ASC eNews Quarterly Newsletter
January 2015

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The Meisner Minute

Greetings once again from the Department of Energy Forrestal Building in your nation's capital. I hope this finds you safely back from the holidays and energized for a challenging and exciting new year. To start, I owe you updates to three activities I introduced in my last newsletter.

First, and this should be old news by now, the Secretary of Energy announced one of the winners in the procurement competition of the collaboration of Oak Ridge, Argonne, and Lawrence Livermore national laboratories, known as CORAL. IBM and its teammates, Nvidia and Mellanox, will deliver two 150–200 petaflop systems to LLNL and ORNL. By the time you read this, I expect that the third member of the CORAL team will announce their industrial partner(s). The IBM bid was surprising in that they teamed with hardware providers from outside the company to provide the winning solution. The resulting system will be a challenge to bring into production. But, it will be exciting to coax performance from its awesome capability and advance our understanding of weapons performance and science.

Second, Congress funded the new element of the ASC Program—Advanced Technology Development and Mitigation (ATDM). A prime motivator for establishing ATDM was to segregate elements of ASC that share the same objectives as the Department's Exascale Computing Initiative (ECI), most of them being ongoing mission activities. However, in funding ATDM, the Department and Congress approved the Program's initiative to begin building new code structures at the labs. This challenging and exciting opportunity presents itself only once every couple of decades. It was made necessary by the new architectures we are encountering that, counterintuitively, result in longer execution time for our existing codes, even when run on faster machines.

It's likely that you have not been hearing much about the ECI, primarily because it has been wrapped up in federal coordination processes. Beginning with the new year, you can expect to see renewed activity. Consequently, the Exascale Seven (E7) leadership team was reconstituted, consisting of the ASC Program executive officers from our labs (LANL, LLNL, and SNL) and the DOE Office of Science Advanced Scientific Computing Research (ASCR) associate lab directors from the DOE labs (ANL, LBNL, ORNL, and PNNL). These are the folks that advise the ECI co-leads, Steve Binkley and me, and direct lab resources to accomplish the objectives of the ECI Program. This same structure will be used to respond to the National Strategic Computing Initiative (NSCI) directions, when they are announced, as the ASC-ASCR team work to integrate ECI and NSCI activities.

Lastly, while there is little news with respect to NSCI, this initiative is proceeding on track. As with any program of such magnitude and organizational complexity, the process is deliberate and time-consuming. Still, I expect that we should see an announcement with regard to this initiative before the next newsletter is published.

As the ASC Program Director, I am excited about the impact your work is having on our stockpile stewardship mission. Results from across the labs illustrate the wide-ranging impact of your work, and also reinforce the professional reputation of the ASC team. As one example, LANL has developed an initial capability to bound the performance effects of physical phenomena that govern boost, which, significantly, can be applied to untested configurations. This advance directly supports a Predictive Capability Framework (PCF) Level-1 milestone in FY15 for pit reuse certification, as well as an FY18 PCF pegpost for evaluating boost predictive capability for nominal primary performance. Achievements at the National Ignition Facility (NIF) are another great example. *Physics World*, an international monthly magazine published by the Institute of Physics, has named NIF's achievement of fuel gain one of its Top 10 breakthroughs of the year. Codes funded through ASC played a critical role in the discovery and testing of insights that resulted in these breakthroughs. Continued research on NIF shows great promise in leading to improvements in our predictive capabilities and a deeper understanding of fusion physics. In addition, SNL is using its full system thermal model of the W78-0 to assess safety margins in fire environments. The model was used to make pre-test predictions, which contributed to successful testing of W78 system hardware. Scientists and engineers at all the NNSA laboratories are finding that significant improvements in experimental testing can be achieved through the use of our tools; and, of course, our tools benefit greatly from the validation data provided by those experiments.

Before closing, I want to recognize Jay Edgeworth for his contributions to the Defense Applications and Modeling elements of the ASC Program as he steps up to other challenges in building advanced manufacturing and joint testing capabilities in Defense Programs.

Rumors you may have heard about my impending retirement are true. My last day will be 30 April. That means I have one more *Minute* to communicate with you. Until then, thanks for your contributions to team ASC and our nation's nuclear deterrent.

