ASC eNews Quarterly Newsletter
September 2014

Contents:
(To go directly to an article, click on its title below.)

The Meisner Minute
New Modeling Code Accurately Calculates Opacity at Record Speeds
New Fluid Model Offers Significant Improvement over Legacy Model
A New Parallel Decomposition Tool for SIERRA Modeling
Exploring the use of Topology Optimization for Component Designs
Progress on the High-Order/Low-Order Algorithm for Thermal Radiative Transport
Testing a New ASC Code Laser Package
ASC Salutes Manuel Vigil
Recent Publications
- Lawrence Livermore National Laboratory
- Los Alamos National Laboratory
- Sandia National Laboratories

The Meisner Minute

Greetings once again. Since my last update, several things have happened. As you all know now the Trinity contract was finally announced shortly after the last Meisner Minute. Cray will be providing the next generation HPC to the program and will be delivering it in two phases. The first phase, slated for delivery late next year, will be very similar to the current Cielo platform and should provide a relatively easy initial transition for our current applications. The second phase, completed approximately a year later, will include Intel accelerators and should be more representative of the direction of future HPC architectures. An interesting feature of the Trinity Advanced Technology System, or ATS, platform is that it will introduce flash memory based burst buffer technology to the HPC community. Speaking of future platforms, bids have been received and evaluated for the follow-on to the Sequoia platform at LLNL. We hope to make an announcement of the vendor for this machine in the near future.

The NNSA senior management team is now complete with the Senate confirmation of Madelyn Creedon as NNSA Deputy Administrator. The other change is the arrival of Brigadier General “S.L.” Davis to Defense Programs, replacing BGen Dawkins who has moved to a position in the National Security Council. I expect this team to remain in place for the remainder of the current administration.

The success of science-based stockpile stewardship has been emphasized by Congress and our leadership on several occasions over the last year. Our program has played a critical role in that success. ASC codes are used to generate the "baseline" response for each weapon in the stockpile, which is used during the Annual Assessment Review (AAR). These baseline models certify the performance of the weapons and underwrite Significant Finding Investigations (SFIs). Several long-standing SFIs were closed (or moved forward significantly) this year with the essential support of ASC codes. Sandia's engineering codes have been used heavily for B61 LEP and W88 Alt design work and will be used to qualify a growing list of components. Los Alamos and Livermore have each deployed a "common model" that successfully simulates a large percentage of past nuclear tests with a common set of ASC integrated design code parameters for each lab. These common models have allowed weapon designers to address several nuclear-test "anomalies," bringing us another step closer to the predictive capability we have been working on since the end of nuclear testing.

On the budget front, it is a new fiscal year and we are once again in continuing resolution through December 11. After that, anyone can guess what might happen and final resolution will likely depend on the makeup of the new Congress. For the time being, the ASC program will continue to operate at the FY 2014 level. Assuming we do get a budget by early next year, ASC should be able to recover from the very large Sequestration reduction in FY13 and begin to fully fund the Advanced Technology Development and Mitigation (ATDM) program element.

Secretary Moniz has been leading the nation's initiative to develop advanced computing technologies and build a useable exascale system by 2023. Recently the Secretary of Energy Advisory Board (SEAB) published a recommendation to the Secretary endorsing an initiative in this area. Additionally, the National Strategic Computing Initiative (NSCI) (sound familiar?) working group commissioned by the President's Office of Science and Technology Policy (OSTP) and led by Rob Leland from SNL, who was on loan to OSTP, concluded its responsibility for authoring an interagency plan for achieving exascale. Further, Congress, especially Senate appropriation and House authorization, continues to encourage the department to pursue exascale, and, as many of you know, twenty-two Senators signed a bipartisan letter of support for the initiative to the President in January. Our national leadership is aligning on computing in a way that has not been seen in decades. But, how it actually shapes up remains a work in progress. Stay tuned.

Finally, I wish to thank everyone who contributed to a series of briefings that were presented to Don Cook in July. While Don has always been supportive of the ASC program, he specifically asked, not for a program update, but for some "deep dives" so that he could understand the emerging challenges to the program as HPC architectures enter a disruptive period of transition to "many-core," accelerators, etc. Don set aside four hours over two days so that he could appreciate the scale of the problems facing the program, and came away with a better understanding of the work that all of you do. Again, thanks to all of you for continuing to build the excellent professional reputation the team all shares.

