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General Comment

See attached file

Attachments

OSTP AI R and D RFI final

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Re: Request for Information on the Development of a 2025 National Artificial Intelligence (AI) Research and Development (R&D) Strategic Plan (Docket ID No. NSF-2025-OGC-0001)

Submitted by: National Lab Directors' Council (NLDC)

Introduction

The United States must secure and sustain AI dominance to protect our national security, drive energy innovation, and uphold our position at the forefront of scientific discovery. Achieving this requires an integrated strategy that combines world-class computing power, scientific expertise and challenges that push AI capabilties to new heights, and collaboration across industry, academia, and government. This approach will allow the U.S. to test, refine, and deploy AI solutions end-to-end for real-world impact.

Success of this approach relies upon strategic allocations of Federal resources to foster strong efforts and robust collaborations among U.S. Departments and Agencies and to incentivize productive partnerships among Federal programs and private sector partners. One set of institutions poised to contribute in this domain is the Department of Energy National Laboratories. These labs are funded principally via Department of Energy (DOE) programs in national nuclear security, basic and applied science, and applied energy. As an integral part of program execution, the labs steward significant experimental and computational capabilities for the nation. In addition, scientists and engineers at each of the 17 DOE labs work closely with faculty members and students in U.S. universities, staff in small and large industrial concerns, and vetted international collaborators. Further, via competitive processes, lab scientists work for government entities beyond the DOE and for industrial and philanthropic partners.

This document describes in greater detail the types and range of technical issues important for the national goals in AI research and development for which DOE national laboratory capabilities are well matched for successful delivery. Specifically, six priority areas for AI research and development are defined; key AI R&D areas needed in order to boost performance in the domains of national security, energy dominance, and scientific leadership.

Before listing the priority directions, we first note that DOE's national laboratories have a proven track record of large-scale partnerships in AI[1] [2] [3] and beyond[4] [5]. As the global AI revolution unfolds, the immense computational power required underscores a critical need for new energy sources, innovative solutions to sustainably fuel its advancement, and specialized AI science that is outside the scope of what industry pursues. The National Labs' vision for AI R&D is a dynamic, two-way process: advances in AI architectures and algorithms accelerate breakthroughs in science with real-world applications in national security and energy, while the challenges these fields pose drive new AI innovations. Sustaining this feedback loop requires DOE's deep domain expertise and the compute and experimental facilities needed to test and deploy ideas from start to finish.

National R&D Priorities

Below, we outline six foundational AI research thrusts to revolutionize the Nation's scientific capability, accelerate the pace of discovery, and create a persistent innovation advantage for the nation. These thrusts are each critical on their own but also deeply interdependent, requiring coordinated strategic federal R&D investments:

1. **AI Agents for Autonomous Science:** Future innovations in national security, energy dominance and scientific discovery will be driven by coordinated AI agent systems that continuously hypothesize, plan, execute, and learn in closed-loop cycles. A key research priority area is the development of multi-agent AI frameworks which combine physics-informed reinforcement learning, optimization methods, and uncertainty-aware methods to autonomously generate, rank, and adapt experimental hypotheses in real time. This approach will supercharge autonomous self-driving labs, scientific instruments and facilities, and will drastically reduce discovery cycles from months to days.
2. **Integrated Digital-Physical Testbeds:** Creating integrated testbeds that combine high-fidelity digital twins with real-world systems is essential for driving AI-enabled discovery. These testbeds will support AI-driven design, optimization, and control across scientific and operational domains. Key research priority areas include development of: (i) validated and verified end-to-end performance models, (ii) automated provenance tracking and metadata frameworks for enormously heterogeneous datasets, and (iii) federated, privacy-preserving AI to enable secure and scalable collaboration across national laboratories, agencies, and industry, protecting sensitive data while accelerating collective innovation.
3. **Architecure Agnostic Scientific Software Ecosystems:** As hardware architectures diversify to include GPUs, TPUs, neuromorphic chips, analog accelerators, and beyond, methodologies must be developed to enable semi-automated adaptation of scientific software and the generation of portable, optimized kernels. Key priority research investments are needed to develop a holistic solution and ensure that AI-driven science

