ASC eNews Quarterly Newsletter
March 2015

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The Meisner Minute

As promised in my last newsletter, this is my final greeting from your nation's capital. I'd like to take this final space to thank each and every member of Team ASC for your dedication to our nation. But before that I owe you an update on two topics.

First, wither NSCI, the National Strategic Computing Initiative? The last time I told you that I expected an announcement before this newsletter was published. As I write this, all I can say is that the NSCI is nearing the finish line, unfortunately, a bit slower than I anticipated. I would point out in my defense that technically I could still be right—NSCI may yet be announced before this newsletter is published, but the details will have to wait to be revealed.

Second, Doug Wade has been rapidly assuming my program director duties (some would say I have been dumping) and has been defending our ASC FY 2016 budget request to Congressional staffers. While it is impossible to know what will ultimately be appropriated, the briefing to all four committees was well received with a fair amount of engagement with the committee staffs. In particular, there is a lot of interest in exascale, the ATDM subprogram, and our interactions with our Office of Science counterparts.

As my tenure comes to an end, I hear several recurring questions. Everybody wants to know if my replacement has been named. The answer is that Kathi Alexander will be performing a national search for my successor. In the meanwhile, Doug Wade will take over. No one is better qualified to lead the program through the technical challenges you are facing.

The second question I get is "Why now?" My answer comes in two parts. First, Wanda and I concluded that it is time to pursue our love of traveling while we still have our health. The second is professional. The program is about to transition into the exascale era in full force. The timing is perfect for someone else to come aboard and set the course for the future.

People invariably asked, "What are you going to do?" Of course, being of sound mind and wanting to stay of sound body, what Wanda (and I) concluded in the "why now" answer above. We plan to travel extensively. Wanda has already booked hotels and bought airline tickets at 10 destinations in the US and abroad.

Lately, I've been asked, "What was your proudest achievement?" Being from your nation's capital, my first temptation is to change the subject to an easier question, "What was your luckiest achievement?" To that I answer, "landing the most awesome job in the computing business—working with incredibly smart and dedicated professionals responding to a national need with a computing capability that would have amazed our nuclear forefathers." My proudest achievement follows from my luckiest. I wrangled highly competitive labs, without breaking their spirit, and got them to work towards a common objective of turning the "Promise of ASCI" into an unprecedented production capability for stockpile scientists and engineers. It took a decade, but a personal sense of satisfaction fell over me when a chorus from the ASC Execs cried for more investment in Commodity Technology Systems—the workhorse systems for DSW and annual assessments--even at the expense of advanced technologies. I almost fell out of my seat. Our successes were positively impacting the mission and putting pressure on us to do more.

As I transition to a new stage of life I am professionally satisfied with the state of the ASC program. My regret is that I am saying a final goodbye to you. But, Wanda and I will sleep well at night knowing that Team ASC continues to serve our great nation. I was proud to have served with you.

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Doug Wade is Acting NNSA ASC Program Director

When Bob Meisner retires at the end of April, Doug Wade will be the Acting NNSA ASC Program Director. ASC executives presented a retirement memento to Bob Meisner at the 2015 ASC Principal Investigators meeting in February.

Caption: L to R: LANL Program Director Bill Archer, NNSA ASC Program Director Bob Meisner, LLNL Program Director Mike McCoy, and SNL Program Director Keith Matzen

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Simulation of Phase Transformation in Materials under Dynamic Compression Paves Way for Next-Generation Hardware

A team of Lawrence Livermore National Laboratory (LLNL) researchers is tackling a long-standing gap in understanding of dynamic materials processes relevant to Stockpile Stewardship. How does a material "know" to change phase once it is shocked? How fast or slow does that phase transformation process proceed, and why? And, if experimental measurements are made during this process, how can we definitively extract information about the phase transition kinetics?

When a material undergoes a phase transition, its physical properties—such as density, compressibility, or sound speed—change dramatically. Iron (Fe), one of the most widely studied materials (experimentally), undergoes a very large change in density when shocked beyond a certain threshold. Multiple shock experiments have been performed on iron throughout the years, in various different geometries, resulting in high-quality datasets. Iron is of tremendous interest to the scientific community for its relevance to planetary physics; indeed, it is believed that the iron at the center of the earth exists in a hexagonal atomic structure, which is different from the cubic structure found at ambient conditions.