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ALE3D Team Commended for Work Conducted for Department of Defense

In a recent email addressed to Lawrence Livermore National Laboratory (LLNL) management, William H. Davis, Deputy Technical Director of the Army's Institute for Multiscale Reactive Modeling (MRSM) at Picatinny Arsenal, acknowledged the superlative technical achievements and broadly appreciated contributions of the Arbitrary Lagrangian-Eulerian (ALE3D) team members for work conducted for the Army's Armament Research, Development, and Engineering Center (ARDEC).

The high-production-level ALE3D computation tool available for both two-and three-dimensional work, is a Department of Energy (DOE)-sponsored ASC Program code developed at LLNL featuring multiphysics and multiscale attributes. Both the DOE and LLNL encourage the use of this simulation capability by the Department of Defense for national security applications.

Davis wrote, "…I wish to commend the following individuals at Lawrence Livermore National Laboratory…These people who are part of the ALE3D team… have worked diligently and to the highest technical standard on the various improvements to the ALE3D code identified to be the MSRM's priorities for modifications to ALE3D in the areas of ParticlePack, detonation shock dynamics, and user-defined functions. These particular areas form the backbone of the MSRM's contribution to the Army's supercomputing efforts in energetics computational technology, and these developments will carry forward this vital and highly extensible capability thanks to the stable and highly supported ALE3D code and its talented development team. Thus the entire Department of Defense as well as the Department of Energy and other government agencies and qualified contractors may use these and associated capabilities for the good of the defense of the United States. I and the staff of the MSRM express unmitigated admiration, as well as gratitude, to this unmatched group of researchers for their enthusiastic and technically superlative support and even more so for their successful efforts to meet a highly accelerated timeline to completion of the contracted functionality in ALE3D."

ALE3D has unique physics and numerical models for application to conventional weapons advancement. The flexible and extensive code framework supports fully integrated hydrodynamics, heat transfer, solid and fluid dynamics, and chemistry models with the ability to capture the physics of high-velocity impact and thermal "cook-off" with the detonation and deflagration of explosives and propellants. Also unique to ALE3D is the fully coupled explicit and implicit time integration allowing the evaluation of short time-scale phenomena such as impact and detonation to the long time-scale thermal and structural loads and response to slow "cookoff."

For more information on ALE3D, see the website
https://wci.llnl.gov/simulation/computer-codes/ale3d

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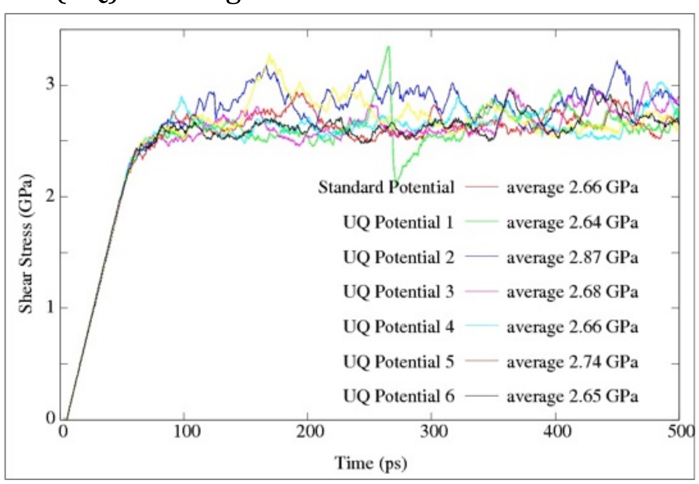
Initial Framework Offers Potential for Uncertainty Quantification in Multiscale Models

Researchers at Lawrence Livermore National Laboratory (LLNL) have begun to address the uncertainty quantification (UQ) challenge associated with the use of a hierarchy of models to bridge quantum- and continuum-length scales.



The model at the continuum level is underpinned by a hierarchy of physics-based models at lower length scales, and just as the parameters of the continuum-level model are passed from the lower scales, so too do the uncertainties propagate along with additional errors due to the necessarily inexact form of the models. At each level, the models describe complex phenomena and are nonlinear in character.