[1] https://www.energy.gov/articles/secretary-wright-leads-ai-collaboration-event-oak-ridge-national-lab
[2] https://openai.com/index/strengthening-americas-ai-leadership-with-the-us-national-laboratories/
[3] https://www.linkedin.com/posts/katrinaemmons_aijam-nationallabs-frontierai-activity-7314033420458741762-V8Nv/
[4] https://www.exascaleproject.org/
[5] https://quantumconsortium.org/members/

remains agile, ready to run on whatever platforms the future brings in both routine and emergency scenarios. The DOE's experience with the Exascale Computing Project offers a foundation to build AI software stacks optimized for DOE AI models and mission-critical applications.

4. **Reliable and Interpretable AI:** In domains where prediction errors have catastrophic consequences, such as nuclear security and energy resource control applications, formal verification techniques must be developed to ensure that AI tools are demonstrably safe and mission ready. Over the past three decades, DOE has established itself as a leader in formal uncertainty quantification (UQ) and verification and validation (V&V) of its modeling and simulation workflows. This methodology has been successfully used for high-consequence decision-making on mission challenges (e.g., national security). The DOE experience just articulated makes it ideally suited to implement these methods for AI by developing the following key priority research directions: (i) Methods for embedding formal verification, safety checks, and robustness requirements directly into the training and deployment process. This includes measuring the model's confidence in its own predictions, validating those estimates under varied conditions, and ensuring system behavior aligns with performance thresholds. (ii) Methods for interpretable, explainable, and causally-grounded AI models, so that humans can understand not only what an AI system predicts, but why it does so. (iii) Methods to better understand AI models from industry and others, enabling responsible modification and optimization when deployed at scale for mission-critical applications.
5. **AI-Ready Data Curation and Multimodal Data Assimilation**: DOE holds a wealth of unique data about the fundamentals of the physical world that are crucial for AI model training. Creating pipelines that curate and fuse multimodal data, ranging from high-resolution simulations, large-scale experiments and sensor streams to historical archives (e.g., underground nuclear test data), and vast corpora of scientific literature and technical reports, will allow training of bespoke AI models to provide strategic advantage for U.S. national security and science endeavors. We must build end-to-end pipelines that transform raw experimental streams into decision-quality insights by first curating and then fusing heterogeneous, multimodal data. Key research priority areas include: (i) self-supervised cleaning algorithms to detect sensor drift, outliers, and format inconsistencies, (ii) physics-informed corrections, (iii) novel mathematical operators and physics-based generative models to reconcile curated streams, and (iv) streaming in-situ analytics with provable latency and memory guarantees to enforce rigorous bounds on imputation error and uncertainty propagation through every stage, closing the loop between measurement and discovery in real time.
6. **Advances to Tackle the Growing Demands of Simulation and AI Workloads:** Both private and public sectors recognize the urgent and daunting need to realize 10–100× gains in performance per watt and scale compute resources to meet AI's exploding demands. The private sector is largely focused on the needs of AI training and inference, not the physics-intensive simulations at the heart of national security, energy security and scientific discovery. Key research priority areas aligned with DOE's core capabilities include: (i) hardware innovation in AI and scientific simulations, including novel accelerator architectures (mixed-precision engines, photonic cores, neuromorphic and

superconducting fabrics) and memory hierarchies optimized for exascale systems; and (ii) new algorithms and software stacks that exploit these hardware advances enabling error-bounded, mixed-precision solvers and in-network aggregation of intermediate results. To support this next wave, DOE is well-positioned to expand siting, power, and cooling infrastructure for AI, for example coupling advanced nuclear reactors with data centers through autonomous design and deployment. To meet national security mission and frontier AI research needs, DOE must deploy one or more large-scale data centers, both classified and open, with 10^5-10^6 GPUs. These integrated investments in hardware, software, and infrastructure will ensure America retains a persistent advantage in frontier AI and mission-critical simulations.

