Artificial Intelligence, Machine Learning, and Data Analytics

NATIONAL ENERGY TECHNOLOGY LABORATORY

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Energy applications for artificial intelligence (AI), machine learning (ML), and data analytics (DA) provide innovative ways to augment the National Energy Technology Laboratory's (NETL's) ongoing mission for the U.S. Department of Energy/Office of Fossil Energy to find more efficient methods to use the Nation's abundant energy resources for a thriving economy, a cleaner environment, and continued energy security.

Artificial Intelligence, Machine Learning, and Data Analytics

Artificial intelligence (AI) refers to machines that can – for a given set of human-defined objectives – learn, predict and make decisions, significantly increasing the speed and efficacy of decision making. Most AI applications use algorithms known as **machine learning (ML)** to find patterns in massive amounts of data. The patterns are then used for making predictions. The automated methods capturing, organizing, and processing the data used by ML are known as **data analytics (DA)**. At the National Energy Technology Laboratory (NETL), these tools are used to accelerate numerous areas of energy technology development.

AI is becoming an increasingly familiar and practical feature of scientific research and development (R&D). It promises to drive growth of the U.S. economy, enhance national security, and improve quality of life. AI has become an important area of interest for NETL and it is making a significant impact in the way that NETL analyzes critical data for decision making related to operating power plants. NETL-sponsored AI innovations improve condition-based monitoring of operational conditions; facilitate new levels of cybersecurity to protect energy assets; and spearhead innovative diagnostic inspections using AI-enabled robots for automated, non-destructive evaluation and repairing power plant boilers.

NETL is also exploring ML applications for use in subsurface energy resource recovery and underground carbon storage. ML can capture the behavior of complex systems through rapid empirical models, quickly providing tools to decision makers with minimum labor and **dramatically lowering the cost of processing monitoring data**. In combination with sensor and control systems, ML also can improve efficiency in natural gas reservoir and subsurface carbon dioxide (CO_2) management and improve risk management, creating **safer conditions and reducing environmental risks**.

Researchers use AI, ML, and DA to create learning algorithms within large datasets to help discover new materials, optimize processes, and run autonomous systems. Computers can find patterns in data that people may overlook, and at speeds that are hundreds to thousands of times faster than traditional human-centric analysis techniques.

Artificial intelligence (AI)

Machines that can learn, predict, and make decisions

Machine learning (ML)

Algorithms that find patterns in massive amounts of data

Data analytics (DA)

Automated method to capture, organize, and process massive amounts of data

Using AI and ML to Improve Electricity Generation

NETL is identifying ways to strengthen and utilize existing fossil energy plants to provide affordable, near-term energy security benefits and support future power and infrastructure needs amidst a changing energy landscape. As these efforts progress, NETL expects **dramatic improvements in cost, efficiency, and environmental performance**.

Plant Maintenance

Dependable, long-term monitoring contributes to power plant reliability but monitoring component condition in real time presents significant technical challenges in key technology development areas. To mitigate these issues, NETL's R&D on predictive maintenance uses data from a diverse set of sensors and applies ML to diagnose emerging faults before they occur, ultimately switching from a culture of preventive maintenance to one of condition-based maintenance.

NETL-funded projects avoid destructive inspections such as cutting open a boiler by conducting non-destructive evaluation (NDE) for damage detection using autonomous robots outfitted with onboard sensor technology, **saving both time and money**. Types of damage detected can include wear, cracks, surface defects, and weld contamination. AI and ML provide smart data analysis (based on historical information and enhanced with real-time measurements) and autonomy and help direct in-situ cleaning and repairs.

ML augmented sensors and controls can also identify operational discontinuities and inform decisions on operational efficiency, **enabling plants to operate more effectively** when required to cycle more frequently than originally engineered.

Digital Twinning

Digital twinning complements ML. NETL is developing a computational model and using visualization to understand and predict the impact of potential process changes in a digital/virtual environment before applying those changes in the real world. A digital twin is also used to replicate wear on engines and turbines, **making maintenance more efficient**. Other NETL-funded projects are using digital twinning to investigate improvements on the flexible operation of existing coal-fired power plants and helping to determine the optimum application of advanced manufacturing techniques to advance rotating detonation engine injector design.