"As multiscale strength modeling begins to deliver validated, physics-based models of the constitutive behavior of solid materials for use in integrated codes, the need for a UQ methodology for multiscale models is growing," said Nathan Barton, leader for the strength and damage effort within the Physics and Engineering Models sub-program of the ASC Program.

Current efforts focus at the smallest length scales, where the quantum mechanical information about atomic bonding is passed via an interatomic potential to the nanoscale systems in which defect (dislocation) mobility is calculated.

"We are developing a framework that uses ASC UQ tools, our potential fitting code, and LAMMPS (the molecular dynamics code used for dislocation mobility calculations)."

For an initial test example, an ensemble of beryllium interatomic potentials was generated based on uncertainties in the quantum mechanical database used for fitting. Those potentials were assessed for "goodness-of-fit" to the data, as well as variations in the resulting mobility (dislocation velocity versus shear stress) and glide mechanisms.

In this sensitivity test, only minor variations in the glide mechanisms were observed. "It is encouraging," added Barton, "that the predicted variations in the key results are typically smaller than the variations in the fitting database, indicating an averaging-out of noise in the database."

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Sandia Completes Second Fracture Challenge

The 2nd Sandia Fracture Challenge (SFC2) focuses on predicting ductile tearing of titanium alloy Ti-6Al-4V under simultaneous competing tensile and shear failure modes at both quasistatic and modest dynamic rates (failures in <1s, comparable to vehicle accident scenarios). Blind predictions have now been reported from 3 internal Sandia teams and 39 external volunteers representing 17 institutions ranging from MIT to École Nationale Supérieure des Mines de Paris. Two separate test labs have now performed the defined experiment. Comparisons between model predictions and experimental outcomes are underway to assess the efficacy of different modeling approaches. All participants are invited to attend a workshop in March at University of Texas at Austin to discuss the results. Also, all teams will present their results at a special symposium organized by Sandia at the 2015 Annual ASME Conference in November 2015.

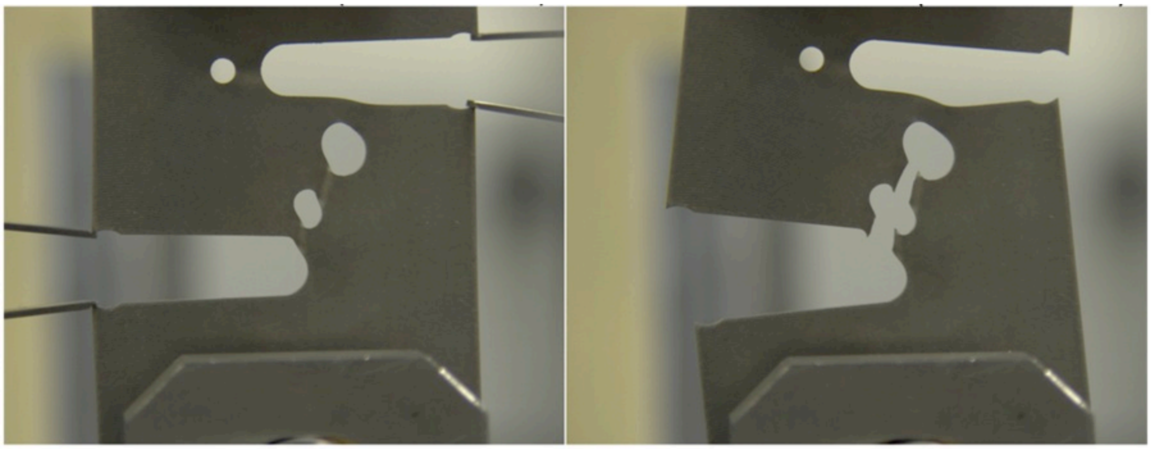

Figure 1: Experimental images taken just before and after unstable crack nucleation and propagation showing failure along the shear path. Of the 14 teams, 10 correctly predicted this path at both slow and fast loading rates.