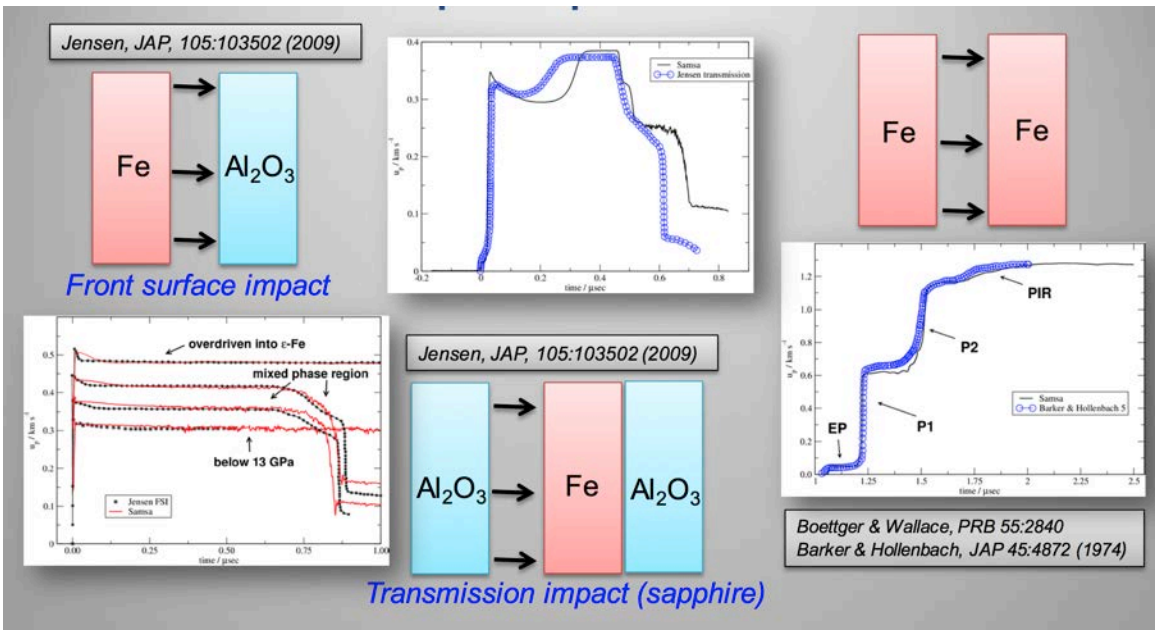
"The real challenge is to formulate a predictive theory for a material that has had its pressure and temperature changed so rapidly that it's in an odd state, far from equilibrium," said Jon Belof, program lead for the LLNL Phase Transition Kinetics effort under ASC/Physics and Engineering Models. "In an attempt to move closer toward equilibrium, the material will change its phase, but when will this process begin and how rapidly will it proceed? This is a very fundamental problem but one that greatly impacts simulation capabilities since the dynamics of the phase evolution greatly dictate the outcome of a simulation, such as overall compression and material strength properties," continued Belof.

The LLNL Phase Transition Kinetics team has developed a general theory for nonequilibrium phase transitions based upon an established approach known as "phase field." Phase field models are mesoscopic in their description of a mixed-phase system and the interface that spatially separates phases. As the phase transition proceeds, heat is transported across the interface and the material volume and sound speed change tremendously. It is in this scenario that the hydrodynamics is perturbed and becomes strongly coupled to the details of the phase transition. In iron, for example, a single shock wave will split into two distinct shock waves that travel at different speeds. Often, this process occurs with a time lag due to the kinetics of the transformation, and it is this time lag that further affects the hydrodynamics.

The Fe phase transition kinetics model has been used to simulate gas-gun experiments undertaken by researchers at Los Alamos and Sandia national laboratories and has been found capable of accurately modeling the phase transition in these experiments. "The dynamic experiments on iron that have been performed to date all have very different loading conditions and geometries," added Belof. "The

fact that we were able to simulate all of these experiments with a common model based on phase field was a pleasant surprise."

The physics of the new LLNL model have been developed into an advanced code prototype named "Samsa." The Samsa code calculates the time-evolution of the phase kinetics and then hands that information off to a multiphysics hydrodynamics code. This "middle-ware" software approach allows for the hydrodynamics and equation of state lookups to happen in a manner that depends upon the nonequilibrium dynamics, without the need for significant modifications to either code. The software architecture developed by the team will enable next-generation computer hardware to not only run existing problems but to now run expanded physics capabilities as presented by material phase transitions.