Power Plant Operations Improvement

NETL is developing and demonstrating the capability to systematically reduce detailed computational fluid dynamics (CFD) simulations of boilers into surrogate models for prognostics and diagnostics during power plant operation. This R&D uses ML to exploit the information available from detailed CFD models in a real-time tool for making practical decisions about how to operate coal plants at part-load.

Other NETL-funded projects are using ML models to improve solid oxide fuel cell (SOFC) geometry, reliability, and degradation.

Transforming Fossil Energy Plants with AI/ML/DA

- Improve maintenance
- Diagnose problems early
- Reduce outages and downtime
- Prevent and detect damage
- Improve flexible operation
- Reduce emissions
- Increase efficiency
- Reduce cost of energy
- Improve cybersecurity

Materials Development

Future coal systems require improved materials to operate in harsh environments, such as extreme pressure, high temperature, and vibration, fatigue, or stress states. NETL's high-performance material development concentrates on advanced manufacturing methods and computational materials modeling to characterize materials properties involved in diverse applications of interest. This includes catalysts and electrocatalysts, solid and liquid membranes for gas capture and separation, oxygen carrier materials, materials for Solid Oxide Fuel Cell applications, and novel nanostructured materials for energy conversion and developing gas sensors.

ML and DA are helping overcome key challenges in developing, modifying, and qualifying new materials. NETL is leading eXtremeMAT, a multi-lab initiative using DA and physics-based models, including quantum mechanics calculations and Monte Carlo simulations to develop and deploy new alloy materials that are affordable and reliable under the harsh environments encountered in power plants.

Cybersecurity

NETL-funded cybersecurity activities use ML and DA to **more robustly detect cyber attacks** on energy generation, transmission, and distribution systems. Captured data provides a baseline that can generate analytical trends and create behavior analysis platforms, providing cybersecurity for fossil power generation infrastructure. Results include predictive anomaly detection methodologies and automated situational awareness of cybersecurity threats within fossil energy power plants.

For power plant control systems, industrial control systems, and electrical grid applications, efforts are underway to address critical cybersecurity threats by leveraging AI and blockchain technologies. Similar applications enable secure energy transactions, increasing grid reliability and implementing a more decentralized energy infrastructure.

Using AI and ML to Advance Subsurface Science

Advances in data collection technologies, more efficient methodologies for data storage, and high-performance computing capabilities create a framework for the broad application of ML and data-driven approaches. This applies to subsurface processes related to the production of oil and gas and the permanent underground storage of CO_2, among others.

Investments by the U.S. Department of Energy's (DOE) Office of Fossil Energy (FE) to develop rapid predictive modeling capabilities using ML algorithms and reduced order models (ROMs) will help build upon and accelerate these industry advances. A rapid "data to knowledge" approach helps operators, regulators, and other stakeholders understand and characterize subsurface processes to **support informed decision making**.

Data Characterization

NETL has made several technological advances related to better understanding subsurface features and geomechanical/geochemical processes. These advanced technologies provide data to better understand reservoir characteristics and their relation to efficient storage of CO_2 and production of oil and natural gas resources. In addition to these enabling technologies, tools, and processes, NETL funds several field-based research projects, acting as data sources for developing ML algorithms, ROMs, and other tools to better evaluate and analyze large datasets.