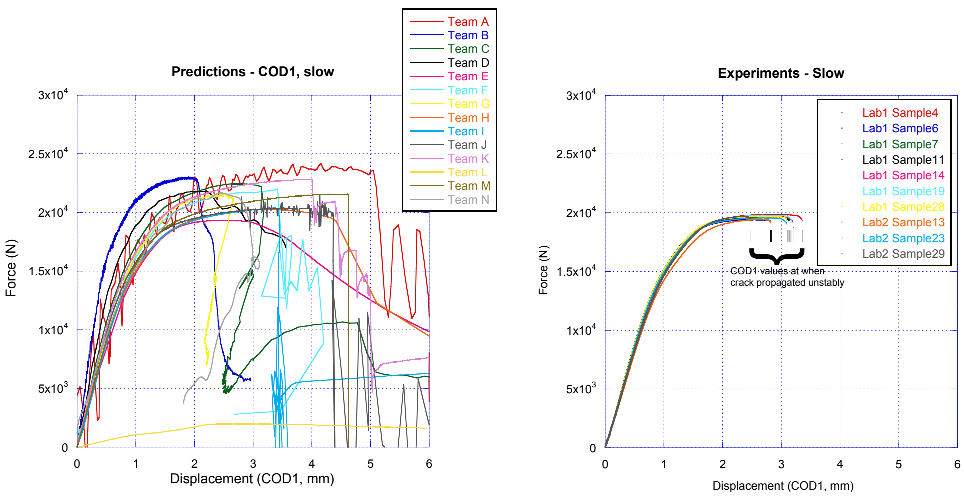

Figure 2: Prediction summary from 14 teams and experimental outcome summary from 2 labs with multiple test specimens.

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Advances in ATDM AgileComponents for Thermal-Mechanical Simulations

Sandia's AgileComponent toolkit has been utilized to demonstrate the ability to do automatic mesh adaptation for large deformation mechanics—a key stepping stone in building next-generation ATDM applications for Nuclear Weapon safety analysis. When mesh adaptation is used during large deformation calculations, it is necessary to adopt a new reference configuration each time the mesh is modified to avoid the complexity of pulling back new adapted element configurations into the original coarse reference space. Figure 1 illustrates a large deformation result, where a new reference configuration was employed at each mesh adaptation step. The coloration on the mesh is the stress field in the *x* direction. Note the non-uniformity of stress in the notch area. This is due to use of the initial coarse mesh elements to define the surface of the notch during the deformation process. Work is underway to adapt the mesh to an approximation of the actual embedded surface geometry and this work will serve to inform our ATDM planning for a future coupled thermal-mechanical safety application with inherent support for next-generation computers.