Caption: Shock-wave propagation experiments in iron (Fe) are depicted for three distinct loading cases: front surface impact (Fe bullet impacting a sapphire target), transmission (sapphire bullet impacting an Fe target) and symmetric transmission (Fe bullet impact Fe target). The black lines in all figures depict the simulation results of the body-centered cubic to hexagonal close-packed Fe phase transition using the new LLNL code, Samsa.

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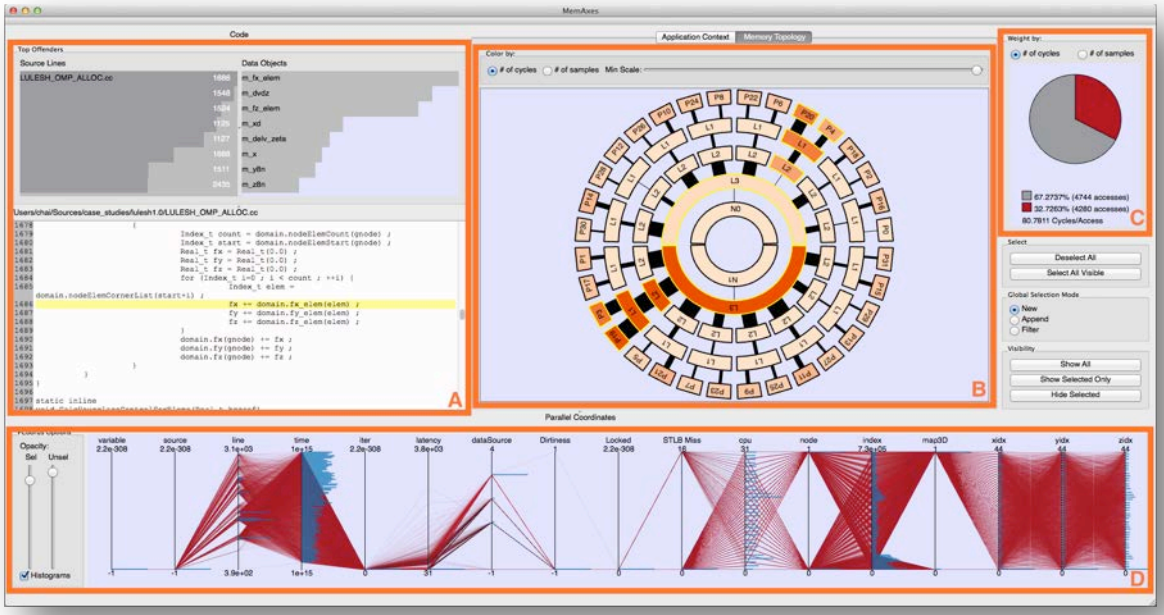
New Tools to Highlight Communication Performance on HPC Platforms

With rising complexity in both systems and applications, maintaining computational efficiency is a continuing challenge for the ASC Program—system architectures are becoming more heterogeneous and diverse; applications are becoming complex, multiphysics simulation frameworks; and optimally mapping one to the other is non-trivial yet critical. New tools are needed to support this task. Two such tools, MemAxes and Ravel, have been developed at Lawrence Livermore National Laboratory (LLNL) to understand and optimize communication and its performance impact, and to play an important role in positively impacting computational efficiency.