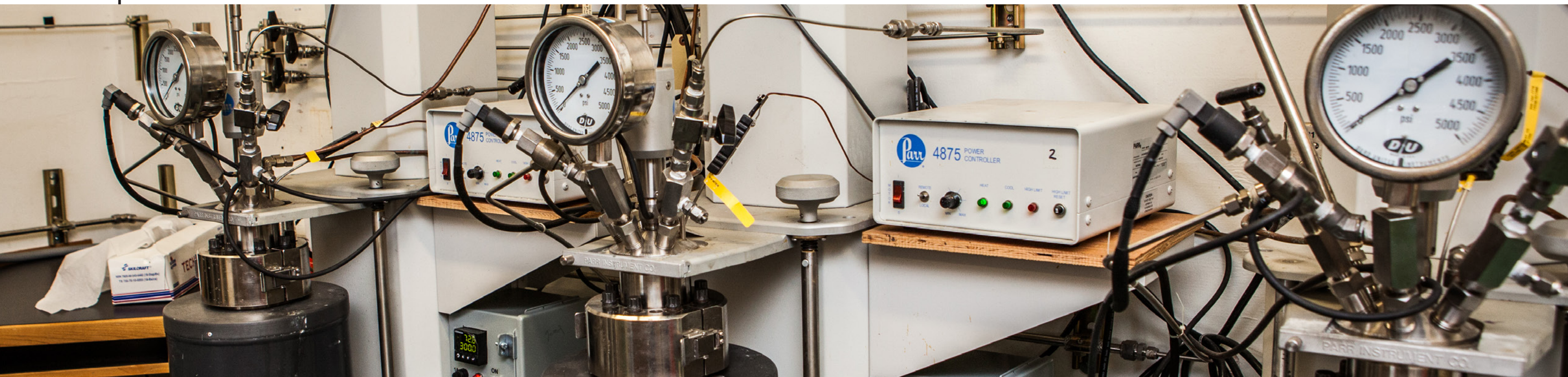
NETL's Regional Carbon Sequestration Partnerships (RCSPs) and Carbon Storage Assurance Facility Enterprise (CarbonSAFE) initiatives focus on characterizing potential CO_2 storage formations and the field demonstration of large-scale CO_2 storage. NETL's Oil & Natural Gas field laboratories are focused on improving extraction of oil and natural gas from both established and emerging resources. The ability to deploy new technologies that collect, analyze, or validate large volumes of subsurface data provides stakeholders the opportunity to **improve decision-making processes and best practices, optimizing resource use and value**.

Predictive Modeling

NETL is developing tools that use DA and ML to better characterize subsurface reservoirs, to more rapidly assess the results of operational choices, and to better predict how the subsurface will respond during operations.

Industry has made significant investments applying DA to subsurface operations in the past several years. NETL plays a key role in accelerating deployment of DA for subsurface problems, particularly by validating them in a field setting. Using ML to develop real-time analytical capabilities with the potential to optimize subsurface operations also can **reduce costs and improve safety during oil and gas extraction and CO_2 storage.**

The greatest potential for transformative impacts in subsurface applications will come from combining ML with physics-based and chemistry-based models. This fundamental change involves leveraging data (measurements), science-based models, and ML to characterize and visualize key reservoir processes, better informing real-time decision making for reservoir management. For the subsurface, this transformational shift can support a myriad of applications, including oil and natural gas production and the long-term storage of CO_2.



Transforming Subsurface Science with AI/ML/DA

- Efficiently analyze large geologic datasets
- Improve understanding of geophysical conditions and reactions to injection/recovery
- Improve subsurface visualization for enhanced characterization
- Improve well integrity and completion design
- Increase hydrocarbon recovery
- Reduce environmental impacts
- Improve dynamic forecasting of reservoir response
- Improve autonomous monitoring and control of injection and production operations

