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March 2013 ASC Newsletter Items – Sandia National Laboratories SAND2013-#####

Sandia Fracture Challenge Results Presented at 2012 ASME Congress Indicate Fracture Models Are Not Yet Predictive

Mid-summer last year, Sandia National Laboratories, in partnership with the US National Science Foundation (NSF) and Naval Surface Warfare Center, launched the Sandia Fracture Challenge. The goal of the Challenge was to benchmark the prediction capabilities for ductile fracture, including physics models, computational methods and numerical approaches currently available in the computational fracture community.

The challenge given to engineering researchers was to predict the onset and propagation of quasi-static ductile fracture of a common engineering alloy in a simple geometry (Figure 1) using modeling and simulation. Twenty-four international research teams initially signed up to participate; however, only 14 teams submitted their predictions before the deadline.

The 14 successful teams presented their methodology and predicted results at a special symposium during the American Society of Mechanical Engineers (ASME) International Mechanical Engineering Congress and Exposition in Houston, TX, November 9-15, 2012.

The methods for fracture prediction taken by the teams ranged from very simple engineering calculations to complicated multi-scale simulations. The wide variation in modeling results presented at the symposium (Figure 2) indicated computational fracture models existing in the mechanics community today are not yet predictive. In addition, predicting ductile failure initiation and crack propagation remains an extremely difficult problem.

Soon after the ASME symposium, discussions began within the research community about how to isolate the shortcomings in computational models and narrow the gaps in predictive capabilities for ductile fracture. A follow-up workshop, hosted by NSF, is in planning stages. It will document the lessons learned from the Sandia Fracture Challenge and define coordinated future R&D activities.

