United States House of Representatives
Committee on Science, Space and Technology
Subcommittee on Energy

Supercomputing and American Technology Leadership
January 28, 2015

Testimony

Roscoe C. Giles, Ph.D.
Chair, Advanced Scientific Computing Advisory Committee (ASCAC)
Office of Science, U.S. Department of Energy

Professor, Department of Electrical and Computer Engineering,
Boston University
roscoe@bu.edu

OPENING

Good morning Mr. Chairman and members of the Subcommittee.
Thank you for inviting me to testify today and thanks for your support for the outstanding scientific and technical activities we are here to discuss.

I am testifying from the perspective of the chair of ASCAC (the ASCR Advisory Committee which reports to the DOE Office of Science under FACA rules. I will refer to several published ASCAC reports as part of my testimony. I will address the value of research supported directly and indirectly by ASCR and also the technological challenges and rewards represented by U.S. leadership in this field.

Science's computing needs have grown exponentially – paralleling the exponential increases in computer power we have seen in recent decades – sometimes pushing the computer industry for new capabilities and sometimes finding novel ways to exploit existing technology. Leadership in scientific and technical computing has been critical to U.S. Leadership in science and technology.

ASCR has enabled DOE scientists to harness unprecedented computing power applied to increasing our understanding of the physical world, designing new materials and devices, and engineering new and improved methods for energy production, utilization, and distribution.

Some recent examples described below include simulations that give us new insight into the behavior of Nuclear Reactors, complex burning flames, materials for Li-Air battery systems, the surface of human skin, and the fate of a Type IIb supernova. Overall, ASCAC has been very pleased with the depth, breadth, and significance of ASCR enabled research.

ASCR achieves these outcomes by: designing and deploying an effective system of world class facilities for computing, data science, and networking in DOE labs; making available expert staff to work with scientists to push the envelope of applications; and supporting research in computer science and applied mathematics leading to key advances in software, hardware and algorithms.

In addition, ASCR has consistently provided leadership to DOE, the nation and the world by accelerating the development of new kinds of computing systems with transformational impact on DOE science and science and engineering more broadly. A productive computing enviroment requires not only the most advanced hardware and software, but also depends on underlying mathematics and algorithms, and a knowledgeable workforce and educational pipeline to create that workforce. ASCR is active in nurturing all elements of the "ecosystem" for scientific computing.

When I last appeared before this subcommittee , others and I testified about the importance of funding the development of "exascale" computing and the dangers to US leadership in computational science if we failed to move expeditiously. I am happy that in the intervening time Congress succeeded in passing such legislation.

In February 2014, ASCAC reported to DOE on the "Top 10 Exascale Research Challenges." I will summarize the conclusions of this report the in testimony below. The report identifies significant challenges which U.S. technology has the ability to address and which will contribute to our technological leadership more broadly.

DOE and ASCR in collaboration with NNSA have planned an exascale computing initiative (ECI) which was provided to ASCAC for review last November. This review is in process with the resulting report due in September 2015.

I think it is critical for the U.S. to maintain and extend its leadership in scientific computing as evidenced in by DOE and ASCR's activities being discussed today.

Background

My name is Roscoe C. Giles and I am a Professor in the Department of Electrical and Computer Engineering at Boston University. I have been involved for many years in leadership roles in computational science and high performance computing and in computational science education.

In particular, I have been a long time member and am currently chair of the DOE Office of Science Advanced Scientific Computing Advisory Committee (ASCAC). I have also been a participant on the recent Secretary of Energy Advisory Board's (SEAB) Task Force on Next Generation High Performance Computing (NG-HPC).

About ASCAC

ASCAC was first constituted in 1999 and is chartered under the Federal Advisory Committee Act (FACA). ASCAC members are appointed by the Undersecretary for Science and are experts in their fields. We report to the Director of the Office of Science in response to formal charges. We are not paid for our work on ASCAC. We hope to provide a useful external, community perspective on the impact, significance, and directions of ASCR efforts. Our committee meetings and reports are public.

Charges to ASCAC range from reviews of program management and effectiveness - for example we supervise regular Committees of Visitors for ASCR research program areas – to major reviews of strategic areas of emphasis and plans, such as the reports on the Exascale Computing and on Data Intensive Science. Charges are generally handled by subcommittees consisting of a few ASCAC members together with selected external participants chosen for their expertise in the specific area of the report.

Additional Materials

The bulk of the written materials I wish to draw to the attention of the Subcommittee are in the form of published ASCAC reports including the latest reports on the Top 10 Challenges for Exascale Research and the Workforce needs and also the Draft Report of the SEAB Next Generation High Performance Computing task force. These are listed on the accompanying citation page. There is also additional information of interest on the DOE ASCR website.

ASCR Overview

ASCR's mission is "*…to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy (DOE).*"

In pursuit of this mission, ASCR has programs and investments that include:

Research:
- Applied Mathematics Research whose fruits are essential for current applications and which provide the algorithmic framework for future applications and systems.
- Computer Science system and software research whose results both enable applications of current systems and chart the direction for future systems.

Facilities:
- Computer, Networking and Data Management facilities to meet the needs of DOE Science programs and their thousands of users.
- Leadership Computing Facilities with unique high-end capabilities made available both to DOE and to the entire nation, including industry (using DOE's long-established user-facility mission).
- Networking and data management facilities increasingly critical to scientific computing and to all large multi-user scientific instruments.

Human Infrastructure & Computational Ecosystem:
- Programs that enable applications scientists from DOE, Industry, and Academia to use effectively use advanced computing for discovery and problem solving.
- Developing the scientific computing and data science workforce

Advancing the Frontiers of Computing:
- Accelerating the development of new computing paradigms, capabilities, and facilities.
- Accelerating the adoption of advanced computing at DOE and in the nation.

In my last appearance before the subcommittee in May of 2013, my testimony focused mainly on ASCR facilities and the need for future exascale class systems. Today, I would like to touch more lightly on the facilities characterization and discuss in more depth some of the impacts of ASCR enabled science and the human infrastructure programs that have made them possible. I will also discuss ASCR's leadership in advancing the future of scientific computing.

Facilities Overview

The **Energy Sciences Network**, or ESnet, is the Department of Energy's high-speed network that provides the high-bandwidth, reliable connections that link scientists at national laboratories, universities and other research institutions, enabling them to collaborate on some of the world's most important scientific challenges. Managed and operated by the ESnet staff at Lawrence Berkeley National, ESnet provides direct connections to more than 40 DOE sites at speeds up to 100 gigabits per second, allowing scientists to manage, share and analyze massive datasets that are the hallmark of 21st century science. Most recently ESnet completed an expansion to Europe that will provide an overall capacity of 340 giagbits per second to support Office of Science experiments and partnerships there. ESnet derives its effectiveness from the extensive cooperation it enjoys with its user community. It is one of the most widely based and successful cooperative efforts within the Department of Energy.