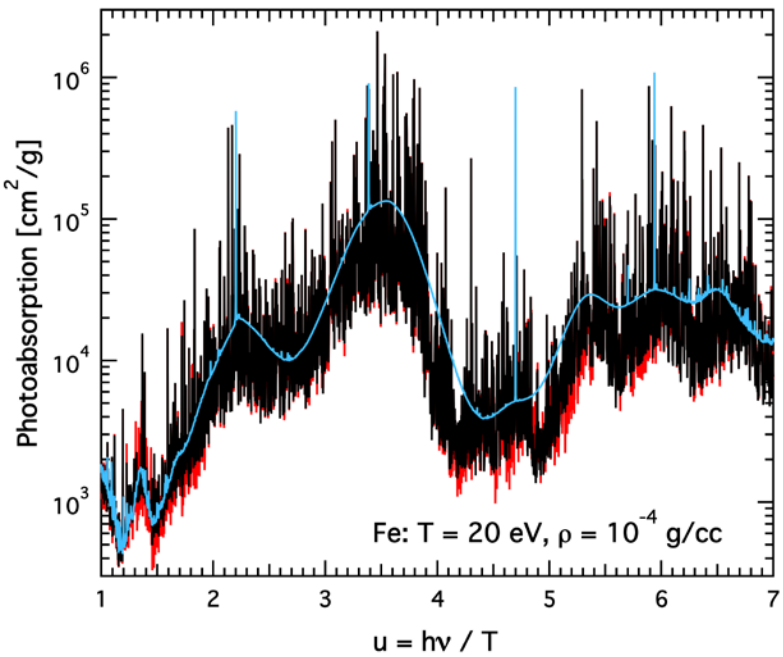
Return to top

New Modeling Code Accurately Calculates Opacity at Record Speeds

A new "random partially resolved transition array" (RPRTA) method of calculating opacity has delivered calculations at a speed greater than 60 times of that which was previously possible using line-by-line methods, and delivered while maintaining current levels of accuracy. Developed by the Radiative and Plasma Properties Team within the ASC Physics and Engineering Models (PEM) sub-program at Lawrence Livermore National Laboratory (LLNL), the new code, Hybrid-RPRTA, is now working on local thermodynamic equilibrium (LTE) opacity solutions for ASC.

"We intend to see how far we can push the code's acceleration versus comparable (but less accurate) super-transition array (STA)-based calculations," said Carlos Iglesias, project principal investigator. "The results will have big implications for inline opacities in high-energy density (HED) design codes, including the efficient development of designer opacity tables for diverse applications."

As LLNL scientists continue to test the new code with validation comparisons to working codes such as OPAL and TOPAZ, they are already moving forward with opacity predictions for full tables. The future looks both fast and accurate for these models.



The opacity of iron at conditions relevant to stellar pulsation. Tables such as this allow ASC scientists to predict the behavior of radiation-hydrodynamic local thermodynamic equilibrium opacities on demand for materials of interest to the ASC Program.

Return to top

New Fluid Model Offers Significant Improvement over Legacy Model

Researchers at Lawrence Livermore National Laboratory (LLNL) have developed an improved model to describe the thermodynamic properties of dense molten materials. This new "Cell Model" describes the smooth transition that a liquid undergoes when heated just above the temperature of melting up to the very highest temperatures where the substance is so hot that forces between particles are of negligible importance.

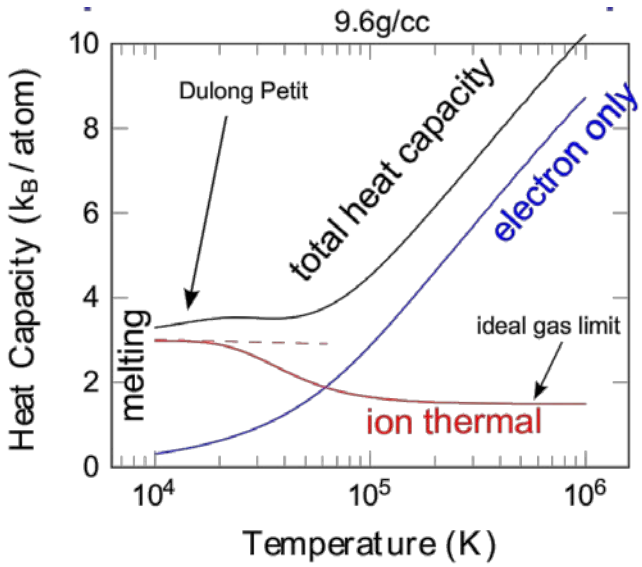
These thermodynamic properties comprise the equation of state (EOS) of the material, which expresses the relationship between the density, the temperature, the pressure, and the energy content of a substance. Tables of numbers representing the EOS are needed as inputs to large-scale simulations of matter being subjected to extreme conditions, such as experiments performed at the National Ignition Facility (NIF). Because many of LLNL's most important applications involve an exceedingly wide range of conditions, those who build EOS models are faced with the task of constructing models that cover many disparate physical regimes; and if the simulations are to run properly, these different regimes must be connected in the model in a manner that is at once mathematically smooth and physically correct.

"These tables of thermodynamic properties represent how materials respond to applied stresses and resist compression when heated," said Lorin Benedict, lead researcher for the project and member of the LLNL EOS theory and modeling team within the Physics and Engineering Models sub-program of the ASC Program. "Our new addition alters the way this material response is modeled in the transition region between liquid and plasma states, and has the potential to impact all of the EOS tables at LLNL."

