SOCIETY for INDUSTRIAL and APPLIED MATHEMATICS

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Society for Industrial and Applied Mathematics Response to Office of Science and Technology Policy Request for Information on the Development of an AI Action Plan

The Society for Industrial and Applied Mathematics (SIAM) is an international community of 14,000 individual members. Almost 500 academic, manufacturing, research and development, service and consulting organizations, government, and military organizations worldwide are institutional members. Our members come from many different disciplines but have a common interest in applying mathematics in partnership with computational science to advance the benefits of artificial intelligence (AI) by improving federal research efforts and applications across sectors, protecting data and privacy, and ensuring reliability and security in computational models and algorithms. Through publications, research, and community, the mission of SIAM is to build cooperation between mathematics and the worlds of science and technology. Thank you for the opportunity to respond to the Request for Information (RFI) on the Development of an Artificial Intelligence (AI) Action Plan.

Federal research investments in AI and related fields, such as computational science, are critical to advance innovation and ensure continued American leadership. AI has the potential to reshape many scientific disciplines as well as other sectors such as health, energy, defense, and education. As applied mathematicians, the SIAM community appreciates efforts both to advance foundational artificial intelligence, as well as to build partnerships that enable specific application areas. In this response, we will focus on several key areas for research and development, infrastructure needs, as well as education and workforce recommendations.

Research and Development

While AI has made tremendous strides over the last few years, further investment is needed to continue the cycle of innovation, ensure AI systems can be built for the particular needs of science and other government missions, and that AI can be relied upon and secure. Federal investment should focus on supporting a broad range of projects and leveraging convergent teams at different sizes to encourage maximum innovation. For example, the National Science Foundation's (NSF) *Mathematical Foundations of Artificial Intelligence* program is enabling small teams of mathematicians, engineers, and computer scientists to address key foundational gaps in the mathematical and theoretical underpinnings of AI to address its current limitations and challenges. These foundational programs should be part of a larger portfolio that also includes major investments, such as the NSF-funded *National AI Research Institutes* and the Department of Energy's (DOE) *Frontiers in Artificial Intelligence for Science, Security and Technology* (FASST) initiative and

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AI Testbeds, that focus on advancing AI in specific application areas. Investments should also continue to be made in fundamental research to develop AI technologies through core programs such as those in NSF's Division of Mathematical Sciences and DOE's Office of Advanced Scientific Computing Research. High-risk, high-reward research that enables major breakthroughs is another critical component of a robust research portfolio at agencies such as the Defense Advanced Research Projects Agency (DARPA) and the Advanced Research Projects Agency for Health (ARPA-H). DARPA has had a longstanding role in pushing the frontiers of AI forward, while ARPA-H has already built an impressive portfolio in computational tools, AI, digital twins, and other computational areas.

AI needs data and data across many agencies requires investment before it can be efficiently used for AI. Investment is needed in research and development to create an integrated suite of data lifecycle methods and tools, informed by the specific needs of federal research communities at the DOE, NSF, National Institutes of Health (NIH), Department of Defense (DOD), and other agencies. Techniques that lead to data harmonization and normalization, such as data cleaning, validation, and error correction must be developed to overcome the natural heterogeneity of data sources which is in inherent conflict with the need for data fusion. Open research questions remain around analyzing highly distributed data sources, enabling data discovery and integration, tracking data provenance, coping with sampling biases and heterogeneity, ensuring data integrity, privacy, security, and sharing, and visualizing massive datasets. The National Institute of Standards and Technology (NIST) also has an important role to play in setting data and AI standards and convening academic, industry, and other stakeholders to share data and AI systems for measurements of reliability, safety, security, and vulnerabilities.