The **National Energy Research Scientific Computing Center** (NERSC) at Lawrence Berkeley Lab is the primary scientific computing facility for the Department of Energy's Office of Science. As one of the largest facilities in the world devoted to providing computational resources and expertise for basic scientific research, NERSC is a world leader in accelerating scientific discovery through computation. More than 5,000 DOE scientists use NERSC systems annually to perform basic scientific research on more than 600 projects spanning a wide range of disciplines. NERSC users consistently publish more than 1,500 peer-reviewed publications each year.

The **Oak Ridge National Laboratory Leadership Computing Facility** (OLCF) was established in 2004 and was charged with developing an unclassified computing resource 100 times more powerful than the systems of the day. Today the OLCF is home to Titan, the United States' fastest and most powerful supercomputer dedicated to open scientific research. Titan ranked as 2nd most powerful computer in the world according to the November 2014 "Top500" list. In 2014, nearly two billion processor processor hours on Titan were awarded to projects from universities, private industry, and government research laboratories, representing a wide array of scientific and engineering research, from climate science to critical materials discovery and to nuclear physics. The OLCF operates a Liaisons program to assist INCITE science teams is porting and optimizing software on the OLCF machines.

The **Argonne Leadership Computing Facility** (ALCF) houses world-class supercomputing resources for open science. It supports a wide range of science and engineering research and serves users from academia, industry, and the national laboratories. ALCF's Mira supercomputer ranked as the 5th most powerful in the world. The ALCF provided over 3 billion processor hours on Mira to researchers in 2014 as well as comprehensive services from training to performance engineering to data analysis, and operates a unique catalyst program to assist the individual science teams to achieve optimal performance and results on ALCF systems from day one.

ASCR Impacts

ASCR's success is ultimately reflected in the scientific productivity, deepening insights, results, and technologies of DOE Science.

There exists a growing stream of scientific successes resulting from the computing capabilities enabled by ASCR. The foundation for this is that ASCR has created an ecosystem that enables and encourages application scientists, computer scientists, and mathematicians to work together on world-class DOE lab computing facilities, in order to solve problems that were considered intractable in the past.

Programs leading to significant science impacts

ASCR's "Scientific Discovery through Advanced Computing" Program (SciDAC) has had three incarnations over the years. In each case the focus has been precisely on enabling applications scientists to use the most advanced ASCR facilities to solve their problems. Successive incarnations of SciDAC have refined how directly DOE Science program offices were involved in the program administration and how the requisite interactions between applications, computer scientists, and mathematicians were managed.

A recent ASCAC Committee of Visitors (2) reaffirmed that "SciDAC remains the gold standard nationally and internationally for fostering interaction between disciplinary scientists and HPC." The current focus of SciDAC is insuring that DOE application scientists are able to effectively execute DOE mission science on the current mid-Petascale generation of supercomputers and the program officers from ASCR and other Science offices work together to fund and manage the program. This is an exemplar of cooperation and collaboration between program offices.

INCITE ("Innovative & Novel Computational Impact on Theory and Experiment") has made resources at leadership computing facilities available competitively to DOE and external scientists and engineers, including industry(9). The fundamental criteria for INCITE awards is the potential to perform transformational computing on the leadership computing facilities at OLCF and ALCF. INCITE awards are open to DOE scientists and also scientist from around the nation and the world.

The leadership computing facilities offer considerable staff support for the implementation and development of projects through the previously mentioned Catalyst and Liaisons programs at ALCF and OLCF. . In this sense, INCITE projects are all partnerships between ASCR and the application research groups.

The ASCR Leadership Computing Challenge (ALCC) programs at the LCF's offer similar access to leading edge facilities and support in a more flexible way which allows additional opportunities for access by DOE applications and discretionary opportunities for access to LCF's by applications, particularly from industry, which are being developed outside the usual DOE and academic scientific circles.

Finally, ASCR SBIR-STTR (Small Business Innovation and Technology Transfer) activities target high-end computing and data science as an enabler of new commercial enterprises.

Some Recent Examples of ASCR Impact

- **2014:** Impossible to compute wheat sequencing now possible in seconds: ASCR research in programming environments, specifically X-Stack DEGAS technologies, has enabled human genome sequencing within 20 seconds, reducing sequencing time by 2X from previous approaches. Wheat genome sequencing, which has been impossible to do, is now possible under 32 seconds using DEGAS.

- **2014: Confirmed: Stellar Behemoth Self-Destructs in a Type IIb Supernova:** For the first time ever, astronomers have direct confirmation that a Wolf-Rayet star died in a violent explosion known as a Type IIb supernova. Using the intermediate Palomar Transient Factory pipeline, supported by resources at NERSC and ESnet, researchers caught supernova SN 2013cu within hours of its explosion. These stars are interesting because they enrich galaxies with the heavy chemical elements that eventually become the building blocks for planets and life.

- **2014: Simulations Shed Light on Pine Island Glacier's Stability.** The rapid retreat of Antarctica's Pine Island Glacier has perhaps reached a point of no return, say three international modeling teams who ran a number of simulations to model the glacier's behavior. To do this work, they relied on three different ice-flow models including BISICLES, a collaborative software package developed in part by ASCR researchers.

Industry, Academia, and the National Labs use ASCR HPC resources to advance basic science and applied research topics in a broad-spectrum of technology areas including: nuclear energy; biofuel production; materials science; enzyme design; photovoltaics; engine combustion; electronics and superconductivity; turbomachinery for wind, carbon –sequestration and gas-turbines; turbulence modeling for noise reduction in wind-turbines and jet engines.

- **Procter & Gamble and Temple University scientists model skin's makeup.** Researchers at Procter & Gamble and Temple University used DOE's Titan to better understand the three-dimensional structure of skin's outermost barrier, the stratum corneum. Access through the INCITE program enabled some major achievements. One is the simulation of 1 million atoms of skin lipid matrix—four separate bilayers, each hundreds of square nanometers and made of ceramides (waxy compounds), fatty acids, and cholesterol in water.

This skin simulation, extending over 2 microseconds, was far too large and complex to have been carried out without OLCF resources. A related achievement is the validation of a state-of-the-art empirical model, the Kasting model, for the permeation of compounds through the stratum corneum. The project's third major accomplishment is the modeling of contact between skin and large concentrations of selected chemical compounds to uncover the mechanism by which compounds disrupt the stratum corneum barrier and are transported through it.

