Testimony for the *Subcommittee on Energy* of the
House Committee on Science, Space, and Technology (117th Congress)

hearing on

Accelerating Discovery: the Future of Scientific Computing at the Department of Energy
Wednesday, May 19, 2021 - 11:00am EDT

By

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Chairperson Bowman and Ranking Member Weber: I appreciate this opportunity to submit testimony for this hearing on the future of scientific computing at the Department of Energy (DOE).

My name is Karen Willcox and I serve as the Director of the Oden Institute for Computational Engineering and Sciences at The University of Texas at Austin, where I am also Associate Vice President for Research and a Professor of Aerospace Engineering and Engineering Mechanics.

I offer my remarks today based on my expertise in scientific computing as well as my extensive interactions with the DOE in multiple capacities, which include serving as the current Co-director of the AEOLUS Mathematical Multifaceted Integrated Capabilities Center (MMICC) funded by the DOE Advanced Scientific Computing Research (ASCR) program, serving as a current member of the External Review Board for the Computing and Information Science Research Foundation at Sandia National Laboratories, and serving as a current member of the Advisory Board for the Advanced Simulation and Computing program at Los Alamos.

I wish to convey to you three main points:

1. **The future of scientific computing must be interdisciplinary**. Its very core must involve computer science, computational science, the mathematical sciences, the domain sciences, and engineering.
2. **The DOE ecosystem that supports mission-driven basic research in scientific computing across the National Laboratories and the Nation's universities is a national scientific treasure** that must be nurtured and bolstered to ensure a secure, sustainable, and competitive future for the Nation.
3. **The future of scientific computing hinges critically on the availability of a highly skilled workforce passionate about addressing the Nation's challenges in science, security, and sustainability.**

The interdisciplinary future of scientific computing

Scientific computing has an unquestionably central role to play in future scientific discovery and technological innovation to address societal grand challenges. The pace at which scientific computing can accelerate discovery and innovation will be limited by the rate at which we address foundational challenges that currently limit the complexity, scale, and trustworthiness of computational analysis, prediction, and decision tools. To address these challenges requires scientific computing research and development that draws on many fields, including computer science, computational science, and the mathematical sciences, and also includes close collaborations with domain scientists and engineers.

Particularly important is the critical role of the field of computational science (sometimes called computational science and engineering). Computational science is an interdisciplinary field that uses mathematical modeling and advanced computing to understand and solve complex problems. Computational science differs from computer science because at its core, computational science involves developing mathematical models and simulations rooted in physical and mechanistic principles, in order to understand, analyze, predict, design, and control natural and engineered systems. Quoting Rüde et al.[1]

> *"Advances in computational science have led to more efficient aircraft, safer cars, higher-density transistors, more compact electronic devices, more powerful chemical and biological process systems, cleaner power plants, higher-resolution medical imaging devices, and more accurate geophysical exploration technologies—to name just a few."*

We can draw insight as to the nature and impact of computational science through the historical example of the finite element method—the workhorse of modern computer-aided engineering analysis and design, and the foundation for the multi-billion-dollar computer-aided engineering (CAE) software industry, which has transformed the practice of engineering. What has it taken to make the finite element method a powerful broadly applicable analysis and design tool that is literally in the hands of every engineer? What has it taken to grow the impact of the finite element method from its origins in engineering structural analysis to its modern-day use in diverse applications from nuclear power plants to subsurface contaminants to polar ice sheets to materials processing to combustion processes and everything in between? A key part of the answer is the decades of investment in foundational mathematical and computational basic research, inspired by and connected to driving applications across engineering and the sciences. This research developed the foundational mathematical theory, such as the error analysis that established the finite element method's reliability,[2] the mathematical formulations that tackled the challenges of numerical stability,[3] and the theory and methods that extended the reach of the finite element method to nonlinear problems.[4]

As we look to the future of scientific computing, the boundaries between computational science and computer science are becoming increasingly blurred. The field of computational science is evolving in the face of increased data in its application domains, while computer science is beginning to impact domains in science, engineering and medicine. The future of scientific computing will involve promising new approaches that span the two fields, such as artificial intelligence (AI) and machine learning, enabled by the increasing amount of scientific data and by advances in scalable algorithms. Indeed, the DOE has been at the forefront of defining the notions of *AI for science*[5] and *scientific machine learning*,[6] with the goal of accelerating research and development breakthroughs in energy, basic science, engineering, medicine, and national security. However, as stated in my recent *Nature Computational Science* perspective piece,[7] when it comes to the development and adoption of AI approaches in scientific and engineering fields we must not lose sight of the need for a balanced investment that goes beyond computer science:

> *"For the last six decades these [scientific and engineering] fields have been advanced through the synergistic and principled use of theory, experiments, and physics-based simulations. Our increased ability to sense and acquire data is clearly a game-changer in these endeavors. Yet in our excitement to define a new generation of data-centric approaches, we must be careful not to chart our course based entirely on the successes of data science and machine learning in the vastly different domains of social media, online entertainment, online retail, image recognition, machine translation, and natural language processing—domains for which data are plentiful and physics-based models do not exist."*

