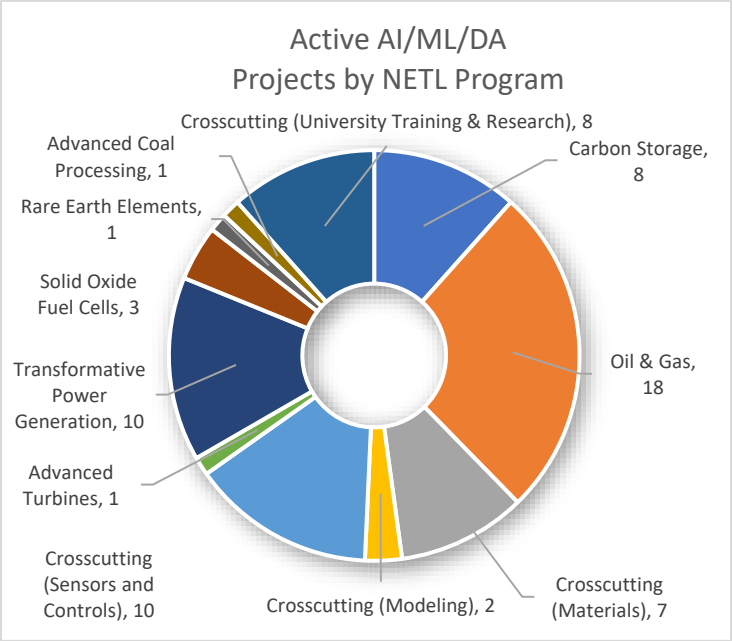
Artificial Intelligence, Machine Learning, and Data Analytics at NETL

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 massive amounts of 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.

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) ongoing mission for the U.S. Department of Energy/Office of Fossil Energy (DOE/FE) to find more efficient methods to use the nation's abundant energy resources for a thriving economy, a cleaner environment, and continued energy security.

69 FE R&D projects with total funding of more than $254 million currently utilize AI, ML, or DA (see chart), including 56 extramural FE projects and 13 internal NETL projects. In addition, there are 23 Office of Electricity and Office of Cybersecurity, Energy Security, and Emergency Response projects managed by NETL.



Transforming Subsurface Science AI/ML/DA can:

- Analyze large geologic datasets efficiently
- 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

Transforming Fossil Energy Plants AI/ML/DA can:

- 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

Applying AI/ML/DA techniques and science-based models helps NETL scientists and projects achieve breakthroughs in meeting the needs of existing U.S. electric power plants, next-generation advanced energy systems, and subsurface operations involving oil and gas operations and carbon storage.

NETL R&D Applications in AI/ML/DA

DOE's fossil energy research and development (R&D) programs are taking advantage of ***new opportunities over a broad range of potential applications for AI, ML, and DA techniques. These techniques help researchers ask more relevant questions and design better experiments to reach development goals at a faster pace. With continued growth in the speed and computational power of supercomputers, these tools are becoming increasingly useful to the energy research landscape.***

The table below shows the AI/ML/DA applications being investigated under fossil energy R&D programs.

AI/ML/DA Application	Fossil Energy R&D Programs										
	Carbon Storage	Oil & Gas	High-Performance Materials	Modeling and Simulation	Sensors and Controls	University Training and Research	Advanced Turbines	Trans. Power Gen.	Solid Oxide Fuel Cells	Rare Earth Elements	Advanced Coal Processing
Predictive Maintenance								X			
Digital Twins				X							
Agent-Based Controls/Online System Identification					X						
Power Plant Components			X				X		X		
Condition-Based Monitoring					X		X	X			
Materials Development			X	X					X		
Cybersecurity					X	X					
Damage Detection						X		X			
Process Optimization and Control			X	X	X	X	X	X	X		
Data Characterization	X	X									X
Predictive Methods	X	X								X	

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.

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).

Global Oil and Gas Infrastructure (GOGI) 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.

Multiphase Flow Science Tools (MFiX)

NETL's suite of multiphase computational fluid dynamics (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. The software is the standard testbed 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 ($CCSI^2$)

The Carbon Capture Simulation for Industry Impact ($CCSI^2$) is a partnership among national laboratories, industry, and academic institutions that develops, deploys, and utilizes state-of-the-art computational modeling and simulation tools. $CCSI^2$'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. $CCSI^2$ 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. $CCSI^2$ 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/Data Analytics

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, CFD, and others. Most of the research projects at NETL use such simulations to save time and resources in support of successful technology development.

