

Department of Energy Artificial Intelligence Initiative for Science, Energy, and National Security

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The Energy Sciences Coalition (ESC) thanks Congress for making U.S. leadership in artificial intelligence (AI) a top priority. As Congress advances AI legislation, ESC recommends that future legislation include Department of Energy (DOE) provisions to execute its unique science, energy, and national security missions and accelerate U.S. innovation to maintain our economic prosperity and global competitiveness.

DOE and its network of 17 national laboratories play a unique leadership role among federal science agencies in advancing innovation and the responsible use of AI and must be included in future AI legislation. A focused DOE AI Initiative should be guided by the vision outlined in the 2023 Advanced Research Directions on AI for Science, Energy, and Security. Over the last five years, under the direction of the DOE Office of Science and the National Nuclear Security Administration, DOE organized a series of workshops to gather input from new and rapidly emerging opportunities and challenges of AI to advance science, energy, and national security. This effort brough together over 1,300 scientists and engineers from national labs, research universities and industry. This resulted in recommendations on how advanced AI systems might be developed over the next 10 years to accelerate scientific research, energy technology development, and improve national security. The scale and opportunity of AI to transform and disrupt how scientific problems are posed and solved also underscore the need to ensure the responsible development and use of safe, security, and trustworthy AI across DOE mission areas. A coordinated DOE program should also follow guidance from the October 2023 Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence, along with the National AI Initiative Act included in the FY 2021 National Defense Authorization Act (Title LV, Section 5501) and the CHIPS and Science Act (Section 10771).

DOE's leadership in AI is based on decades of investment in supercomputing and advanced scientific experimental facilities, data management and communications infrastructure, and the scientific workforce. DOE builds and operates the world's fastest and most capable supercomputers, including the world's first exascale computers which can perform more than 1,000,000,000,000,000,000 operations or tasks per second (a 1 followed by 18 zeroes). These

The Energy Sciences Coalition (ESC) is a broad-based coalition of organizations representing scientists, engineers and mathematicians in universities, industry and national laboratories who are committed to supporting and advancing the scientific research programs of the U.S. Department of Energy (DOE), and in particular, the DOE Office of Science.

calculations, along with scientific data from other state-of-the-art facilities such as light sources, accelerators, and genomics centers produce tremendous amounts of data, which is key for AI and machine learning applications across various scientific and national security areas. DOE has developed unique data management infrastructure to store, review, and use this data to meet DOE missions. It also stewards key data repositories with information not just from DOE, but industry and other federal agencies, which are high-quality, public resources that make it easier for industry, academia, federal agencies, and other users to find and access data for scientific and technological discoveries. This includes data repositories for materials, biology and environmental research as well as energy data for residential and commercial buildings, geothermal, solar, wind, marine, and hydrokinetic applications. DOE is also one of the largest federal sponsors of STEM research, education and workforce development, including in applied mathematics and computer science, that serve as the foundations to understand generative AI and large-scale language models, such as ChatGPT.

A focused, dedicated AI Initiative is needed to fully leverage this unique DOE infrastructure and expertise to meet the nation's science, energy, and national security challenges. AI can play a major role in finding important scientific and technological solutions, such as the search for new quantum materials for quantum computing, sensing, and networking applications; new nuclear and fusion reactor designs; streamlined nuclear weapons designs to maintain the nation's nuclear deterrent; prediction and early detection of nuclear proliferation in countries of concern; predictable ways to engineer microbes and plants for a sustainable bioeconomy; and improved climate models to improve resiliency and mitigate the worst effects of extreme weather events. These advances must also take into account the responsible development of AI focused on challenges related to AI technology, such as explainability, validation, security, and privacy; implementation such as transparency, safety engineering, and ethics; and applications, such as AI-human interactions, education, and job impacts. DOE is well equipped to address both the opportunities and challenges, working in partnership with other federal agencies and industry partners.