- **Related Publication**: M. Paloncyova, R.H. DeVane , B.P. Murch, K. Berka, M. Otyepka, "Rationalization of Reduced Penetration of Drugs through Ceramide Gel Phase Membrane," *Langmuir*, **30** (46) 13942-13948 (2014); DOI: 10.1021/la503289v. Published: NOV 25 2014
- https://www.olcf.ornl.gov/2014/11/14/procter-gamble-and-temple-university-scientists-model-skins-makeup/

- **"The Complexities of Combustion" (Jackie Chen, SNL).** Researchers from Sandia National Laboratories, including PI Jackie Chen and team member Ankit Bhagatwala, employed the direct numerical simulation code (DNS) known as S3D on Titan to simulate a jet flame burning dimethyl ether, an oxygenated biofuel, in an attempt to match the conditions of a companion experiment at The Ohio State University (OSU).

  The jet flame configuration is used to probe fundamental turbulent flame physics associated with local extinction, where parts of the flame extinguish, and are subsequently re-ignited through turbulent mixing, a finite-rate chemical process that may occur in practical combustors including that may occur in practical combustors including diesel jet flames. If researchers can identify strategies to minimize flame extinction, this will greatly enhance efficiency and minimize undesired emissions in combustion devices such as engines. While Chen's team has simulated jet flames in the past, the latest simulations on Titan were a breakthrough for two reasons: the inclusion, for the first time, of dimethyl ether (DME), a more complex and oxygenated fuel, and the highest Reynolds number ever achieved by the team, 13,050, which is a measure of the turbulent mixing intensity.

  The increased Reynolds number allows the team to resolve a wider range in turbulence scales with detailed chemistry, a major breakthrough when trying to match experimental conditions and also for evaluating turbulent mixing and combustion models. "These simulations represent the first time we've incorporated DME and the highest Reynolds number ever achieved in a fully resolved reacting direct numerical simulation," said Ramanan Sankaran, an OLCF scientific liaison who assists Chen's team with their simulations on Titan.

- **Related Publication:** A. Bhagatwala, Z. Luo, H. Shen, J. Sutton, T. Lu and J. H. Chen, "Numerical and experimental investigation of turbulent DME jet flames," *Proc. Combust. Inst.* **35**, 1157-1166 (2015).
- https://www.olcf.ornl.gov/2014/11/11/the-complexities-of-combustion/

- **Westinghouse-CASL team wins major computing award for reactor core simulations on Titan.** The Consortium for Advanced Simulation of Light Water Reactors (CASL) team, led by Fausto Franceschini of Westinghouse and Andrew Godfrey of ORNL, performed core physics simulations of the Westinghouse AP1000 pressurized water reactor (PWR) core using CASL's Virtual Environment for Reactor Application (VERA).Westinghouse is deploying the AP1000 worldwide with eight plants currently under construction in China and the United States.

- The simulations, performed on Titan's Cray XK7 system, produced 3D, high-fidelity power distributions representing conditions expected to occur during the AP1000 core startup and used up to 240,000 computational units in parallel. One of the neutron transport components of VERA, the Exnihilo code suite developed at ORNL, was used for the simulations. The code includes deterministic transport solvers such as Denovo, which can take advantage of Titan's NVIDIA graphics processing unit accelerators, as well as a new stochastic transport module known as Shift.

  The results included as many as one trillion particle histories per simulation to reduce statistical errors and provide insights that improve understanding of core conditions, helping to ensure safe startup of the AP1000 PWR core.
  - https://www.olcf.ornl.gov/2014/07/02/westinghouse-casl-team-wins-major-computing-award-for-reactor-core-simulations-on-titan/
  - Thomas M. Evans, Wayne Joubert, Steven P. Hamilton, Seth R. Johnson, John A. Turner, Gregory G. Davidson, and Tara M. Pandya**, "**Three-Dimensional Discrete Ordinates Reactor Assembly Calculations on GPUs", ANS MC2015 - Joint International Conference on Mathematics and Computation (M**&**C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method, Nashville, TN, April 19–23, 2015, American Nuclear Society, LaGrange Park, IL (2015).
  - F. Franceschini, B. Oelrich Jr., J. Gehin,, "Simulation of the AP100 First Core with VERA", Nuc. Eng. Inter. 59, (718), 33-35 (2014):

- **Converting Greenhouse Gas CO_2 Into Fuel and Useful Chemicals** *(Victor Batista, Yale University)***.** Scientists using supercomputers at the National Energy Research Scientific Computing Center (NERSC) have discovered a mechanism that drives the conversion of the greenhouse gas carbon dioxide (CO_2) into usable fuels and chemicals. This mechanism holds the promise of being able to provide carbon-neutral fuels and furthering the goal of U.S. energy independence. The simulations run at NERSC reveal that, unexpectedly, the CO_2 conversion process is initiated by a reaction with hydrogen atoms bound to a platinum metal surface. Other mechanisms had been proposed before these simulations settled the issue. The findings will be useful in the design and development of new technologies that can generate fuels that are consumed without producing CO_2.
    - http://www.nersc.gov/news-publications/news/science-news/2013/turning-greenhouse-gases-into-gold/
    - http://pubs.acs.org/doi/abs/10.1021/jz400183z

- **More Efficient Thin Film Solar Cells** *(Yanfan Yan, U. Toledo).* Researchers have made a discovery that could lead to less expensive, more easily fabricated thin-film solar cells using supercomputer simulations performed at the National Energy Research Scientific Computing Center (NERSC). Scientists had known that treating cadmium-telluride (CdTe) solar cells with cadmium-chloride improves efficiency, but the detailed mechanism had been unknown until a team of researchers combined simulation and experimental analysis to show that the enhanced efficiency occurs when chlorine atoms substitute for many of the tellurium atoms near grain boundaries. Thin-film CdTe solar cells are considered a rival to currently used silicon-based photovoltaic systems because of their theoretically low cost per power output and ease of fabrication, but their efficiency has lagged that of traditional materials. This new understanding could be used to guide the engineering of high-efficiency CdTe materials.
    - http://www.nersc.gov/news-publications/news/science-news/2014/atomic-switcheroo-explains-origins-of-thin-film-solar-cell-mystery/
    - http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.112.156103

- **A Previously Undiscovered Molecular Turn Leads Down the Path to Type 2 Diabetes***.* Computing resources at the ALCF have helped researchers determine how proteins misfold to create the tissue-damaging structures that lead to type 2 diabetes. The researchers combined experiments and computation to understand the chemical pathway. The simulations located an entire step that had been missing, an intermediate step in which transient rigid fibrils form, then morph into floppy protein loops, which finally take the form of more tough fibrils and stack up to form the damaging amyloid fibril .

With the new understanding and access to Mira, future work could target a possible treatment, such as designing an inhibitor to interfere with the harmful pathway. In addition, the research collaboration can apply the method to determine the intermediate steps in similar diseases such as Alzheimer's that are linked to the formation of amyloid fibrils.