Appendix: Active NETL AI/ML/DA Projects

Program	Performer	Project Title	Project Number	NETL Technology Manager
Advanced Coal Processing	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	COAL DATA – Building the American Coal Database tool for beneficiating coal and coal waste streams	FWP-1022432	Joseph Stoffa
Carbon Storage	University of Texas at Austin	Development of a Framework for Data Integration, Assimilation, and Learning for Geological Carbon Sequestration	FE0026515	Mark McKoy
Carbon Storage	New Mexico Institute of Mining and Technology	Improving Subsurface Stress Characterization for Carbon Dioxide Storage Projects by Incorporating Machine Learning Techniques	FE0031684	Mark McKoy
Carbon Storage	Sandia National Laboratories (SNL)	FWP Support for: Identification of Faults Susceptible to Induced Seismicity: Integration of Forward and Joint Inversion Modeling, Machine Learning, and Field Calibrated Geologic Models	FWP-18-021006	Mark McKoy
Carbon Storage	Los Alamos National Laboratory (LANL)	Support for Regional Initiative to Accelerate CCUS Deployment in Midwestern and Northeastern USA	FWP-FE-1142-19-FY20	Mark McKoy
Carbon Storage	Los Alamos National Laboratory (LANL)	Southeast Regional Carbon Storage Partnership: Phase IV	FWP-FE-1143-19-FY20	Mark McKoy
Carbon Storage	University of Illinois at Urbana-Champaign	Identification of Faults Susceptible to Induced Seismicity	FE0031685	Mark McKoy
Carbon Storage	Pennsylvania State University	Integration of Seismic-Pressure-Petrophysics Inversion of Continuous Active-Seismic Monitoring Data for Monitoring and Quantifying CO2 Plume	FE0031544	Mark McKoy
Carbon Storage	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Carbon Storage Data FWP, Task 27.0 Next Generation Development, Deployment, and Modernization of Database, Tools, Online Viewer, and Atlas; Task 28.0 Curation of Carbon Storage R&D Products Through Advanced Data Computing Solutions; Task 29.0 CS Digital Core Data Management Tool	FWP-1022465	Mark McKoy
Crosscutting (High Performance Materials)	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	eXtremeMAT - Accelerated Design and Manufacture of Next Generation Extreme Environment Materials	FWP-1022433	Briggs White

Program	Performer	Project Title	Project Number	NETL Technology Manager
Crosscutting (High Performance Materials)	Pennsylvania State University	High Throughput Computational Framework of Materials Properties for Extreme Environments	FE0031553	Briggs White
Crosscutting (High Performance Materials)	Missouri State University	Multi-modal Approach to Modeling Creep Deformation In Ni-Base Superalloys	FE0031554	Briggs White
Crosscutting (High Performance Materials)	Oak Ridge National Laboratory (ORNL)	Components Fabricated by Additive Manufacturing	FWP-FEAA128	Briggs White
Crosscutting (High Performance Materials)	University of Maine	Ultrasonic Measurements of Temperature Profile and Heat Fluxes in Coal-Fired Power Plants	FE0031559	Briggs White
Crosscutting (High Performance Materials)	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Advanced Alloy Development	FWP-1022406	Briggs White
Crosscutting (High Performance Materials)	Carnegie Mellon University	Computer vision and machine learning making the processing-microstructure- property connection in heat resistant alloys	UCFER-04-20	Sydni Credle
Crosscutting (Modeling, Simulation, and Analysis)	Southwest Research Institute	Digital Twin Model for Advanced Manufacture of a Rotating Detonation Engine Injector	FE0031644	Sydni Credle
Crosscutting (Modeling, Simulation, and Analysis)	NETL, CMU, SNL, WVU, LBNL	IDAES - Institute for the Design of Advanced Energy Systems	FWP-1022423	Sydni Credle
Crosscutting (Sensors and Controls)	Siemens Corporation	Novel Temperature Sensors and Wireless Telemetry for Active Condition Monitoring of Advanced Gas Turbines	FE0026348	Sydni Credle
Crosscutting (Sensors and Controls)	Georgia Tech Research Corporation	Real-Time Health Monitoring for Gas Turbine Components using Online Learning and High Dimensional Data	FE0031288	Sydni Credle
Crosscutting (Sensors and Controls)	Southern Company Services, Inc.	Operational Technology Behavioral Analytics	FE0031640	Sydni Credle