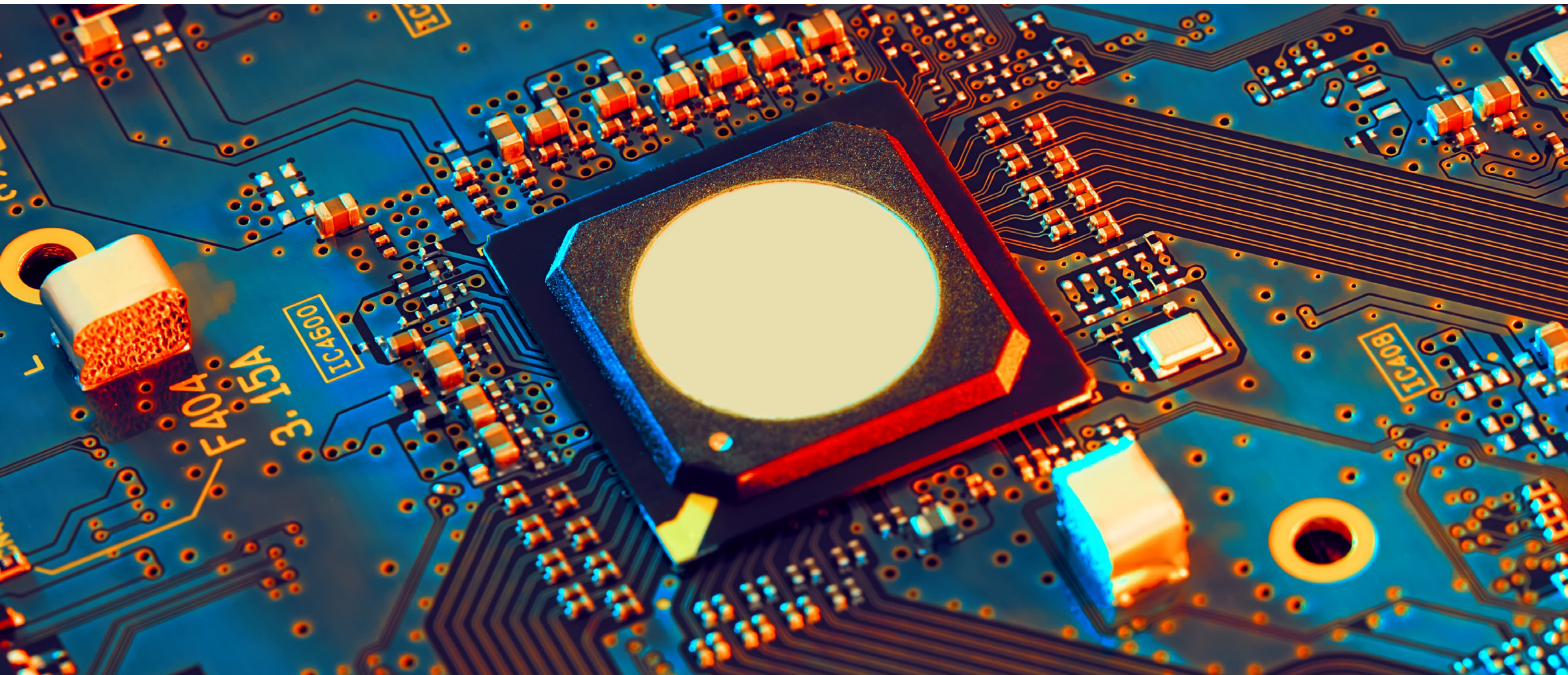
Science-Informed Machine Learning for Accelerated Real-Time (SMART) Decisions Initiative

DOE's Carbon Storage and Oil & Natural Gas Programs created the Science-Informed Machine Learning for Accelerated Real-Time (SMART) Decisions in the subsurface initiative to support real-time analysis leading to dramatic improvements in subsurface visualization, dynamic forecasting, and autonomous control.

This initiative:

- Improves operations in complex subsurface systems;
- Builds on prior investments in empirical models and ML, advanced sensors and data management, and predictions of subsurface system behavior; and
- Focuses on real-time visualization, real-time forecasting, and rapid data to knowledge.

A better understanding of these dynamic processes will help improve the production efficiency of oil and natural gas resources and facilitate the safe, efficient storage of CO_2 in the subsurface.



NETL Predictive Modeling Tools that Leverage AI/ML/DA

NETL utilizes an extensive suite of predictive modeling tools that leverage AI/ML/DA in support of the DOE/FE mission.

IDAES
Institute for the Design of Advanced Energy Systems

The Institute for the Design of Advanced Energy Systems (IDAES)

The Institute for the Design of Advanced Energy Systems (IDAES) is a resource for developing and optimizing innovative advanced energy systems via process systems engineering tools and approaches. The open source IDAES computational framework supports developing new concepts for energy systems. Due to the complexity of energy systems and an increasing need to operate dynamically, IDAES models support tightly coupled multi-scale optimization of processes with the bulk power system, while incorporating uncertainty quantification techniques. This includes a process model library and optimization-based ML tools for creating thermophysical property models, reaction models, and general surrogate models.

Offshore Risk Modeling (ORM) Suite

NETL's Offshore Risk Modeling (ORM) suite supports DOE goals for offshore spill prevention and data-driven risk assessments for oil and natural gas industry activities. ORM improves offshore oil and gas operational strategies and resource assessments using novel DA, ML, and advanced visualization techniques optimized for the offshore. ORM can be used in daily operations as well as long-term planning to improve decision making, and it helps ensure that the United States is prepared for future rapid response needs (e.g., hurricane impacts, oil spill scenario planning).