- **2014: Decreasing time to solution for supersonic turbomachinery** *(R. Srinivansan, Ramgen Power Systems LLC)* Cost-effective methods to capture and store power-plant carbon emissions are a principle barrier to widespread application of CCS. Simulations at OLCF transformed Ramgen's process for designing cost effective carbon capture and sequestration turbomachinery, cutting the projected time from concept to commercial testing by at least two years and the cost by over $4 million. Based off previous HPC simulations at OLCF, Ramgen has been able to complete initial testing of a 13,000-horsepower CO2 compressor, with an additional stage of ongoing technology development utilizing HPC resources. This compressor is projected to reduce the capital costs of CO2 compression by 50 percent and produce a minimum of 25 percent savings in operating costs. Applying these cost savings to a new 400-megawatt clean coal plant would result in significant annual operating cost savings.
    - https://www.olcf.ornl.gov/2012/08/14/ramgen-simulates-shock-waves-makes-shock-waves-across-energy-spectrum/
    - https://www.olcf.ornl.gov/2014/06/13/ramgen-takes-turbomachine-designs-for-a-supersonic-spin-on-titan/

- **2014 Materials Science for Wind Energy –1 Million Molecule Freezing Water Droplet Simulation for Non-Icing Surfaces** *(M. Yamada (GE) at OLCF)*. One of the factors restricting the growth of wind energy is that many of the world's windiest places are cold as well. Just as ice growth on aircraft wings limits aircraft operation, ice growth on wind turbine blades will reduce their efficiency, or require that the turbine be shut down. Re-engineering the surface of the turbine blades may solve this problem, but requires fundamental understanding of how ice forms on the blades. While previous computer simulations of freezing had used around 1,000 molecules, GE understood that much larger simulations were needed to study icing on wind turbines. Using Titan, GE simulated hundreds of water droplets, each including one million molecules for 6 different surfaces under a range of temperatures. These represent the most comprehensive simulation of water freezing on a surface ever performed The results will guide future testing in developing new anti-icing materials.
    - https://www.olcf.ornl.gov/2013/10/25/titan-propels-ge-wind-turbine-research-into-new-territory/

- **Predictive Materials Modeling for Li-Air Battery Systems.** Lithium-air (Li-air) batteries are viewed as a possible game changer for electric vehicles, but realizing their enormous potential is a very challenging scientific problem that requires the development of new materials for electrodes and electrolytes. With this INCITE project, scientists from Argonne and IBM Research are teaming up to use Mira to better understand the physical and chemical mechanisms needed to make Li-air batteries a reality.

  With the potential to store up to 10 times the energy of a Li-ion battery of the same weight, Li-air batteries are particularly appealing to researchers because of their theoretical energy density. But developing a viable Li-air battery is a long-range effort that requires scientific breakthroughs in materials design, chemistry, and engineering.

  One of the most significant hurdles is finding suitable materials for Li-ion-conducting electrolytes, which enable the transport of ions between the anode and the cathode and promote the diffusion of oxygen from the environment into the electrochemical cell.

  In a recent study, IBM researchers focused on the zirconium-containing, garnet-like lithium-lanthanum-oxide, known as LLZO (Li7La3Zr2O12), a promising material for solid-state electrolytes. To observe Li-ion migration, the team needed to simulate time scales in nanoseconds rather than picoseconds. They were able to achieve this factor-of-a-thousand improvement by implementing a highly efficient parallel version of metadynamics (a tool for accelerating rare events, such as mapping the conductivity of a material regardless of its complexity) into their simulations and by taking advantage of Mira's substantial power with full machine runs. This enabled the researchers to obtain, for the first time, the free-energy profile for Li-ion conductivity in LLZO. One of their key findings was that the presence of vacancies in cubic LLZO is crucial to lowering its activation energy and enhancing its Li-ion conductivity.

  IMPACT
  This project is providing insight into the complexities of the Li-air battery at the molecular level, including an understanding of the microscopic mechanism for high Li-ion conductivity. The results will help to inform the design of new materials for Li-air electrolytes and electrodes. If realized, Li-air batteries could enable widespread deployment of electric vehicles, greatly reducing U.S. dependence on foreign oil.

- **Improving Aircraft Engine Combustor Simulations.** A jet engine combustor combines air flowing faster than a hurricane with swirling fuel to generate the extraordinary release of heat that ultimately powers the aircraft. Understanding these complex physical and chemical interactions is critical to fuel efficiency and emissions performance, but physical testing can be difficult and time consuming.

Computer simulation of the complex physics of a combustor creates a "virtual test," thus reducing the need for physical testing. Pratt & Whitney explored leading-edge combustor design methods using the Argonne Leadership Computing Facility as part of DOE's INCITE program.
IMPACT

This INCITE project led to improved capabilities and reduced solution times for 3-D combustor simulations. The work has been a key enabler for the depth of understanding needed to meet emissions goals. INCITE simulation technologies were applied to Pratt & Whitney's next-generation, low-emission Geared Turbofan™ engine. This groundbreaking engine delivers unprecedented reductions in emissions, noise, and cost of ownership compared to engines of the previous state of the art.

- **Simulations of Electrochemical Oxide Interfaces at Mesoscale:** Electrochemical interfaces are responsible for the success of electrochemical energy conversion/storage systems, such as fuel cells and batteries, as well as the failure of materials caused by corrosion. This project aims to elucidate nanoscale and mesoscale mechanisms associated with electrochemical processes occurring at reactive material interfaces. Breakthroughs in the fundamental understanding of these interfaces are necessary in the design and development of novel oxide materials for energy applications.

  Dynamical electrochemical processes combine the remarkable complexity of many interfacial reactions, transport phenomena, and microstructural evolution with the formidable subtleties of material defect chemistry at the interface. Focusing on material synthesis and electrochemical interfaces, project researchers set out to understand these behaviors at the atomistic and molecular levels during an electric field-assisted oxide-sintering process.

  Sintering—the process of welding together two metal powders at a diminished liquid phase—is well established, though the processes governing electric field sintering phenomena at the nanoscale were largely unexplored. Using representative oxide models of zirconia and ceria variants, researchers have shown that electric field-assisted sintering can be used to design oxide materials with modifications that would affect their functional properties.

  Using an INCITE award, Argonne researchers conducted calculations of the atomistic scale and interfacial properties of nanoscale oxides and oxide heterostructures. Results have helped explain experimentally observed improvements in oxide quality resulting from the electric field-assisted sintering process.

- **Intensity-Dependent Dynamics in Fermilab and CERN Accelerators** *(James Amundson, Fermilab):*
  Particle accelerators are an enabling technology for both basic research (e.g., studying the fundamental constituents of matter and the structure of nuclei) and the applied sciences (e.g., probing the structure of materials). Accelerator technologies also have broad economic and societal impact. DOE-originated accelerator technologies are behind the tens of thousands of accelerators that are at work every day producing particle beams in hospitals and clinics, in manufacturing plants and industrial laboratories, in ports and printing plants and, literally, on the ships at sea. Adding them all up, some 30,000 particle accelerators operate in the world today in medicine, industry, security and defense and basic science. The market for medical and industrial accelerators exceeded $3.5 billion dollars a year in 2009, and it is growing at more than ten percent annually. All digital electronics now depend on particle beams for ion implantation, creating a $1.5 billion annual market for ion-beam accelerators. All the commercial products that are processed, treated or inspected by particle beams have a collective annual value of more than $500 billion.

