SOCIETY for INDUSTRIAL and APPLIED MATHEMATICS
3600 Market Street, 6th Floor
Philadelphia, PA 19104-2688 USA
Phone +1-215-382-9800
Fax +1-215-386-7999
www.siam.org • siam@siam.org

Testimony by Dr. James Crowley
Executive Director, Society for Industrial and Applied Mathematics (SIAM)

Testimony on Supercomputing and American Technology Leadership
before the
Subcommittee on Energy
Committee on Science, Space, and Technology
United States House of Representatives, Washington, DC

January 28, 2015

My name is Jim Crowley, and I am the Executive Director of the Society for Industrial and Applied Mathematics (SIAM). I have served as Executive Director of SIAM since 1995.

SIAM has over 14,000 members, including applied and computational mathematicians, computer scientists, numerical analysts, engineers, statisticians, and mathematics educators. They work in industrial and service organizations, universities, colleges, and government agencies and laboratories all over the world. In addition, SIAM has over 500 institutional members—colleges, universities, corporations, and research organizations. SIAM members come from many different disciplines, but have a common interest in applying mathematics in partnership with computational science towards solving real-world problems.

Thank you very much for the opportunity to testify today and for highlighting the critical work of the Department of Energy (DOE) Office of Science and the Office of Advanced Scientific Computing Research (ASCR). I would like to emphasize how much SIAM appreciates your Committee's continued leadership on and recognition of the critical role of the Office of Science and its support for mathematics, science, and engineering in enabling a strong U.S. economy, workforce, and society. The DOE Office of Science supports basic research to address pressing challenges in energy, computing, physical sciences, and biology. This support has been critical to the applied mathematics and computational science community. DOE was one of the first federal agencies to champion computational science as one of the three pillars of science, along with theory and experiment, and SIAM deeply appreciates and values DOE activities.

The Role of Mathematics and ASCR in Meeting Energy Challenges

ASCR supports research to develop new modeling, simulation, and data tools and to connect those tools to researchers across the Office of Science and DOE for use in solving scientific and energy challenges. Modern life as we know it – from search engines like Google to the design of modern aircraft, from financial markets to medical imaging – would not be possible without the techniques developed by mathematicians and computational scientists. Likewise, the Department of Energy depends on mathematical and computational techniques to advance science and engineer new energy solutions.

3600 Market Street, 6th Floor
Philadelphia, PA 19104-2688 USA
Phone +1-215-382-9800
Fax +1-215-386-7999
www.siam.org • siam@siam.org

The nation faces critical challenges in energy, including in energy efficiency, renewable energy, improved use of fossil fuels and nuclear energy, future energy sources, and reduced environmental impacts of energy production and use. As DOE and the research community design a long-term strategy to tackle these issues, the tools of mathematics and computational science (theory, modeling, and simulation) have emerged as a central element in designing new materials, predicting the impact of new systems and technologies, and better managing existing resources.

To tackle many of these challenges, DOE must be able to understand complex systems such as the US power grid, the behavior of nanomaterials relevant to energy, and the dispersion of nuclear radiation after a disaster. These and other complex systems have high levels of uncertainty, lack master plans, and are susceptible to breakdowns that could have catastrophic consequences. Understanding complex systems helps mitigate these risks and facilitate the development of controls and strategies to make systems more efficient.

Applied mathematics and computational science play a key role in predictive modeling and analysis to understand complex systems. Already, mathematical and computing researchers using these tools have made substantial progress improving our understanding across fields such as genomics, biofuels, materials fabrication, and nuclear security.

Activities within ASCR play a key role in supporting research that begins to fulfill these needs through programs such as the Applied Mathematics program, the Scientific Discovery through Advanced Computing (SciDAC) program, and programs to maintain the pipeline of the computational workforce. These programs have a long history of not only developing novel mathematical methods and algorithms but also taking these the next step and developing robust software that is used by DOE, the academic community, and industry.

Mathematics and the Development of Exascale

SIAM supports ASCR's new all-in approach on research to develop exascale computing, noting that investments in mathematical modeling, algorithm research, and software development are essential to realizing the full benefits of this next generation of high performance computers and to transferring their capabilities to industry for broad economic benefit.

While achieving exascale computing has the potential to allow for revolutionary advances in many fields critical to solving our energy challenges, getting to exascale and realizing its benefits requires overcoming significant computing challenges, including in applied mathematics. ASCR is currently supporting research to address these challenges, which are described below.