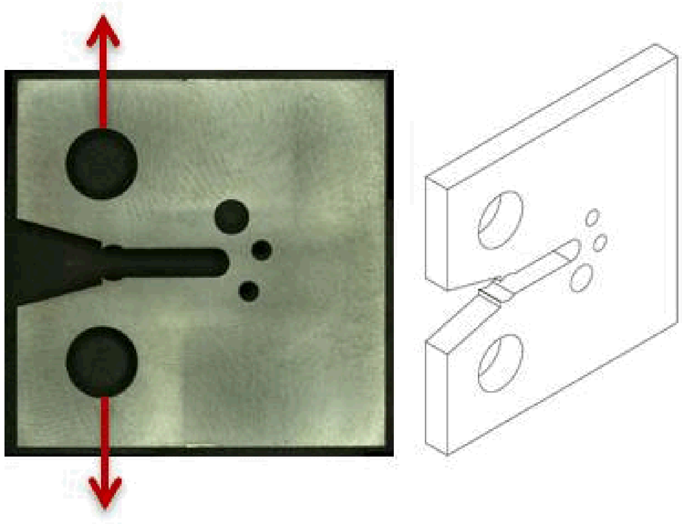

Figure 1: Sandia Fracture Challenge Specimen

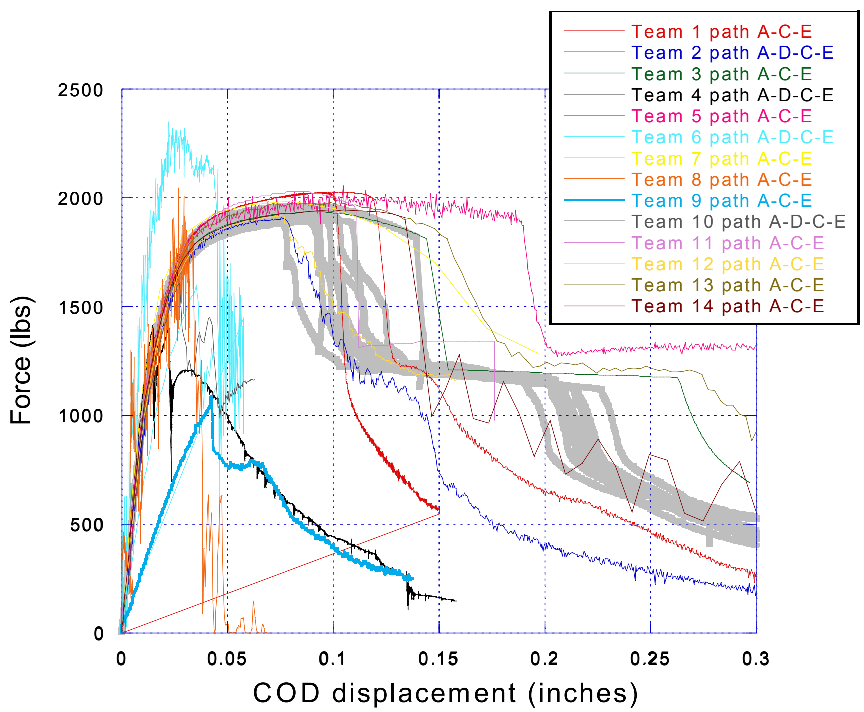

Figure 2: Comparison between the modeling results (in various colors) and experiment (in gray)

ACES and NERSC form partnership for next-generation supercomputers, an unprecedented collaboration between NNSA and the Office of Science

The Alliance for Computing at Extreme Scale (ACES), a collaboration between SNL and LANL, and the National Energy Research Scientific Computing Center (NERSC) at LBNL have fully integrated as a team as they work towards their respective next-generation supercomputer deployments. The goal of the new alliance is to acquire two supercomputers, Trinity and NERSC-8, using a common set of technical requirements and a single procurement process. In addition to strengthening the partnership between NNSA and the DOE Office of Science (DOE/SC) in the area of high performance computing, there are a number of advantages to combining the acquisition strategy. It leverages shared technical and risk management expertise and saves industry time and money in responding to a single request for proposal and a single set of requirements. There are also benefits associated with shared experiences in production operations.

Trinity will be the next-generation supercomputer to provide high performance computational resources in support of NNSA's Stockpile Stewardship Program mission. Driving Trinity's architectural requirements is the need to increase ASC predictive capabilities. Cielo and Sequoia (the current machines at LANL and LLNL) are unable to support the higher fidelity models, both in geometry and physics, needed to provide necessary predictions.

NERSC-8 will increase DOE ability to support rapidly increasing computational demands of the entire spectrum of DOE/SC computational research. It will also transition DOE scientific applications to more energy-efficient architectures. The NERSC-8 deployment will support well-established fields that already rely on large-scale simulation, but are moving to incorporate additional physical processes and higher resolution. It will also support scientific discovery performed using a very large number of individual, mutually independent compute tasks.

The ACES and NERSC team will issue a formal Request for Proposals in the third quarter of calendar year 2013, and plans to have contracts in place by the end of the year. Deployments are planned for late 2015 to early 2016.

Sandia, Los Alamos and NERSC host joint mini-app deep dive with NVIDIA's Developer Technologies Group

Hardware and software experts from NVIDIA's Developer Technologies Group recently visited Sandia for a deep-dive on mini-application performance and porting activities. Attendees from ACES and NERSC learned the very latest developments in NVIDIA's hardware solutions and approaches to optimizing codes for high-performance GPU architectures. NVIDIA also presented several optimization activities where they are using key ASC and ASCR mini-applications to inform future hardware designs. This gave the laboratories the opportunity to learn how modifications to the algorithms or programming models will improve future application performance.

The visit by NVIDIA builds upon a strong and growing collaboration between ACES and NERSC as the laboratories increasingly focus on the opportunities for co-designing future Exascale systems. The laboratories also continue active engagement with leading industry vendors to identify future application characteristics and requirements to enable hardware designers to improve performance, lower power requirements and increase machine reliability. Follow-up discussions from the NVIDIA visit are also helping to refine requirements for future directive-based programming models, a key facet of utilizing existing investment in legacy application codes, as well as programmer tools such as mathematics libraries and runtime systems.

Both ACES and NERSC plan to continue broad industry engagement over the coming year through on-going collaboration and discussion based upon research and analysis being performed on in-house prototype hardware and software systems.

Mantevo 1.0 release, co-design via miniapps and the launch of mantevo.org portal

Sandia researchers, along with colleagues from LLNL, LANL, the Atomic Weapons Establishment, NVIDIA, Intel and AMD, announced the first official release of the Mantevo suite of mini applications and mini drivers on December 14, 2012. The community portal (mantevo.org) for accessing Mantevo packages and related capabilities launched simultaneously.

