Use Case Name	Agency	Bureau/Department	Summary of Use Case	Stage of System Development Life Cycle	Date Development/Acquisition Began	Date Implemented	Contact Name	Contact Email	Developer Information	Consistent with EO 13960	AI Techniques Used	Training Data Origin	Releaseable to the Public
Groundwater Modeling	U.S. Department of Energy	Office of Legacy Management	Groundwater modeling includes parameter estimation			2003-01-01	Kathleen Whysner	kathleen.whysner@lm.doe.gov	Commercial-off-the-shelf			Target levels orginate in the LM data sets	Yes
Memorandum of Understanding Between the US DOE and US NRC on Cooperation in the Area of Operating Experience and Applications of Data Analytics (Signed June 2021)	U.S. Department of Energy	Office of Environment, Health, Safety & Security	The purpose of the Memorandum of Understanding (MOU) between the US DOE and US NRC on cooperation in the area of operating experience and applications of data analytics (Signed June 2021) is to efficiently use resources and to avoid needless duplication of effort by sharing data, technical information, lessons learned, and, in some cases, the costs related to the development of approaches and tools, whenever such cooperation and cost sharing may be done in a mutually beneficial fashion. The technical areas for collaboration include, those related to operating experience and safety data collection and analysis, including operational events, occupational injuries, hazardous substance releases, nuclear safety, radiation protection, equipment failure, accidents and accident precursors, trending analysis, and risk-informed decision-making. Applications of data analytics in the analysis of operating experience and safety data, including data visualization and analysis, artificial intelligence, machine learning, natural language processing, predictive analytics, and other advanced analysis techniques, user interface design, and deployment, and decision-making using data analytics tools.		2021-06-01	2021-06-01	Felix Gonzalez	felix.gonzalez@hq.doe.gov	In-house			N/A	Yes
Soil Moisture Modeling	U.S. Department of Energy	Office of Legacy Management	Use multisource machine learning to model soil moisture within the lysimeter embedded within a disposal cell		2022-10-03	2023-03-01	Annette Moore	annette.moore@lm.doe.gov	Commercial-off-the-shelf			In situ data from the lysimeter	Yes
SMMM	U.S. Department of Energy	Brookhaven National Laboratory	AI/ML is being used to evaluate measurements in real-time during simultaneous experiments on two beamlines and then drive subsequent data collection on both of the beamlines to maximize the scientific value generated per time.		2020-05-01		Phil Maffetone	pmaffetto@bnl.gov	In-house			Government datasets	Yes
Machine Learning for Autonomous Control of Scientific User Facilities	U.S. Department of Energy	Brookhaven National Laboratory	BNL will work alongside SLAC, to implement ML algorithm(s) into NSLS-II Operations to interpret accelerator data more intelligently. We intend to train said algorithms with 5+ years of archived device-data from accelerator components, records of previous fault causes (to connect to data-symptoms) and stored beam current.		2020-01-01		Kerstin Kleese Van Dam	kleese@bnl.gov	In-house			Government datasets	Yes
Automated sorting of high repetition rate coherent diffraction data from XFELS	U.S. Department of Energy	Brookhaven National Laboratory	"Coherent X-rays are routinely provided today by the latest Synchrotron and X-ray Free-electron Laser Sources. When these diffract from a crystal containing defects, interference leads to the formation of a modulated diffraction pattern called ""speckle"". When the defects move around, they can be quantified by a correlation analysis technique called X-ray Photon Correlation Spectroscopy. But the speckles also change when the beam moves on the sample. By scanning the beam in a controlled way, the overlap between the adjacent regions gives redundancy to the data, which allows a solution of the inherent phase problem. This is the basis of the coherent X-ray ptychography method which can achieve image resolutions of 10nm, but only if the probe positions are known. The goal of this proposal will be to separate ""genuine"" fluctuations of a material sample from the inherent beam fluctuations at the high data rates of XFELs. Algorithms will be developed to calculate the correlations between all the coherent diffraction patterns arriving in a time series, then used to separate the two sources of fluctuation using the criterion that the ""natural"" thermal fluctuations do not repeat, while beam ones do. We separate the data stream into image and beam ""modes"" automatically."		2021-07-01		Kerstin Kleese Van Dam	kleese@bnl.gov	In-house			Government datasets	Yes
Machine Learning for Linac Improved Performance	U.S. Department of Energy	Fermi National Accelerator	In Linacs at FNAL and J-PARC, the current emittance optimization procedure is limited to manual adjustments of a few parameters; using a larger number is not practically feasible for a human operator. Using machine learning (ML) techniques allows lifting this restriction and expanding this set. Our goal is to integrate ML into linac operation - and in particular RF control to achieve a more optimal longitudinal emittance and lower overall losses.				Kiyomi Seiya	kiyomi@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
AI Denoising	U.S. Department of Energy	Fermi National Accelerator	This program aims to develop generative models for quickly simulating showers of particles in calorimeters for LHC experiments				Kevin Pedro	pedrok@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks, Hierarchical Generative Model	experimental data, open-source	Yes
Next-Generation Beam Cooling and Control with Optical Stochastic Cooling	U.S. Department of Energy	Fermi National Accelerator	This program leverages the physics and technology of optical stochastic cooling (OSC) to explore new possibilities in beam control and sensing. The planned architecture and performance of a new OSC system at IOTA should enable turn-by-turn programmability of the high-gain OSC. This capability can then be used in conjunction with other hardware systems as the basis of an action space for reinforcement learning (RL) methods. The program aims to establish a new state of the art in beam cooling and a flexible set of tools for beam control and sensing at colliders and other accelerator facilities.				Jonathan Jarvis	jjarvis@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
In-storage computing for multi-messenger astronomy in neutrino experiments and cosmological surveys	U.S. Department of Energy	Fermi National Accelerator	This project aims to address the big-data challenges and stringent time constraints facing multi-messenger astronomy (MMA) in neutrino experiments and cosomological surveys. Instead of following the traditional computing paradigm of moving data to the compute elements, it does the opposite to embed computation in the data where processing is performed in situ. This will be achieved through emerging computational storage accelerators on which ML algorithms may be deployed to execute MMA tasks quickly so alerts can be disseminated promptly.				Michael Wang	mwang@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes

hls4ml	U.S. Department of Energy	Fermi National Accelerator	This project develops hardware-software AI codesign tools for FPGAs and ASICs for algorithms running at the extreme edge.		2021-08-10		Nhan Tran	ntran@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
Streamining intelligent detectors for sPHENIX/EIC	U.S. Department of Energy	Fermi National Accelerator	This project develops real-time algorithms for event filtering with tracking detectors for nuclear physics collider experiments.				Nhan Tran	ntran@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
In-pixel AI for future tracking detectors	U.S. Department of Energy	Fermi National Accelerator	This project explores novel AI-on-chip technology for intelligent detectors embedded with sensing technology				Farah Fahim	farah@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
SONIC: AI acceleration as a service	U.S. Department of Energy	Fermi National Accelerator	This project focuses on integration of AI hardware for at-scale inference acceleration for particle physics experiments.				Nhan Tran	ntran@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
High-Velocity AI: Generative Models	U.S. Department of Energy	Fermi National Accelerator	This project has two parts: 1. generating adversarial examples and then using domain adaptation and other techniques to improve the robustness of AI classification algorithms against those attacks (focusing on astrophysics/cosmology applications); 2. using AI algorithms to improve the output of low-quality classical simulation engines to deliver a high-quality result at high speed.				Kevin Pedro	pedrok@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks, Hierarchical Generative Model	experimental data, open-source	Yes
Uncertainty Quantification and Instrument Automation to enable next generation cosmological discoveries	U.S. Department of Energy	Fermi National Accelerator	This project will develop AI-based tools to enable critical sectors for near-future cosmic applications. Uncertainty quantification is essential for performing discovery science now, and simulation-based inference offers a new approach. The automated design and control of instrumentation will be important for improving the efficiency of planning and executing cosmic experiments.				Brian Nord	nord@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
READS: Real-time Edge AI for Distributed Systems	U.S. Department of Energy	Fermi National Accelerator	This project will develop and deploy low-latency controls and prediction algorithms at the Fermilab accelerator complex				Kyle Hazelwood	kjh@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
Simulation-based inference for cosmology	U.S. Department of Energy	Fermi National Accelerator	This project will develop and use simulation-based inference to estimate cosmological parameters related to cosmic acceleration in the early and late universe — via the cosmic microwave background and strong gravitational lensing, respectively. This will produce an analysis pipeline that can be deployed for next-generation cosmic surveys.				Brian Nord	nord@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
Extreme data reduction for the edge	U.S. Department of Energy	Fermi National Accelerator	This projects develops AI algorithms and tools for near-sensor data reduction in custom hardware.		2021-08-10		Nhan Tran	ntran@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks, Novel Spectroscopic Technology	experimental data, open-source	Yes
Machine Learning for Accelerator Operations Using Big Data Analytics / L-CAPE	U.S. Department of Energy	Fermi National Accelerator	Big data analytics for anomaly prediction and classification, enabling automatic mitigation, operational savings, and predictive maintenance of the Fermilab LINAC				William Pellico	pellico@fnal.gov	In-house		Artificial Intelligence, Big Data, Neural Networks	experimental data, open-source	Yes
Geo Threat Observable for structure cyber threat related to the energy sector	U.S. Department of Energy	Idaho National Laboratory	Collection of open source threat inforamtion related to cyber issues in the energy sector, collected stored in graphdb and used in machine learning for similarities of threat enabling better reuse of cyber protections.		2019-10-01		Rita Foster	Rita.Foster@inl.gov	In-house			Open source threat intelligence collected, NLP used to scrape information off of cyber incident reports and websites, some data from cyber sensors, threat feeds and some data from manual threat analysis activities.	Yes
Deep Learning Malware Analysis for reusable cyber defenses.	U.S. Department of Energy	Idaho National Laboratory	The INL uses machine learning (feed forward neural network) on a large data set of translated malware binaries in graph structures to identify commonality between malware.		2017-10-01		Rita Foster	Rita.Foster@inl.gov	In-house			Data for malware binaries come mainly from open source malware repositories collected; @DisCo application dissassembles and stores into a graph db for management and vector embedded queries to identify common malware functions useful for cyber defenses.	Yes
Biology, genomics, and synthetic biology	U.S. Department of Energy	Lawrence Livermore National Laboratory	Combining experimental and computational methods to perform fundamental and applied research in genomics, molecular toxicology, nanotechnology, host–pathogen biology, structural biology, genetics, microbial systems, and medical countermeasures				Kris Kulp	Kulp2@llnl.gov	In-house			in-house	Yes
Innovation methods, processes and promising practices that can affect the speed and effectiveness of innovation processes at scale.	U.S. Department of Energy	Lawrence Livermore National Laboratory	Computational approaches that lead to faster insights into the development and deployment of large scale operations				Charity Follett	follett2@llnl.gov	In-house			in-house	Yes
Cyber security, data storage, and data management technologies	U.S. Department of Energy	Lawrence Livermore National Laboratory	Data-processing pipelines and user interfaces to process and aggregate large, bulk, and possibly unstructured datasets allowing for search and export of data for further analysis in secure way				Brad Hart	hart14@llnl.gov	In-house			in-house	Yes
Advanced materials science, engineering, and exploration relevant to the other key technology focus areas	U.S. Department of Energy	Lawrence Livermore National Laboratory	Enabling machine learning based technology to specialized materials for superior performance for scientific research and manufacturing systems				Bob Maxwell	maxwell7@llnl.gov	In-house			in-house	Yes

Natural and anthropogenic disaster prevention and mitigation	U.S. Department of Energy	Lawrence Livermore National Laboratory	Leveraging a broad, multimodal data stream to predict and understand natural disaster scenarios for the purposes of prevention and mitigation				Tarabay Antoun	antoun1@llnl.gov	In-house			in-house	Yes
Advanced energy, batteries, and industrial efficiency	U.S. Department of Energy	Lawrence Livermore National Laboratory	Leveraging data science to navigate design space for better batteries and energy storage as well as scale up of various technologies				Tony VanBuuren	vanbuuren1@llnl.gov	In-house			in-house	Yes
Quantum computing and information systems	U.S. Department of Energy	Lawrence Livermore National Laboratory	Machine learning and quantum computing applied towards optimization, quantum chemistry, material science, and cryptography				Eric Schwegler	schwegler1@llnl.gov	In-house			in-house	Yes
AI/ML and other software advances	U.S. Department of Energy	Lawrence Livermore National Laboratory	Model architecture development research, including workflows, algorithm and performance optimization				Jim Brase	Brase1@llnl.gov	In-house			in-house	Yes