By comparing directly to a series of Path Integral Monte Carlo and Density Functional Theory Molecular Dynamics simulations of carbon, the new Cell Model has lead to significant improvements in the high-temperature liquid EOS over previous models currently in wide use. Carbon was chosen as the first test case because simulations on carbon were already available, and because an improved EOS was needed due to the increased use of diamond samples in experiments at NIF.

"In order to improve the extrapolation of the ion-thermal component from temperatures near the melting curve all the way to the ultra-high temperature limit, we've developed a new physically based model that we've tested against advanced quantum simulations for carbon," said Alfredo Correa, one of the developers of the Cell Model. "We were researching models of global applicability and mathematical smoothness, and the model we have now constructed is less ad hoc than previous approaches, because it is derivable from basic physical laws."

More detailed information can be found in "Multiphase equation of state for carbon addressing high pressures and temperatures," *Phys. Rev. B* 89, 224109 (published June 30, 2014). (http://journals.aps.org/prb/abstract/10.1103/PhysRevB.89.224109)



The heat capacity of liquid carbon as a function of temperature, as represented by the new Cell Model. The heat capacity describes the propensity of a material to absorb energy when heated. The Cell Model was recently used in the construction of an equation of state for carbon.

Return to top

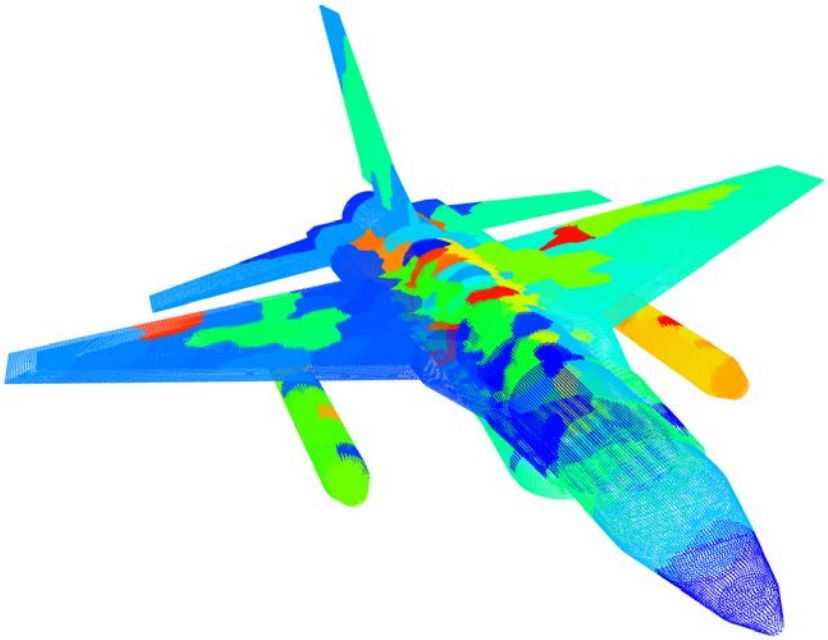
A New Parallel Decomposition Tool for SIERRA Modeling

An important new capability for large-scale, realistic calculations at Sandia was developed by the Zoltan2 and SIERRA Toolkit teams resulting in massively parallel graph-based mesh partitioning technology as part of the design-to-analysis tool chain. This new tool enables partitioning of much larger meshes for Sierra than was ever possible before and can dramatically shorten the time required to pre-process a mesh before parallel simulations are run. This capability was made possible by combining algorithms in Zoltan2 and the mesh creation and manipulation capabilities of SIERRA's new Toolkit.

The joint team investigated several known and anticipated technical issues in achieving load-balanced partitions. Specifically considering mesh proximity in the graph model, for example, accounts for the computational demands of mechanical contact in structural dynamics and solid mechanics simulations. Also, both parallel partitioning strategies and in-node coloring algorithms were investigated, in preparation for performance studies on multithreaded computing hardware.

The new capability provides unprecedented performance to SIERRA users. For example, parallel partitioning of a mesh with 8 billion elements on 4000 processors of Chama required less than 5 minutes. In comparison, partitioning a typical problem for 400 processors using our serial decomposition tool requires several hours of CPU time. Further R&D efforts will investigate the use of this capability as an in-core rebalancing tool, which will be a critical part of being able to run large-scale simulations on

next-generation compute platforms. (POCs: Manoj Bhardwaj, mkbhard@sandia.gov; Karen Devine, kddevin@sandia.gov)



