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Modern AI, a Critical Enabler for DOE

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Exceptional advances in artificial intelligence (AI) over the past decade have led to unprecedented transformation and opened new doors for scientific discovery, energy resilience, and national security within the Department of Energy's (DOE's) purview. AI is increasingly critical to all DOE mission areas and even changing how we do science.[1] Modern AI is no exception. Modern AI represents the collection of astounding advances in AI, from recent advances in deep learning and deep reinforcement learning to generative AI. These approaches are driving an era of enlightenment. The most recent advances, in generative AI, offer specific algorithms that do more than categorize or discriminate data—they generate a range of potential results. Often, these algorithms are trained on large unlabeled data to expand their capabilities. Among these algorithms, foundation models[2] and large language models have emerged as powerful tools for generating human-like text and demonstrating impressive capabilities in various applications. The Gordon Bell Special Prize for COVID-19-related research was awarded to a joint laboratory, industry, and academic team in 2022 for training large language models to discover variants of the SARS-CoV-2 virus.[3] Other modern AI methods include diffusion models that turn text descriptions into visual imagery (still or video), generative adversarial networks, and variational autoencoders. The strategic use of modern AI in the U.S. is critical to maintaining our national security, economic robustness, and scientific leadership. DOE is primed to rapidly transform its scientific endeavors in this nascent era.

Discoveries in biological science, physical science, and acceleration of carbon cycle closure are possible with modern AI. Laboratories could be automated, enabling scientists to generate automation scripts and robust experimental designs that create plans to explore experimental space more efficiently.[4] Autonomous experimentation will facilitate closed-loop scientific discovery (e.g., hypothesis generation and refinement, planning and execution of experiments). One application will be to generate high-throughput data using AI-driven and autonomous phenotyping systems. The data will be suitable for training generative models for digital twins of biological systems across scales (e.g., from pathways to single-cell systems and microbial communities), thereby enabling digital distributed biomanufacturing. Modern AI possesses the potential to revolutionize climate simulations by processing an unprecedented number of complex variables and larger (unlabeled) datasets compared to existing methodologies. This ability is crucial to decoding intricate, nonlinear climate systems and could yield valuable insights into the factors contributing to climate change. Foundation models could enable prediction and control of material behaviors at atomic and molecular levels, pioneering a new era of physical science. These models could predict the optimal arrangement of atoms to deliver desired properties, like greater strength, higher conductivity, or enhanced biocompatibility, enabling the application-specific material design such as carbon capture and conversion. For example, modern AI could enhance the properties of materials such as metal-organic frameworks, membranes for superior carbon capture efficiency, or new catalysts that increase the CO_2 conversion rate.

Modern AI is a crucial enabler for applied energy missions. AI will be instrumental in managing and coordinating microgrids and energy storage solutions, bolstering resilience in fluctuating demand or potential disruptions. Modern AI will be used to optimize cybersecurity and energy generation, distribution, and consumption across various forms of renewable energy, such as wind, solar, and hydroelectric power. This approach will enable more accurate

[1] https://www.science.org/content/article/ai-changing-how-we-do-science-get-glimpse
[2] https://arxiv.org/pdf/2108.07258.pdf
[3] https://www.biorxiv.org/content/10.1101/2022.10.10.511571v1.full.pdf
[4] https://www.synthace.com/blog/chatgpt-for-biology-experiment-design-and-automation

prediction of energy production based on weather patterns and adjust grid operations accordingly to maintain security and stability and reduce waste. Leveraging materials discovery will significantly affect catalysis for energy storage materials and increase energy storage system capacity by orders of magnitude. These advances contribute to the vital goal of achieving net-zero carbon emissions.

AI-driven innovation will span the national security, nuclear security, and nonproliferation enterprise. In this new era, we must operationalize and deploy AI using advanced data fabrics to meet the challenge posed by our strategic competition. A defense nuclear nonproliferation foundation model would be game-changing in our ability to leverage data from high-consequence systems to derive new insights to defend our nation. Moreover, modern AI combined with simulations can advance the development of digital twins of devices and systems that close the gap between materials properties and system performance (e.g., enhancing key attributes in vital materials used in nuclear and other high-consequence systems[5]). As cyber-enabled threats increasingly challenge our nation's infrastructure, having AI tools in our arsenal will be paramount.

AI can optimize laboratory operations. AI holds the potential to accelerate progress, optimize resource utilization, and enhance decision-making within laboratory environments. For example, AI can play a pivotal role in achieving net-zero carbon emissions when laboratories can identify energy consumption patterns, make real-time adjustments, and implement energy-saving measures. Generative AI can provide natural language interfaces that make complex repositories of policies and procedures easily accessible to staff (i.e., hazard databases, material safety data sheets) and synthesize opportunities (i.e., peer-reviewed publications, proposal calls). AI-powered code generation can automate repetitive tasks, facilitate rapid prototyping, and assist in bug detection. These applications have the potential to boost productivity and accelerate the delivery of quality software solutions. Further, AI can be an enabler for staff embracing diversity and inclusivity in how they respond to opportunities, form new teams, and recruit new scientists to join the national laboratories.

Responsible and ethical use of trustworthy AI is paramount. Many U.S. agencies are developing approaches for the responsible use and development of trustworthy AI.[6,7] DOE must approach the implications of modern AI from its unique perspectives and accountabilities while aligning with existing and future regulation.[8,9,10] Responsible and ethical AI frameworks prioritize and instantiate fundamental human and societal values defined by principles of accountability, transparency, and privacy, while limiting unintended bias. Adopting components of existing normative frameworks could benefit the DOE by using metrics and approaches that are measurable and interpretable by global stakeholders. A responsible, ethical, and trustworthy AI framework will help stakeholders build confidence in AI systems. Moreover, well-developed and understood standards, training, and policies offer flexible ways to mitigate risks and manage ethical concerns.

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[5] https://pubs.aip.org/aip/pop/article/28/4/042709/263543/Cognitive-simulation-models-for-inertial

[6] https://www.ai.mil/docs/RAI_Strategy_and_Implementation_Pathway_6-21-22.pdf

[7] https://www.nist.gov/artificial-intelligence

[8] https://oecd.ai/en/dashboards/countries/UnitedStates

[9] https://www.federalregister.gov/documents/2020/12/08/2020-27065/promoting-the-use-of-trustworthy-artificial-intelligence-in-the-federal-government

[10] https://www.whitehouse.gov/ostp/ai-bill-of-rights/

Harnessing the power of modern AI can significantly accelerate scientific discovery, catalyze innovation, and streamline policy-making in critical areas for DOE. Their rapid and efficient use can keep the U.S. at the forefront of global scientific advancement, bolster our leadership in formulating and strategically steering international standards, and maintain our competitive edge in the market for next-generation technologies. Our nation's competitors are actively exploiting the advantages of generative AI; corresponding U.S. investment is needed to avoid falling behind in the global scientific and technology arena and to lead the community such that AI develops in ways consistent with U.S. values. Hence, the strategic use of modern AI within the U.S. is critical to maintaining our national security, economic robustness, and scientific leadership.

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