High-performance computing, semiconductors, and advanced computer hardware	U.S. Department of Energy	Lawrence Livermore National Laboratory	Novel computer hardware architecture/configurations that can perform at the edge and/or in harsh environments				Terri Quinn	Quinn1@llnl.gov	In-house			in-house	Yes
Robotics, automation, and advanced manufacturing	U.S. Department of Energy	Lawrence Livermore National Laboratory	AI is being used for accelerating hardware development and interpretation of sensor data to improve process reliability				Eric Douss	Douss1@llnl.gov	In-house			in-house	Yes
To use ML to help identify promising oxygen carrier materials.	U.S. Department of Energy	National Energy Technology Laboratory	A combination of experimental data and computational results will be used both to understand O2 production and to develop a machine learning model that can be used to identify promising carrier compositions. These compositions will be evaluated on two primary criteria, performance and ability to be synthesized. Once the model has identified promising candidates, these materials will be synthesized and compared to existing carriers. This new data will then be used to refine the models.				Jerry Carr	jerry.carr@netl.doe.gov	In-house		Other	Unknown	Yes
Machine learning based identification of current hazardous offshore metocean and bathymetric conditions that can impact safe offshore energy operations	U.S. Department of Energy	National Energy Technology Laboratory	Build off user testing and further refine analytical logic to develop Version 2 of the OGA smart tool for release on EDX. Continue refinements to offshore hazard models, including wave and turbidity current models. Draft manuscripts detailing the OGA Tool models and algorithms. Assemble a metocean and seafloor database for release with the OGA Tool Version 2 online; strategize web-hosted versions of the OGA Tool and database.		2019-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Big Data, Neural Networks, Other	government datasets, citable publications, open-source datasets	Yes
Reduce computational cost of CFD simulations that screen for more efficient intensified solvent contactor geometries.	U.S. Department of Energy	National Energy Technology Laboratory	Collaborate with Subtask 4.3 Machine Learning Support to reduce the computational complexity of validated CFD calculations using Deeper Fluids (DF), graph neural networks (GNNs), or similar ML approaches. Further development of ongoing process modeling/optimization ultimately informed by the CFD reduced order models (ROM) will also be a focus.		2021-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Neural Networks, Other	Unknown	Yes
To drive insights on the power system reliability, cost, and operations during the energy transition with and without FECM technologies	U.S. Department of Energy	National Energy Technology Laboratory	Commercially available models will be used to generate predictive scenarios		2018-04-01		Steve Richardson	steven.richardson@netl.doe.gov	In-house		Big Data	Unknown	Yes
To drive insights on the dependencies between the natural gas and electricity sectors to increase reliability of the NG system	U.S. Department of Energy	National Energy Technology Laboratory	Commercially available models will be used to generate predictive scenarios		2018-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Big Data	Unknown	Yes
AI/ML methodology for rapid design of sorbents tuned to specific ash impoundment and/or landfill requirements.	U.S. Department of Energy	National Energy Technology Laboratory	Computation of the descriptors (atomic property-weighted radial distribution functions) that will be used for the ML portion of the task; Fitting of a machine-learned model for the prediction of B sorption; Optimization and computational design of a sorbent for maximum sorption of B as a function of B concentration in the aqueous solution; Force field generation for an additional pollutant (if needed); Sorption calculations and ML fitting for the second pollutant (TBD); Optimization and computational design of a sorbent for maximum sorption of the second pollutant as a function of pollutant concentration in the aqueous solution.		2021-04-01		Steven Richardson	steven.richardson@netl.doe.gov	In-house		Other	In-house calculations and publications	Yes
To enhance the SimCCS toolset to better account for existent infrastructure and to more broadly engage other user bases to improve toolset performance and applicability.	U.S. Department of Energy	National Energy Technology Laboratory	Continue development of the SimCCS toolset, which is utilized to determine optimal placement for CO2 pipeline rights of way (ROW) and infrastructure in a machine-learning driven methodology that that considers environmentally sensitive areas, Justice40 considerations, and utilization of existent infrastructure.		2022-08-01		Johnathan E. Moore	johnathan.moore@netl.doe.gov	In-house		Artificial Intelligence	Unknown	Yes
To create and apply machine learning algorithms to predict carbon dioxide enhanced oil revoery improvements with rich gas in the Bell Creek Field and other selected fields.	U.S. Department of Energy	National Energy Technology Laboratory	Create models with ML algorithms to predict CO2 EOR improvements with rich gas in the Bell Creek Field and other selected fields. The results of these models will be compared with the predictions of CMG's reservoir simulations models.		2019-10-01		Robert Noll	robert.noll@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
Data platform to expedite access and reuse of carbon ore data for materials, manufacturing and research	U.S. Department of Energy	National Energy Technology Laboratory	Data platform to expedite access and reuse of carbon ore data for materials, manufacturing and research. Assembled using data science, NLP methods, and hosted in virtual, multi-cloud platform for online analytics.		2018-04-01		Steve Richardson	steven.richardson@netl.doe.gov	In-house		Natural Language Processing, Other	Unknown	Yes
Computational methods for the characterization of CO2 chemisorption in amine-functionalized MOFs.	U.S. Department of Energy	National Energy Technology Laboratory	Databases of MOFs will be screened using computational methods to identify promising MOFs. Software will be further developed to allow for the addition of desirable functional groups (amines) to metal centers and/or ligands of MOFs. The team will calculate the reaction enthalpy for CO2 sorption in amine functionalized MOFs and further computational methods for the characterization of CO2 chemisorption in amine-functionalized MOFs will be developed.		2022-04-01		Viktoria L Pretzman	laura.pretzman@netl.doe.gov	In-house		Other	In-house calculations and publications	Yes
ML-based approaches to improve site characterization efforts	U.S. Department of Energy	National Energy Technology Laboratory	Demonstrate application of ML-based approaches to improve site-characterization efforts performed during the pre-injection phase using data from either IBDP (for which data are currently available) or other opportunistic field demonstration or commercial projects (for which data may become available) and develop value of information guidelines. Demonstrate how ML-based rapid forecasting can be used to help with pre-injection reservoir management decisions under data uncertainties. Demonstrate how a visualization platform with ML-based models can help regulators (and other stakeholders, such as site developers) to		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	EDX - government datasets	Yes

To develop low cost conversion of coal to graphene	U.S. Department of Energy	National Energy Technology Laboratory	Demonstrate the techno-economical feasibility of a 250 ton/day manufacturing facility to convert coal to high-quality graphene. The core technology is based on flash joule heating (FJH) to convert various coals to graphene. Machine learning algorithms will map out the correlation of processing parameters with the final product (graphene yield, quality, dimensions).		2021-03-01		Jason Montgomery	jason.montgomery@netl.doe.gov	Contracted		Natural Language Processing, Neural Networks	Unknown	Yes
To implement machine learning to predict aerodynamic and combustion characteristics in hydrogen turbine	U.S. Department of Energy	National Energy Technology Laboratory	Design rules and reduced models will be formulated by combining high fidelity simulations of chemically reacting flow, stochastic modeling techniques, reduced modeling through machine learning and testing of injector configurations. These can be used in an industrial setting to predict the aerodynamic and combustion characteristics in hydrogen turbine combustors based upon which design decisions are made.		2021-09-15		Seth Lawson	seth.lawson@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To automate development of proxy models for power generation combustion systems.	U.S. Department of Energy	National Energy Technology Laboratory	Detailed CFD of large combustion systems will be performed. From the results, machine learning will be used to develop fast proxy models which can will provide results close to the CFD results, but in a small fraction of the time. These fast models will then be used in real-time digital twin models of the power plant, which can be used to help the power plant operator to spot instrumentation failures or cyberattacks on the plant.		2021-10-01		Steve Richardson	steven.richardson@netl.doe.gov	In-house		Other	Unknown	Yes
To implement unsupervised learning based interaction force model for nonspherical particles in incompressible flows	U.S. Department of Energy	National Energy Technology Laboratory	Develop a neural network-based interaction (drag and lifting) force model. A database will be constructed of the interaction force between the non-spherical particles and the fluid phase based on the particle-resolved direct numerical simulation (PR-DNS) with immersed boundary-based lattice Boltzmann method (IB-LBM). An unsupervised learning method, i.e., variational auto-encoder (VAE), will be used to improve the diversity of the non-spherical particle library and to extract the primitive shape factors determining the drag and lifting forces. The interaction force model will be trained and validated with a simple but effective multi-layer feed-forward neural network: multi-layer perceptron (MLP), which will be concatenated after the encoder of the previously trained VAE for geometry feature extraction.		2020-08-01		Richard Dunst	richard.dunst@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes
To develop 5G integrated edge computing platform for efficient component monitoring in coal-fired power plants	U.S. Department of Energy	National Energy Technology Laboratory	Develop an on-demand distributed edge computing platform to gather, process, and efficiently analyze the component health data in coal-fired power plants. Given that edge computing servers are closer to the field devices in modernized power plants, the efficiency of edge computing service with respect to dynamic orchestration, resource data collection, and health information monitoring will be investigated for timely detection of remote faults and to perform diagnosis.		2021-08-23		Robie Lewis	robie.lewis@netl.doe.gov	Contracted		Big Data	Unknown	Yes
To identify and characterization REE-CM hot zones using machine learning-aided multi-physics.	U.S. Department of Energy	National Energy Technology Laboratory	Develop and field demonstrate a machine learning (ML)-aided multi-physics approach for rapid identification and characterization of REE-CM hot zones in mine tailings with a focus on coal and sulfide mine tailings or other processing or utilization byproducts, such as fly ash and refuse deposits.		2023-01-01		Heather Dougherty	heather.dougherty@netl.doe.gov	In-house		Artificial Intelligence	Unknown	Yes
To implement boiler health monitoring using a hybrid first principles-artificial intelligence model	U.S. Department of Energy	National Energy Technology Laboratory	Develop methodologies and algorithms to yield (1) a hybrid first-principles artificial intelligence (AI) model of a PC boiler, (2) a physics-based approach to material damage informed by ex-service component evaluation, and (3) an online health-monitoring framework that synergistically leverages the hybrid models and plant measurements to provide the spatial and temporal profile of key transport variables and characteristic measures for plant health.		2019-09-01		Maria Reidpath	maria.reidpath@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
Development of AI/ML methods	U.S. Department of Energy	National Energy Technology Laboratory	Develop quality, reliability, and version control standards for SMART software. Continue development of AI/ML methods for use by the 2A and 2C activities, including Modeling anomalies due to local heterogeneity coupled with an enhanced capacitance-resistance model (CRM) and Bayesian Belief Network (BBN) modeling integrated with geochemistry. Continue development of advanced computational approaches with modeling using the most advanced general purpose PDE/ODE physics-informed neural network (PINN) tool developed by NVIDIA and accelerate training PINNs using Wafer Scale Engine (WSE) by Cerebras Systems Inc.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	EDX - government datasets	Yes
Develop and demonstrate reinforcement learning approach for time-varying control for flexible hydrogen and power production.	U.S. Department of Energy	National Energy Technology Laboratory	Efforts on IES control will include the development of a dynamic optimization-based nonlinear model predictive control (NMPC) framework. NMPC approaches for optimizing cell thermal management and maximizing IES efficiency under set-point transition will be developed for flexible operation. Reinforcement learning (RL) approaches will also be developed for optimal control policy selection and learning-based adaptive control. There are opportunities for improved learning through interaction with the electrolyzer in addition to learning from the MPC action. Multi-policy approaches will be developed for control, independently by RL or in concert with MPC, or even for scheduling the operating policy. The ultimate goal is to develop operational strategies and an NMPC and RL control framework for optimizing IES performance under flexible hydrogen and power production scenarios, while minimizing physical and chemical degradation over long-term operation.		2022-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Other	Open-source and publications	Yes
Neural networks used to compensate a drone-mounted magnetic sensor for maneuvering of the drone.	U.S. Department of Energy	National Energy Technology Laboratory	Electromagnetic technology development and optimization for cased wells. Scalable solutions—getting to 100,000 wells/year through drone technology and ML technology. NETL will develop ML algorithms to compensate magnetic data for the maneuvering of drone aircraft. Magnetic noise can limit sensitivity of detection and resolution of anomalies in the magnetic data. The ML algorithms will reduce attitude- and heading-induced noise in drone magnetic surveys.		2022-04-01		Brian Dressel	brian.dressel@netl.doe.gov	In-house		Neural Networks, Other	Datasets provided by private sector collaborators	Yes