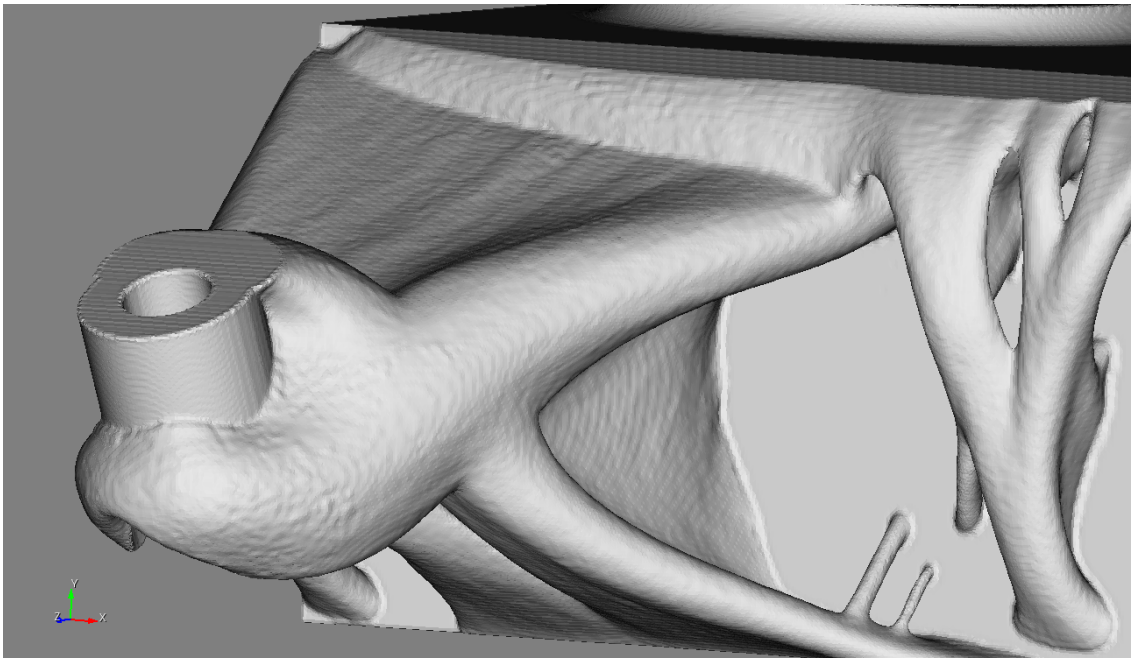
Example of a mesh decomposition of complex F16 model.

Return to top

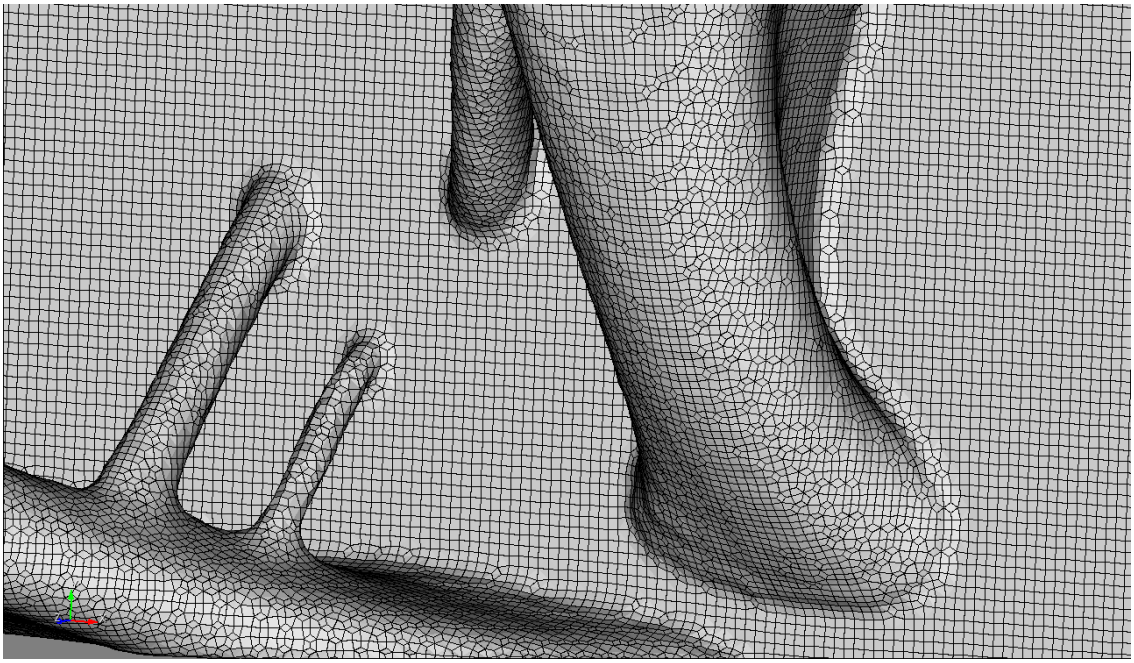
Exploring the use of Topology Optimization for Component Designs