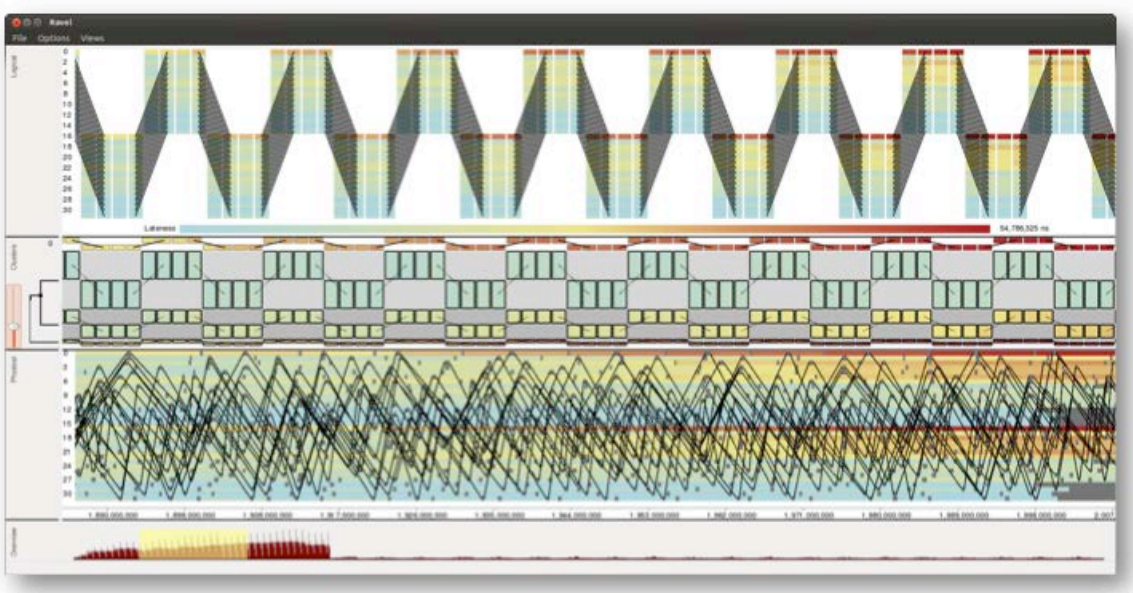
MemAxes allows computational scientists to visualize on-node memory traffic through an easy-to-view graphical interface that shows memory access data mapped to application and machine characteristics, including the node and memory topology, location within the simulated mesh, and affected data structures and code locations. A case study using LULESH, the Livermore Unstructured Lagrangian Explicit Shock Hydrodynamics code, solved optimization of on-node locality problems by mapping the computation to the cores close to the data it accesses. With memory access becoming one of the most dominant factors for both performance and energy, MemAxes and its unique ability to see memory traffic mapped to intuitive displays can help address computational efficiency.

Ravel is a trace visualization tool that shows message details for inter-process communication based on the message passing interface (MPI). Often, a physical timeline view of computing messages can create a “hairball” of data, and new techniques were needed to unravel this mess of information. Ravel approaches this challenge by extracting a virtual timeline, which allows concurrent events to be lined up, creating an easier-to-interpret picture. Ravel accomplishes this by first identifying phases and time slices to create the virtual timeline, then maps physical time information onto the virtual timeline to expose bottlenecks, and finally applies clustering based on these metrics to achieve scalability with respect to the number of MPI processes used. A case study using Ravel to optimize communication patterns showed reduced communication time for large laser plasma code at LLNL by a factor of five at large scale. Overall, Ravel provides a critical contribution to making message trace approaches intuitive for the user, even for complex message patterns and at large scale.

“Visualization techniques are powerful not only for analyzing and understanding data generated by our ASC codes, but also for helping to analyze performance of the codes. Both of these tools provide novel ways to help scientists identify features and unravel issues related to using advanced hardware and software at scales where efficiency is essential,” said Becky Springmeyer, LLNL lead for Computational Systems and Software Environment.



Caption: MemAxes interface showing data structures and code (window A), memory system topology (window B), and a parallel coordinates view for interactive metric selection (window D).



Caption: The Ravel interface with virtual timeline on top, the cluster view below that, followed by the original “hairball” view created by using a physical timeline. The bottom row shows a summary of the timing metrics for interactive selection.

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First Trinity Hardware: Testbeds Delivered

As part of the Trinity contract, the first hardware was delivered in early February. Two Application Regression Testbeds (ARTs) were delivered; one to Los Alamos National Laboratory (LANL) and one to Sandia National Laboratories (SNL) as part of the Alliance for Computing at Extreme Scale (ACES) partnership. In addition, a System Development Testbed (SDT) was delivered to LANL.

The ART systems (named Trinitite at LANL and Mutrino at SNL) will be used for application development and testing in their respective unclassified networks. Each ART system will initially have 100 Haswell nodes. When they become available early in the calendar year 2016, an additional 100 Intel Knight's Landing (KNL) nodes will be installed in each system. The Trinitite system is the first water-cooled system at LANL. It will provide operational experience prior to the larger installation of the Trinity system in the Metropolis Center for Modeling and Simulation at LANL.

The SDT system (named Gadget) will be used primarily for systems software development and testing ahead of the main Trinity delivery. The initial delivery of Gadget will have 20 Haswell nodes with an additional 20 KNL nodes as they become available in early 2016. During the next few weeks, all of the testbeds will undergo acceptance testing.

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LANL FOUS Program Manager Hal Armstrong Retiring

After 35 years of service at Los Alamos National Laboratory, Hal Armstrong is retiring in March 2015. Hal has served as the Facilities, Operations, and User Support (FOUS) Program Manager for the past 6 years and has done an outstanding job leading this critical ASC Program area that provides the infrastructure and staffing for the computer centers. FOUS is a focal point of the ASC Program, requiring interactions with line management; other program elements such as Platforms, CSSE, and Integrated Codes; and the user community. A recent example of the complexity Hal has dealt with was balancing funding of the SCC Cooling Project at the Metropolis Center for Simulation and Computing with the rest of the service needs of the program.