To provide natural gas leak detection and quality control	U.S. Department of Energy	National Energy Technology Laboratory	Employing machine learning techniques to train sensing systems to quantify the concentration of natural gas species, distinguish between natural gas at different parts of the processing pipeline, and distinguish natural gas from natural and man-made interfering sources such as wetlands and agriculture.		2020-04-01		Joseph Renk	joseph.renk@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes

To design, develop, and demonstrate an AI-integrated physics-based attack resilient proactive system.	U.S. Department of Energy	National Energy Technology Laboratory	Enable "defense-in-depth" cyber-physical system (CPS) security and resiliency for the distribution grid. The recipient will design, develop, and demonstrate a vendor-agonistic scalable Artificial Intelligence Integrated Attack-Resilient Proactive System (AI-ARPS) for utility distribution grid systems including advanced distribution management system (ADMS) and DER management system (DERMS) applications.		2022-10-01		J. Clark Robinson	clark.robinson@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To apply machine learning methods to explore the inter-well uncertainty in the Goldsmith Landreth San Andres Unit and to update reservoir models.	U.S. Department of Energy	National Energy Technology Laboratory	Engineered water can lower interfacial tension and minimize capillary forces that gravity can push the oil up and out of the matrix. This proposal is to test this technology in the field scale, in Goldsmith Landreth San Andres Unit. Apply history matching of flexible interface-based reservoir models and ML methods such as generative adversarial networks that provide new methods to explore the inter-well uncertainty and to update the reservoir models.		2019-10-01		Anthony Zammerilli	anthony.zammerilli@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
Use AI to process large sensor datasets for identification and classification of NG pipeline conditions and methane leaks	U.S. Department of Energy	National Energy Technology Laboratory	Focused on development of advanced data analytic techniques and methods for distributed OFS technology, including AI and ML, for identification of signatures and patterns representative of hazards, defects, and operational parameters of the natural gas pipeline network.		2022-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes
ML-based reduced order models of reservoir response to Co2 injection into saline and/or hydrocarbon-bearing formations - as the basis for integrated assessment modeling of leakage risk (e.g., SACROC)	U.S. Department of Energy	National Energy Technology Laboratory	Generally, the approach used by NRAP researchers to address these questions is to develop a robust, science-based integrated assessment framework that links fast forecasting models of CO2 storage system components (e.g., storage reservoir; leakage pathways including wells, faults, and fractured caprock; intermediate formations; and receptors of concern, including groundwater aquifers and the atmosphere). Superimposed on this system model are various fit-for-purpose analytical capabilities that support analyses in support of stakeholder decision making for questions related to site-specific risk evolution, risk-based area of review delineation, conformance assessment, and post-injection site monitoring In Task 2.0, researchers will augment and expand this functionality to demonstrate relevance to industry-standard site risk management methods (i.e., bowtie analysis framework) and to understand containment performance and leakage risk for scenarios where a site transitions from CO2 utilization for EOR to dedicated CO2 storage. To ensure that risk assessment efforts are informative to real geologic storage deployment scenarios, NRAP researchers will engage with a diverse set of stakeholders to establish an appropriate modeling and risk assessment design basis.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	Unknown	Yes
Transform reservoir management decisions through rapid analysis of real time data to visualize forecasted behavior in an advanced control room "human-in-the-loop" format.	U.S. Department of Energy	National Energy Technology Laboratory	Improve low-fidelity model performance by transfer-learning with high-fidelity data, and reduce uncertainty by combining high-fidelity and lower-fidelity models for improved UQ performance.		2020-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Other	Unknown	Yes
Natural Language Processing	U.S. Department of Energy	National Energy Technology Laboratory	Information and articles on energy storage will be gathered and reviewed. Developed natural language processing (NLP) algorithms will be used to help categorize and understand various energy storage efforts in the R&D communities. Additionally, trends within the discovered and selected topical focus areas in energy storage will be examined. This will provide a view of energy storage R&D, which is not biased or limited to known search terms.		2022-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Big Data, Natural Language Processing, Other	Literature Metadata from Semantic Scholar Academic Graph	Yes
To apply machine learning and data analytics techniques to integrated subsurface datasets to predict key reservoir properties and compare various fields across the area of study and to correlate vintage data with new data and address the distribution of fractures and vugs.	U.S. Department of Energy	National Energy Technology Laboratory	Laboratory experiments will be used to optimize a CO2 flood composition specific to HTD rock properties, and subsequently design and simulate injection scenarios that offer wettability alteration, foaming, and reduced surface tension. This work will improve oil recovery from matrix porosity and mitigate the impact of fracture zones. The optimized design will be implemented and tested in a Trenton/Black River field. The results will provide strategies to improve oil recovery in complex carbonate formations in the Michigan Basin as well as in other carbonate plays.		2019-10-01		Kyle Clark	kyle.clark@netl.doe.gov	Contracted		Artificial Intelligence, Big Data	Unknown	Yes
DOE AI Data Infrastructure System	U.S. Department of Energy	National Energy Technology Laboratory	Leveraging generative AI and cloud enabled data infrastructure to improve CCS user experience and connectivity producing an adaptive user interface that streamlines connection of CCS stakeholders to what matters to them.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Artificial Intelligence, Big Data, Other	Open-source and government datasets	Yes
To drive insights on environmental performance of the natural gas system to inform effective mitigation strategies	U.S. Department of Energy	National Energy Technology Laboratory	Life Cycle Analysis models will be used to define and estimate environmental parameters/performance		2018-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes
To improve control of hybrid SOFC-gas turbine power systems.	U.S. Department of Energy	National Energy Technology Laboratory	Machine learning algorithms are being developed and compared to other control methods for SOFC-gas turbine hybrid power generation systems.		2021-10-01		Steve Richardson	steven.richardson@netl.doe.gov	In-house		Other	Unknown	Yes
To create reduced order models for predicting long term performance degradation behavior of fuel cells and electrolyzers.	U.S. Department of Energy	National Energy Technology Laboratory	Machine learning algorithms are being used to analyze large datasets of microstructural and perfromance degradation simulations of various electrode microstructres to develop reduced order models that can be used for long-term perfromance degradation predictions of large area fuel cell/electrolysis cells and cell stacks. The reduced order models can be used for dynamic simulations that can more accurately mimic the changing loading conditions of the modern grid.		2019-07-01		Steve Richardson	steven.richardson@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes
To develop a novel platform for secure data logging and processing in fossil fuel power generation systems using blockchain and machine learning to reduce down time for fossil energy power plants, limit reductions of power and reduce cost for repairs.	U.S. Department of Energy	National Energy Technology Laboratory	Machine learning model development will consist of traditional machine learning and deep learning algorithms implementation for anomaly detection. Machine learning server will be used to develop the traditional models using One-Class Support Vector Machine (SVM) and K-Mean Clustering and deep learning models using Recurrent Neural Network (RNN) and its various implementations like Long Short-Term Memory (LSTM), Gated Recurrent Unit (GRU), Generative Adversarial Network (GAN), and Autoencoders using the sensor data collected from secure sensor network.		2019-09-01		Heather Hunter	heather.hunter@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes

Creation of polymer datasets and inverse design of polymers with targeted backbones having High CO2 permeability and high CO2/N2 selectivity.	U.S. Department of Energy	National Energy Technology Laboratory	Machine learning models were developed to predict CO2 permeability and CO2/N2 selectivity of polymers. Novel methods were developed to generate polymer datasets. Furthermore, a novel machine learning technique is being developed to inverse design the polymers that will have targeted properties.		2022-04-01		Viktoria L Pretzman	laura.pretzman@netl.doe.gov	In-house		Other	Approximately 400 research papers	Yes
To leverage disparate data to update assessments, analytics, and infromation for NATCARB and CS Atlas	U.S. Department of Energy	National Energy Technology Laboratory	ML Is utilized to parse and generate additional data and information that can be parsed and labeled to provide additional inputs for geologic carbon storgae assessments from multiple sources.		2018-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Other	Unknown	Yes
To drive insights on pipeline maintenance and repair strategies to reduce incidents of pipeline leakage; support evaluation of use and reuse strategies	U.S. Department of Energy	National Energy Technology Laboratory	ML will be used to develop a pipeline risk assessment geospatial model and support evaluation of use and reuse opportunities.		2022-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes
To drive insights using machine learning-based dynamics, control, and health models and tools developed by NETL to gain valuable operational data, insights, and	U.S. Department of Energy	National Energy Technology Laboratory	ML will be used to develop dynamics, controls, and health models for operating power generation facilities		2018-04-01		Steve Richardson	steven.richardson@netl.doe.gov	In-house		Other	Unknown	Yes
ML-based proxy models and multi-level data driven fracture network imaging to support rapid decision making.	U.S. Department of Energy	National Energy Technology Laboratory	ML-based proxy-models of fracture network, HF geometry, HF properties, bottomhole pressure and drainage volume contribute to fracture network, production forecast and well drainage volume visualizations.		2020-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Other	Unknown	Yes
Use ML to enable a geophysical monitoring toolkit, and assimilate real-time modeling and data.	U.S. Department of Energy	National Energy Technology Laboratory	ML-enabled rapid and autonomous geophysical monitoring and real-time modeling and data assimilation tools (along with visualization and decision-support frameworks), work together to radically improve pressure and stress imaging.		2020-01-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	Unknown	Yes
Advanced subsurface imaging, lower energy cost, impacts, and improved resolution	U.S. Department of Energy	National Energy Technology Laboratory	More detailed analysis and simulation of a closed cycle pulsed MHD generator will be performed in this subtask. The numerical code will be used to produce an optimized system which achieves a 10 MWe power output over a 10s duration with a total duty cycle of 2 minutes. The expected output of this task is an optimized concept as a function of the various input and design parameters for the system (e.g., magnet size, pebble bed heater size).		2021-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Big Data, Neural Networks, Other	government datasets, citable publications, open-source datasets	Yes
Advanced subsurface imaging, lower energy cost, impacts, and improved resolution	U.S. Department of Energy	National Energy Technology Laboratory	More detailed analysis and simulation of a closed cycle pulsed MHD generator will be performed in this subtask. The numerical code will be used to produce an optimized system which achieves a 10 MWe power output over a 10s duration with a total duty cycle of 2 minutes. The expected output of this task is an optimized concept as a function of the various input and design parameters for the system (e.g., magnet size, pebble bed heater size).		2019-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Artificial Intelligence, Other	Government datasets and open-source	Yes
Advanced subsurface imaging, lower energy cost, impacts, and improved resolution	U.S. Department of Energy	National Energy Technology Laboratory	More detailed analysis and simulation of a closed cycle pulsed MHD generator will be performed in this subtask. The numerical code will be used to produce an optimized system which achieves a 10 MWe power output over a 10s duration with a total duty cycle of 2 minutes. The expected output of this task is an optimized concept as a function of the various input and design parameters for the system (e.g., magnet size, pebble bed heater size).		2021-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Neural Networks, Other	First principles acoustic simulations ('high fidelity') using commercial software, COMSOL	Yes
To provide insights into opportunities to beneficiate and use hydrocarbon infrastructure for alternative uses such as offshore carbon storage.	U.S. Department of Energy	National Energy Technology Laboratory	Multiple big data-driven AI/ML models will be used to evaluate geologic, geospatial, and infrastructure related information to inform predictions using natural language processing, Artificial Neural Networks, and possibly bayesian networks as well.		2021-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes
AI/ML may be needed to extract data from text, image and tabular-based resources. NEWTS is partnering with university teams to use ML to fill in data gaps using predictive models.	U.S. Department of Energy	National Energy Technology Laboratory	NEWTS data requirements and database structure needs will be established by reviewing datasets and literature on energy-water streams. Data sources will be identified from regulatory agencies, government monitoring programs, as well as open-source literature. Metadata of each source will be compiled into a data catalog for tracking and reference. Datasets, including high-quality composition data for relevant streams, will be collected and downloaded. Acquired data will be processed into a structured format based on the prioritization of datasets to be included in NEWTS. Data acquisition and processing might entail the application of ML (e.g., natural language processing) to efficiently resurrect data trapped in historical reports (e.g., PDFs) or other unstructured formats. One research product of this subtask will be a release of the data catalog, which will be made available on		2022-04-01		Viktoria L Pretzman	laura.pretzman@netl.doe.gov	In-house		Natural Language Processing, Other	Unknown	Yes
To evaluate current infrastructure throughout a study area and evaluating future infrastructure needs to accelerate the deployment of CCUS	U.S. Department of Energy	National Energy Technology Laboratory	One key task focuses on evaluating current infrastructure throughout the Initiative study area and evaluating future infrastructure needs to accelerate the deployment of CCUS. LANL will utilize its unique technologies for this project focusing on SimCCS, with a minor consulting role using NRAP and machine learning algorithms.		2019-10-01		Dawn Deel	dawn.deel@netl.doe.gov	In-house		Artificial Intelligence	Unknown	Yes
Demonstrate the robust performance of our ML method in a commercial-scale synthetic data and integrate image-to-image mapping with convolutional neural networks	U.S. Department of Energy	National Energy Technology Laboratory	Our method quickly incorporates streaming observations for accurate and timely forecasts with uncertainty quantification, taking reservoir simulation data as inputs and incorporating real-time observation streams for accurate, timely geological carbon storage forecasts. Computation effort is distributed over many machines, facilitates coupled inversions using many ML models, and allows for ML-Driven optimization and sensitivity analysis		2020-01-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Neural Networks, Other	Unknown	Yes
To develop drag models for non-spherical particles through machine learning	U.S. Department of Energy	National Energy Technology Laboratory	Produce comprehensive experimental and numerical datasets for gas-solid flows in well-controlled settings to understand the aerodynamic drag of non-spherical particles in the dense regime. The datasets and the gained knowledge will train deep neural networks to formulate a general drag model for use directly in NETL MFiX-DEM module. This will help to advance the accuracy and prediction fidelity of the computational tools that will be used in designing and optimizing fluidized beds and chemical looping reactors		2020-09-01		Omer R. Bakshi	omer.bakshi@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes

To fill critical data gaps in big data analytics and machine learning applications to inform decision making and improve the ultimate recovery of unconventional oil and natural gas resources.	U.S. Department of Energy	National Energy Technology Laboratory	Project will conduct numerical analysis of all-digital pressure sensing technology will be used to create a synthetic dataset with downhole pressure sensor readings for each stage and will be analyzed statistically with DA to integrate with software.		2019-10-01		David Cercone	david.cercone@netl.doe.gov	Contracted		Artificial Intelligence, Big Data	Unknown	Yes
To design, proto-type and demonstrate a miniaturized implementation of a multi-process, high-spatial-resolution monitoring system for boiler condition management.	U.S. Department of Energy	National Energy Technology Laboratory	Project will develop control logic for automated control of bituminous coal-fired boiler. Plant operational data will be compared against monitoring data to determine when different sensor output from a miniaturized high temperature multi-process, high-spatial-resolution monitoring system signifies damaging conditions in that region of the boiler, and what operational changes can be made to eliminate the damaging condition. The control logic will be developed for automated control of soot-blowing and other boiler operations		2018-10-01		Richard Dunst	richard.dunst@netl.doe.gov	Contracted			Unknown	Yes
To provide combustion performance and emissions optimization through integration of a miniaturized high-temperature multi process monitoring system	U.S. Department of Energy	National Energy Technology Laboratory	Project will develop control logic for automated control of lignite coal-fired boiler. Plant operational data will be compared against monitoring data to determine when different sensor output from a miniaturized high temperature multi-process, high-spatial-resolution monitoring system signifies damaging conditions in that region of the boiler, and what operational changes can be made to eliminate the damaging condition. The control logic will be developed for automated control of soot-blowing and other boiler operations		2018-10-01		Omer R. Bakshi	omer.bakshi@netl.doe.gov	Contracted			Unknown	Yes
Development of new machine learning-based process modeling capabilities that assess the viability and efficiency, with uncertainty quantification, of the chemical processes involved in the carbon fiber production and its output quality	U.S. Department of Energy	National Energy Technology Laboratory	Provide sub-pilot-scale verification of lab-scale developments on the production of isotropic and mesophase coal-tar pitch (CTP) for carbon fiber production, using coals from several U.S. coal-producing regions. An extensive database and suite of tools for data analysis and economic modeling, with an associated web-based community portal, will be developed to relate process conditions to product quality, and to assess the economic viability of coals from different regions for producing specific high-value products.		2020-06-01		Christian Robinson	christian.robinson@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
Analysis to Assess Offshore CCS Trends and Gaps	U.S. Department of Energy	National Energy Technology Laboratory	Providing expertise, input, and support for the development of a DOE (NETL/FECM) carbon storage technical resources catalog that facilitates searching for information about datasets, models and tools, publications and reports, and competencies resulting from DOE-FECM/NETL's offshore and CSP activities. this project will complete a review and analysis of knowledge and data resources resulting from international offshore CCS projects. Outcomes of this analysis are expected to include the integration of key data and tools into the EDX-hosted Open Carbon Storage Database and DisCO2ver platform (in development via the EDX4CCS FWP), as well as geo-data science based analysis and recommendations on geologic and metocean insights from international studies and their alignment or relevance to U.S. Federal offshore settings.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	Open-source	Yes
Initial case study using regulatory compliance (well integrity testing, fluid compositionali data, geographic, and geologic information from oil and gas wells in the Wattenberg Field, Denver Basin, central Colorado, USA	U.S. Department of Energy	National Energy Technology Laboratory	Researchers will apply artificial intelligence/machine learning (AI/ML) techniques to national-scale well characterization and integrity test datasets to yield new insights into leakage potential.		2022-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Other	Unknown	Yes
UNET and other approaches for ML-based inversion	U.S. Department of Energy	National Energy Technology Laboratory	Researchers will develop a design basis for risk-based monitoring considering data dimensionality, uncertainty, and inter-tool/module connectivity, and define the components of the monitoring design optimization tool (DREAM) to be incorporated into NRAP-Open-IAM and the SMART platform.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Artificial Intelligence, Other	Unknown	Yes
To develop a wireless, distributed data acquisition and interpretation system foe seismic monitoring and carbon storage characterization.	U.S. Department of Energy	National Energy Technology Laboratory	Resensys plans to develop a wireless, distributed data acquisition and interpretation system tailored for monitoring and characterization of seismic activity at carbon storage sites. The seismicity data collected in real time during the CO2 storage site characterization and sequestration processes combined with advanced signal processing and Artificial Intelligence and Machine Learning (AI/ML) methodologies provide an understanding of natural seismicity risks prior to any CO2 injection, prior to making large investments in developing the storage project.		2022-06-27		Ashley Urosek	ashley.urosek@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To research and develop physics-aware and AI-enabled cyber-physical intrusion response for the power grid.	U.S. Department of Energy	National Energy Technology Laboratory	Responding to anomalous cyber and physical events in a timely manner requires fusing data from both cyber and physical sensors into actionable information. Thus, cyber-physical intrusion response research will be conducted that leverages cyber and physical side data and models with artificial intelligence (AI) as a scalable approach to maintain or regain power system resilience under anomalous incidents such as cyber threats.		2022-10-01		Bob Hayes	robert.hayes@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To implement sensor-driven deep learning/artificial intelligence for power plant monitoring	U.S. Department of Energy	National Energy Technology Laboratory	Sensor-driven deep learning/artificial intelligence for intelligent health monitoring capabilities that occur at the sensor (embedded computing) or base station (edge computing). Will give power plant operators more prediction tools about scheduling maintenance. Focus is on a high-priority in-situ boiler temperature measurement system that relies on chipless RFID technology and much-needed temperature, pressure, environmental, and water quality industrial sensors.		2021-08-16		Robie Lewis	robie.lewis@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes
To drive insights on water recovery from cooling tower plumes	U.S. Department of Energy	National Energy Technology Laboratory	Study of plume formation and collection on mechanical (induced) draft cooling towers, partly in a high-fidelity controlled environment and partly on a full-scale industrial cooling tower. It will start by building the needed laboratory setup and installing various sensors on the lab cooling tower. At the same time a computational fluid dynamics (CFD) model will be implemented to get precise full-scale plume models. Using the insights into power-plant plume characteristics the project will iterate on and experimentally test electrodes and collectors, which make up modular panels, on the lab cooling tower. What has been learned from the full-scale plume modeling and sensor data analysis will then be applied to develop a design model to build the optimal collection apparatus for given working conditions		2019-10-01		Heather Hunter	heather.hunter@netl.doe.gov	Contracted			Unknown	Yes

To use AI to calibrate the simulation model by matching simulation data with production history data.	U.S. Department of Energy	National Energy Technology Laboratory	Task 2 - Together with GEM, CMG's intelligent optimization and analysis tool, CMOST Artificial Intelligence (AI), will be used to calibrate the simulation model by matching simulation results with production history data. . Based on the data sets, a series of simulation cases will be generated to perform parameter estimation using a systematic approach. As simulation jobs complete, the results will be analyzed using CMOST AI to determine how well they match production history. An optimizer will then determine parameter values for new simulation jobs.		2019-10-01		David Cercone	david.cercone@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To automate RDE image analysis, machine learning for RDE image analysis is being employed.	U.S. Department of Energy	National Energy Technology Laboratory	The expected outcome of this project will be extensive experimental data that can provide valuable insight in RDC design, coupling RDC with turbomachinery, model validation, and next generation combustion sensors that use artificial intelligence and computer vision. Design of an optimized inlet to maximize pressure gain in an RDE relies on an understanding of the coupling between the inlet plenums (fuel and air), the combustor annular channel, and the exhaust diffusor. This creates a challenge for CFD as the models are significant and computationally expensive. NETL is continuing a collaboration with the University of Michigan to accelerate reacting flow CFD modeling using machine learning (ML).		2022-04-01		Brian Dressel (acting)	brian.dressel@netl.doe.gov	In-house		Other	Unknown	Yes
To develop and create an autonomous robotic inspection system.	U.S. Department of Energy	National Energy Technology Laboratory	The goal of the project is to prevent negative environmental and socioeconomic impacts of coal waste (coal ash and tailings) by developing an aerial robot-enabled inspection and monitoring system of active and abandoned coal ash and tailings storage facilities. The first objective of this project is the development of a programmable drone, equipped with several complementary sensors, that will autonomously inspect several structures of a storage facility. The second objective of this project is to create artificial intelligence-based hazard detection algorithms that will use multispectral and georeferenced images (i.e., thermal and visual) and 3D Point Clouds data collected by an autonomous drone to detect hazards in the storage facility structure that would indicate uncontrolled leakage to the environment or lead to the potential failure of the structure.		2022-10-01		Jason Hissam	jason.hissam@netl.doe.gov	Contracted		Artificial Intelligence, Robotic Processing Automation (RPA)	Unknown	Yes