A collaborative team of designers, analysts, modelers, and code developers at Sandia has recently demonstrated topology optimization-based design-through-analysis and design-through-manufacturing processes for a weapon component. Topology optimization is a method of computationally generating structures that optimizes the amount and placement of material in order to satisfy a design goal (strength/weight). This capability, developed as part of a Laboratory Directed Research and Development (LDRD) initiative, was used to generate a potential candidate design for the B61-12 Actuator and Pulse Battery Assembly (APBA) housing that would increase the natural frequency of the first vibrational mode. The design geometry is quite organic-looking as is typical of optimized designs, so non-traditional tools were required to go from the design to analysis and manufacture. As part of the workflow, new capabilities in the Cubit geometry and meshing toolkit were employed to extract the optimized shape, edit and smooth rough features, and export the resulting triangulation. The recently developed “Sculpt” meshing algorithm was used to generate an all-hex mesh for analysis and the triangulation exported from Cubit was used directly for additive manufacturing (3D printing) of the design. The modal analysis performed with SIERRA indicated an increase of 32% in the natural frequency of the first vibrational mode.

This initial exercise demonstrated the exciting potential of using topology optimization to affect weapon design. It also helped identify the key computational and workflow pieces required to realize true performance-based design. (POC: Brett Clark, bwclark@sandia.gov).



33 million all-hex finite element mesh of the APBA generated using Sculpt (mesh lines not shown).



Zoomed-in view of hex mesh.

Return to top

Progress on the High-Order/Low-Order Algorithm for Thermal Radiative Transport

Los Alamos has been developing the High-Order/Low-Order (HOLO) algorithm for solving a variety of complex multi-physics systems, and the algorithm has shown promising results. The Transport Methods Project has an ongoing effort to incorporate this methodology into the Eulerian Application Project (EAP) code base for accelerating thermal radiative transfer (TRT) problems. The HOLO algorithm has been deployed in EAP software, coupled with both the Monte Carlo-based Jayenne software and the Sn-based Capsaicin software.

Frequently, a stiff nonlinearity due to absorption and re-emission of TRT problems is simplified through linearization. This linearization introduces “pseudo-scattering”, which may result in increased computational time and decreased accuracy. A key idea of the HOLO algorithm is to remove this linearization and to treat the stiff coupling in a simpler (lower-order, LO) system.

The HOLO algorithm employs two different (i.e., kinetic and continuum) descriptions of transport process and casts them as a physics-based multi-level system. The LO system is obtained by taking the moments of the original TRT equation. The closure of the LO system can then be derived such that it accounts for both the discretization mismatch and transport effects. This “discrete consistency” between HO and LO solutions enables algorithmic acceleration that can be greater than an order of magnitude (Figure 1).

A part of our current effort is extending the algorithm to more complex multi-physics problems. Due to availability of the consistent LO system, the majority of multi-physics coupling can be carried out through the LO system, consequently enabling the isolation of the HO TRT system. By eliminating the linearization simplification, our HOLO algorithm removes a stability constraint. This permits choosing the time-step size with accuracy the only constraint, as opposed to stability (Figure 2).