As Congress advances legislation, ESC recommends the following policy proposals for DOE provisions:

- Cross-cutting R&D program. ESC recommends a broad, whole-of-DOE effort that focuses on unique DOE science, engineering, energy, and national security missions. This program should support fundamental science, early-stage engineering and prototyping of AI hardware and software technologies, and the deployment of AI applications to advance science, energy, and national security. This program should also include flexible and diverse funding mechanisms to drive innovation, mitigate risks, and scale up activities across a range of disciplines, including single principal investigator and small research group grants for high-risk and innovative paths and prototypes; medium-sized efforts to tackle specific grand challenges such as Energy Frontier Research Centers and Scientific Discovery through Advanced Computing (SciDAC) centers; and large-scale consortia of universities, national labs, and industry to integrate, test, and deploy AI systems. A key component would be the safe, reliable, and transparent use of AI, including privacy issues.
- Joint leadership by the Office of Science and National Nuclear Security Administration (NNSA). ESC recommends that leadership of an AI Initiative be jointly shared by the DOE

Office of Science and NNSA to simultaneously address unique science and national security missions. The DOE Office of Science should coordinate closely with DOE's applied energy offices to develop energy-specific applications and ensure AI platforms are integrated across DOE missions. The Exascale Computing Initiative serves as a successful model of DOE Office of Science and NNSA collaboration and partnership in designing, building, and operating the first exascale supercomputers. DOE Office of Science and NNSA jointly funded co-design teams made up of over 1,000 scientists, engineers, and other experts from DOE national laboratories, academia, and industry to work together on hardware, software, and applications. This coordinated framework, coupled with a robust research and deployment effort at scale, is what is needed to drive innovation in AI.

- National Science, Energy, and National Security Hubs. ESC recommends the launch of at least 8 large-scale innovation hubs focused on advancing unique AI applications for DOE science, energy, and national security missions. These large-scale teams of DOE national labs, universities, industry, and other research organizations bring together unique DOE research expertise, infrastructure, and workforce to have significant impact. STEM education and workforce development as well as fostering connections across a wide range of disciplines ranging from physicists and engineers to computer scientists would be an important element of this consortia and would complement science and technology research and development efforts. Industry is making significant investments in AI and driving innovation, but focused on applications central to industry rather than DOE mission areas in science, energy, and national security. ESC recommends up to \$35 million per year for each Hub over 10 years to tackle the opportunities and challenges of AI for DOE missions.
- AI Computing Infrastructure and Integrated Data Management. ESC recommends significant investments in AI computing infrastructure, such as AI accelerators for hardware and software development. Custom-designed AI hardware and software for DOE computing infrastructure will push the boundaries of technology development and applications and help drive innovation in the private sector. ESC also recommends investments in integrated data management leveraging DOE's vast unclassified and classified data sets to make it available to researchers, industry, state and local governments, communities, and other users to accelerate the pace of innovation and application development and help with decision-making. DOE should also partner with other federal agencies, including the Department of Commerce to evaluate and mitigate national and global security risks associated with AI systems and the National Science Foundation to coordinate the development of the National AI Research Resource (NAIRR) and other accessible AI data infrastructure.
- STEM Education and Workforce Development. ESC recommends boosting targeted investments at DOE in AI STEM education and workforce development. DOE can scale up existing programs, such as the Computational Science Graduate Fellowship Program and the Early Career Research Program, or further expand traineeships to have dedicated tracks for AI to meet the growing gap in an AI-skilled and -trained workforce.
- Authorized funding levels to maintain U.S. competitiveness. ESC recommends at least \$1 billion a year for a DOE AI Initiative that includes the program elements highlighted above, including investments at the DOE Office of Science, NNSA, and the applied energy offices. This level of investment is consistent with Section 10771 of the *CHIPS and Science Act*, authorizing \$11.2 billion in research, development, and demonstration activities at DOE in the 10 key technology areas, including AI.

Thank you for your consideration of this critically important initiative.

Sincerely,

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ESC Membership

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