



Artificial Intelligence and Machine Learning for Energy Applications

NETL leverages artificial intelligence (AI) and machine learning (ML) to drive advancements across its research portfolio. By integrating AI/ML with high-performance computing and advanced data analytics, NETL accelerates innovation in next-generation energy systems, materials discovery, predictive modeling, and infrastructure resilience. These efforts are anchored by specialized AI/ML capability centers and expertise, including the Science-Based Artificial Intelligence/Machine Learning Institute (SAMI) and the Center for Artificial Intelligence and Machine Learning (CAML). These capabilities strengthen the nation's energy systems and increase the productivity and impact of American science and engineering.

R&D Applications

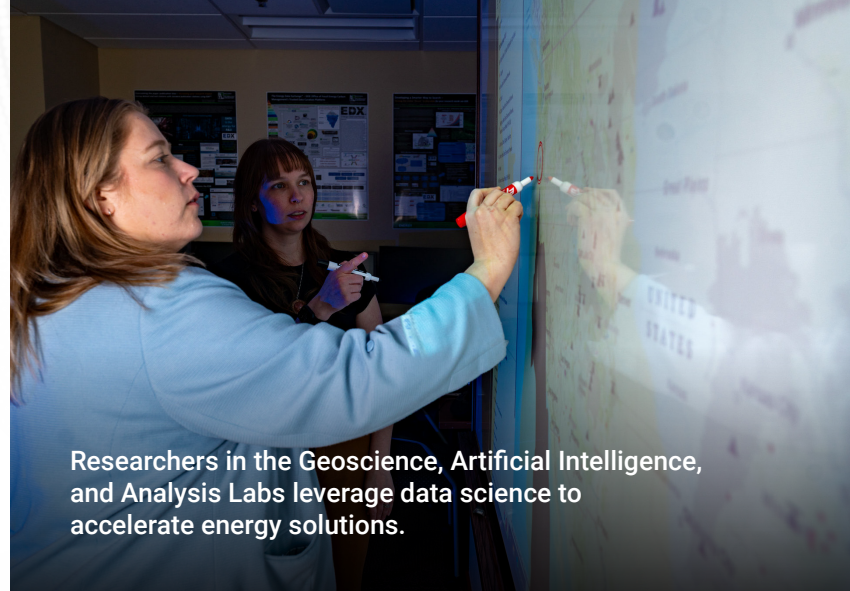
- Resource Discovery and Characterization
- Geospatial Intelligence
- Power Generation
- High-Performance Materials
- Advanced Turbines
- Energy Infrastructure Integrity
- Simulation-Based Engineering
- Cyber-Physical Systems
- Sensors and Controls
- Process Modeling
- Decision Science

Faster Simulations, Smarter Energy Solutions

NETL's ongoing collaboration with Cerebras Systems is transforming scientific computing through pioneering wafer-scale engine research. As a successful public-private partnership, this project leverages NETL's deep domain expertise to aid in the development of cutting-edge AI hardware. This capability significantly shortens R&D timelines, reduces costs, and accelerates the delivery of next-generation energy technologies.



The high-performance Joule 3.0 Supercomputer accelerates energy technology development.



Researchers in the Geoscience, Artificial Intelligence, and Analysis Labs leverage data science to accelerate energy solutions.



Research Highlights

Joule 3.0 Supercomputer Accelerates Energy Technology Development and Advanced AI/ML Simulation

Joule 3.0, NETL's high-performance computing system, delivers 6.11 petaflops of peak performance, enabling advanced modeling for energy research while operating within a highly efficient modular data center. In 2027, NETL will expand its capabilities with the opening of the Computational Science and Engineering Center, which will house Joule 3.0 and provide a hub for advanced computing, AI/ML applications, and systems simulation to accelerate energy technology development.

NETL's SAMI Drives Responsible AI and Collaborative Innovations in Energy Research

Established in 2020, NETL's SAMI accelerates the development and deployment of responsible, trustworthy AI and ML across the laboratory's Centers of Excellence. SAMI provides targeted technical assistance to R&D projects, driving strategic AI applications to solve grand challenges, establishing ethical governance guidelines, and ensuring data integrity and secure repository access. Through these collaborative ventures, alongside crosscutting webinars, developer hackathons, and tech talks, SAMI actively cultivates workforce expertise and fosters the interdisciplinary partnerships necessary to deliver high-performance, data-secure energy solutions.

EDX Spatial Integrates AI To Simplify Geospatial Mapping and Regional Energy Planning

NETL's Energy Data eXchange® (EDX®) is a secure, scalable, cloud native platform providing data access and research collaboration for both DOE users and external partners. EDX Spatial extends the core functionality to include geospatial mapping capabilities, providing private and public access to interactive data, web-based maps, and data dashboards and visualizations. With over 1,000 streaming data layers, EDX Spatial enables users to query and analyze complex data without specialized software or skills. With the upcoming EDX Spatial Assistant, users will be able to use an AI-powered chat bot to help create maps and solve geospatial questions.

Accelerating Real-Time Subsurface Decision Making

Through the SMART (Science-Informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications) initiative, NETL is developing its unified simulation platform consisting of several tools and modules to enable real-time physics-based simulation of coupled subsurface processes. ML-based tools provide quantitatively accurate results at a fraction of the computational cost of process-based simulations, and enable rapid real-time decision support.

Publications

- Creason, C. G., Justman, D., Rose, K., Montross, S., Bean, A., Mark-Moser, M., & Thomas, R. B. (2023). A geo-data science method for assessing unconventional rare-earth element resources in sedimentary systems. *Natural Resources Research*, 32(3), 855-878.
- Ding, J., Fan, S., Liu, G., & Tao, C. (2025). Advancing AI-driven drilling in deep offshore unconventional reservoirs: Progress and prospects. SSRN, 5765908. <http://dx.doi.org/10.2139/ssrn.5765908>.
- Justman, D., Creason, C.G., Montross, S., Mark-Moser, M., Thomas, R.B., Bean, A., & Rose, K. (2021). *Supplementary data for technical report: Towards a geo data science method for assessing rare earth element occurrences in coal and other sedimentary systems*. National Energy Technology Laboratory. <https://edx.netl.doe.gov/dataset/supplementary-data-ree-sed-trs>.
- Tiwari, S. P., Shi, W., Budhathoki, S., Baker, J., Sekizkardes, A. K., Zhu, L., Kusuma, V. A., Hopkinson, D. A., & Steckel, J. A. (2024). Creation of polymer datasets with targeted backbones for screening of high-performance membranes for gas separation. *Journal of Chemical Information and Modeling*, 64(3), 638-652. <https://doi.org/10.1021/acs.jcim.3c01232>
- Wenzlick, M. (2024). *AI/ML challenges and opportunities in materials development*. National Energy Technology Laboratory. <https://doi.org/10.2172/2438427>.

NETL is a U.S. Department of Energy (DOE) national laboratory dedicated to innovating and accelerating the nation's energy solutions in hydrocarbons, geothermal energy, and critical minerals production. The Lab further strengthens its impact by engaging with industry, academia, and other stakeholders through four strategically located Centers of Excellence: Coal, Critical Minerals & Advanced Alloys, Oil & Gas, and Geothermal. With research sites in Albany, Oregon; Morgantown, West Virginia; and Pittsburgh, Pennsylvania, NETL operates as one laboratory to create advanced energy technologies that support DOE's mission and enable affordable, reliable and, secure energy to fuel human prosperity.



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