Research focused on the intersection of modeling and AI can unlock tremendous progress in scientific discovery. The current theory and practice of AI struggles to incorporate physical models and constraints. Formulations of new AI algorithms structured to include physical models, rather than having to "learn" the physics, will allow the designs of new classes of AI applications optimized exactly for the scientific tasks that require them. To do this will require advances in such formalisms as projection operators that enforce physical principles, data structures that encode symmetries and constraints, and the construction of physical priors and their injection into mathematical models.

Many scientists are exploring ideas and developing new insights, but the field of scientific machine learning is still evolving. Alphafold13, Google's breakthrough technology for predicting protein conformations, showcased the potential for ML to outperform traditional scientific approaches. Other potential roles for ML in science include automatically monitoring and running experiments or series of experiments, improved methods for

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combining simulation results and experimental data, and the generation of new hypotheses from data. Quite likely, the most important ideas have not yet been thought of. Many AI models focus on prediction accuracy without a focus on explainability. For scientific applications, prediction without insight is seldom enough. A key area of exploration is the development of interpretable models and algorithms that provide insight into why and how a model produces a particular output. This requires investment in techniques for explainable AI models. Artificial intelligence and machine learning have enormous potential to impact the processes of scientific research, but broad investments in mathematics and computing will be required to realize these opportunities.

A particular area of promise for AI innovation is at the intersections of AI and health. AI holds tremendous promise to revolutionize biomedical research in the understanding of chronic diseases, diagnostics, and development of treatments. Health agencies, such as the NIH, lag physical science agencies in their AI investments and need a focused initiative to take advantage of this promising technology while addressing privacy and other issues. An AI initiative could invest in potential research moonshots to develop AI that will truly work and be trustworthy for health applications. Further research is also needed to address AI use in healthcare to accelerate the development and deployment of reliable AI that provides accurate diagnosis and treatments for all patients. AI is accelerating at such a speed that NIH needs to keep up with the advancements of this emerging field and related technology like digital twins. In absence of dedicated funding, NIH may fail to adapt to AI that could shape the future of the U.S. healthcare system. OSTP should also encourage participation of relevant Health and Human Service agencies including NIH, Centers for Disease Control (CDC), and the Food and Drug Administration (FDA) in NSF's National Artificial Intelligence Research Institutes program to address these challenges.

Another promising area is the intersection of AI and the basic science, energy, and national security missions of DOE. Additional research funding is needed to fully realize the potential of AI for these applications. Current and past successes, such as the development of a digital twin for a nuclear power plant to aid in inspections and maintenance, and AI-based screening and design of functional materials for harsh environments, including fusion reactors, are just the tip of the iceberg of what the incredible developments AI can bring to these areas.

New mathematical foundations are needed for the development of AI methods that are explainable and reliable. Foundational work is also needed in the following topical areas:

- Adversarial AI, cybersecurity, and how to address other security challenges.
- Data Sparse AI: Data that are available to large language models are starting to reach a limit and this will hinder further innovation without new methods.

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Furthermore, individuals and organizations are likely to protect the data they produce, further making data accessibility harder. Generative models that are based on first principles understanding can be used to augment measured data. This is even more important in scientific applications wherein large amounts of data will never be available.

- Energy Efficient AI: Current AI techniques cannot simply continue on their path of energy consumption; it is not sustainable. New mathematical and algorithmic techniques are needed to develop more efficient use of AI subsystems.

Infrastructure

AI research requires large-scale infrastructure that keeps advancements out of reach for many beyond the most highly resourced companies. The federal government can help advance a more robust ecosystem for AI innovation and enable university and national lab research efforts through investments in federal AI infrastructure that are available to users through a competitive process to make sure the most promising research gains access. At NSF, the *National AI Research Resource* (NAIRR) pilot is underway following a task force effort initiated in the first Trump Administration. The pilot will end in FY 2026 and NSF should look to build the full NAIRR that will revolutionize AI capabilities. At DOE, in addition to the *National Laboratory AI Testbeds*, a facility or facilities should be established to ensure that researchers have access to experimental non-traditional hardware that will inform a holistic codesign cycle between manufacturers and users of transformative computing technologies. As the non-traditional computing hardware industry evolves and the roles of different enterprises change, the government should remain open to establishing new types of collaborations and relationships with both existing and emerging industrial partners. These new devices will likely be initially employed as accelerators, so their ability to integrate with existing high-performance computing (HPC) platforms must be part of the design process. Investments are also needed in research and development collaborations between computational scientists and computer vendors to ensure development of future energy efficient computing platforms that meet the needs of the computational science community.