  Fermilab researchers are using ALCF resources to perform complex accelerator simulations aimed at reducing the risks and costs involved in developing the world's highest-intensity particle beams.

  The future of high-energy physics requires running today's accelerators at intensities that are higher than ever. Both Fermilab and CERN strive to accurately understand intensity-dependent effects in their accelerator complexes. Such understanding requires detailed numerical modeling that goes beyond the capabilities of desktop machines and simple clusters. This project is working to simulate these accelerators with unprecedented fidelity.

  The Fermilab Recycler and Main Injector form the final high-energy stage of the Fermilab accelerator complex. During each acceleration cycle, the Recycler receives protons in six batches from the Booster. The simulations carried out by this INCITE project have captured theoretically predicted instabilities in the high-intensity neutrino beams that will be produced, including demonstrating the existence of an instability in the Fermilab Booster, a kind of instability generated by bunch-to-bunch effects that could potentially shut down the whole beam. These kinds of insights will help in the planning of a high-intensity beam project called the Fermilab Proton Improvement Plan II, which will create neutrino beams for the Long Baseline Neutrino Facility, and help considerably in the next phase of research at CERN's LHC.

  IMPACT
  While it is generally understood that particle accelerators are used to discover the fundamental matter of the universe, high-intensity beams in accelerators around the world allow scientists to explore the structure and

function of matter and materials more tangible to our everyday lives. The results can advance research in fields as diverse as materials science and renewable energy, as well as drive the long-term development of ideas once thought unfeasible, such as the transmutation of nuclear waste.

Presentations:

- "Accelerator Beam Dynamics on Multicore and GPU and MIC Systems," SIAM Conference on Parallel Processing for Scientific Computing, February 18–21, 2014, Portland, Oregon.
- James Amundson, "Transverse Instabilities in the Fermilab Booster," 16th Advanced Accelerator Concepts Workshop (AAC 2014), July 2014, San Jose, California.
- Eric Stern, "Developments in Synergia Space-Charge-Induced Resonance Trapping," 16th Advanced Accelerator Concepts Workshop (AAC 2014), July 2014, San Jose, California.

- **Increasing efficiency for automobiles through improved under-hood packaging**.

  Improving the air flow through the engine compartment of an automobile can reduce the drag and improve the efficiency of the vehicle in the same way improving the air flow around the automobile can. However, the engine compartment must also be arranged in a way that all engine components receive adequate cooling. The complexity of the problem is so large that Ford used the Jaguar and Titan supercomputers to perform accurate simulations of air flow through more than 50 million individual computational cells. More than 1,600 individual simulations were used to understand the effects of different packaging arrangements and different driving conditions. The results showed enough potential for improving automobile efficiency that Ford both updated its automobile design methods, and began improving its own high-performance computing capability.

  (Additional note: Ford has published papers based on the methods used in these simulations.)

- **In an EERE funded Project, GM and Ford study improved engine efficiency through High-Performance Computing**

  The auto manufacturers, the national laboratories, and the DOE's Office of Energy Efficiency and Renewable Energy have a long history of working together to develop simulations of engine operations that can be used to improve the efficiency of internal combustion engines without compromising their power or reliability. Both GM and Ford, with support from EERE and Oak Ridge National Laboratory, are currently using Titan's computational capability to test strategies for improving engine efficiency. GM is using OpenFOAM, an open-source computational fluid dynamics (CFD) code, to simulate new concepts for fuel injectors. These simulations will help GM develop “spark-ignited direct injection,” or SIDI, which will improve the combustion efficiency of engines. Ford is using the commercial CFD code Converge to study the effects of exhaust gas recirculation (EGR), a process which improves fuel efficiency. Simulating EGR requires simulating the engine over multiple combustion cycles, greatly increasing the complexity of the simulation. In both cases, GM and Ford are not only using their simulations to improve engine operations, but are using their experience to develop software that will let other users perform simulations using Titan more effectively.

Example SBIR Activities

Industries are increasingly using modeling and simulation to improve productivity. Commodity IT is becoming more parallel and Industry can benefit from tools, software, and libraries developed in the HPC community. ASCR SBIR investments target small businesses that harden HPC tools and software, including those developed by ASCR researchers, to improve industry access to advanced HPC methods.

Success Examples:

Optimization Algorithms for Power Applications (*Ziena Optimization LLC*). Ziena, a US small business, used ASCR SBIR funds to integrate HPC decision algorithms for power applications into their optimization software program. Test results showed over 50% decreased solution time. The Ziena product is being tested by the European Commission. If successful, Ziena’s product will become the leading optimization solver engine for managing power grids in Europe.

2014 Computational Fluid Dynamics Simulations and Real-Time Analysis (*David Philips, Cascade Technologies Inc*). Cascade Technologies increased usability of high-fidelity HPC CFD codes for non-HPC specialists by integrating the code into standalone web based “apps”. The resulting product enabled faster analysis, reduction in wasted compute hours, and increased data provenance for end-users. Since the recent product launch, over 30 commercial, government, and academic users have benefited from the system.

2013 Graphical HPC Application for Product Simulation (*Robert M O’Bara, Kitware Inc*). Kitware developed easy-to-use Computational Model Building framework that connects users to HPC simulation codes. Kitware’s product provides the ability to create and run proof-of concept product simulations and allows easily scaling to higher-end systems. The Army Corps of Engineers Engineering Research and Design Center are early adopters of the new product.

2013 Big Data Tools for Energy Materials (*Tal Sholklapper, Voltaiq*). Companies developing batteries and related technologies perform extensive cyclic testing, generating enormous quantities of data. Entrepreneurs at Voltaiq are used ASCR SBIR funds to develop cloud-based software to address a Big Data problem in energy materials sector. The new software product can dramatically increase the pace of battery innovation and development for thousands of organizations working in the battery sector.

ASCR Partnerships with other DOE Offices

The Office of Advanced Scientific Computing Research is currently working directly with DOE programs in Nuclear Energy and the Office of Electricity, which maintains resources that are used by EERE programs in Vehicles Technology and Wind Energy. ASCR has partnered with the Office of Electricity and Argonne National Laboratory to perform fundamental research on simulating the electrical grid that will allow development of strategies for making the grid both flexible enough to integrate renewables, and secure enough to provide energy to the nation. In Vehicles Technology, ASCR super-computers are used as part of industrial partnerships designed to increase fuel economy without compromising engine performance. ASCR computing capabilities have also been used by companies in wind energy that are bringing technology to market.