Mantevo packages are small programs that embody one or more performance impacting elements of large-scale production applications. Mantevo 1.0 includes eight packages, including seven miniapplications: CloverLeaf, CoMD, HPCCG, MiniFE, MiniGhost, MiniMD, and MiniXyce, and one minidriver: EpetraBenchmarkTest.

While Mantevo miniapps have been around for several years, energy efficiency concerns are driving change at all levels of computing. Co-design has become an essential activity in order to jointly answer questions about how memory, processor, operating system, programming model and application designs can advance simultaneously. Miniapps have emerged as a critical central component in the co-design process, representing concrete, yet malleable, proxies for large-scale applications, enabling rapid exploration of a very complex design space.

The collection of Mantevo reference implementations continues to grow. The base implementation of each Mantevo miniapp includes OpenMP, MPI and sequential execution. As a part of our advanced systems testbed efforts, many other models are also supported, including AVX, CUDA, OpenACC, OpenCL, Intel TBB, qthreads and KokkosArray.

For more information, or to download these packages, visit the following links.

Mantevo website: http://mantevo.org
Mantevo Suite 1.0 download: http://mantevo.org/download.php

ASC Salutes Jeremy Templeton

The Verification and Validation (V&V) subprogram of ASC is pretty important. After all, we want to be highly confident in the predictions we make about the safety, security, and reliability of the weapons in the stockpile.

Sandia's engineering researcher Jeremy Templeton wants to provide confidence in the safety of nuclear weapons systems in abnormal thermal environments.

State-of-the-art uncertainty quantification theory brings that confidence.

Quantifying margins and uncertainties analysis begins by working with systems engineers to understand the relevant safety themes and environments of concern. Analysts then obtain as much information as possible regarding the weapon's design. This includes information such as the materials used and the knowns and unknowns about parts configuration. "All this information is used to build a realistic model for the heat transport physics throughout the system," said Templeton.

After quantifying algorithm accuracy through rigorous verification methods, assessment of the impact of physical uncertainties on system response begins. "This helps us learn which parameters are important to determining the behavior of the systems and which are not, helping us make the best use of limited experimental and computational resources," he said.

These results provide the basis for validation testing. Predictivity of the model is assessed quantitatively to confirm the assumptions made in the modeling process, followed by tens of thousands of targeted simulations. These simulations show how the system meets the defined safety requirements probabilistically.

Templeton's work, and that of his team, in this area has inspired an LDRD project in a seemingly unlikely area – calibrating the engineering models of gas turbine engines. The idea is to inform models using high fidelity data and use computationally efficient methods to impact the engine design cycle, leading to increased efficiency and reduced emissions.

"I also work on developing multi-scale and multi-physics coupling methods for atomistic and continuum descriptions of physical phenomena," he said. "The goal is to understand the fundamental behavior of electrical energy storage systems at a molecular level."

Templeton has worked with the Sandia portion of the ASC program for five years. He came to Sandia after completing his Ph.D. in Mechanical Engineering at Stanford University. His thesis was in the area of turbulent flows, developing new wall models for large-eddy simulation (LES) using optimal control theory. “We demonstrated orders-of-magnitude computational savings in some canonical flows with minimal reduction in accuracy as compared to LES without wall models,” he said.

“I enjoy working at the intersection of physics, statistics, and computation,” said Templeton.“The constant process of learning and improvement makes work a lot of fun. I particularly like having the opportunity to think deeply about hard problems, such as how to assess very rare events, and then putting those ideas into practice to solve a real problem.”

His contributions at Sandia are noteworthy. “Jeremy and the teams he’s led have brought an outstanding level of rigor to the verification and validation of full systems thermal analysis for the W87,” said Greg Wagner, manager of the Thermal/Fluid Science and Engineering Department. “He’s pulled in some of the most up-to-date techniques in uncertainty quantification theory and used them to have impact on a very applied problem, setting an example that can be followed by other analysis teams across the labs.”

Wagner further observed, “I’m always impressed with Jeremy’s range of knowledge, his creativity, and his willingness to share his expertise. When I want help thinking through a tough problem, to talk about ideas for new projects, or to get some technical coaching or mentorship for a less experience staff member, Jeremy is always the first person I turn to.”

Wagner’s comments are quite a statement about the value Templeton brings to the ASC program, and the confidence we can have in our predictions about the safety of nuclear weapons systems in abnormal thermal environments.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.