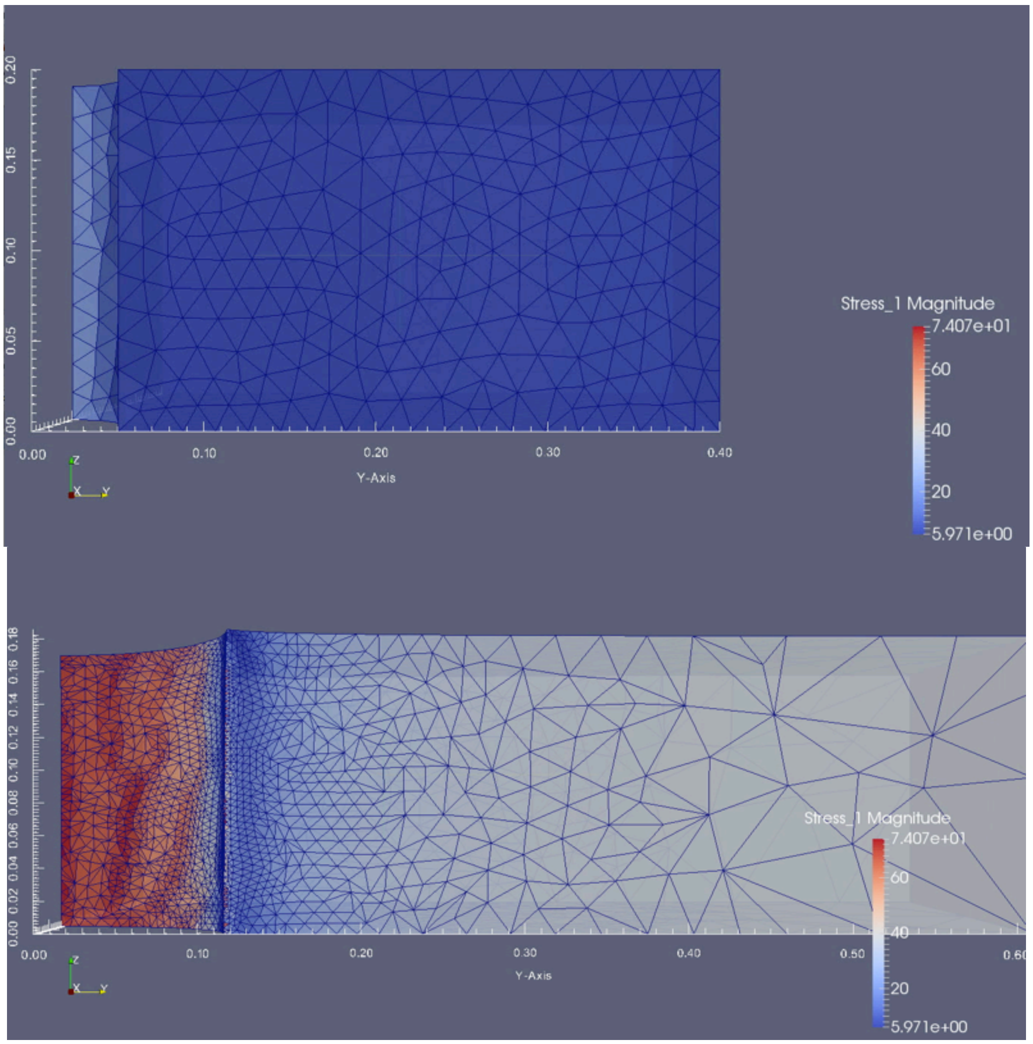

Figure 1: Images illustrating the stress field for an adaptive elasticity problem, where a new reference configuration is employed each time the mesh is adapted. The top image shows the notched bar at the first time step, the lower image shows the result near the end of the calculation.

Sandia's ATDM program has also implemented an AgileComponent-based topological optimization capability and demonstrated a multi-objective and multi-loadset topological optimization. The current capability computes the design that is Pareto optimal in mechanical stiffness and thermal conduction, i.e., the design for which mechanical stiffness cannot be improved without sacrificing thermal conductivity and vice versa. This tool can be used to generate Pareto optimality curves that represent the boundary between feasible and infeasible performance requirements. The demonstration in Figure 2 shows the power of the AgileComponent infrastructure for rapidly building new capabilities that have embedded analysis and optimization using the power of automatic differentiation. This demonstration showcases how Sandia's ATDM program will leverage these capabilities for future ATDM applications for Directed Stockpile Work.

