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The Center for AI @PNNL

PNNL's Leadership in Artificial Intelligence

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Amid the ongoing AI revolution, Pacific Northwest National Laboratory (PNNL) is advancing the frontiers of scientific discovery, energy resilience, and national security by applying AI to global issues. Through internal workforce development, PNNL has rapidly scaled the number of technical staff able to apply AI techniques to DOE mission problems: more than 1,200 individuals have been trained in lab-taught "bootcamps," and hundreds of our government sponsors and stakeholders have also participated. Today, more than 20 percent of our research staff are applying AI to their missions or developing new AI approaches, while maintaining focus on its ethical applications. PNNL has developed foundational expertise and forward-learning capability in AI through deliberate internal investments and sponsored programs across all our mission areas. Our core AI capabilities focus on applying AI technologies to the breadth of PNNL's science, energy, and security domains. We also focus on unique specializations in AI that address grand scientific challenges in support of the nation to operationalize AI through scalable, assured, and fieldable methods.

Discoveries in biological science, physical science, and acceleration of carbon cycle closure. PNNL has developed methods to generate biochemical property libraries and candidates for metabolomic identification using variational autoencoders. Foundation models trained from scientific literature, and fine-tuned with DOE unique data resources, will enable multimodal data extraction to provide contextual knowledge representations that empower scientists and engineers with knowledge that was previously extraordinarily tedious and laborious to extract. PNNL has been investing in Foundation Models for Scientific Discovery in Chemistry through its Laboratory-Directed Research and Development program, which has demonstrated early success in integrating scientific literature and physical science knowledge to reason at unprecedented scales. Physics-Informed Learning Machines (PhILMs), funded by DOE/Advanced Scientific Computing Research, was the first center in the U.S. to address physics-informed neural networks and the embedding of physical constraints in neural network models. DEEPXDE, developed under PhILMs, has more than 100,000 downloads. The pioneering activities in PhILMs focus on modern AI in our new center: SEA-CROGS. Preliminary outcomes include new AI architectures that integrate generative AI with operator learning to advance scientific computing. PNNL led a Basic Research Needs workshop that defined the foundations of scientific machine learning and has been a key contributor to the AI for Earth System Predictability road map.

Modern AI is a crucial enabler for applied energy missions. Securing grid operations is essential to our future. PNNL has developed novel approaches for cybersecurity using large language models to identify new potential vulnerabilities and ways to defend against them. In partnership with Google Brain, PNNL created the capability to reduce power disruption during emergencies through adaptive power grid management in real time with deep learning. A new software application called Smart-PGSim uses AI to efficiently solve power grid simulations crucial for planning and optimizing electricity delivery. A first-of-its-kind method for automated control leverages AI advances to support grid optimization. Researchers use physics and modern AI learning for energy-efficient building control. In a PNNL study, deep reinforcement learning, a form of autonomous AI, proved effective in preventing 95 percent of cyberattacks. The results show promise in using more intelligent cybersecurity in proactive cyber-defense of the nation's power grid. Modern AI approaches developed by PNNL and published in *Nature Materials Degradation* have enabled a better understanding of material corrosion in alloys, which is critical for equipment characterization and maintenance in critical infrastructure. Our AI model advances energy storage research by developing digital twins for batteries.

AI-driven innovation spanning the national security, nuclear security, and nonproliferation enterprise. PNNL created what the U.S. Special Operations Command

describes as its first and only operational AI system supporting 24/7 mission operations. This state-of-the-art scalable and fielded capability leverages data-fabric and data-mesh concepts for high-throughput modern AI and data fusion for pattern-of-life characterization across 10 years of multimedia data. For another U.S. organization, PNNL is developing novel geospatial analytics and computer vision algorithms for high-altitude airborne sensors, leading innovation in few-shot learning for complex sensor geometries and target distances not previously achieved by prior performers (large incumbents). These PNNL-developed algorithms are deployed in the sponsor's largest mission-critical system. Assuring AI-enabled high-consequence systems is critical to their operational use. PNNL staff were featured in a DOE podcast discussing AI assurance and they developed measures to detect AI assurance issues and devise solutions addressing these challenges (e.g., diffusion models, model editing, data poisoning). The National Academies of Science, Engineering, and Medicine led an AI workshop co-organized by PNNL for the U.S. Army on *AI and Justified Confidence* to investigate opportunities for the U.S. Army to improve security, reliability, and transparency to foster soldier trust in AI-enabled command-and-control operations. AI is also being applied in the nuclear enterprise. Specifically, AI-enabled physics and process models are enhancing U.S. capabilities for early detection and materials characterization. Leveraging fine-tuned large language models to enhance discovery and disruption proliferation and elicit pathways is now possible. For example, the PNNL-developed NukeLM led to the discovery of new potential proliferation pathways.

Optimized laboratory operations using AI. PNNL was the first DOE national laboratory to gain programmatic access to OpenAI's most advanced model (GPT-4) through our strategic partnership with Microsoft. This, along with the instantiation of several open-source and other large language models, created a powerful set of testbeds for PNNL staff to prototype and develop innovative use cases using generative AI. One early use case piloted at PNNL is a generative-enabled help desk assistant. Trained on a vast repository of 12,000 IT TechDesk articles, this assistant generates first-draft email responses to more than 10,000 inbound support emails received annually. The goal is to extend this capability to other areas, such as HR benefits, to realize significant efficiencies for both support staff and their customers. In the realm of software development, PNNL engineering teams are actively piloting GitHub Copilot. This intelligent tool accelerates development by providing suggestions and auto-generating code, enhancing productivity, and enabling developers to focus on higher-level tasks.

Responsible and ethical use of trustworthy AI. Understanding and upholding the ethical use of AI is front and center at PNNL. PNNL has developed a holistic approach for Trusted and Responsible AI and created tools that assist in achieving accountability, transparency, fairness, and robustness. PNNL has contributed to the IEEE Ethics Certification Program for Autonomous and Intelligent Systems and is the only national laboratory to do so. Now through IEEE, PNNL is authorized to certify autonomous and intelligent systems in a range of Trustworthy and Ethical AI standards, and PNNL also contributed to the IEEE CertifAIed process and has a CertifiAIed lead assessor on staff.

The strategic value of modern AI for DOE and our nation's strategic competitiveness is immense and cannot be overstated. These groundbreaking methods bring great promise for advancement across whole-of-government missions. Investment and application of modern AI is a commitment to maintaining our nation's competitiveness on the global stage. PNNL has been committed to building an AI-ready research enterprise, delivering impact in foundational and applied AI research and engineering critical to DOE and national security sponsors. As we embrace the AI era, we are charting the course for a more innovative, secure, and prosperous future.

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