As computing power increases to the exascale, the potential gains from applying advanced simulation to applied technologies and key scientific problems also increases. Because of the challenges of preparing simulations to operate at the exascale, the DOE has already funded three exascale co-design centers: the Center for Exascale Simulation of Advanced Reactors (CESAR), the Center for Exascale Simulation of Combustion in Turbulence (ExaCT), and the Exascale Co-design Center for Materials in Extreme Environments (ExMatEx). CESAR's work will allow both simulation of new reactor designs, and create capabilities that will allow existing reactors to be operated safely and reliably. The capabilities ExaCT develops for simulation turbulent combustion using exascale simulation can be used to develop predictive models used to improve the efficiency of all combustion powered systems, including aircraft, automobiles, and coal and natural gas fired power plants. Finally, the discovery and design through simulation of materials that can operate at high temperatures and high pressures will benefit a range of technology areas, including combustion, nuclear energy, fuel cells, and concentrated solar power. These three examples are not the only potential impacts of exascale computing and ASCR is working with programs within the Office of Science and throughout DOE to identify specific challenges and opportunities for a wide array of applications.

Workforce Development

ASCAC, along with the other Office of Science Advisory Committees, was recently asked to identify disciplines in which significantly greater emphasis in workforce training at the graduate or postdoctoral levels is necessary to address workforce gaps in current and future Office of Science mission needs. Professor Barbara Chapman of the University of Houston led our workforce subcommittee whose report (3) concluded that:

> "Simulation and computing are essential to much of the research conducted at the DOE national laboratories. Experts in the ASCR-relevant Computing Sciences, which encompass a range of disciplines including Computer Science, Applied Mathematics, Statistics and domain sciences, are an essential element of the workforce in nearly all of the DOE national laboratories.
>
> Results of data analyzed are that the Computing Sciences workforce recruitment and retention activities are below the level necessary to sustain ASCR facilities and maintain DOE's high standards of excellence for innovative research and development. In particular, the findings reveal that:
>
> - All large DOE national laboratories face workforce recruitment and retention challenges in the fields within Computing Sciences that are relevant to their mission…
> - Insufficient educational opportunities are available at academic institutions in the ASCR-related Computing Sciences that are most relevant to the DOE mission.
> - There is a growing national demand for graduates in ASCR-related Computing Sciences that far exceeds the supply from academic institutions. Future projections indicate an increasing workforce gap and a continued underrepresentation of minorities and females in the workforce unless there is an intervention.
> - The exemplary DOE Computational Science Graduate Fellowship (CSGF) program, deemed highly effective in every one of multiple reviews, is uniquely structured and positioned to help provide the future workforce with the interdisciplinary knowledge, motivation, and experiences necessary for contributing to the DOE mission.
> - The DOE laboratories have individually developed measures to help recruitment and retention, yet more can be done at the national level to amplify and extend the effectiveness of their locally developed programs.
>
> The subcommittee recommendations:
>
> - Preserve and increase investment in the DOE CSGF program *(discussed in detail below)* while developing new fellowship programs modeled after the CSGF program to increase opportunities for more high-quality students, particularly students from underrepresented populations and demographics, in the computing sciences.

- Develop a recruiting and retention program that increases DOE's visibility on university and college campuses, establish uniform measures across DOE laboratories to improve the attractiveness of careers in DOE laboratories, and examine the laboratory funding model and its impact on recruiting and retention.
- Establish a DOE-supported computing leadership graduate curriculum advisory group to identify and raise visibility of graduate level curricular competencies specifically required to fulfill DOE's Computing Sciences workforce needs.
- Expand support for local laboratory programs, collect workforce data pertaining to the ASCR-related Computing Sciences, and encourage greater inter-laboratory sharing of information about locally successful programs and workforce related data.
- Working with other agencies, develop a strategic plan with programs and incentives to pro-actively recruit, mentor and increase the involvement of significantly more women, minorities, people with disabilities, and other underrepresented populations into active participation in CS&E careers."

The Computational Science Graduate Program (CSGF)

Since its inception in 1991 the DOE Computational Science Graduate Fellowship (CSGF) has played a vital role in ensuring a sufficient supply of skilled interdisciplinary scientists and engineers who can effectively address the Department's most complex challenges using the most advanced scientific modeling and simulation tools. CSGF has fulfilled not only the growing demand for these skills to address DOE mission needs, but has helped to meet the significant growth in national demand by industry, academia, and other government agencies, as these institutions increasingly seek highly trained, computationally skilled scientists and engineers. In recent years, CSGF also has begun to produce trained scientists who can deal with the challenges "big data."

The CSGF program, which is funded jointly by the DOE Office of Science's Office of Advanced Scientific Computing (ASCR) and the National Nuclear Security Administration (NNSA), is viewed as an exemplar in providing doctorate-level training of computational scientists and engineers who have the interdisciplinary knowledge and skills most relevant to the DOE mission areas. CSGF participants are selected competitively through vigorous review and the program provides for four years of support to graduate students and requires an approved interdisciplinary graduate program of study and research practicum with computational scientists at a DOE laboratory. In short, CSGF aims to create a new kind of scientist that is unobtainable presently from traditional academic programs that do not expose students to real-world computational-science applications.

As mentioned above, the Office of Science, in the past year, tasked its Advisory Committees, including ASCAC (7), to provide their respective expert assessments of the disciplines in which significantly greater emphasis in workforce training at the graduate level is necessary to address gaps in the current and future Office of Science workforce needs. All six committees, including ASCAC and representing disciplines from chemistry, materials, biological systems science, and climate science to high energy physics, nuclear physics, fusion and plasma sciences, identified computational sciences as in need of greater emphasis in workforce training.

The resounding multigenerational success of the CSGF program gives evidence to the impact the ASCR can have on the workforce. (Indeed, we have just had our first CSGF Alum join ASCAC this year).

I respectfully urge the Science Committee to put its weight behind this important workforce development endeavor.

Maintaining World Leadership in Computing

ASCR has consistently provided leadership to DOE, the nation and the world by accelerating the development of new kinds of computer systems with transformational impact on DOE science and science and engineering more broadly.

DOE has been a leader

Since the 1950s, DOE and its predecessor organizations have been at the forefront of scientific computing. Although this grew out of the national imperatives associated with nuclear weapons, it was recognized early on that high-performance computing had an essential role in the physical sciences and civilian research in applied mathematics and scientific computing was started in the organizations that have evolved into the Office of Science today. In the 1990s, as massively parallel computing established new frontiers in scientific computing, ASCR brought these tools to the U.S. scientific community, culminating in the petascale computers in use today. During this same time, ASCR supported development of cluster-based computing tools that are in widespread use today in research laboratories, universities and industries.