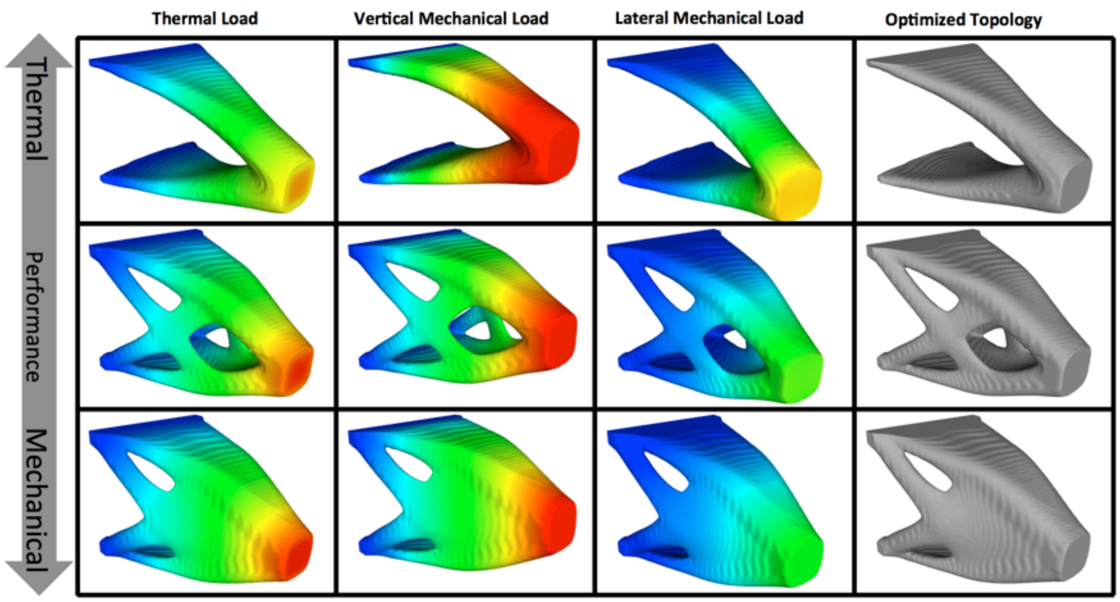

Figure 2: Example of topological optimization using AgileComponents with multiple objectives and loading conditions. The middle row shows an optimal configuration considering multiple objectives and its performance across a thermal load and two mechanical loading cases.

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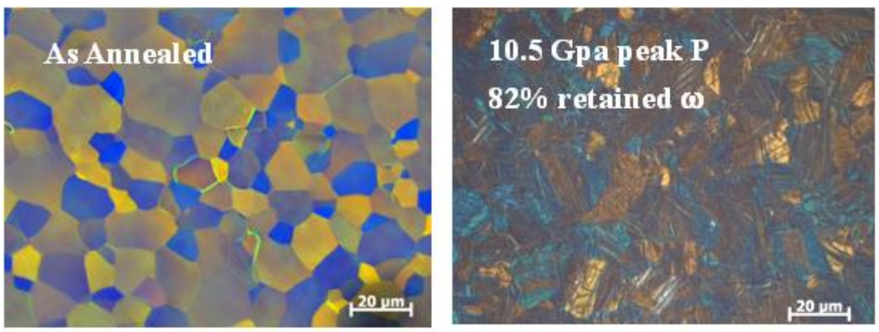
Understanding Relevant Physics Across Scales through an Integrated Approach

The ASC PEM Materials Project at Los Alamos National Laboratory is working to better understand and capture meso-scale physics within the context of continuum-scale material deformation, damage, and failure modeling capabilities in the ASC Program. Dislocation evolution, phase transformations, porosity nucleation and growth, and similar phenomena are inherently meso-scale physical processes, with mechanisms occurring at length scales associated with the atomic lattice or grain boundaries of the material. Yet it is exactly these meso-scale phenomena that dictate the bulk features of the continuum-scale mechanical response of many materials relevant to the ASC Program.

Without a proper accounting and representation of the meso-scale physics, our continuum-scale models will be, at best, empirical, and fully lacking in predictive capability. For example, one fundamental mechanism that permits plastic flow in metals is dislocation motion, which involves the evolution of defects or irregularities in the atomic lattice of the material. If one does not accurately capture this meso-scale behavior, and represent this behavior within our continuum-scale models for strength, then our continuum-scale model is missing much of the physics that allow us to be predictive. The challenge, therefore, in the continuum-level modeling required for our Integrated Code (IC) strategy, is not only the incorporation of meso-scale physics, but the proper understanding of the most relevant physical mechanisms and the development of models the span the length scales involved, along with appropriate implementation strategies, which may require scale-coupling algorithms.

We still lack a fundamental understanding of many of the physical mechanisms occurring at the meso-scale and contributing to the continuum-scale material response characteristics. The ultimate challenge is working across the Science Campaigns, and the Physics and Engineering Models, the IC, and the Verification & Validation (V&V) program elements to develop an integrated approach to understanding the relevant physics, developing the best multi-scale models, properly implementing these models into IC, and working with the V&V and design communities to ensure proper model testing and use.



Understanding retained phases in shocked polycrystalline metals is a current area of research

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70 Years of Computing at Los Alamos