To provide integrated boiler management through advanced condition monitoring and component assessment.	U.S. Department of Energy	National Energy Technology Laboratory	The Integrated Creep-Fatigue Management System represents an online boiler damage monitoring system applicable to creep and fatigue. The system will be configured to allow connectivity to the plant data historian (e.g., OSISoft:PI) and to commercial finite element software (e.g., ANSYS and Abaqus). In addition to configuring interaction with finite element software, existing damage mechanism monitoring modules will also be deployed using online analytical calculations. This functionality will be applied to terminal tubes entering the boiler header for which the combined mechanisms of creep and oxidation can be calculated without the need for a finite element analysis.		2019-01-01		Barbara Carney	barbara.carney@netl.doe.gov	Contracted			Unknown	Yes
Solving Field Equations on the Wafer Scale Engine	U.S. Department of Energy	National Energy Technology Laboratory	The intent is to develop a collocated, finite volume code to allow maximum mesh flexibility and support advanced CFD capabilities found in modern CFD codes like Fluent, OpenFOAM, and MFiX. NETL will take a metered approach to development towards a fully reacting CFD capability on the WSE. EY22 will be filled with API capability expansions needed to support general purpose CFD applications, such as general purpose finite volume formulations, collocated grid capabilities (Rhie & Chow Interpolation), bit stuffing to save memory when dealing with cell types, general purpose boundary conditions, etc. In addition, the code will be benchmarked in a series of tests towards a fully reacting CFD capability that will support problems of interest to FECM.		2022-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Big Data, Other	Generated from CFD on the fly during training	Yes
Using time-series classification to assist in automated analysis of sensor data taken during experiments on the MHD test channel.	U.S. Department of Energy	National Energy Technology Laboratory	The measurements of chemical composition will be combined with resistance measurements to validate CFD models of the MHD channel system. Specifically, validated CFD models will be able to separate the contribution of the bulk and boundary layer resistance to the overall resistance of the MHD channel.		2021-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Other	Experimentally obtained data	Yes
To develop and validate sensor hardware and analytical algorithms to lower plant operating expenses for the pulverized coal utility boiler fleet	U.S. Department of Energy	National Energy Technology Laboratory	The objective is to develop and validate sensor hardware and analytical algorithms to lower plant operating expenses for the pulverized coal utility boiler fleet. The focus is on relatively inexpensive new "Internet of Things" technologies to minimize capital investment. Three technologies will be explored for demonstration and full-scale testing in a coal-fired power plant. The first focuses on gas and steam temperature control issues at low load. The second uses sensors and analytic algorithms for monitoring coal pulverizer operation at lower loads to reduce the minimum firing capability of coal burners. The third investigates new sensors and advanced controls to better balance air and fuel at each burner enabling reduction in the minimum firing capability of coal burners.		2018-01-01		Diane Revay Madden	diane.madden@netl.doe.gov	Contracted			Unknown	Yes
To leverage ML models to increase the size and complexity of problems that can be optimized within IDAES.	U.S. Department of Energy	National Energy Technology Laboratory	The objective is to leverage ML models as surrogates for complex unit operations or to bridge between scales to increase the size and complexity of models that can be optimized within IDAES.		2021-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Other	Unknown	Yes
To realize next generation solid-state power substation.	U.S. Department of Energy	National Energy Technology Laboratory	The objective of the proposed project is to realize next generation solid-state power substation (SSPS) incorporating machine learning, cyber-physical anomaly detection, and multi-agent distributed networked control. The project will have the following capabilities: distributed control and coordination coupled with localized intelligence and sensing, autonomous control for plug-and-play, automatic reconfiguration, recovery, and restoration enabling decoupled, asynchronous, and fractal systems.		2022-10-01		Joseph Dygert	joseph.dygert@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To develop innovative biomonitoring and remediation of heavy metals using phytotechnologies.	U.S. Department of Energy	National Energy Technology Laboratory	The objective of the work is to utilize algal- and cyanobacterial-based phycotechnologies to address pervasive heavy metal contamination from coal combustion product (CCP) impoundments at the Savannah River Site. Novel bioindicators will be developed to gauge the potential for phytoremediation to restore legacy impoundment sites.		2023-01-25		Heather Hunter	heather.hunter@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes

To use computational tools to optimize the design of solid CO2 sorbents.	U.S. Department of Energy	National Energy Technology Laboratory	The objective of this project is to use computational tools to optimize the design of solid CO2 sorbents based on functionalized PIM-1 (or other porous, glassy polymers) impregnated with molecular primary amines. The expected outcome of this project is to inform, via computational methods, which polymer structure and which molecular amines can lead to a solid sorbent in which CO2 loading capacity, CO2 heat of adsorption, and overall CO2 mass transfer rate are optimal at extremely low CO2 partial pressures while amine leaching has been minimized.		2022-04-01		Viktoria L Pretzman	laura.pretzman@netl.doe.gov	In-house		Other	In-house calculations and publications	Yes
To accelerate discovery of protection system and laser processing of protective coatings on CMC for hydrogen turbines.	U.S. Department of Energy	National Energy Technology Laboratory	The objectives of this project are to design, process, and validate a laser-manufactured, integrated, and graded bond coat-environmental barrier coat-thermal barrier coat (BC-EBC-TBC) system that can effectively protect and lead to the use of Silicon Carbide fiber/Silicon Carbide (SiCf/SiC) matrix CMCs in next-generation hydrogen-fueled turbines.		2023-02-03		Omer R. Bakshi	omer.bakshi@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To develop an AI-driven integrated autonomous robotic visual inspection (RVI) platform.	U.S. Department of Energy	National Energy Technology Laboratory	The overall objective of the research is to develop an AI-driven integrated autonomous robotic visual inspection (RVI) platform that can perform real-time defect identification, dynamic path planning, and safe navigation in a closed-loop manner. The		2023-02-01		Adam Payne	adam.payne@netl.doe.gov	Contracted		Artificial Intelligence, Robotic Processing Automation (RPA)	Unknown	Yes
Use ML to reduce high-fidelity physical models to a fast calculation that requires minimal effort to initiate.	U.S. Department of Energy	National Energy Technology Laboratory	The platform will combine an intuitive user interface and visualization capabilities from gaming software with the speed and enhanced detail in evaluating reservoir dynamics and processes through ML /reduced order model approaches. Advancements made with ML will alleviate the need for both the expert user and the computational infrastructure and make understanding subsurface fluid flow accessible to the everyday user with a moderate level of understanding of the physics of the system. ML will allow the experts to reduce the high-fidelity physical models to a fast calculation that requires a minimal amount of effort to initiate, but allows a user to investigate their own scenarios without the need for predetermined models. Application of the platform will rapidly enhance the experience base required for deploying and managing commercial-scale projects, particularly for CO2 storage projects where field experience is limited, because of the anticipated intuitive translation of subsurface dynamics in real-time.		2020-01-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	Unknown	Yes
To provide an effective quality assurance method for additively manufactured gas	U.S. Department of Energy	National Energy Technology Laboratory	The primary goal of this project is to develop a cost-effective quality assurance (QA) method that can rapidly qualify laser powder bed fusion (LPBF) processed hot gas path turbine components (HGPTCs) through a machine learning framework which would assimilate in-situ monitoring and measurement, ex-situ characterization, and simulation data. The project technical deliverable will be a rapid QA tool capable of: i) building a metadata package of process-structure-property data and models intended for LPBF-processed HGPTCs by mining both simulation and in-situ/ex-situ characterization data; and ii) qualifying online/offline a manufactured component by inputting simulation with/without in-situ monitoring data to the developed algorithms to predict porosity and fatigue properties. The target application of this QA tool will be advanced HGPTC produced by LPBF in Inconel 718. Data mining techniques will be developed to consolidate and analyze the heterogeneous big data stemmed from the aforementioned methods of upfront simulation, online monitoring and post-build characterization, and thus enabling a collaborative learning about the process-microstructure-properties relationship. The resultant QA package includes a process-structure-property database and machine learning tools for using LPBF metal AM to fabricate HGPTC. The developed metadata package enables online/offline qualification of additively manufactured turbine components by inputting simulation with/without in-situ monitoring data to the developed machine learning algorithms to predict porosity and fatigue properties.		2019-10-01		Mark C. Freeman	mark.freeman@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To deploy dynamic neural network optimization to minimize heat rate during ramping for coal.	U.S. Department of Energy	National Energy Technology Laboratory	The primary objective of the proposed work is to 1) deploy dynamic neural network optimization (D-NNO) to minimize heat rate during all phases of operation (ramping, low load, and high load) at a coal power plant. The project will build a high-fidelity, systems-level, dynamic model of the plant for a rapid prototyping environment for the D-NNO and to allow researchers to better understand the dynamic phenomena that occur during ramping and at various plant loads, and Commercialize D-NNO as a readily-available software application by working with an industry-proven software platform. The plant will be perturbed over time to allow machine learning (ML) models to be fitted to the plant's response data.		2019-10-01		Barbara Carney	barbara.carney@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes
To create a data-driven multiscale phytotechnology framework for identification and remediation of leached-metals-contaminated soil.	U.S. Department of Energy	National Energy Technology Laboratory	The project objectives are to integrate satellite remote sensing, machine learning and image processing, geological engineering models, and soil science and plant pathology to: 1) identify potential leaching of metals from coal ash impoundments (Phase I), and 2) propose locally adaptable phytoextraction approaches to remediate contaminated regions (Phase II).		2022-10-01		Heather Hunter	heather.hunter@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To develop a general drag model for assemblies of non-spherical particles created with artificial neural networks	U.S. Department of Energy	National Energy Technology Laboratory	The project plans to develop a more accurate artificial neural network (ANN)-based method for modeling the momentum exchange in fluid-solid multiphase mixtures to significantly improve the accuracy and reduce the uncertainty of multiphase numerical codes and, in particular, of MFiX, by developing and providing a general and accurate method for determining the drag coefficients of assemblies of non-spherical particles for wide ranges of Reynolds numbers, Stokes numbers, and fluid-solid properties and characteristics. The research team will achieve this goal by conducting numerical computations with a validated in-house CFD code and using artificial intelligence methods to develop an ANN that will be implemented in TensorFlow and linked with the MFiX code.		2020-09-01		Adam Payne	adam.payne@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes

Using AI/ML to replace conventional geophysics inversion - does the process quicker than the typical method. Make geophysical results more user-friendly.	U.S. Department of Energy	National Energy Technology Laboratory	The project will deploy a high sensitivity atomic magnetometer (potassium magnetometer or helium 4 magnetometer) on a sUAS platform. Baseline surveys using the sUAS platform with the magnetic receiver payload will be flown at the same CarbonSAFE site that baseline ground surveys were performed in EY21. Results of the forward modeling performed in EY20 will determine whether MT or CSEM (or both) methods will be tested. Using AI/ML to replace conventional geophysics inversion - does the process quicker than the typical method. Make geophysical results more user-friendly.		2020-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Neural Networks	Government models	Yes
To develop and evaluate a general drag model for gas-solid flows via physics-informed deep machine learning	U.S. Department of Energy	National Energy Technology Laboratory	The project will evaluate the performance of several ANN algorithms for machine learning, pertinent to the deep neural network (DNN) algorithms. The DNN candidates will include random forest (RF), BPNN, XGBoost, and other supervised deep neural network algorithms. The best DNN algorithm will be identified by ranking of these algorithms' performance. The Recipient will integrate the deep learning ANN model (DNN model) into the multiphase flow simulation software MFiX-DEM, which is part of the NETL's open source CFD suite of software MFiX. The DNN based drag model developed on TensorFlow will be implemented using NETL's existing software links between MFiX and TensorFlow.		2020-08-01		Heather Hunter	heather.hunter@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes
