Simulations Summit Summary

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On Wednesday, October 13th, we held a Simulations Summit here in Washington, where I hosted more than 70 leaders of academia, industry, the government, and national research laboratories to discuss policies and plans for bringing science and simulations to bear on stimulating and accelerating national competitiveness. Fundamentally, I wanted to address two questions: How can we more effectively deploy existing simulation capabilities, and how do we continue to improve these capabilities over the next decade and beyond? The summit served to promote awareness of the current capabilities and successes of simulations in widely varying sectors of our economy, and illuminated the current state of hardware, software, and methodologies so that we can accurately define the barriers that we face.

The Simulations Summit began with a series of keynote addresses, which were followed by three panel discussions among leaders in the application of high-performance computing to simulation challenges. The first keynote address was by Ernest Moniz, former Under Secretary of the Department of Energy and Professor of Physics at MIT. Dr. Moniz laid out the history of supercomputing and simulations within the Department and in the nation. In the mid-90's the Department began the Accelerated Scientific Computing Initiative (ASCI) to address the Stockpile Stewardship challenge of eliminating the need for nuclear testing through simulation. The focused, definite goal of the ASCI program enabled the Department to establish the U.S. as the global leader in high-performance computing (HPC). Dr. Moniz emphasized key structural features that led to the success of the ASCI program: its focus on the high-end of the computing spectrum, the creation of key commercial partnerships, the existence for a robust support environment, and deliberate use of modeling and simulation for validation and verification as well as uncertainty quantification. The success of ASCI informed the development of the Scientific Discoveries through Advanced Computing (SciDAC) program within the Department's Office of Science, which paired mathematicians with computer scientists to accelerate innovation in simulations. SciDAC's mission was to develop the hardware and software necessary to achieve terascale computing in order to bring simulations to bear on ten broad scientific challenges. Congress created the Office of Advanced Scientific Computing Research (ASCR) in 2003 to work with industry to develop the next generation of high-performance computers. ASCR continues to advance the simulations capabilities at DOE national labs expand the accessibility of these national resources.

Horst Simon, Deputy Director of Lawrence Berkeley National Lab, gave the audience some perspective on the current state of scientific computing. The United States is the clear leader in high-performance computing, with 90% of HPC platforms produced by U.S. technology and most of the work performed on supercomputers using software developed by U.S. researchers. The Jaguar system at Oak Ridge National Lab had been the world's most powerful computer since 2009, and has a top speed of 1.75 petaflops. However, there is growing competition in high-performance computation globally, with increased investments by China, Japan, Europe, and others. Indeed, a decade ago China had little presence in high-performance computing, and has recently announced the development of world's most powerful computer, the Tianhe-1A , capable of achieving 2.5 petaflops. While China's fastest computers use U.S.-made hardware, they are also developing their own processor lines and are expected to announce a machine capable of petaflop performance using these components within the next 18 months.

Secretary Chu's keynote address stressed the importance of simulations and high-performance computing to U.S. competitiveness in science. Secretary Chu described the scientific breakthroughs that have come as a result of U.S. investment in simulations in areas from climate modeling to biology to material science. He noted that scientists will be using simulations to better understand how plants turn solar energy into chemical energy at the Joint Center for Artificial Photosynthesis. Secretary Chu emphasized that simulations have yet to be fully brought to bear on several critical issues, including building design. Sharon Glotzer of the University of Michigan, who delivered the final keynote, built on the Secretary's comments by delving into the use of simulation to design novel materials, and the beneficial feedback in materials science between these simulations and experimental validation.

The first panel at the Simulation Summit included representatives from Proctor and Gamble, Ford Motor Company, Lockheed Martin, and Caterpillar who outlined the current opportunities and challenges for simulations to benefit manufacturing. Thom Lange from P&G described how they use in-house computing power to eliminate portions of the design and manufacturing cycle. P&G uses computing technology that is about a decade behind the state-of-the-art DOE computers, and depends on continued advancement of the cutting edge in order to pull its technology forward. Bertley Moberg from Ford agreed, noting that the cost of physical prototypes continues to increase while the cost of simulations goes down. All panelists noted that one of the biggest barriers to simulations was imposed by limitations in software. Most manufacturers use commercially available code as much as possible, though this constrains the possible applications of the simulations. When the company identifies a need that is not met commercially, they often partner with the DOE national labs through either cooperative research and development agreements or programs such as INCITE to develop necessary software. These projects not only benefit the private industry partner, but they also advance DOE missions.

Senior leaders from Harvard, the University of Michigan, the University of Illinois, and the University of Chicago described state-of-the-art education and training programs focused on generating a computationally-skilled workforce. Thom Dunning from UIUC pointed out that while most universities offer computer science courses, few provide opportunities for undergraduate students to perform simulations using HPC in any meaningful way. Don Lamb of the University of Chicago agreed, noting that the apprenticeship model currently dominates education in high-performance computing. Dr. Dunning described a new Virtual School of Computational Science and Engineering, a virtual organization that pools the expertise of faculty and staff from multiple universities and national labs to offer summer courses for graduate students, with access to petascale computing power.

The third discussion panel focused on the interactions and potential for cooperation among industry, academia, national laboratories, and computing manufacturers. William Madia of Stanford University focused his remarks on the importance of simulation to promote U.S. competitiveness. In particular, he emphasized that simulation efforts should focus high-impact, industry-driven problems in order to have material impacts. Dimitri Kusnezov of the National Nuclear Security Administration drew attention to the different strengths and motivations of each player in the world of simulations and high-performance computing. Effective promotion and deployment of simulation will depend on building collaborative structures that build on the strengths of each player. Peter Ungaro of Cray, a manufacturer of supercomputers, discussed the challenge of meeting the needs of both the very high end (such as DOE's drive to maintain world leadership in HPC) and industrial users. The needs of these different classes of customers will shape collaborations aimed at different classes of problems. Thom Mason, Director of Oak Ridge National Laboratory, framed his remarks by focusing on CASL, the Consortium for Advanced Simulation of Light Water Reactors, an Energy Innovation Hub funded by DOE. Dr. Mason suggested that CASL, which brings together industry, academia, electric utilities, and the national lab, will be successful because it has a set of very clear deliverables driven by the industry's needs.

At the conclusion of the Summit, it was evident that a golden moment has presented itself to continue U.S. leadership in simulations, but concerted action and continued DOE leadership are necessary to turn this opportunity into reality. In his summary remarks, Nick Donofrio, IBM Fellow Emeritus and a pioneer in the development and use of high-performance computing told attendees, "If we are going to be the leaders of economic growth and development and continue to drive our standards of living up then we are going to have to do it with our intellectual capabilities – and this is a manifestation of that. We will have to do it in a nonlinear fashion. Every time we have won it has been because we were more innovative, while others followed the semi-logarithmic plots and stayed on the curve."