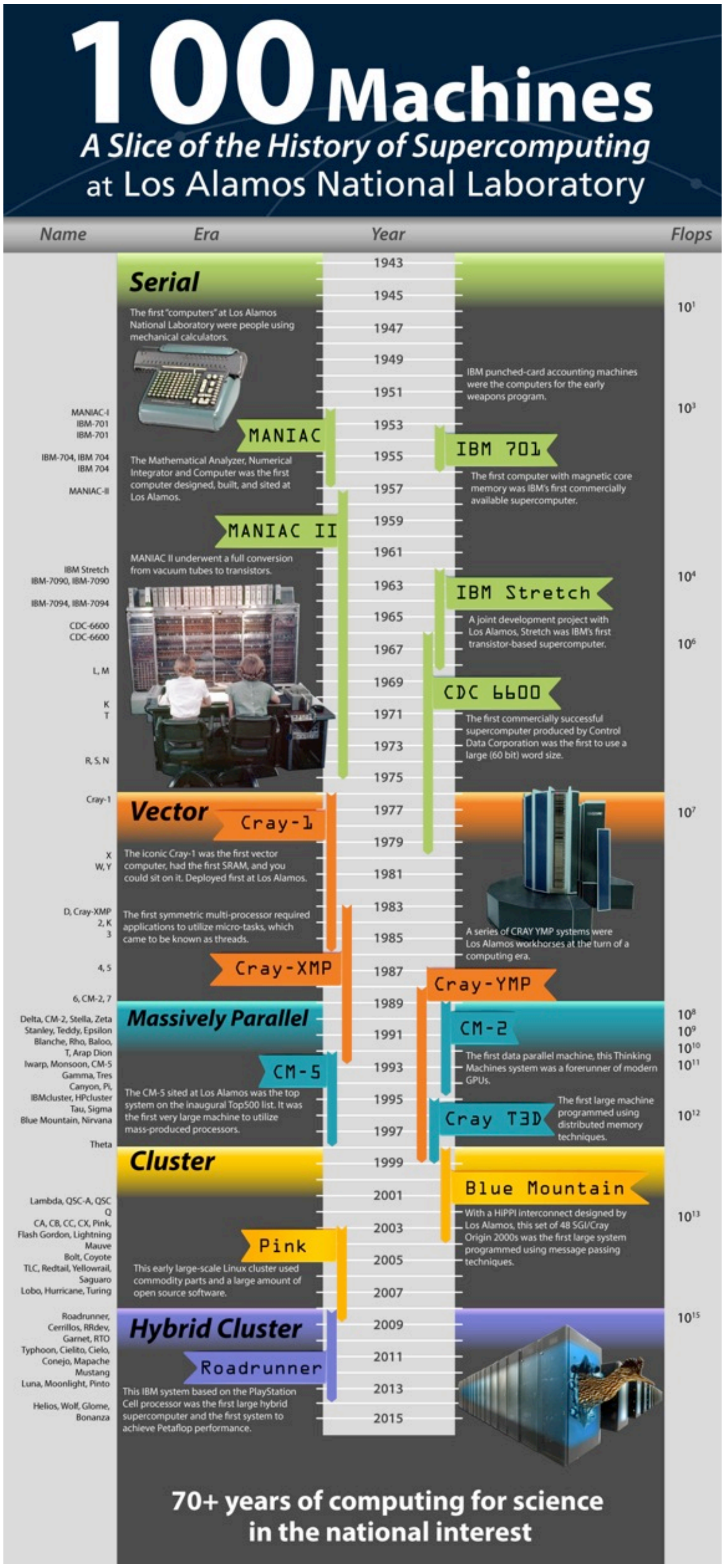
Los Alamos established its first computing center in 1944 when Stanley Frankel and Eldred Nelson connected IBM 405 punch card accounting machines (PCAM) with 605 multiplier units. The PCAM were used to carry out the implosion calculations for the first generation of nuclear weapons. The very first calculations on the ENIAC were thermonuclear burn simulations carried out by Los Alamos staff with John von Neumann. Thereafter, Los Alamos hijacked every government-owned first-generation computer to carry out evermore-complicated thermonuclear simulations leading up to the first thermonuclear tests in the 1951 Greenhouse events and the 1952 Ivy Mike event.

Also in 1952 was commissioning of MANIAC, the first electronic computer sited at Los Alamos. With the commissioning of the Bonanza system in 2014, Los Alamos computer centers have installed 100 supercomputers since MANIAC! The first part of the serial era, 1944 to 1966, was dominated by IBM systems such as the IBM 701.