GOGI

Global Oil and Gas Infrastructure Database

The Global Oil and Gas Infrastructure (GOGI) database demonstrates novel DA and ML methods and tools developed by NETL to rapidly and efficiently find, access, integrate, and use internet data to map and assess global oil and gas infrastructure. The GOGI database is funded by the United Nations Environment Programme (UNEP) and 10 of the world's largest oil and gas companies to improve infrastructure maintenance and reduce their environmental footprint.

MFiX

Multiphase Flow Science Tools (MFix)

NETL's suite of multiphase CFD code, called Multiphase Flow with Interphase eXchanges (MFiX), is developed for modeling reacting multiphase systems. This open source suite of software tools has more than three decades of development history and more than 5,000 registered users worldwide. This software is the standard test bed for comparing, implementing, and evaluating multiphase flow constitutive models. In a project called "CFD for Advanced Reactor Design (CARD)," NETL's in-house MFiX group uses AI to accelerate CFD codes.

Carbon Capture Simulation for Industry Impact (CCSI2)

The Carbon Capture Simulation for Industry Impact (CCSI2) is a partnership among national laboratories, industry, and academic institutions that develops, deploys, and utilizes state-of-the-art computational modeling and simulation tools. CCSI2's open source, R&D 100 award-winning computational toolset provides end users in industry with a comprehensive, integrated suite of scientifically-validated models with uncertainty quantification, optimization, risk analysis, and intelligent decision-making capabilities. CCSI2 utilizes a variety of ML methods within its Framework for Quantification of Uncertainty and Surrogates (FOQUS), helping generate optimal experimental designs that maximize the learning from costly laboratory and pilot scale experiments, reducing technical risk. CCSI2 also employs DA and ML to accelerate the solution of complex models for the detailed design of novel carbon capture devices and components that utilize advanced manufacturing to enable process intensification.

NETL Capability Centers for AI/ML/DA

NETL established and leads the Science-Based Artificial Intelligence/Machine Learning Institute (SAMI), a joint institute for AI and ML. NETL has created SAMI's required computational infrastructure, including the Joule 2.0 supercomputer, the Watt computer for data analysis, and the Energy Data eXchange (EDX), supporting the entire life cycle of data with secure, private, collaborative workspaces for research projects. NETL also is investing in new infrastructure to support SAMI, including the Center for Artificial Intelligence and Machine Learning (CAML) at NETL-Pittsburgh and a Computational Science and Engineering (CSE) Center at NETL-Morgantown.

Science-Based Artificial Intelligence/Machine Learning Institute (SAMI)

The Science-based Artificial Intelligence/Machine Learning Institute (SAMI) combines the strengths of NETL's fossil energy subject matter experts, computational scientists, and data scientists with experts in AI/ML at external institutions. SAMI is supported by NETL's supercomputer and AI/ML computer hardware. SAMI accumulates ML knowledge in analytical projects; enhances data handling functions, including curation, management, and data transformation; and combines physics-based modeling and AI/ML to address previously unanswerable problems. SAMI supports lab initiatives in fossil energy integration, optimization, and resiliency and real-time decision science for the subsurface, as well as NETL's effort to develop and screen materials for carbon capture.

Center for Artificial Intelligence and Machine Learning (CAML)

NETL's Center for Artificial Intelligence and Machine Learning (CAML) houses computer hardware and software allowing researchers to explore problems using AI and ML. The center features a machine designed to house, transport, and process up to 19 petabytes of data using cutting-edge algorithms developed by NETL and external collaborators.

Center for Computational Science and Engineering (CSE)

NETL is home to Joule 2.0, which is among the fastest, largest, and most energy-efficient supercomputers in the United States. The powerful 4-petaflop system allows researchers to simulate energy technologies at various scales with the help of physics-based models such as density functional theory, molecular dynamics, Monte Carlo simulations, microkinetic models, phase-field models, computational fluid dynamics, and others. Most of the research projects at NETL use such simulations to save time and resources in support of successful technology development.