To use advanced machine learning techniques to analyze static and dynamic measurements of proppant distribution and fracture geometry data.	U.S. Department of Energy	National Energy Technology Laboratory	The project will use advanced ML techniques to analyze static and dynamic measurements of proppant distribution and fracture geometry data from thousands of microchips injected with proppant near the wellbore.		2019-10-01		Robert Noll	robert.noll@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To leverage machine learning and predictive analytics to advance the state of the art in pipline infrastructure integrity management.	U.S. Department of Energy	National Energy Technology Laboratory	The purpose of this project is to leverage advances in machine learning and predictive analytics to advance the state of the art in pipeline infrastructure integrity management using forecasted (predicted) pipeline condition, using large sets of pipeline integrity data (periodic nondestructive inspection, NDI) and continuous operational data (e.g., sensor data used to monitor flow rate and temperature) generated by oil and gas (O&G) transmission pipeline operators.		2018-10-01		Eric Smistad	eric.smistad@netl.doe.gov	In-house		Artificial Intelligence	Unknown	Yes
To detect leaks and creaks.	U.S. Department of Energy	National Energy Technology Laboratory	The relevant research has been focused on demonstrating applicability of novel machine learning based approaches to two major challenges associated with safe management of large-scale geologic CO2 storage operations, early detection of leaks (i.e., by detecting small leaks) and early detection of induced seismicity (i.e. by detecting small seismic signals).		2022-08-01		Johnathan E. Moore	johnathan.moore@netl.doe.gov	In-house		Artificial Intelligence	Unknown	Yes
To perform reconstruction of the 3D temperature field using Neural Networks with measured and known propagation paths.	U.S. Department of Energy	National Energy Technology Laboratory	The sensor will first be tested up to 300 □C. For high-temperature tests, the Recipient will use Alstom's Industrial Size Burner Test Facility (ISBF) or another appropriate facility. The high-temperature sensor will be first tested from room temperature to 1,800 □C. The results will be compared with data obtained using other methods such as surface acoustic wave (SAW), thermocouples, and optical fiber sensors. A 3D temperature mapping will be created by fusing the high-temperature sensor data. The Recipient will test the system's survivability in a boiler environment. A high-temperature sensing array will be tested to map the temperature distribution within an exhaust pipe. The sensor array will be tested at one 6'' port or a similar location. The Recipient will also perform reconstruction of the 3D temperature field using Neural Networks with measured and known propagation paths.		2020-09-04		Robie Lewis	robie.lewis@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
Using ML to design sensing materials which can work under harsh environments.	U.S. Department of Energy	National Energy Technology Laboratory	The team proposes to develop an ML approach that relies upon established experimental and theoretical evidence to gain a comprehensive ML model and boost the gas sensing material design. The essence of this approach will be to assess materials' optimal performance at a specific condition, such as temperature, pressure, and radiation levels. The development of the package will occur in several steps: (1) building a materials database from various sources; (2) using ML techniques to build, evaluate, and optimize an ML model; (3) predicting the temperature dependence of sensing properties, such as gas selectivity, for FECM relevant gas species to screen the materials in the material bank, or proposing new sensing materials; and (4) exploring the gas sensing mechanisms suited for high-temperature application for those predicted most promising gas sensing materials.				Steven Richardson	steven.richardson@netl.doe.gov	In-house		Other	Materials Project publications	Yes
To drive insights into solid oxide cell performance and degradation through big data analysis and computer vision	U.S. Department of Energy	National Energy Technology Laboratory	The team uses deep learning models to analyze large banks of high-dimensional simulation results, determine the most impactful input parameters, produce tailored recommendations for industrial manufacturers, and ultimately generate a reduced-order model for predicting long-term performance of solid oxide cells. The team is also developing computer vision models to extract critical high-resolution information from easily obtained low-resolution or 2D microstructural data, and also using computer vision to super-resolve that low-resolution data, producing full sets of high-resolution 3D data from low-resolution 3D tomography or even from 2D micrographs. The team has recently developed and published a generative adversarial network model for generating high-fidelity synthetic microstructural data of solid oxide cells. Machine learning is also used in the team's reduced order phase field simulations of microstructural changes.		2022-04-01		Brian Dressel (acting)	brian.dressel@netl.doe.gov	In-house		Big Data, Hierarchical Generative Model, Neural Networks, Other	Generated in-house and generally published or a part of published work	Yes

To drive insights into solid oxide cell performance and degradation through big data analysis and computer vision	U.S. Department of Energy	National Energy Technology Laboratory	The team uses deep learning models to analyze large banks of high-dimensional simulation results, determine the most impactful input parameters, produce tailored recommendations for industrial manufacturers, and ultimately generate a reduced-order model for predicting long-term performance of solid oxide cells. The team is also developing computer vision models to extract critical high-resolution information from easily obtained low-resolution or 2D microstructural data, and also using computer vision to super-resolve that low-resolution data, producing full sets of high-resolution 3D data from low-resolution 3D tomography or even from 2D micrographs. The team has recently developed and published a generative adversarial network model for generating high-fidelity synthetic microstructural data of solid oxide cells. Machine learning is also used in the team's reduced order phase field simulations of microstructural changes.		2022-04-01		Brian Dressel (acting)	brian.dressel@netl.doe.gov	In-house		Neural Networks, Spatio-temporal Graph Neural Networks, Other	Publications	Yes
Database will be utilized to demonstrate targeted biocide strategies using AI to assess large DNA datasets.	U.S. Department of Energy	National Energy Technology Laboratory	The team will develop a public DNA database that will advance knowledge in produced water management. This project consists of two phases: (1) the development and launching of the database, and (2) the demonstration of applicability of the database by conducting a network analysis. The work will be pursued as defined in the phases below. The fully characterized streams will be used by other FWPs to estimate overall resource recovery and will be used by other FWPs as training set for machine learning (ML) models to predict compositions when only limited measurements can or have been completed for the produced water.		2022-04-01		Viktoria L Pretzman	laura.pretzman@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes
Data discovery, processing, and generation using machine learning for a range of CCS data and information	U.S. Department of Energy	National Energy Technology Laboratory	The team will focus on supporting ongoing geospatial data collection and publishing efforts leveraging the new EDX++ cloud computer capabilities through ArcGIS Enterprise Portal. The use of Arc Enterprise Portal will support the development of the Carbon Matchmaker tool, as well as support the release of a new version of GeoCube, which will be host to the updated Carbon Storage Open Database and NATCARB completed in EY21. NETL is supporting DOE-FECM in developing and releasing a survey and map for the Carbon Matchmaker, a tool developed to enable stakeholders to self-identify carbon dioxide related activities (production, utilization, storage, direct air capture, and infrastructure/transportation) to identify and connect stakeholders and support national collaborative opportunities. The ArcGIS Enterprise Portal will be leveraged to build out a new version of GeoCube with the migration of hundreds of spatial data layers into the new platform. The migration of data to an Arc Enterprise based GeoCube will enable easier version control for data integration and curation.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Big Data, Natural Language Processing, Other	Open source, government datasets, citable publications, and other open-source datasets (such as data published as a result of government funded research)	Yes
Fluid migration from well-to-well communication will be inputted in AI to determine a costs-benefit analysis	U.S. Department of Energy	National Energy Technology Laboratory	This project will develop an ML algorithm to predict the time when a growing fracture will reach the monitored well. The ML workflow will be trained on the distinctive tensile strain signature that precedes the growing fracture. The new workflow will be designed to work in conjunction with the fracture warning ML workflow developed in EY21. Together, these workflows will: (1) provide an early warning of well-to-well communication, (2) predict the measured depths where the communication will happen, and (3) provide an estimated time until the beginning of well-to-well communication.		2021-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Artificial Intelligence, Big Data, Other	Unknown	Yes
Using recursive neural networks and using fiber optic cables to recognize strain patterns and warn operators a fracture is coming.	U.S. Department of Energy	National Energy Technology Laboratory	This project will develop an ML algorithm to predict the time when a growing fracture will reach the monitored well. The ML workflow will be trained on the distinctive tensile strain signature that precedes the growing fracture. The new workflow will be designed to work in conjunction with the fracture warning ML workflow developed in EY21. Together, these workflows will: (1) provide an early warning of well-to-well communication, (2) predict the measured depths where the communication will happen, and (3) provide an estimated time until the beginning of well-to-well communication.		2021-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Neural Networks, Other	Government data and proprietary datasets provided by industry consortium	Yes
Rokbase Geologic Core Data Tool	U.S. Department of Energy	National Energy Technology Laboratory	This project will develop the platform through which the DOE OGFL data are easily accessible, searchable, and described, enabling future R&D, sustainable resource planning, and responsible stewardship of the team's national resources. NETL's expertise in developing geo-data science, ML, visualization, online data mining and integration, and advanced analytics through scientific computing (including high performance computing and big data computing methods) and virtualized environments can be leveraged to support further intelligent analytics for offshore systems.		2021-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Neural Networks, Other	Government datasets	Yes
Advanced model to forecast offshore landslide risks and marine geohazards	U.S. Department of Energy	National Energy Technology Laboratory	This research will use data and models from the Offshore Risk Modeling (ORM) with intelligent databases, artificial intelligence (AI)/ML, big data, and other advanced computing technologies to address offshore subsurface natural-engineered system challenges, such as characterization and mapping of geologic hazards, safe operations, equipment reliability, and environmental assessments.		2018-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Big Data, Natural Language Processing, Other	Open-source	Yes
Computational capabilities to support experimental efforts	U.S. Department of Energy	National Energy Technology Laboratory	This subtask will leverage NETL's in-house computational capabilities and existing university collaborators to support experimental efforts by providing atomic-level DFT and microkinetic modeling calculations for catalyst systems. This work provides atomic-level details on reaction energetics and establishes key structure-property relationships used to optimize catalyst structure and formulation.		2021-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house			Synthetic data generated using first-principles method	Yes
Use ML to analyze the existing H2 and natural gas pipelines to identify the key parameters that can enable the H2 transport and storage at a large scale	U.S. Department of Energy	National Energy Technology Laboratory	This task aims to use geo-data science methods and geospatial information science to analyze the existing H2 and natural gas pipelines to identify the key parameters that can enable the H2 transport and storage at a large scale. The results can help to justify the importance of real-time pipeline monitoring and recommend optimized sensor deployment strategies to support smart maintenance and methane emissions reduction goals.		2022-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes

Demonstrate how ML-based approaches can help operators during active injection and post-injection monitoring	U.S. Department of Energy	National Energy Technology Laboratory	To demonstrate how ML-based approaches can help operators during active injection and post-injection monitoring, it is necessary to understand their needs and identify how ML-based approaches can potentially meet or support those needs. Task 4 will establish data-sharing protocols between SMART and the operator to create an exchange mechanism that is not intrusive to the operator and provides updates from ML results designed to enhance the operator decision process. Demonstrate application of ML-based approaches to improve site-monitoring and operations efforts performed during injection and post-injection phases, e.g., using IL-ICCS data, and developing value of information guidelines.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	EDX - government datasets	Yes
To develop artificial intelligence-enabled tools (ArtIT) for cyber hardening of power grids.	U.S. Department of Energy	National Energy Technology Laboratory	To develop a novel resiliency framework for power grids by integrating different theories, such as closed-loop controls, security, agility, formal reasoning and synthesis, machine learning, and laboratory setup demonstration. The framework will provide enhanced resiliency to wide-area control operations in cyberattacks.		2022-10-01		J. Clark Robinson	clark.robinson@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To develop and demonstrate drone-based geophysical and remote-sensing technologies to quantify critical minerals (CM).	U.S. Department of Energy	National Energy Technology Laboratory	To develop and demonstrate drone-based geophysical and remote-sensing technologies to quantify critical minerals (CM) in coal, coal related, unconventional and secondary sources or energy related waste streams. Drone-based geophysical surveys and remote sensing combined with artificial intelligence/machine learning (AI/ML) analytics for real-time integration and analytics has potential to transform characterization and monitoring for CM from conventional and secondary resources.		2023-02-09		Christian Robinson	christian.robinson@netl.doe.gov	In-house		Artificial Intelligence, Robotic Processing Automation (RPA)	Unknown	Yes