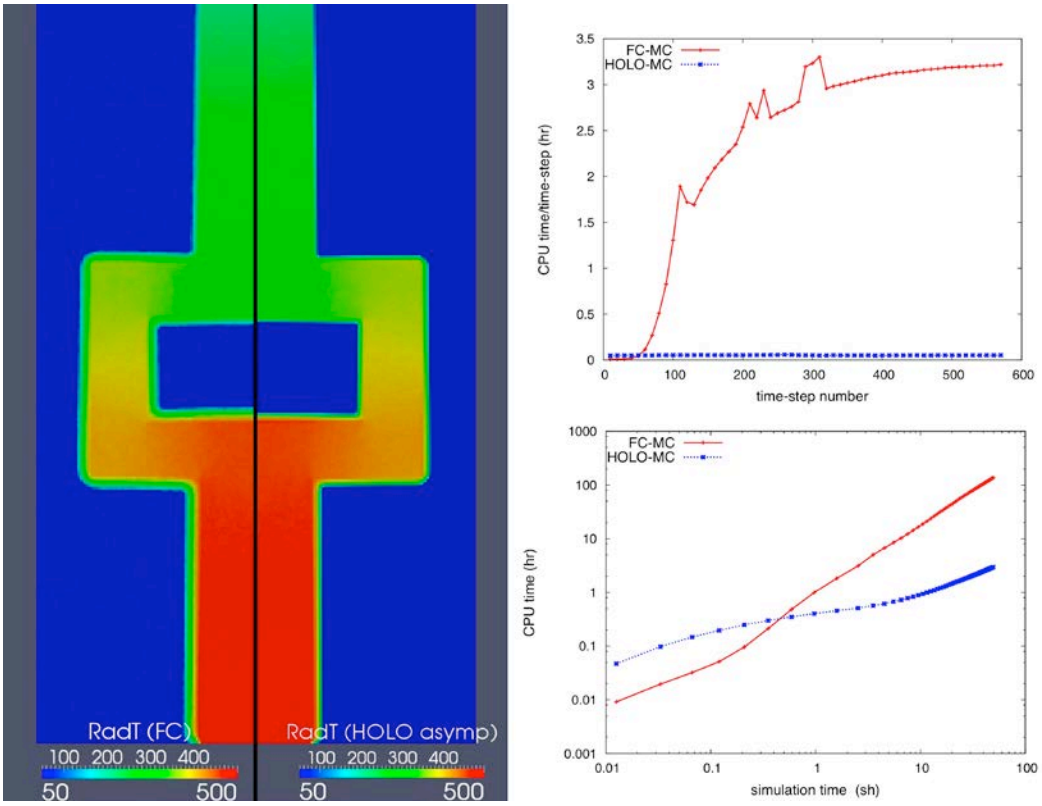


Figure 1: Efficiency comparison between HOLO-MC and IMC. A factor of 40 algorithmic acceleration is observed in this 2D grey TRT problem. On the left, radiation flows through an optically thin, "crooked pipe." The plots on the right show the corresponding efficiency gains of HOLO-MC, compared with those from the standard algorithm, FC-MC.

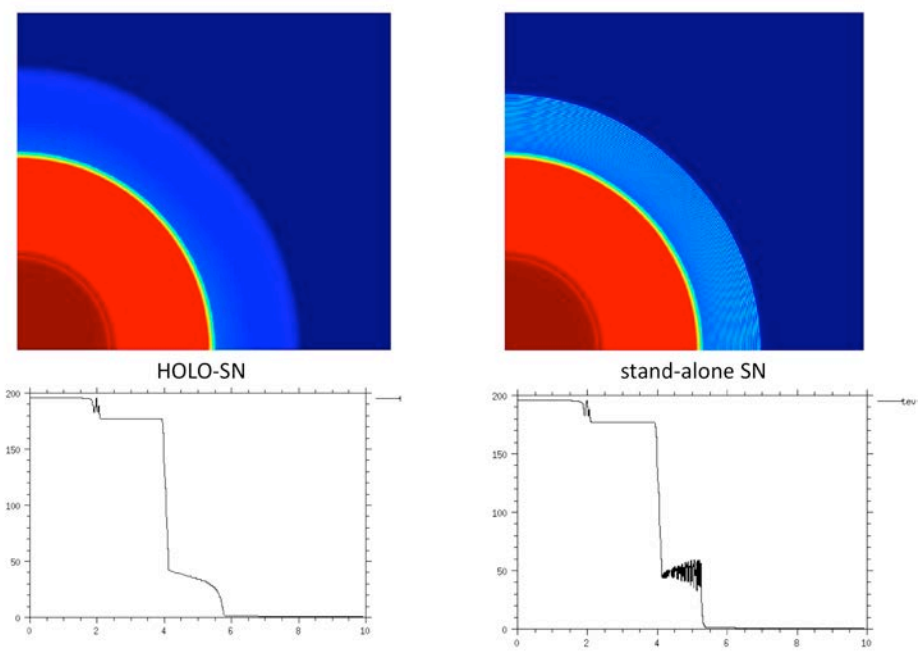


Figure 2: Radiation hydrodynamics example comparison between HOLO (left) and standalone Sn (right). Standalone Sn exhibits unphysical oscillation due to instability caused by linearization.

Lastly, the HOLO approach is well-suited to mapping multi-physics codes onto advanced computer architectures. Many current multi-physics algorithms employ “loose” multi-physics coupling among physics models, and solved via sequential, “lock-step” execution, through “operator splitting.” This approach requires many communication synchronization points, and each physics package typically uses the entire machine allocation, which leads to a potential inefficiency in future heterogeneous computer architectures. With the HOLO algorithm, more efficient, asynchronous operator splitting is possible (Figure 3). In addition, nonlinear coupling across the physics models is carried out through the LO system, eliminating splitting errors. This LO solve can use a small number of compute nodes. On the other hand, multiple HO solvers can be executed asynchronously, which may use a majority of the remaining compute nodes. This approach also enables efficient load balancing. The concept of mapping the HOLO algorithm to heterogeneous computer architectures was developed during the COCOMANS, LANL LDRD-DR project.