Program	Performer	Project Title	Project Number	NETL Technology Manager
Crosscutting (Sensors and Controls)	Expert Microsystems	Hybrid Analytics Solution to Improve Coal Power Plant Operations	FE0031753	Sydni Credle
Crosscutting (Sensors and Controls)	Sonalysts, Inc.	Metaphortress: A Situational Awareness Platform	SC0018729	Sydni Credle
Crosscutting (Sensors and Controls)	West Virginia University Research Corporation	Boiler Health Monitoring using a Hybrid First Principles-Artificial Intelligence Model	FE0031768	Sydni Credle
Crosscutting (Sensors and Controls)	General Electric (GE) Company	Deep Analysis Net with Casual Embedding for Coal Fired Power Plant Fault Detection and Diagnosis	FE0031763	Sydni Credle
Crosscutting (Sensors and Controls)	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Advanced Sensors and Controls: Task 5.1 - Development and Testing of Agent Based Controls for Power Systems	FWP-1022427	Sydni Credle
Crosscutting (Sensors and Controls)	National Rural Electric Cooperative Association	Generation Plant Cost of Operations and Cycle Optimization Model	FE0031751	Sydni Credle
Crosscutting (Sensors and Controls)	Sporian Microsystems, Inc.	A Spectroscopy-Based, Online, Real-time Monitoring System with Integrated Machine Learning for Liquid Phase Selenium in Coal Power Plant Effluent Streams	SC0020797	Sydni Credle
Crosscutting (University Training & Research)	University of Texas at San Antonio	A General Drag Model for Assemblies of Non-Spherical Particles Created with Artificial Neural Networks	FE0031894	Sydni Credle
Crosscutting (University Training & Research)	University of Missouri	A Robotics Enabled Eddy Current Testing System for Autonomous Inspection of Heat Exchanger Tubes	FE0031645	Sydni Credle
Crosscutting (University Training & Research)	Colorado School of Mines	AI Enabled Robots for Automated Nondestructive Evaluation and Repair of Power Plant Boilers	FE0031650	Sydni Credle

Program	Performer	Project Title	Project Number	NETL Technology Manager
Crosscutting (University Training & Research)	Florida International University	Secure Data Logging and Processing with Blockchain and Machine Learning	FE0031745	Sydni Credle
Crosscutting (University Training & Research)	Florida International University	Development of a Pipe Crawler Inspection Tool for Fossil Energy Power Plants	FE0031651	Sydni Credle
Crosscutting (University Training & Research)	University of Texas at El Paso	Autonomous Aerial Power Plant Inspection in GPS-Denied Environments	FE0031655	Sydni Credle
Crosscutting (University Training & Research)	New Mexico State University	A Lizard-Inspired Tube Inspector (LTI) Robot	FE0031649	Sydni Credle
Crosscutting (University Training & Research)	Florida International University	Development and Evaluation of a General Drag Model for Gas-Solid Flows Via Physics-Informed Deep Machine Learning	FE0031904	Sydni Credle
Oil & Gas	Southwest Research Institute (SwRI)	Smart Methane Emission Detection System Development	FE0029020	Jared Ciferno
Oil & Gas	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Offshore Research: Task 3.0 Assessing Current and Future Infrastructure Hazards; Task 5.0 Geohazards & Subsurface Uncertainty Smart Modeling; Task 6.0 Infrastructure and Metocean Technology; Task 10.0 Smart Models to Optimize Use or Reuse of Platforms for EOR; Task 11.0 Integrated Geologic and Techno-Economic Assessment of Offshore Systems for CO2-EOR Deepwater/Ultradeep Water	FWP-1022409	Roy Long
Oil & Gas	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Natural Gas Infrastructure: Task 2.0 Sensor Devices and Enabling Technologies; Task 7.3 Geospatial Analytics for Optimized Sensor Deployment and Utilization; Task 7.5 Geo-Data Science to Assess and Identify Pipeline Reuse & Optimization Opportunities for EOR	FWP-1022424	Jared Ciferno

Program	Performer	Project Title	Project Number	NETL Technology Manager
Oil & Gas	Pacific Northwest National Laboratory (PNNL)	Novel Signatures from Deployed Sensors for Natural Gas Transmission Pipelines	FWP-72954	Jared Ciferno
Oil & Gas	University of North Dakota Energy and Environmental Research Center (UNDEERC)	Improving Enhanced Oil Recovery Performance Through Data Analytics and Next-Generation Controllable Completions	FE0031790	Jared Ciferno
Oil & Gas	Battelle Memorial Institute	Chemically Enabled Carbon Dioxide Enhanced Oil Recovery in Multi-Porosity, Hydrothermally Altered Carbonates in the Southern Michigan Basin	FE0031792	Jared Ciferno
Oil & Gas	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Onshore Unconventional Resources	FWP-1022415	Jared Ciferno
Oil & Gas	WVU	Marcellus Shale Energy and Environment Laboratory (MSEEL)	FE0024297	Jared Ciferno
Oil & Gas	University of Utah	Improving Production in the Emerging Paradox Oil Play	FE0031775	Jared Ciferno
Oil & Gas	University of Wyoming	Unlocking the Tight Oil Reservoirs of the Powder River Basin, Wyoming	FE0031779	Jared Ciferno
Oil & Gas	Clemson University	All-digital Sensor System for Distributed Downhole Pressure Monitoring in Unconventional Fields	FE0031781	Jared Ciferno
Oil & Gas	Battelle Memorial Institute	Using Natural Gas Liquids to Recover Unconventional Oil and Gas Resources	FE0031782	Jared Ciferno
Oil & Gas	University of Kentucky	Conasauga Shale Research Consortium	FE0031783	Jared Ciferno
Oil & Gas	University of Kansas Center for Research, Inc.	A Novel “Smart Microchip Proppants” Technology for Precision Diagnostics of Hydraulic Fracture Networks	FE0031784	Jared Ciferno
Oil & Gas	University of North Dakota Energy and Environmental Research Center (UNDEERC)	Carbon Dioxide Enhanced Oil Recovery Improvement In Conventional Fields Using Rich Gas	FE0031789	Jared Ciferno
Oil & Gas	University of Texas at Austin	Engineered Water for Improved Oil Recovery from Fractured Reservoirs	FE0031791	Jared Ciferno
Oil & Gas	University of New Mexico	Solid State Mixed-Potential Electrochemical Sensors for Natural Gas Leak Detection and Quality Control	FE0031864	Jared Ciferno