To develop high fidelity tools which run in near real time not only help in the field to guide and optimize complex operations but can be used as digital twins	U.S. Department of Energy	National Energy Technology Laboratory	To develop high fidelity tools which run in near real time not only help in the field to guide and optimize complex operations but can be used as digital twins for cyber security and cyber-physical modeling.		2018-04-01		Steve Richardson	steven.richardson@netl.doe.gov	In-house		Big Data	Unknown	Yes
To build the first data analytics and artificial intelligence field laboratory for unconventional resources in the Powder River Basin, focusing on optimization of hydraulic fracture stimulations through the use of multiple diagnostic technologies.	U.S. Department of Energy	National Energy Technology Laboratory	To establish a tight oil Field Laboratory in the Powder River Basin and accelerate the development of three major unconventional oil resources through detailed geologic characterization and improved geologic models leading to significant advances in well completion and fracture stimulation designs specific to these three formations. Utilize multi-variate analysis to understand the interrelationship between completion and stimulation controls on well productivity.		2019-10-01		Eric Smistad	eric.smistad@netl.doe.gov	Contracted		Artificial Intelligence, Big Data	Unknown	Yes
To apply machine learning applications to map carbon ore, rare earth element, and critical mineral resources	U.S. Department of Energy	National Energy Technology Laboratory	To identify information gaps, GIS and machine learning applications will be used to map carbon ore, rare earth element, and critical mineral resource infrastructure, and market data in consultation with NETL geospatial modeling activities. Research needs and technology gaps will be assessed, and resources targeted for sampling and characterization. This effort will provide a complete Northern Appalachian carbon ore, rare earth element, and critical mineral value chain basinal assessment to enable quick development of commercial projects.		2021-10-01		Eric Smistad	eric.smistad@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
Using natural language processing to explore and extract information from historical literature/pdfs	U.S. Department of Energy	National Energy Technology Laboratory	Training and adaptation of natural lanaguage processing algorithms to improve exploration and extraction of information from old, historical scientific literature. Extraction of knowledge and data, as well as preservation of key information.		2020-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Big Data, Natural Language Processing, Other	Unknown	Yes
Advanced Image Segmentation	U.S. Department of Energy	National Energy Technology Laboratory	U-Net CNN segmentation to isolate pore and fluid from computed tomography scans of multiphase transport in cores.		2018-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Neural Networks, Other	Unknown	Yes
Machine Learning for geophysical data inversion	U.S. Department of Energy	National Energy Technology Laboratory	Use machine learning to generate synthetic seismic and gravity data, and data driven inversion for leak detection		2018-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	Unknown	Yes
Machine learning for legacy well evaluation	U.S. Department of Energy	National Energy Technology Laboratory	Use machine learning to identify common attributes that correlated to well integrity issues to prioritize for monitoring and remediation.		2018-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	Unknown	Yes
Using AI to improve predcitions of subsurface properties, analyze multi-variate inputs, address knowledge and information gaps to improve predictions and modeli	U.S. Department of Energy	National Energy Technology Laboratory	Use of AI methods such as fuzzy logic, neural networks, tensor flow, and natural language processing to assist with knowledge and data exploration, transformation and integration, as well as modeling and analysis of multi-variate data used in the resource assessment method to improve outputs and predictions.		2022-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Artificial Intelligence, Big Data, Other	Open-source and government datasets	Yes
Machine learning to process multi-model data and information to aid in the identification of undocumented orphaned wells	U.S. Department of Energy	National Energy Technology Laboratory	Use of machine learning to process and analyze trends and patterns in known well data to predict undocuemnted orphaned wells, as well as machine learning approached to process different imagery based data to further classify and characterize additional undocuemented orphaned wells within the Appalachain Basin		2022-04-01		Brian Dressel	brian.dressel@netl.doe.gov	In-house		Big Data, Other	government datasets (state and federal)	Yes
To analyze data and derive insights and improve predictions to forecast wellbore kick events to reduce loss of control events.	U.S. Department of Energy	National Energy Technology Laboratory	Use of neural networks and/or AI cluster data analysis methods to improve detection and forecasting of wellbore and drilling related loss of control events, known as kicks, to imrpove real-time detection and prediction of these conditions.		2018-04-18		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Neural Networks, Other	Unknown	Yes
To use data analytics and machine learning techniques to advance understanding of the characteristics of the Emerging Paradox Oil Play	U.S. Department of Energy	National Energy Technology Laboratory	Using data analytics and machine learning techniques to advance understanding of the characteristics of the entire Parardox oil play through integration of geologic and log-derived “electrofacies” models and upscaling to 3D seismic data and propagation through the seismic volume.		2019-10-01		Stephen Henry	stephen.henry@netl.doe.gov	Contracted		Artificial Intelligence, Big Data, Neural Networks	Unknown	Yes
To help automate data integration and exploration for geologic core properties related information.	U.S. Department of Energy	National Energy Technology Laboratory	Using natural language processing, deep learning neural networks, and possibly tensor flow for image analytics.		2020-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Big Data, Natural Language Processing, Other	Unknown	Yes
Machine learning to tool and model applications for CCS needs	U.S. Department of Energy	National Energy Technology Laboratory	Utilze and apply different machine learning approaches to help model and analyze Class VI well regulatation data, CCS infrastructure optimization, CCS data visualization, and interaction with “really big” (petabyte-scale) datasets used for CCS resource characterization and risk reduction (e.g., reflection seismic surveys) within the EDX multi-cloud ecosystem.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Big Data, Other	Open-source and government datasets	Yes
Machine learning to refine and analyze data for CCS needs	U.S. Department of Energy	National Energy Technology Laboratory	Utilze and apply different machine learning approaches to process data and generate new derivative data products that help address CCS stakeholder data-needs for resource evaluation, risk assessment, supply chain, social and environmental justice evaluations, regulatory compliance, and more.		2022-04-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Big Data, Other	Open-source and government datasets	Yes

To verify and validate testing of advanced power generation technologies	U.S. Department of Energy	National Energy Technology Laboratory	Verification and validation testing with direct support and collaboration from operating power plants with advanced power generation technologies and prime mover and downstream systems using near-real-time data, resulting in better informed plant operators, and reduced disruptions, while meeting changing service demands based on enhanced operating flexibility		2021-06-11		Omer R. Bakshi	omer.bakshi@netl.doe.gov	Contracted		Artificial Intelligence, Big Data	Unknown	Yes
Use of machine learning models to produce surrogates for efficient optimization	U.S. Department of Energy	National Energy Technology Laboratory	We consider the use of machine learning models to produce surrogates for efficient optimization. The IDAES implementation will be demonstrated on a real-scale design problem focused on carbon capture (e.g., rigorous MEA model), or an integrated energy system.		2022-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Other	Open-source and publications	Yes
Using ML to build predictive models of branching processes and develop novel algorithms for automated MIP solver tuning	U.S. Department of Energy	National Energy Technology Laboratory	We will collect dual gaps obtained as a result of using different branching strategies and feed them into ALAMO, Pysmo, and other machine learning approaches to build predictive models of branching processes as a function of carefully chosen instance features. These models will then be deployed as part of the IDAES platform to facilitate optimization of advanced integrated energy systems. o Currently, tuning MIP solvers for a particular application is approached by ad-hoc trial-and-error methods that are tedious and often ineffective, limiting design engineers to solution of small problems. To address this challenge and facilitate the solution of energy systems currently intractable, we propose to develop novel algorithms for automated MIP solver tuning through the use of machine learning.		2022-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Other	Open-source and publications	Yes
Develop, integrate, and automate the reduction of CFD models while preserving acceptable levels of accuracy. In general for CCSI2, this work intends to focuse on CFD applications.	U.S. Department of Energy	National Energy Technology Laboratory	Will leverage state-of-the-art, physics-based deep learning (DL) models to learn generalizable surrogates that may be used in place of CFD models to predict quantities required for downstream optimization. The products from this subtask can be immediately leveraged by other subtasks that are seeking to speed up their CFD simulation models to streamline their downstream analyses. Addtionally, improvements to the ML/AI interface in FOQUS. Includes support for vector variables in the ML/AI plugin and support for additional surrogate model tools (e.g., PyTorch, Sci-kit Learn) and additional normalization function forms in the ML/AI plugin.		2022-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Neural Networks, Other	Unknown	Yes
To employ machine learning to study the dependence of electrochemical performance on microstructural details	U.S. Department of Energy	National Energy Technology Laboratory	With a significant number of images. The Recipient will build deep learning methods at the object detection stage using the Region Based Convolutional Neural Network (RCNN) or You Only Look Once (YOLO) class of algorithms, the heart of which is a deep learning image classifier. Deep learning algorithms will also be built using convolutional layers followed by residual layers to extract feature vector descriptors in the second stage. In the third and fourth stages of affinity and association, a recurrent neural network approach can be used to build a tracker. All of these approaches require a large training set that will enable sophisticated models to be built to handle the complexity of the application. With a limited number of images. In the case that there is are a limited number of images, the Recipient will still be able to follow the processing pipeline. The recipient will determine a suitable approach, with concurrence from the project manager. Two potential approaches include: • Transfer learning: training the image classifier in the object detector on images of similar quality and appearance, and • Match filtering: detection, feature extraction, and matching based on traditional image processing and computer vision techniques.		2021-09-10		Evelyn Lopez	evelyn.lopez@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes
With sensor technologies and network developed, in the future, AI/ML may be used to accelerate data processing of sensor data from the sensor network.	U.S. Department of Energy	National Energy Technology Laboratory	With sensor technologies and network developed, in the future, AI/ML may be used to accelerate data processing of sensor data from the sensor network to identify and predict risks and failures in plugged wells.				Sandra Borek	sandra.borek@netl.doe.gov	In-house			N/A	Yes
Online real time system Identification	U.S. Department of Energy	National Energy Technology Laboratory	Work will focus on using SI to monitor the condition of a power plant boiler at different process states. SI algorithms will be implemented within an MPC to provide continuous adaptability as the power plant ramps through the entire range of operating loads. Once the control algorithm has been developed to be effective on representative models, it will be tested on a high-fidelity commercial power plant simulator or on a real power plant facility. The online SI techniques will be tested on historical power plant data, dynamic models (including a power plant simulator), power generating equipment including laboratory pilot-scale power systems, and on power plants where feasible.		2021-04-01		Steven Richardson	steven.richardson@netl.doe.gov	In-house		Artificial Intelligence, Big Data, Other	Industrial power plant (obtained under MOU) and NETL's Hyper test facility (government)	Yes
To expore and analtze hydrogen-fueled rotating detonation engines using advanced turbulent combustion modeling and high-fidelity simultion tools.	U.S. Department of Energy	National Energy Technology Laboratory	(1) analysis of injector design effects on RDE parasitic combustion; (2) understanding the impact of RDE ignition mechanism and initial transients on the ensuing detonation wave behavior; (3) deployment and assessment of machine learning assisted turbulent combustion models for predictive and computationally-efficient RDE CFD simulations; and (4) development of a highly scalable high-order CFD modeling framework for scale-resolving simulations of full-scale RDEs and investigation of TCI and wall boundary layer effects.(1) analysis of injector design effects on RDE parasitic combustion; (2) understanding the impact of RDE ignition mechanism and initial transients on the ensuing detonation wave behavior; (3) deployment and assessment of machine learning assisted turbulent combustion models for predictive and computationally-efficient RDE CFD simulations; and (4) development of a highly scalable high-order CFD modeling framework for scale-resolving simulations of full-scale RDEs and investigation of TCI and wall boundary layer effects.		2022-10-01		Matthew Adams	matthew.f.adams@netl.doe.gov	In-house		Artificial Intelligence	Unknown	Yes