Emergence of Data Science

During the last decade, there has been increased recognition of the importance of data, often referred to as "big data" across both the research and commercial domains. In the commercial domain, this is apparent though the rise of Google, Facebook, and Twitter, to name just a few. In the scientific domain, DOE Office of Science has been at the forefront of applications of large data in the physical sciences, including data taken at large scientific facilities, such as the Large Hadron Collider, and observational data, such as taken by terrestrial-based telescopes. ASCR has actively supported these developments through applied mathematics and computer science research in the management and manipulation of large scientific datasets. The ESnet system, operated by ASCR, provides the backbone capability for the manipulation of these large datasets across U.S. scientific institutions.

ASCR High End Computing Development Activities

After an extraordinary series of community workshops, engaging DOE applications scientists and engineers, computer scientists, mathematicians, industry representatives and academics, ASCR developed the foundations for the "exascale" initiative: to build the technology – hardware, software, applications frameworks— that would allow for a machine to deliver a computational capability of 10^{18} operations per second and, along the way, enable remarkable advances at all intermediate scales of computing of relevance to science and industry. Key requirements of such computers is that they be energy efficient (goal is 20 megawatts), readily programmable, and reliable over the long run times of DOE's applications.

The term "extreme-scale computing" is used more broadly to refer to leadership systems across these scales, ranging from embedded processors to leadership facilities that will host exascale computers. A recent report from the National Research Council titled "The Future of Computing Performance: Game Over or Next Level?" (11) highlighted the importance of leadership in extreme-scale computing for US competitiveness.

Next Generation Computing Reviews and Reports

ASCAC: Exascale Computing

In 2009, ASCAC was charged with reviewing ASCR's body of work on exascale computing. Dr. Robert Rosner of the University of Chicago led our subcommittee on this charge. We delivered our review report – "The Opportunities and Challenges of Exascale Computing" (8) in Fall 2010. We found the case for exascale compelling and recommended that ***"DoE should proceed expeditiously with an exascale initiative so that it continues to lead in using extreme scale computing to meet important national needs."***

ASCAC: Data Intensive Science

In 2012 ASCAC was asked to consider the synergies between "big data" and the development of exascale computing. Professor Vivek Sarkar of Rice University chaired a subcommittee to address this issue. In 2013, ASCAC delivered the report "Synergistic Challenges in Data-Intensive Science and Exascale Computing." (5)

Its findings included:

1. There are opportunities for investments that can benefit both data-intensive science and exascale computing.
2. Integration of data analytics with exascale simulations represents a new kind of workflow that will impact both data-intensive science and exascale computing.

3. There is an urgent need to simplify the workflow for data-intensive science.
4. There is a need to increase the pool of computer and computational scientists trained in both exascale and data-intensive computing.

Recommendations included:

1. The DOE Office of Science should give high priority to investments that can benefit both data-intensive science and exascale computing so as to leverage their synergies.
2. DOE ASCR should give high priority to research and other investments that simplify the science workflow and improve the productivity of scientists involved in exascale and data-intensive computing.
3. DOE ASCR should adjust investments in programs such as fellowships, career awards, and funding grants, to increase the pool of computer and computational scientists trained in both exascale and data-intensive computing.

ASCAC: Top 10 Exascale Research Challenges

In July 2013, ASCAC was charged to identify "a list of no more than 10 technical approaches (hardware and software) that will enable the development of a system that achieves the Department's exascale goals, particularly the usability goals for the Department's mission critical applications."

Professor Robert Lucas of the University of Southern California Information Sciences Institute chaired a subcommittee of experts to respond to this charge. The report entitled "Top 10 Exascale Research Challenges" (4) was completed on February 10, 2014.

The Top Ten Exascale System Research Challenges
(not in a particular order):

1. Energy efficiency: Creating more energy-efficient circuit, power, and cooling technologies.
2. Interconnect technology: Increasing the performance and energy efficiency of data movement.
3. Memory Technology: Integrating advanced memory technologies to improve both capacity and bandwidth.
4. Scalable System Software: Developing scalable system software that is power-aware and resilience-aware.
5. Programming systems: Inventing new programming environments that express massive parallelism, data locality, and resilience
6. Data management: Creating data management software that can handle the volume, velocity and diversity of data that is anticipated.
7. Exascale Algorithms: Reformulating science problems and redesigning, or reinventing, their solution algorithms for exascale systems.
8. Algorithms for discovery, design, and decision: Facilitating mathematical optimization and uncertainty quantification for exascale discovery, design, and decision making.
9. Resilience and correctness: Ensuring correct scientific computation in face of faults, reproducibility, and algorithm verification challenges.
10. Scientific productivity: Increasing the productivity of computational scientists with new software engineering tools and environments.

In addition to the list the subcommittee strongly felt that it should give voice to the community's assessment of the importance of next generation computing to DOE and the nation. ASCAC concurred and provided the additional findings and recommendations below:

Findings:

1. <u>Exascale computing is critical for executing the DOE mission.</u>
   ASCAC reafffirms its findings from previous reports that leadership in high performance computing (HPC) is critical to achieving the DOE mission of ensuring U.S. leadership in science, engineering, and national security. In the

last six years, this has been documented in many exascale reports from Office of Science programs, the National Nuclear Security Administration, and other U.S. government agencies.

2. U.S. national leadership is at risk.
   Without aggressive investment and technical innovation in HPC, the U.S. risks falling behind rapidly emerging international competitors, not all of whom are friendly to U.S. interests. This in turn threatens to undermine the nation's intellectual leadership in a broad range of science, its economic position, and its security.

3. The U.S. has the technical foundation to create exascale systems.
   The U.S. semiconductor and HPC systems industries are capable of developing the necessary technologies for an exascale computing capability by the early part of the next decade, based largely on evolving commercially driven component fabrication, systems integration, and software engineering capabilities. However, for a truly effective and productive exascale computing capability, the U.S. government will need to focus investments on the research, development, and integration of HPC technologies that will otherwise not be created solely by commercial drivers.

4. An evolutionary approach to achieving exascale will not be adequate.
   The dramatic improvements essential to achieving effective exascale computing will not be satisfied by incremental extensions to today's conventional practices. Commercial market drivers do not provide a viable general path to delivering necessary scalability, time and energy efficiency, and user productivity including performance portability to future generation exascale class computers.

5. The U.S. government's continuous leadership and investment are required to create exascale systems.
   The U.S. computing industry is unlikely to develop effective exascale computer systems without U.S. government investment and focused mission goals. Innovation, sometimes of an incremental nature, and in other areas revolutionary, will be required under DOE direction to enable U.S. leadership in advanced HPC.

Recommendations:

1. DOE should invest in a program of continuous advancement in HPC.
   Exascale is only the next milepost in a half-century of continuous progress towards increasing capability in computational science. The U.S. government requires a stable, long-term investment strategy to ensure continuous U.S. leadership in HPC beyond today's petascale performance regime, extending to exascale and beyond. In the immediate future, much of that research investment should be focused on the top ten challenges identified within this report.