We must recognize that energy, environmental, and nuclear challenges by their very nature require *predictions* that go well beyond the available data. There is a critical need to *quantify uncertainty* and our associated confidence in predictions; there is a critical need to make *informed decisions that account for risk*. The future of scientific computing will only address these needs through balanced investment in the foundational mathematical sciences and in computational science, along with data science and computer science. We must also not underestimate the criticality of continuing to invest in *experimental research and development*; advancing discovery through scientific computing requires validated computational models. Again, we can look to examples from our scientific past and appreciate that advances in time/space resolved experimental diagnostics have contributed significantly to establishing trust and credibility in physics-based computational models, because of the ability to do meaningful comparisons and validations at small scales.

The value of the DOE's mission-driven basic research ecosystem

The DOE research and development ecosystem is uniquely positioned to play a leading role in addressing these challenges and in crafting a strong interdisciplinary future for scientific computing.

The National Laboratories exemplify a culture of careful, measured, validated, and verified research that addresses vital scientific and technical application domains. Their leadership in scientific computing is complemented by their world-leading experimental and scientific user facilities. The growing efforts to support research that cuts across computational and experimental domains are essential to the future of scientific computing, and here DOE plays a unique role.

DOE support for basic research at National Laboratories and at the Nation's universities has fostered interdisciplinary computing research in a way that community-driven basic research has struggled to achieve.

As one example, I highlight the Mathematical Multifaceted Integrated Capabilities Center (MMICC) program of DOE ASCR. The Applied Mathematics Program invests $9M per year to fund three MMICC centers. The focus of these centers is on basic research in applied mathematics, but strongly driven by application needs. For example, our current AEOLUS MMICC, led by The University of Texas at Austin, is addressing basic mathematical research needs to enable predictive modeling, optimal process control, and optimal experimental design for applications in advanced materials and additive manufacturing. Over the past eight years, the MMICC program has been transformational in how it has shaped my basic research portfolio. What are the crucial elements? (1) The size of the center is large enough to bring together a diverse team that includes mathematicians, computer scientists, computational scientists, engineers, and domain experts, spanning universities and National Laboratories. This in turn enables a much-needed holistic research approach for increasingly complex systems. (2) The long funding horizon (4 or 5 years) provides the stability to invest in challenging high-payoff basic research ideas. It also provides the opportunity for PhD students to truly integrate with the team and the project. (3) The mission-driven nature of the center goals challenges my mathematical research to target problems that practitioners actually care about, yet the focus on basic research permits the research to lay long-lasting foundations that may ultimately impact a broad range of problems.

This notion of mission-driven cross-cutting mathematical research has been a mainstay of the DOE Applied Mathematics Program. It has provided, and will continue to provide, the rigorous mathematical and computational underpinnings that are essential to advancing scientific computing.

The criticality of the workforce

Achieving this future vision for scientific computing hinges critically on the availability of a highly skilled workforce passionate about addressing the Nation's challenges in science, security, and sustainability. The challenges in front of us include (1) training the workforce with the interdisciplinary skills that cut across the mathematical sciences, computing, and domain sciences, and (2) ensuring a strong, diverse pipeline of highly trained professionals who remain committed to scientific and engineering domains, rather than being lured away by more lucrative positions in commercial and business sectors.

The Oden Institute at The University of Texas at Austin has a globally recognized interdisciplinary graduate program in Computational Science, Engineering, and Mathematics (CSEM).[8] The CSEM program is unique in that we sit outside the usual departmental and school structure; our students are truly trained at the interfaces. A critical part of that training is the immersive research experience enabled by basic research grants, such as the MMICC program I described earlier, or the Predictive Science Academic Alliance Program (PSAAP).[9] Our graduate students work with collaborators from the National Laboratories and from industry partners. They engage in internships. They are immersed in the notion of basic research that targets societal grand challenges together with a culture of rigorous mathematically grounded approaches and a culture of high performance computing at scale. This prepares them to contribute to some of the Nation's most pressing scientific and technological challenges. For example, under our previous Diamond MMICC center, we trained scores of doctoral students and postdoctoral researchers, many of whom have gone on to careers in academia and the National Laboratories.[10]

Maintaining a strong investment in DOE basic research funding for universities, while also continuing to support the collaborative and academic alliance programs at the National Laboratories, is absolutely critical to addressing the Nation's future workforce needs.

Summary

Scientific computing will play a central role in future scientific discovery and technological innovation to address societal grand challenges. Scientific computing has and will thrive in an ecosystem that fosters interdisciplinary basic research and that provides the culture, environment, and resources needed to train a highly skilled workforce passionate about addressing the Nation's challenges in science, security, and sustainability. The DOE has been uniquely strong in providing this ecosystem in the past decades, and, with the proper support, is well positioned to do so in the future.

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[8] https://www.oden.utexas.edu/graduate-studies/
[9] https://psaap.llnl.gov/
[10] http://dmd.mit.edu/young-gems