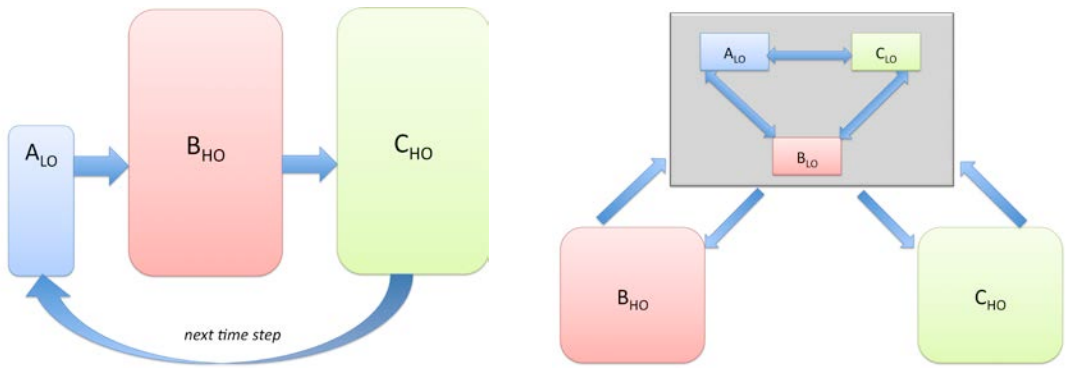


Figure 3: sequential (left) and asynchronous (right) operator splitting approaches to solve multiphysics problems. The sequential method requires B_{HO} to finish before C_{HO} may begin. The asynchronous approach allows for B_{HO} and C_{HO} to be computed at the same time, and linearizations to be removed by iterating across the low-cost, LO solution steps.

Return to top

Testing a New ASC Code Laser Package

Laboratory for Laser Energetics (LLE – University of Rochester) and LANL scientists recently implemented the laser package from the LLE DRACO code (J.A. Marozas, http://www.lle.rochester.edu/pub/viewgraph/PDF/PR/PRMAROZASAPS06.pdf) into the xRAGE code as part of the strategy to make xRAGE able to run all types of high energy density (HED) experiments. This laser package has been used extensively by LLE scientists to model direct drive experiments, primarily at the Omega laser. At Los Alamos, we have been testing the laser package on several direct drive capsules with different shell thicknesses fielded at Omega. The xRAGE simulations use a turbulent mix model, surface roughness, and other physics needed for HED experiments. The simulations have initial zone sizes of 0.25 to 0.5 microns. The capsules have shell thicknesses between 7.5 and 29.3 microns and typical outer diameters of 870 microns. The simulated physics performance of these capsules is similar to previous good matches. The usage of lasers and surface roughness creates spikes in the density profile, as shown

in Figure 1. These spikes have been seen by LLE scientists using the DRACO code. Density plots are shown for a thin (7.5-micron shell) and thick (29.3-micron shell) capsule in Figure 2, which clearly shows that the thin shell capsule is broken up while the thick shell capsule is intact, which is consistent with experimental data. The computer run time is about 15% to 30% longer with lasers than without, but can easily achieve nearly the same wall clock time by increasing the number of processors.

We thank H. Herrmann and Y. Kim of LANL for permission to use unpublished data.

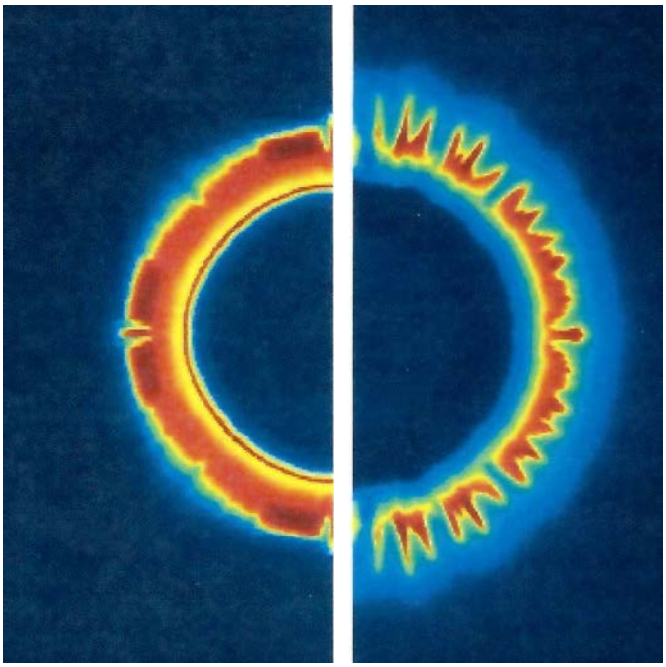


Figure 1. Density plots for an 18.7-micron-thick capsule without lasers or surface roughness (left panel) and with lasers and surface roughness (right panel). These images were taken about 200 ps before bang time. The image frames are 160 microns wide.