2. DOE should invest in the U.S. industrial base to catalyze the foundation for exascale systems.
   DOE should invest in extending commercial semiconductor, communications, systems integration, and software technologies to prepare the U.S. industrial base for its role and contributions in future HPC scientific, engineering and national security missions. All of these exascale components must be developed by and be available from U.S. sources, otherwise the supply chain is vulnerable to interdiction by foreign powers, which in turn could threaten the nation's security.
3. DOE should invest in exascale mathematics and system software responsive to DOE missions and other U.S. government requirements.
   The mathematical algorithms needed for many DOE missions are unique, and must be reinvented to function at exascale. As with today's Leadership-class systems, much of the software infrastructure of an exascale system will be unique to its scale and the missions for which DOE will deploy it. Therefore, DOE must invest in robust and scalable mathematical algorithms, operating systems, runtime systems, and tools for the management of the data that will be generated and/or processed.

SEAB: Next Generation Computing Task Force

The DOE Secretary of Energy Advisory Board (SEAB) was charged in December 2013 by Energy Secretary Moniz to "review the mission and national capabilities related to next generation high performance computing," including exascale computing. Specifically, SEAB was requested to examine and report on the justification for an exascale computing initiative, related basic research necessary to enable next generation high performance computing, the current state of technology and plans for an exascale program in DOE, the role of DOE in leading the development of exascale computing, and the implications of data centric computing for exascale computing. I was a participant in this task force.

SEAB provided its draft report (10) on August 10, 2013 (http://energy.gov/seab/downloads/report-task-force-next-generation-high-performance-computing) and its final report is expected to be released at the March 2015 SEAB meeting.

SEAB concluded in its preliminary report that investable needs exist for an exascale class machine; significant, but projectable technology development can enable one last "current" generation machine; "classical" high end simulation machines are already significantly impacted by many of the data volume and architecture issues; data-centric at the exascale is already important for DOE missions; common challenges and under-girding technologies span computational needs; the DOE National Labs are an important and unique resource for the development of next generation high performance computing and beyond; a broad and healthy ecosystem is critical to the development of exascale and beyond systems; and it is timely to invest in science, technology and human investments for “Beyond Next”.

SEAB’s recommendations in its preliminary report to Secretary Moniz include the following:

1. DOE, through a program jointly established and managed by the NNSA and the Office of Science, should lead the program and investment to deliver the next class of leading edge machines by the middle of the next decade. These machines should be developed through a co-design process that balances classical computational speed and data-centric memory and communications architectures to deliver performance at the 1-10 exaflop level, with addressable memory in the exabyte range.
2. This program should be executed using the partnering mechanism with industry and academia that have proven effective for the last several generations of leadership computing programs. The approximate incremental investment required is $3B over 10 years.
3. DOE should lead, within the framework of the National Strategic Computing Initiative (NSCI), a co-design process that jointly matures the technology base for complex modeling and simulation and data centric computing. This should be part of a jointly tasked effort among the agencies with the biggest stake in a balanced ecosystem.
4. DOE should lead a cross-agency U. S. Government (USG) investment in “over-the-horizon” future high performance computing technology.
5. DOE should lead the USG efforts to invest in maintaining the health of the underlying balanced ecosystem in mathematics, computer science, new algorithm development, physics, chemistry, etc.

ASCR path toward exascale

And, indeed, ASCR has been working in partnership with industry, lab personnel, and the community to move us along the path to exascale. Some program elements have included:

- Establishment of Co-Design centers to exploit a key element of effective extreme computing applications – the guided interplay of application/hardware/software in the design of systems.
- Computer Science Research: X-Stack software to develop tools for extreme scale systems, Advanced Architectures
- Applied Mathematics Research: Uncertainty Quantification, Extreme Scale Algorithms
- Prototypes: (joint with NNSA) FastForward, Design Forward
- Community: Exascale Research Conferences

The Exascale Computing Initiatiative (ECI)

DOE's plan for its Exascale Computing Initiative (ECI) was provided to ASCAC for review(1) on November 21, 2014 (http://science.energy.gov/~/media/ascr/ascac/pdf/meetings/20141121/Exascale_Preliminary_Plan_V11_sb03c.pdf). ASCAC's review is scheduled to be complete by September 2015.

A key strategy in the ECI is to work jointly with U.S. computer companies on the path to exascale computing. This effort is embodied in the FastForward program, which presently seeks to develop critical technologies needed to deliver next-generation affordable and energy-efficient technologies for extreme scale computing for the next decade. FastForward is joint between DOE Office of Science and National Nuclear Security Administration (NNSA) and involves participation by computing industry leaders, including AMD, Cray, IBM, Intel and NVIDIA. FastForward will be followed by successive R&D efforts that integrate these technologies into first single node prototypes and eventually into full exascale systems. Deployment is planned for the 2023 time frame.

Concurrently, DOE and NNSA are, through the ECI, developing the systems and applications software required to effectively use the planned exascale systems. Additionally, research is underway to develop new approaches for realizing the full potential of the expected increase in parallelism in exascale computers.

The next steps in facilities

In the interim until an ECI facility is available to do science, ASCR continues to deploy more powerful super computer facilities, reflecting the state of the art on the path to exascale.

The Collaboration of Oak Ridge, Argonne, and Lawrence Livermore (CORAL) was established by DOE to leverage supercomputing investments, streamline procurement processes and reduce costs to develop supercomputers that will be five to seven times more powerful when fully deployed than today's fastest systems in the US. DOE announced in November 2014 (http://energy.gov/articles/department-energy-awards-425-million-next-generation-supercomputing-technologies) its plans million to build two state-of-the-art supercomputers at the Department of Energy's Oak Ridge and Lawrence Livermore National Laboratories, respectively. Both CORAL awards leverage IBM's Power Architecture, NVIDIA's Volta GPU and Mellanox's Interconnect technologies to advance DOE's priority research initiatives for national nuclear deterrence, technology advancement, and scientific discovery. Oak Ridge National Laboratory's (ORNL's) new system, Summit, is expected to provide at least five times the performance of ORNL's current leadership system, Titan. Lawrence Livermore National Laboratory's (LLNL's) new supercomputer, Sierra, is expected to be at least seven times more powerful than LLNL's current machine, Sequoia. Argonne National Laboratory will announce its CORAL award at a later time.

Conclusions

- DOE through ASCR has enabled truly great computational science serving national needs modeling for the nation transformational impacts of modeling, simulation, and data science on our knowledge and well-being.
- ASCR has pioneered the development of next generation computing for the use of science. Confronting and overcoming the challenges of exascale technology will be a benefit to DOE science and the nation.
- U.S. Leadership in next generation computing should not be squandered.
- Thanks for your continuing support to grow the US capabilities and capacity and expertise in high end computing.