The transition to transistors, but still serial systems, was dominated by the Control Data Corporation (CDC) 6600 and 7600 systems from 1966 to 1976. The vector era was next with Cray systems providing production computing from 1976 until 1998. These systems provided the simulation support for shrinking the size of U.S. nuclear weapons so they could be used in tactical weapon systems and on ballistic missiles.

With the end of nuclear testing came the Accelerated Strategic Computing Initiative (ASCI) program that ushered in the massively parallel era with commercial clusters such as the SGI Blue Mountain system commissioned in 1998. The massively parallel clusters are providing simulations today on the Cray Cielo and Luna systems. The simulations are a key part of the Stockpile Stewardship Program that strives to keep the stockpile safe, secure, and reliable without nuclear testing.

Los Alamos is moving into a new, as yet unnamed, era as Moore's Law is reaching its limits. The next generation of systems has two paths to provide more parallelism. The hybrid path couples fast, but limited, accelerators with powerful traditional processors. This path was first shown to be viable in 2009 by the Los Alamos/IBM Roadrunner system, the first system to achieve 1 petaflop performance. The many cores path uses many lightweight cores to achieve the desired computing power. The Cray Trinity system that Los Alamos is installing in 2015 exemplifies the many cores systems. With Trinity, Los Alamos computing power will have increased by 16 orders of magnitude from 1943! See the figure "100 Machines: A Slice of the History of Supercomputers at Los Alamos National Laboratory." Today's transition to the next generation of systems is an exciting time for everyone involved in computing at Los Alamos, and reminds us of the proud history that we are building upon.



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ASC Salutes: Ian Karlin

Should the national ASC Program take an evolutionary approach to adapting its simulation codes for the next-generation platforms? Or would something bold—revolutionary, even—be more appropriate? These are the questions that Computer Scientist Ian Karlin grapples with every day since earning his PhD only three short years ago and joining Lawrence Livermore National (LLNL) as a member of the scientific and technical staff.

Considering an evolutionary approach, Ian and other LLNL scientists have studied how well the large, integrated multiphysics code HYDRA performs on ASC's advanced technology system, Sequoia. As described in a talk Ian gave at the International Supercomputing Conference last June in Leipzig, Germany, he and the other scientists were surprised to find that neither floating point instruction nor bandwidth were the performance limiting factors. Instead, parts of the code were limited by non-floating point instructions or memory latency (the delay between when data is requested by the processor and when it begins to arrive). These findings helped the team assess vendor proposals for the 2014 multilab CORAL procurement (Oak Ridge and Argonne national laboratories with LLNL) for the next ASC supercomputer, Sierra, to be sited at LLNL and due for production use in 2018.

Considering the more revolutionary approach, Ian leads the computer science team within the LLNL Laboratory Directed Research and Development (LDRD) Strategic Initiative, SHOCX. The team is assessing the suitability of higher order finite element methods for future computing platforms. These methods have a higher compute intensity than do current codes, which may make them better suited for future machines where data movement capabilities will be small relative to compute capabilities. Ian's work on this multidisciplinary team has motivated algorithmic changes to reduce data motion and better prepare LLNL's BLAST code for future machines.

Prior to joining LLNL's technical staff, Ian worked at LLNL as a post-doctoral researcher under Physicist Bert Still in Weapons and Complex Integration (WCI). As part of a multi-institution team, Ian evaluated the performance portability of different programming models for ease of application tuning with minimal impact to the code base. The ability to tune code for diverse machines with minimal changes will be important for application developer productivity as ASC codes need to run efficiently on ASC capability platforms as well as capacity clusters at LLNL.

"Ian is an expert in computer architecture, performance analysis, and code optimization," said Still. "In short, he knows what to measure, how to interpret the results, and how to use the results to improve the code. These are critical skills for the ASC integrated codes in facing the challenges presented by next-generation architectures, and Ian will be a key player in helping to address them."

The ASC Program looks forward to Ian's next programming approach—both evolutionary *and* revolutionary.

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Recent Publications

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12. Isaacs, K.E., Gamblin, T., Bhatele, A., Bremer, P-T., Schulz, M., Hamann, B. (2014). "Extracting logical structure and identifying stragglers in parallel execution traces," ACM SIGPLAN Symp. on Principles and Practices of Parallel Programming (PPoPP'14), Orlando, FL, Feb. 15–19.
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