Program	Performer	Project Title	Project Number	NETL Technology Manager
Oil & Gas	NETL, NAESB, Industry partners	Use of digital methods (DL) for natural gas contract execution	N/A	Jared Ciferno
Oil & Gas	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Natural Gas Hydrate Research	FWP-1022410	Joseph Stoffa
Rare Earth Elements	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Rare Earth Elements from Coal and Coal By-Products Task 9.0: Development of a Sedimentary REE Resource Assessment Method	FWP-1022420	M.A. Alvin
Solid Oxide Fuel Cells	Oak Ridge National Laboratory	Reliability of Materials and Components for Solid Oxide Fuel Cells - Task 5: Non-Conventional SOFC Geometries; Task 4: Advanced Manufacturing of SOFC	FWP-FEAA121	Shailesh Vora
Solid Oxide Fuel Cells	Pacific Northwest National Laboratory	SECA Core Technology Program - PNNL - Task 2: SOFC Modeling	FWP-66841	Shailesh Vora
Solid Oxide Fuel Cells	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Solid Oxide Fuel Cells Task 2: Cell and Stack Degradation Evaluation and Modeling	FWP-1022411	Shailesh Vora
Transformative Power Generation	GE Steam Power, Inc.	Extended Low Load Boiler Operation to Improve Performance and Economics of an Existing Coal Fired Power Plant	FE0031546	John Rockey
Transformative Power Generation	University of Utah	Deployment of Dynamic Neural Network Optimization to Minimize Heat Rate During Ramping for Coal	FE0031754	John Rockey
Transformative Power Generation	National Energy Technology Laboratory (NETL) Research Innovation Center (RIC)	Transformational Technologies for New and Existing Plants (TTNEP) Task 3.0: Optimizing Dynamics for Performance and Reliability; Task 4.0: Sensors, Diagnostics, and Control for Performance and Reliability; Task 6.0: CFD-Based Reduced Order Model	FWP-1022461	John Rockey
Transformative Power Generation	Clemson University	Test and Validate Distributed Coaxial Cable Sensors for In Situ Condition Monitoring of Coal-Fired Boiler Tubes	FE0031765	John Rockey
Transformative Power Generation	Microbeam Technologies, Inc.	Demonstration of Multi-Gamma Based Sensor Technology for As-Fired Coal Property Measurement	FE0031750	John Rockey
Transformative Power Generation	Electric Power Research Institute, Inc.	Integrated Boiler Management through Advanced Condition Monitoring and Component Assessment	FE0031683	John Rockey

Program	Performer	Project Title	Project Number	NETL Technology Manager
Transformative Power Generation	Reaction Engineering International	Development of Miniaturized High-Temperature Multi-Process Monitoring System	FE0031682	John Rockey
Transformative Power Generation	Reaction Engineering International	Combustion Performance and Emissions Optimization Through Integration of a Miniaturized High-Temperature Multi Process Monitoring System	FE0031680	John Rockey
Transformative Power Generation	West Virginia University Research Corporation	High Temperature Electrochemical Sensors for In-Situ Corrosion Monitoring in Coal-Based Power Generation Boilers	FE0031548	John Rockey
Transformative Power Generation	Microbeam Technologies, Inc.	Improving Coal Fired Plant Performance through Integrated Predictive and Condition-Based Monitoring Tools	FE0031547	John Rockey
Turbines	University of Pittsburgh	An Effective Quality Assurance Method For Additively Manufactured Gas Turbine Metallic Components Via Machine Learning From In-Situ Monitoring, Part-Scale Modeling, and Ex-Situ Characterization Data	FE0031774	Richard Dennis