielo was deployed for stockpile stewardship, and it has excelled as a stable and reliable platform for running capability computing campaigns for the tri-lab weapons community, particularly for problems that cannot be resolved at less than near-petascale size. Cielo's architecture allowed easy migration of the existing integrated weapons codes, thus extending the ability to conduct critical simulations while the code teams work to adapt the codes to the changing computing architectures. The examples shown in this article illustrate that Cielo is excelling at the job for which it was intended.

LANL ASC Projects Showcased in Stockpile Stewardship Quarterly

Since February 2011, the Office of Stockpile Stewardship, NA-11, has published the "Stockpile Stewardship Quarterly" (SSQ). Four ASC researchers at LANL are featured in the February 2013 issue. Alek Zubelewicz in the Physics and Chemistry of Materials Group and coauthor Abigail Hunter in the Lagrangian Codes Group at Los Alamos contributed the article titled "Fracture Model for Beryllium and Other Materials." Another LANL author, Kim Molvig, contributed the article titled "Knudsen Layer Reduction of Fusion Reactivity." Molvig in the Verification and Analysis Group and coauthor Nelson Hoffman is in the Plasma Theory and Applications Group.

To see the articles, go to the LANL public website at http://www.lanl.gov/asc and look under Documents.

Los Alamos National Laboratory
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