Driving National Security, Energy Dominance and Scientific Leadership with Frontier AI Research

Advancing the R&D priorities articulated above will enable U.S. national security, energy dominance and scientific leadership. A few key exemplars are as follows:

- **National Security**: Develop secure, domain-specific AI tools to enhance national security measures, including detection of nuclear proliferation, safeguarding critical materials, accelerating weapons modernization and customization, advancements in cybersecurity, and addressing issues such as hard targets or concept to deployment systems all reduced by years. These AI tools will help realize game-changing long-term goals such as deterrence on demand, making bioweapons obsolete, developing a reliable extreme weather event advisor, and improving our understanding of space, oceans, and earth.
- **Energy Dominance:** Integrating advances realized through the R&D priorities above, we will achieve energy dominance by driving innovations to reduce energy costs, unlock next-generation energy resources, and win the AI race with reliable, resilient energy generation. Key applications include (i) grid autonomy for secure, reliable planning and operations; (ii) autonomous design, licensing, and operation of advanced nuclear (fission / fusion) technologies; and (iii) a virtual data subsurface framework to accelerate discovery, management and efficient extraction of energy resources such as American critical minerals, geothermal, hydrogen, energy storage solutions, and traditional oil and gas reserves.
- **Scientific Leadership**: The deep integration of AI agents, robotics, computing and the world's most powerful collection of computational and experimental facilities at the DOE labs is expected to enable researchers to address the nation's most pressing challenges at a scale, speed, and accuracy far beyond what can be envisioned today. The foundational AI research directions described above are required to develop a digitally connected, AI-orchestrated, automated, and smart ecosystem of DOE's experimental and computational facilities across the complex. Such a unified and world-unique, AI-enabled 'Science and Innovation' platform would accelerate breakthroughs on 'over the horizon' challenges that are intractable today, creating new industries and strengthening America's competitive position in critical science and technology areas.

Leveraging DOE's Unique Capabilities for National AI Advancement

In a constrained budget environment, the temptation may be to rely solely on commercial R&D or narrower academic grants to advance AI. But the path to U.S. leadership in AI for science, energy, and security demands infrastructure, integration, and mission focus. DOE laboratories fill a critical niche for partnering with industry, academia, and other federal agencies by delivering:

- **Computational science:** DOE national laboratories have a history of advancing the nation's computational capabilities and platforms in the national interest, with a long history of successful partnerships with industry and academia.
- **Unique datasets:** DOE national laboratories are home to vast scientific data repositories, knowledge bases, analysis platforms, and related activities with the expertise to manage and develop their use.
- **World unique scientific facilities:** DOE exascale computing systems and world-unique experimental user facilities form the cohesive environment necessary for generating high-quality scientific data to train and validate AI models.
- **Mission-Driven S&T in the national interest:** Under national energy, security, and scientific mandates, the DOE pursues high-risk, long-horizon R&D and publishes (as appropriate) all code, data, and methods under open licenses—amplifying impact across industry and academia.
- **Multidisciplinary By Design:** By co-locating computer scientists, applied mathematicians, domain experts, and engineers, the DOE labs eliminate barriers to interaction and accelerate translation of foundational advances into production grade AI systems.
- **Proven Accelerators of Industry Innovation:** Partnering with DOE labs gives U.S. industry access to unmatched expertise, advanced technologies, and world-class facilities, accelerating technology roadmaps, de-risking product development, and expanding into high-impact sectors like energy, manufacturing, and security, all while strengthening global competitiveness.
- **Workforce:** In partnership with universities and industry, the DOE can create national AI workforce training hubs that specifically focus on scientific innovation at the largest scales and mission critical applications.

For eight decades, DOE laboratories have tackled society's grandest "big science" challenges—from the dawn of nuclear modeling to the first leadership class exascale simulations—and demonstrated their ability to mobilize rapidly against emerging crises as the government's agile "science weapon"[6] [7] [8]. Today, DOE national labs stand poised to integrate AI with national security, scientific discovery, and energy innovation in ways that will define American competitiveness and security for decades to come.

[6] https://covid19-hpc-consortium.org/

[7] https://science.osti.gov/nvbl

[8] https://www.energy.gov/articles/doe-advancing-safe-and-secure-ai-research-infrastructure-through-national-artificial