Prior to becoming the LANL ASC FOUS Program Manager, Hal led various high-performance computing (HPC) teams, including the high-performance storage system (HPSS) Team Leader. He was the deputy group leader for the HPC Systems group and also the LANL HPSS Executive Committee Representative.

Paul M. Weber, currently in the HPC Systems Integration group at LANL, will be acting FOUS program manager. Paul joined LANL as an undergraduate student in 1998 and has developed a career in high-performance computing through his participation in many software- and systems-focused activities. Paul joined LANL's HPC Division in 2006 as an HPC consultant, and subsequently migrated into the role of data visualization specialist, where he focused on user support, R&D, outreach, and the management of HPC Division's advanced visualization facilities. Most recently, he has been involved in the redesign and refurbishment of LANL's Powerwall Theater and in the deployment of state-of-the-art in situ visualization capabilities to ASC simulation codes.

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Breakthrough Mesh Optimization Technology Enhances Reliability of Auto Hex-meshing Capabilities

Sculpt is a relatively new parallel application for automatically generating all-hex meshes for complex geometric models. Its major benefit is its ability to avoid the time-consuming interactive geometry preparation common with traditional hex meshing tools and is capable of producing meshes of upwards of one billion elements in just minutes.

Sculpt utilizes a mesh optimization technique that guarantees identical meshes regardless of the number of processors used to generate the mesh. This procedure has in some cases produced a small number of poor quality elements, which can sometimes render the mesh unusable for analysis.

To address this issue, scientists at Sandia National Laboratories have developed a new MPI-based algorithm, known as parallel coloring that isolates and improves poor quality elements while still maintaining parallel consistency. A study that included more than 50 CAD models meshed using Sculpt's new smoothing procedures produced computable mesh quality (minimum scaled Jacobian greater than 0.2) in over 90 percent of the models. This improved from about 50 percent where parallel coloring was not used. These results illustrate the effectiveness and reliability of Sculpt in providing a practical meshing solution for real-world simulation for large-scale models.

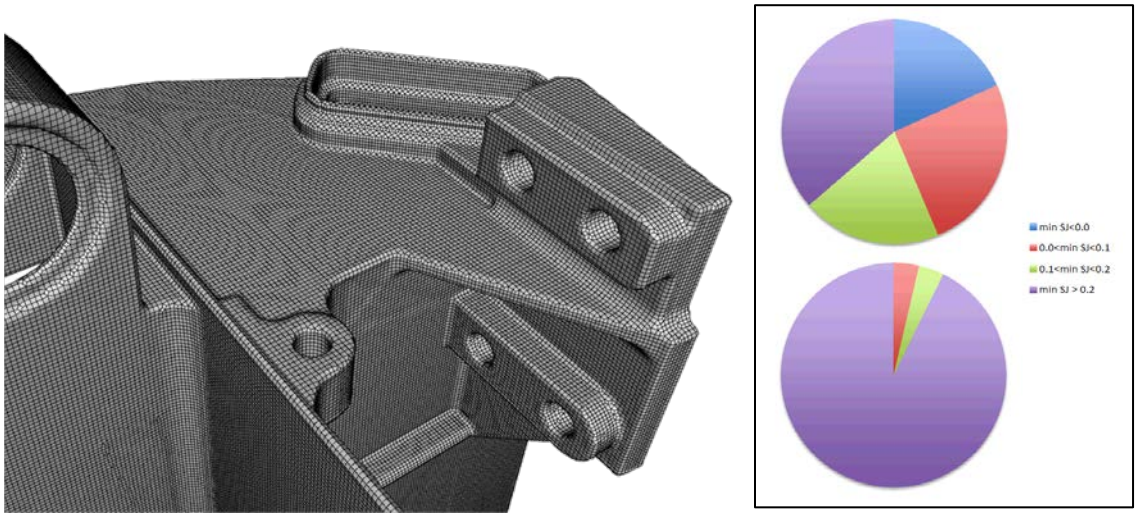

Figure: Improvement in minimum Scaled Jacobian mesh quality metric before (top chart) and after (bottom chart) optimization using the Coloring algorithm.