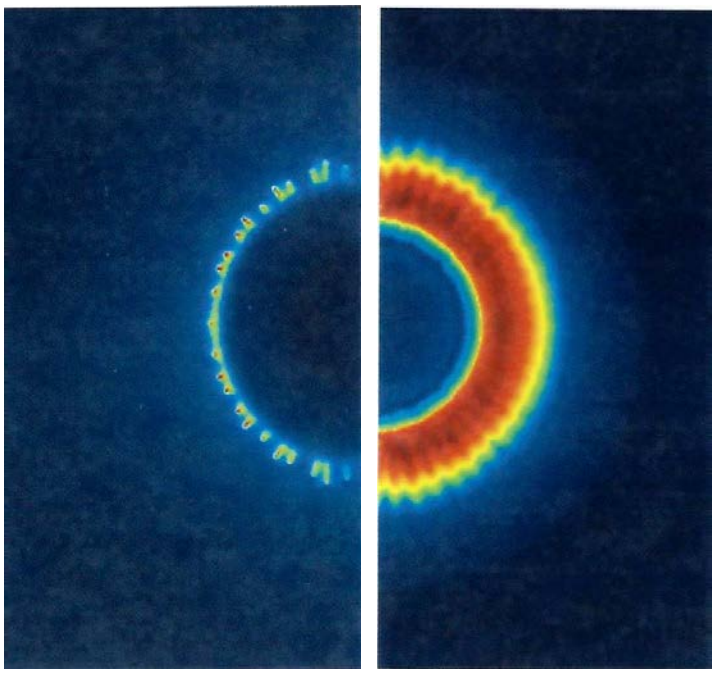


Figure 2. Density plots for a 7.5-micron-thick capsule (left panel) and a 29.3-micron-thick capsule (right panel). These images were taken about 200 ps before bang time. Note the broken up shell of the 7.5-micron-thick capsule, while the shell is intact for the 29.3-micron-thick capsule. The image frames are 340 microns wide.

Return to top

ASC Salutes Manuel Vigil

Manuel Vigil is the Trinity Project Director for the acquisition and project management of the Trinity Advanced Technology System. He is also the Platforms Program Manager for LANL's ASC Program. With more than 40 years of service, Manuel has made significant contributions to the ASC Program and high performance computing at LANL.

Over the past 14 years Manuel led the planning, acquisition, system integration, and project management efforts for the ASCI Blue Mountain, ASC Q, ASC Roadrunner, Cielo, and Trinity High Performance Computing platforms. Each of these platforms made possible significant advancements in stockpile stewardship simulations.

As acquisition and deployment of large supercomputer systems became more complex, Manuel began developing and implementing formal project management processes for HPC, and he became a certified Project Management Professional (PMP) in 2005. He has a unique ability to manage and execute large complex systems, and match technology to meet users' needs. Manuel has developed a national reputation for being able to bring together and lead teams and work with stakeholders from various organizations to successfully execute large, complex supercomputer projects.

Manuel's leadership has played a major role in the success of the partnership between Sandia and LANL as part of the New Mexico Alliance for Computing at Extreme Scale (ACES). This partnership led to the deployment of Cielo, the first major supercomputer acquired and deployed by ACES. This monumental task required strong leadership and the ability to integrate different cultures to deploy a successful platform for ASC users.

The Trinity platform acquisition partnered LANL, Sandia, and the National Energy Research Scientific Computing Center (NERSC) to develop technical requirements and to evaluate and select systems for ACES and NERSC.

In 2004, while on assignment to ASC Headquarters, Manuel led the development of a pilot ASC process for implementing DOE Order 413.3 (Project Management for the Acquisition of Capital Assets) for ASC supercomputer acquisitions, a process that is still the basis for the acquisition of today's ASC platforms. As a project manager, Manuel established strong vendor relationships that significantly contributed to technological advancements to meet users' needs.

Manuel has a bachelor's degree in mathematics from New Mexico Highlands University and a master's degree in computer science from University of New Mexico. He grew up in Northern New Mexico in a farming community with 17 brothers and sisters. Connection to his family has always been at the forefront of his daily life. As the father of three sons, Manuel was a scout master and a coach for numerous sports. Manuel's other interests include hiking, fishing, biking, and genealogy work. Manuel just celebrated 37 years of marriage to his wife, Prescilla. They enjoy spending time with their granddaughters.

Return to top

Recent Publications

Lawrence Livermore National Laboratory

Ahn, D.H., M.J. Brim, B.R. de Supinski, T. Gamblin, G.L. Lee, M.P. LeGendre, B.P. Miller, A. Moody, M. Schulz (2013). "Efficient and Scalable Retrieval Techniques for Global File Properties," Proc. of the Int. Parallel and Distributed Processing Symp. (IPDPS'13), Boston, MA, LLNL-PROC-554055, May 20-24.

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Cleveland, M., N. Gentile (2013). "A Radiating Shock Evaluated Using Implicit Monte Carlo Diffusion," Proc. Int. Conf. on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, Sun Valley, ID, May 5-9, p. 2398.

Cleveland, M., N. Gentile (2013). "Teleportation Error in Frequency-Dependent Hybrid Implicit Monte Carlo Diffusion," Proc. 23rd Int. Conf. on Transport Theory, Santa Fe, NM, Sept. 15-20.

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