At the hardware level, computer chips must change in radical ways to achieve exascale speeds, such as containing 100 times more processing elements than today. This will require new breakthroughs in algorithm development to take advantage of parallelism on the chip as well as

3600 Market Street, 6th Floor
Philadelphia, PA 19104-2688 USA
Phone +1-215-382-9800
Fax +1-215-386-7999
www.siam.org • siam@siam.org

parallelism between computational nodes comprised of multiple chips. In order to achieve high rates of performance, algorithms that minimize data movement, possibly by increasing the relative number of computations, will be the most efficient. Algorithm developers will need to take these facts into account as they develop multi-scale, multi-physics algorithms.

Utilizing exascale to study complex systems will require the construction of new predictive mathematical models of large, nonlinear dynamic networks that span several spatial and temporal scales. Understanding and manipulating these systems will require large, multi-scale, nonlinear, and hybrid models, which either do not exist or are in their infancy today. Simulations carried out at finer scales often will require the modeling of physical effects that are ignored in current simulations, which requires both the development of new mathematical models as well as new algorithms to run them. DOE is additionally supporting research in uncertainty quantification, which will allow the confidence in computational forecasts and predictions to be measured.

In addition to allowing revolutionary advances in modeling and simulation, exascale can potentially be utilized to manage ever-growing data volumes in science, from DNA sequence data to information on materials from DOE's light source facilities. These data need to be stored in databases that are easily accessible and searchable, requiring increasingly sophisticated and scalable data mining algorithms. In addition, the data from heterogeneous sources need to be integrated, within databases as well as within models. Once accessible in databases, the typically high dimensional data sets need to be analyzed using advanced mathematical and statistical methods.

Co-design of hardware, software, and applications are critical for successful exascale development so that each component of an exascale computer is optimized in an integrated fashion. ASCR Co-Design Centers are addressing the challenge of designing exascale systems to enable a variety of predictive mission and science outcomes. To achieve co-design requires frequent interactions among hardware architects, systems software experts, designers of programming models, and implementers of the science applications that provide the rationale for building extreme-scale systems.

Mathematical and computational scientists with appropriate awareness and ability to tackle interdisciplinary exascale challenges will be essential to realizing the benefits of exascale. Programs should be implemented to ensure this pipeline of mathematicians and computational scientists at the undergraduate, graduate, post-doctoral, and early career levels. In addition, programs that encourage interdisciplinary collaboration between computational scientists and domain scientists are essential to incentivizing these collaborations, which are crucial for the realization of exascale's scientific benefits. Programs that support partnerships, workshops, travel to technical conferences, and summer internships also help to create a new community of researchers more alert to and equipped to conduct interdisciplinary research.

SOCIETY for INDUSTRIAL and APPLIED MATHEMATICS
3600 Market Street, 6th Floor
Philadelphia, PA 19104-2688 USA
Phone +1-215-382-9800
Fax +1-215-386-7999
www.siam.org • siam@siam.org

Supporting the Pipeline of Mathematicians and Computational Scientists

Before I close my testimony, I would like to discuss an important workforce development program within ASCR. SIAM is grateful to Congress for its support of the Computational Sciences Graduate Fellowships (CSGF), a critical program that maintains the pipeline of the computational science and engineering workforce. Researchers trained in computational science and working in universities, national laboratories, and industry are central to DOE's mission and essential to propel advances in DOE mission-critical fields such as nanotechnology, biofuels, genomics, and materials fabrication. CSGF helps ensure the existence of an adequate supply of scientists and engineers with strong computational research experience and close ongoing ties to DOE to meet future national workforce needs.

The CSGF has a long history of success at DOE. Connections to the national labs are integral to CSGF's success, as fellows train at DOE national labs and program requirements are closely tied to DOE mission needs. A 2011 Committee of Visitors (COV) report[1] evaluating CSGF found that the program has been highly successful at producing alumni with strong computational research experience and close ongoing ties to DOE. CSGF is a valuable program and a unique source of talent in the area of computational science where high performance computing is applied to challenging and important science and engineering problems.

Conclusion

The programs in the Office of Science, particularly those discussed above, are important elements of DOE's efforts to fulfill its mission. They contribute to the goals of dramatically transforming our current capabilities to develop new energy supplies and improve energy efficiency to ensure energy independence and facilitate DOE's effort to increase U.S. competitiveness by training and attracting the best scientific talent into DOE laboratories and the American research enterprise.

I would like to conclude by thanking you again for your ongoing support of the DOE Office of Science and the actions you have already taken to enable DOE and the research and education communities it supports, including thousands of SIAM members, to undertake the activities that contribute to the health, security, and economic strength of the U.S. The DOE Office of Science is critical to maintaining our competitive edge in science and technology.

I appreciate the opportunity to provide testimony to the Committee and am happy to answer any questions.

[1] http://science.energy.gov/~/media/ascr/ascac/pdf/reports/ASCAC_CSGF_Report_2011-Final.pdf