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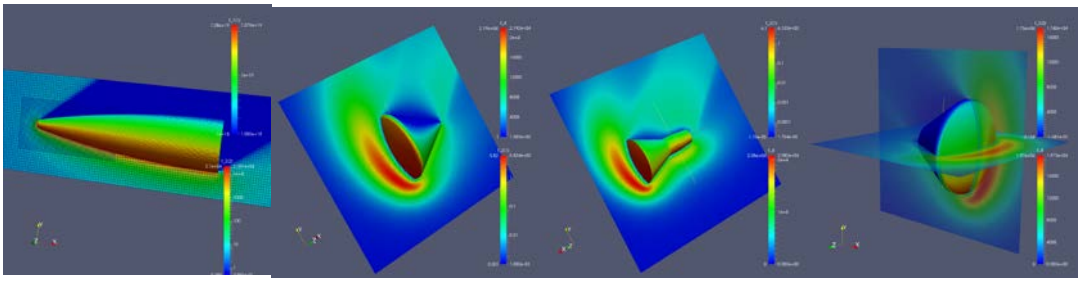
Chemically Reacting Flows Simulated with SPARTA 3D DSMC Code for Classic Re-entry Vehicle Geometries

Chemically reacting, thermal-nonequilibrium rarefied gas dynamics simulations have been completed for a variety of altitudes and flow speeds for a number of re-entry vehicle geometries using the recently implemented, advanced chemistry models with SPARTA, a recently developed 3D Direct Simulation Monte Carlo code suitable for current and next-generation high-performance computing architectures. The selected flight conditions are such that established continuum (CFD) approaches are not as predictive due to the rarefaction of the flow and the nonequilibrium chemical activity. These simulations were performed in preparation for a scheduled ASC Level-2 milestone and demonstrated all of the capabilities that will be needed (chemical reactions, adapted grids, restart files, massively parallel processing, I/O, and post processing on Sequoia).



Generic ogive Apollo capsule Gemini capsule Orion capsule

Figure: Examples of chemically reacting flow fields simulated with SPARTA for four classic re-entry vehicle geometries.

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ASC Salutes: Eric Keiter

Infeasible, against common wisdom, unattainable… As scientists and engineers we're often confronted with these mindsets and as is our nature, we thrive on stepping up to these types of challenges. When Eric Keiter joined Sandia National Laboratories (SNL) in 1998 with a PhD in Material Science, he not only took on the naysayers but succeeded in grand fashion. Eric was one of the innovators and the current project lead of the ASC code Xyce, one of the world's first parallel circuit simulators and a critical tool for electrical component design and qualification for current and future Life Extension Programs (LEPs) and Alts.

Eric was instrumental in the development, "from the ground up," of the Xyce parallel circuit simulator, which disproved the then-conventional wisdom the electrical design automation (EDA) community held of the infeasibility of parallel circuit simulation. During the development of Xyce from its inception in 1999, Eric has mentored and recruited many of the current and former Xyce developers over the lifespan of the project. In 2006, Xyce was integrated within the Qualification Alternatives to the Sandia Pulse Reactor (QASPR) project and has become one of the cornerstones for the integrated experimental and modeling & simulation capability that will be required to deliver qualification evidence to current and future nuclear weapon (NW) LEPs and Alts. One of the pinnacles of the Xyce project was receiving the prestigious R&D 100 Award in 2008, further establishing SNL as a world-class institution for electrical simulation.

Eric's contributions to QASPR go beyond the Xyce circuit code; he is the inventor of novel analytical radiation aware compact models that are critical for NW applications. Eric is "the" expert at Sandia and a leading developer internationally of these models. His expertise is recognized by national and international professional societies where he has been the subcommittee chair of Technical Program Committees for multiple IEEE circuit simulation conferences and is a Senior Member of the IEEE. He is also the Sandia representative within the Compact Model Coalition, an organization that establishes industry standards for compact modeling. During his time at Sandia, Eric has developed mastery within the areas of compact modeling, circuit and system simulation algorithms, modular code structuring, coding and software development, and the flow of simulation-based designs, making him one of the few people worldwide to have this breadth of mastery. This expertise and the success of Xyce led to Eric's promotion to a Distinguished Member of Technical Staff in 2014.

Eric has a bachelor's degree in mathematics and physics from Augustana College and a Master's and PhD degree in Materials Science from the University of Wisconsin-Madison. He grew up in various university towns in the Midwest, having

a pair of chemistry professors for parents. Eric is married and has a young son. His hobbies include competitive swimming, photography, and playing the piano.

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Recent Publications

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