NATIONAL ENERGY TECHNOLOGY LABORATORY

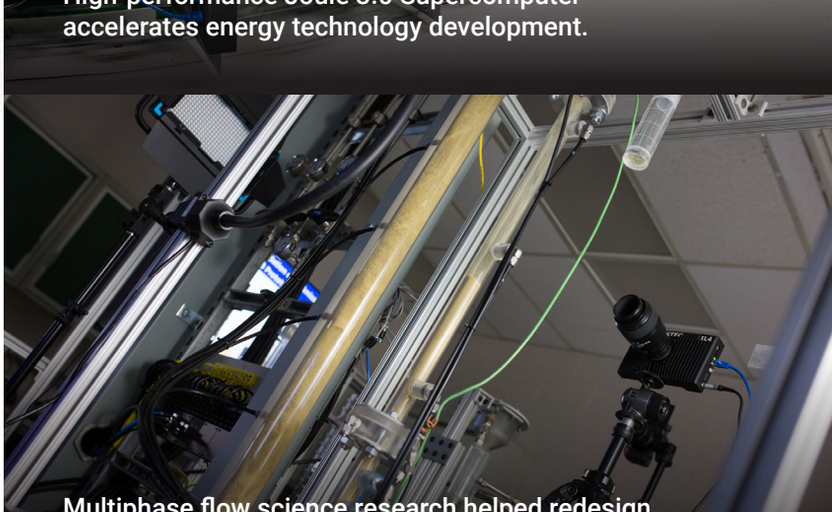
Artificial Intelligence and Machine Learning for Energy Applications

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 capabilities strengthen the security, reliability and affordability of the nation's energy systems.

R&D Applications

- Oil and Natural Gas
- Critical Minerals and Rare Earth Elements
- Advanced Coal Processing
- Subsurface Science
- High-Performance Materials
- Simulation-Based Reactor Design
- Sensors and Controls
- Advanced Turbines
- Power Generation
- Solid Oxide Fuel Cells

High-performance Joule 3.0 Supercomputer accelerates energy technology development.



Multiphase flow science research helped redesign DOE Environmental Management's Integrated Waste Treatment Unit.

Faster Simulations, Smarter Energy Solutions

NETL's ongoing collaboration with Cerebras Systems is transforming scientific computing. Advanced processor architectures can run complex energy simulations up to 470 times faster than traditional supercomputers. This capability significantly shortens R&D timelines, reduces costs and accelerates the delivery of next-generation energy technologies.

Research Highlights

NETL's Hybrid Performance (HyPer) Facility Increases Power Production Efficiency and Flexibility

NETL's HyPer facility was created to support U.S. Department of Energy efforts to research highly efficient power generation technologies that can reduce U.S. dependence on foreign sources of oil and other energy feedstocks. The facility simulates expensive developing technologies and combines them with specific hardware for a cyber-physical system approach. The HyPer facility also serves as a test bed for new sensor and advanced control methods that could improve the performance of existing power plants.

eXtremeMAT Consortium Accelerates Materials Qualification

Through the eXtremeMAT Consortium, NETL led the development of accelerated testing protocols using AI/ML to predict material degradation rates 5 to 10 times faster than traditional methods. These advancements reduced alloy qualification timelines for fossil energy systems by up to 50% and were successfully validated under real-world extreme environment conditions above 1,100°C.

Joule 3.0 Supercomputer and Computational Science and Engineering (CSE) Center

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 CSE 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.

Accelerating Real-Time Decision Making in the Subsurface

Through the Science-informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications (SMART) initiative, NETL developed the Unified Simulation Module (USM) to enable real-time simulation of coupled subsurface processes, supporting rapid decision-making for carbon storage and management. ML surrogate models under SMART reduced uncertainty in CO_2 storage efficiency estimates by up to 30%, while the SMART Visualization and Decision Support Platform integrates field data with predictive modeling to enhance operational control.

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.
- Epting, W. K., Lei, Y., Mason, J. H., Abernathy, H. W., Kalapos, T., & Hackett, G. A. (2021). Optimization of SOFC electrode microstructures with long term performance modeling and machine learning. ECS Transactions, 103(1), 909.
- 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, 5/24/2021, https://edx.netl.doe.gov/dataset/supplementary-data-ree-sed-trs.
- Rose, K., Bauer, J.R., and Mark-Moser, M., 2020, A systematic, science-driven approach for predicting subsurface properties, Interpretation, 8:1, 167-181 https://doi.org/10.1190/INT-2019-0019.1.
- Tiwari, S. P., Shi, W., Budhathoki, S., Baker, J., Sekizkardes, A. K., Zhu, L., Kusuma, V. A., Hopkinson, D. A., and 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.

NETL is a U.S. Department of Energy (DOE) national laboratory dedicated to innovating and accelerating the nation's energy solutions in hydrocarbon, geothermal energy and critical minerals production. 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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