Investments are needed in foundational models as well as the research, software tools, and system management tools needed to enable complex workflows that combine simulation with machine learning so that AI can better work with existing HPC computing infrastructure supported. This is primarily a role for DOE along with some investments from NSF and DOD.

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Partnerships

Computational science has always been an interdisciplinary endeavor, drawing on mathematics, computer science, and application domains. With the growth in the importance of data science and AI, the field is becoming even broader. National Laboratories, academia, and industry all have specific strengths to benefit AI research and development. Many of the most pressing scientific and societal challenges can only be solved through the efforts of multidisciplinary, multi-institutional teams. The federal government should create incentives for interdisciplinary education and research collaboration that engage National Laboratories, academia, and industry.

Establishment of additional coordination and engagement between the applied mathematics and computational science community and the wide-ranging federal healthcare and biomedical research will improve the nation's preparedness, health systems, drug development and approval pathways. For example, NIH and FDA recently collaborated with NSF on a program to catalyze the development of digital twins for biomedical and healthcare technologies to improve clinical trials. The Administration should encourage these kinds of collaborations to bring together researchers from computer science, applied math, and engineering along with those in health operations, behavioral science, regulatory science, and biomedical research to foster new ways to evaluate medical devices, better modeling for disease preparedness, and development of new tools. This model can be adapted to other agencies and application areas to further additional applications. The NSF *National AI Research Institutes* are another good model for interagency collaboration and involve the partnership of several agencies, including the United States Department of Agriculture (USDA), Department of Homeland Security (DHS), Department of Education (ED), and DOD. More agencies should be encouraged to join this program to harness breakthrough research for addressing their unique mission needs.

Education and Workforce

Finally, as an organization representing thousands of researchers and educators from hundreds of academic institutions, SIAM is well aware of the AI R&D workforce challenges facing the nation. The potential limitations posed by workforce shortages could significantly constrain our ability to maintain our leadership in AI amid an international environment that is growing increasingly competitive. Federal science agencies have a critical role to play in sustaining the vitality of AI R&D in the U.S. through their support of research and education programs. SIAM recommends that the Action Plan includes support for programs like NSF's *NSF Research Traineeships (NRT), Graduate Research Fellowships (GRF)*, *Research Experiences for Undergraduates (REU),* and *CAREER* awards as well as DOE's *Computational Science Graduate Fellowship* program. These programs

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are crucial to the training and professional development of the next generation of the mathematical researchers and computational scientists who will underpin U.S. competitiveness in AI in future decades. Agencies should also look for opportunities to pursue partnerships and offer internships that give students exposure to National Laboratories, intramural research, or defense challenges. Exposure to federal laboratories has proven to be an effective way to inspire students at all levels to pursue careers in federal service, which is an important avenue alongside industry and academic workforce needs.

Undergraduate curricula are critically important to ensuring American preeminence in AI through education in the mathematical foundations of machine learning. SIAM recommends that the action plan commits to supporting the integration of data science and modeling into undergraduate STEM coursework in order to improve students' familiarity with these subjects as they seek to successfully enter the AI workforce, use AI in their scientific or engineering careers, and shape future innovations. The Administration should also consider ways to develop AI technology for new ways of upskilling and retraining the workforce as large sectors evolve through increasing use of AI.

Sincerely,

Carol Woodward	Suzanne L. Weekes	Alejandro Aceves
President	Chief Executive Officer	Vice President for Science Policy

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