SOCIETY for INDUSTRIAL and APPLIED MATHEMATICS

Official Written Testimony for Fiscal Year 2025: DOE Office of Science Submitted by: Dr. Sven Leyffer, President, SIAM; Dr. Alejandro Aceves, Vice President for Science Policy, SIAM; Dr. Suzanne L. Weekes, Executive Director, SIAM Submitted to: Subcommittee on Energy and Water Development, Committee on Appropriations, United States Senate, April 26, 2024

Summary: This written testimony is submitted on behalf of the Society for Industrial and Applied Mathematics (SIAM) to ask you to continue your support of the Department of Energy (DOE) Office of Science with funding of $9.5 billion in fiscal year (FY) 2025. In particular, we urge you to provide $418.5 million for Mathematical, Computational, and Computer Sciences Research in the Advanced Scientific Computing Research (ASCR) program within the Office of Science. We also emphasize the importance of support for graduate students through the Computational Sciences Graduate Fellowship and request that $20 million be provided in FY 2025.

Written Testimony: On behalf of SIAM, we submit this written testimony for the record to the Subcommittee on Energy and Water Development Appropriations of the United States Senate.

SIAM has approximately 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.

SIAM appreciates your Committee's leadership on and recognition of the critical role of the Department of Energy (DOE) Office of Science and its support for mathematics, science, and engineering in enabling a strong U.S. economy, workforce, and society. 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.

SIAM is grateful for the strong funding that the Office of Science received in FY 2024, and we join with the research community to request that you continue this momentum by providing the Office of Science with $9.5 billion for FY 2025. The requested amount is necessary for ensuring continued support for areas such as mathematics and scientific research to help address national priorities, foster economic growth, and create jobs.

Advanced Scientific Computing Research-- Activities within the Advanced Scientific Computing Research (ASCR) program play a key role in supporting research that begins to fulfill the needs described above. **Within the overall amount for the Office of Science, SIAM requests that $418.5 million be provided for Mathematical, Computational, and Computer Science Research within the Office of Advanced Scientific Computing Research (ASCR), which is $128 million above the FY 2024 enacted level and consistent with the President's FY 2025 Budget Request.** This level of funding would enable ASCR to transition funding from the Exascale Computing Project that is now nearing completion back into marquee foundational research programs. These programs have been heavily underfunded during the years of the Project and the increased funding will enable DOE to address challenges in next generation computing systems, develop and utilize Artificial Intelligence/ Machine Learning technologies in simulations and data intensive applications, and make progress on other basic research priorities. Basic research in applied mathematics and computational science is needed to ensure the long-term health and viability of the high-performance computing (HPC) ecosystem that the Department of Energy (DOE) relies on for conducting groundbreaking discovery science while

supporting increased investment in priority areas such as quantum computing and artificial intelligence.

Core research activities within ASCR enable the development of critical tools for computational science, modeling, and data analysis that enhance advanced computing capabilities and seed new areas of research with potential for revolutionary advancements. Sustained investment in basic research ultimately enabled the global leadership in HPC that the U.S. currently enjoys. While our strength in HPC is exemplified by the groundbreaking deployment of the exascale systems, this position is increasingly being challenged by China and other countries.

Computational science has long been an essential part of DOE's scientific enterprise, but the near future is unusually ripe with opportunities. With the deployment of the Exascale computing systems ASCR is uniquely positioned to support a broad array of research and initiatives from other programs in the Office of Science and all of DOE. To ensure these systems are used to the maximum benefit it is vital that DOE has a clear strategy on future roles ASCR will play, how to maximize its impact, and how to use ASCR's capabilities to support cross-cutting DOE initiatives such as the Energy Earthshots. While the Exascale computers are currently the strongest in the world, and an accomplishment many years in the making, it is in ASCR's mission to continue to drive U.S. technological leadership and the future of supercomputing, and to always be looking towards what comes next. To accomplish this effectively ASCR needs to clearly layout its vision for the future of advanced computing.

Supporting the Pipeline of Mathematicians and Scientists-- SIAM is grateful for Congress's strong support of the Computational Sciences Graduate Fellowships (CSGF) in FY 2022, providing a $5 million increase after it had been flat funded since FY 2015, but **requests**

that $20 million be provided for the Computational Science Graduate Fellowship (CSGF) in FY 2025 within the overall amount for research. Researchers trained in computational science and working in universities, national laboratories, and industry are essential to propel advances in many DOE critical research areas. This program is critical to 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 increase we are requesting to CSGF reflects the growing need for an expanded workforce in emerging areas of importance to DOE such as artificial intelligence and data science. As international competition in science and engineering intensifies, maintaining U.S. leadership in these areas will increasingly depend on our ability to cultivate a scientific workforce with strong research experience and close ties to DOE. An increase in funding to CSGF would also enable ASCR to address a consistent oversubscription in the program and advance diversity, equity, and inclusion through expanded outreach to minority serving institutions.

In addition to CSGF, this level of funding for the research program would support increases for the Reaching a New Energy Sciences Workforce (RENEW) initiative, started in FY 2022, and continued support for the Accelerate and FAIR initiatives, which would further broaden and diversify the applied mathematics and computer science research communities by increasing opportunities for students and institutions that are currently underrepresented.

The Role of Mathematics in Meeting Health, Energy, and Security Challenges--Support for applied mathematics and computational science is critical to sustaining the nation's global scientific and technological leadership, energy production capabilities, and national security. By exploiting DOE's world class supercomputing capabilities, mathematicians and computational scientists supported by the abovementioned programs pioneer new modeling and

simulation techniques that enable substantial breakthroughs in materials synthesis, energy distribution, and human physiology among other complex areas where laboratory experiments or field observations are too costly, time consuming, or simply insufficient. This was demonstrated recently in the midst of the novel coronavirus pandemic. Researchers at Oak Ridge National Laboratory (ORNL) developed a computational model of the novel coronavirus. They then ran the model on ORNL's supercomputer, *Summit*, and were able to identify 77 molecular compounds that could serve as the basis for therapeutic drugs to counter COVID-19.[1]

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 sources of energy 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 headquarters and laboratories, the American research enterprise, and the clean energy economy.

Thank you again for your ongoing support of the DOE Office of Science. The DOE Office of Science needs sustained annual funding to maintain our competitive edge in science and technology, and therefore we respectfully ask that you continue your support of these critical programs. We appreciate the opportunity to provide testimony to the Committee on behalf of SIAM and look forward to providing any additional information or assistance you may ask of us during the FY 2025 appropriations process.

[1] https://chemrxiv.org/articles/Repurposing_Therapeutics_for_the_Wuhan_Coronavirus_nCov-2019_Supercomputer-Based_Docking_to_the_Viral_S_Protein_and_Human_ACE2_Interface/11871402/3