Geochemically Informed Leak Detection (GILD)	U.S. Department of Energy	National Energy Technology Laboratory	A Bayesian Belief Network has been developed to interogate the altered geochemistry around a potential CO2 leakage site. The use of the BNN and site specific parameters will reduce the percentage of false positives with this method.		2018-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Artificial Intelligence, Other	Unknown	Yes

To develop a deep-learning Artificial Intelligence model for analysis of fundamental combustion characteristics	U.S. Department of Energy	National Energy Technology Laboratory	A deep-learning Artificial Intelligence model will be pursued for rapid analysis of detailed fundamental combustion characteristics that support the design and troubleshooting process of H2-containing fuel combustor development.		2021-08-01		Matthew Adams	matthew.f.adams@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes
Prediction of gasification gas yield and compositions using machine learning	U.S. Department of Energy	National Energy Technology Laboratory	A machine learning (ML) model will be developed to aid in investigating and optimizing of gasification with various feedstocks like waste plastic, waste coal, biomass and MSW. Database on the gasification will be built from main resources of literature, prior experiments in NETL, and new generating experiments in NETL. AI/ML will be a part of the project. It combines with experimental study to accelerate development of gasification applying to variour feedstocks including waste plastics, waste coal, MSW and its mixture. The ML will have more impact as the big database will be built.		2021-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Big Data, Other	Open source, journal publication, own lab experiment results	Yes
To implement novel SSC-CCS sensing technology and associated condition-based monitoring (CBM) software for improved understanding of the boiler tube failure mechanisms	U.S. Department of Energy	National Energy Technology Laboratory	A preliminary condition-based monitoring (CBM) package with graphic user interface (GUI) will be developed. This CUI will allow the operators to view the current and historical signals of temperature profiles of the boiler tube at specific sensor locations. Combining the pre-existing conditions and the opinions from designers/operators/experts' experiences, the system will be integrated with EPRI's Boiler Failure Reduction Program to provide assessments on the health conditions of the boiler tubes, warnings/diagnoses on potential failures and locations, and suggestions on maintenance locations and schedules.		2019-10-01		Richard Dunst	richard.dunst@netl.doe.gov	Contracted			Unknown	Yes
Develop fast predictive models using novel machine-learning based methods.	U.S. Department of Energy	National Energy Technology Laboratory	Accurate, fast predictive ML models form the foundation for the virtual learning platform. Generating training data then developing ML based models enables a Virtual Learning Environment (VLE) for exploring and testing strategies to optimize reservoir development, management & monitoring prior to field activities.		2020-01-01		M. Kylee Underwood	mary.underwood@netl.doe.gov	In-house		Other	Unknown	Yes
To help automate data discovery and preparations to support a range of CS models, tools, and products	U.S. Department of Energy	National Energy Technology Laboratory	AI & ML are used to help collect and process data from multipel sources to further integrate and characterize infromation to provide additional data and infromation to support a range of carbon storage work		2018-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Big Data, Natural Language Processing, Other	Unknown	Yes
AI used to interpret sensor data.	U.S. Department of Energy	National Energy Technology Laboratory	AI is being used to classify sensor data. An AI algorithm was written and trained with a wide range of known sensor conditions to enable automatic classification of sensor data into likely constituent gas concentrations.		2021-04-01		Steven Richardson	steven.richardson@netl.doe.gov	In-house		Other	In-house generated sensor data fabricated in the lab, tested, then generate the testing data	Yes
To accurately predict alloy & component performance extrapolated to conditions where experimental results to do not exist.	U.S. Department of Energy	National Energy Technology Laboratory	AI/ML will be used to interrogate databases comprised of experimental data, literature data, and synthetic data generated improved physics based models to generate reduced order models to accurate predict materials the performance of materials and components under extreme environments (temperature, atmosphere) and complex loading (cyclical, triaxial) for long service life durations.		2019-04-01		Steve Richardson	steven.richardson@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes
To drive insights on emissions from natural gas production, storage, and transmission to determine how best to reduce emissions	U.S. Department of Energy	National Energy Technology Laboratory	AI/ML will be used to recognice patterns in well integrity records that could predict failure events		2018-04-01		Sandra Borek	sandra.borek@netl.doe.gov	In-house		Big Data, Other	Unknown	Yes
To develop an Artificial intelligence-based model for rotating detonation engine designs	U.S. Department of Energy	National Energy Technology Laboratory	An artificial intelligence-based model will be used to develop low-loss rotating detonation engine (RDE) designs for use in power generation using natural gas/syngas mixtures. The model formulation will enable full-scale RDE calculations over 100-1000 detonation cycles.		2019-10-01		Mark C. Freeman	mark.freeman@netl.doe.gov	Contracted		Artificial Intelligence	Unknown	Yes
To drive insights through data-driven predictive modeling to forecast the remaining lifespan and future risk of offshore production platforms.	U.S. Department of Energy	National Energy Technology Laboratory	An Artificial Neural Network and Gradient Boosted Regression Tree were developed and applied to predict the remaining lifespan of production platforms. These big data-driven models resulted in predictions with scored accuracies of 95–97%.		2018-04-01		Christy Pecyna	christy.pecyna@netl.doe.gov	In-house		Artificial Intelligence, Big Data, Neural Networks, Other	Unknown	Yes
ANN Submodels of Reaction Physics	U.S. Department of Energy	National Energy Technology Laboratory	ANN development of flow physics for code acceleration		2022-04-01		Jerry Carr	jerry.carr@netl.doe.gov	In-house		Other	High-fidelity computer simulations using in-house open-source software, MFiX	Yes
To demonstrate multi-gamma based sensor technology for as-fired coal property measurement	U.S. Department of Energy	National Energy Technology Laboratory	Applying an advanced multigamma attenuation (MGA) sensor to accurately and precisely measure coal properties at the point of injection into burners. One research objective is to perform MGA testing and databases development for neural network developed fingerprinting of coal properties. This will include neural network refinement with MGA data and to upgrade Microbeam's Combustion System Performance Indices (CSPI) – CoalTracker (CT) program with MGA-based neural network algorithms.		2019-10-01		Andrew Downs	andrew.downs@netl.doe.gov	Contracted		Artificial Intelligence, Neural Networks	Unknown	Yes
Applications of Natural Language Processing and Similarity Measures for Similarity Ranking	U.S. Department of Energy	Office of Environment, Health, Safety & Security	"EHSS has been developing applications of natural language processing (NLP) and similarity measures for advanced information retrieval and searching of datasets (e.g., SQL databases, CSV files, reports) as well as estimating similarities between records within a dataset or records between different datasets. Similarity search has been successfully applied to efficiently search DOE COVID-19 Hotline questions and answer database, searching DOE annual site environmental reports, similarity between DOE occurrence reporting and processing system and lessons learned, and AIX data. Similarity measures can also be used to identify opportunities for resource prioritization and prediction. As of October 2021, the tool runs locally by the principal investigator on project based, as requested or as a desktop application. Initial developments were initiated to move to a web-based application but not completed due to lack of user need and resources."		2021-10-01	2010-10-01	Felix Gonzalez	felix.gonzalez@hq.doe.gov	In-house			As Needed or Requested	Yes

Data Analytics and Machine Learning (DAMaL) Tools to enhance the analysis of Environment, Safety and Health (ES&H) data: Classification, Robotic Process Automation and Data Visualization	U.S. Department of Energy	Office of Environment, Health, Safety & Security	"The EHSS Data Analytics Machine Learning (DAMaL) tools, classification, robotic process automation and data visualization tool, uses natural language processing (NLP) and classification algorithms (i.e., random forests) to automate the classification of records, visually provide insights in the trends and provide an indication of importance and risk. The tool leverages artificial intelligence (AI) to analyze the text of the DOE environment, safety, and health (ES&H) and operating experience dataset records (e.g., occurrence reporting and processing system, fire protection, lessons learned, accident and injury reporting system, contractor assurance system CAS) and identifies important topics that can be used by an analyst to drill down and further explore potential safety issues in the DOE operations. As of October 2021, the tool has been deployed in the DAMaL tools website. Expected to continue to maintain, develop documentation (e.g., users analysis guides), improve and enhance, and increase data sources.		2018-08-01	2018-08-01	Felix Gonzalez	felix.gonzalez@hq.doe.gov	Contracted			DOE ES&H Occurrence Reporting and Processing System (ORPS)	Yes
Data Analytics and Machine Learning (DAMaL) Tools for Analysis of Environment, Safety and Health (ES&H) data: Similarity Based Information Retrieval	U.S. Department of Energy	Office of Environment, Health, Safety & Security	"The EHSS Data Analytics Machine Learning (DAMaL) tools, similarity-based information retrieval tool, uses natural language processing (NLP) and cosine similarity to leverage artificial intelligence (AI) to increase the efficiency of a user to find important records in the DOE environment, safety, and health (ES&H) datasets (e.g., occurrence reporting and processing system, fire protection, lessons learned, accident and injury reporting system, contractor assurance system CAS). The tool has no restriction on the text query, provides NLP options to the user (e.g., stemming or lemmatization) and could be used to improve decision-making in job planning activities, identifying hazards, and obtaining insights from operating experience and lessons learned data discovery and analysis, accident investigations among other areas. As of October 2021, Tool developed and deployed in the DAMaL tools website. Expected to continue to maintain, develop documentation (e.g., users analysis guides), improve and enhance, and increase data sources.		2018-08-01	2021-10-01	Felix Gonzalez	felix.gonzalez@hq.doe.gov	Contracted			The approach utilized is not supervised machine learning and does not require training data. Data used is from EHSS ES&H databases.	Yes
Data Analytics and Machine Learning (DAMaL) Tools to enhance the analysis of Environment, Safety and Health (ES&H) data: Unsupervised Machine Learning Text Clustering	U.S. Department of Energy	Office of Environment, Health, Safety & Security	"The EHSS Data Analytics Machine Learning (DAMaL) tools, unsupervised machine learning clustering tool, uses natural language processing (NLP) and clustering algorithms (i.e., k means, DBSCAN and dimensionality reduction approaches) to leverage AI to analyze the text of the DOE environment, safety, and health (ES&H) and operating experience dataset records (e.g., occurrence reporting and processing system, fire protection, lessons learned, and accident and injury reporting system, contractor assurance system CAS). The tool identifies recurrent and important topics that can be used by an analyst to drill down and further explore potential recurrent safety issues in the DOE operations. As of October 2021, the tool has been partially deployed in the DAMaL tools website. Development is mostly complete with use case in Fire Protection Trending and Analysis completed and undergoing review of report. Expected to continue to maintain, develop documentation (e.g., users analysis guides), improve and enhance, and increase data sources.		2018-08-01	2018-08-01	Felix Gonzalez	felix.gonzalez@hq.doe.gov	Contracted			Unsupervised Machine Learning does not need training data. Data used is from EHSS ES&H databases.	Yes
AI-Based Chat Bot	U.S. Department of Energy	Office of the Chief Information Officer	The OCIO EITS Service Desk is exploring the ability to use AI chat bots to interact with end-users. We are looking to have a single bot architecture that is highly tuned to IT system languages to properly handle the terms that may be used in an enterprise environment. The primary benefit would be to make knowledge more available to the end-users in a consumable manner. Additionally, it would connect to ITSM workflows that could automate basic functions such as request an account, provide permissions, or create an MS Teams site as examples. Additionally, the technology needs to provide a significant amount of feedback to the EITS Service Desk on unanswered questions, questions dropped, ineffective responses, incorrect responses, etc.		2022-09-30		Tony Castellano	Tony.Castellano@hq.doe.gov	Commercial-off-the-shelf			OJT	Yes
Advancing Market-Ready Building Energy Management by Cost-Effective Differentiable Predictive Control	U.S. Department of Energy	Pacific Northwest National Laboratory	An AI based differentiable programming framework for domain aware data efficient predictive modeling and AI based control policy synthesis as well as methods for safety verification and online learning. Domain aware deep learning models are used for learning and predicting the response of building systems and components and for optimizing the building energy system response to provide resilient operation and sustained energy efficiency.		2022-10-01		Draguna Vrabie	draguna.vrabie@pnnl.gov	In-house			Simulated data generated by this project based on building simulations, and open-sourced by PNNL as well as real data collected and shared with PNNL by the project's industry partners	Yes
Adaptive Cyber-Physical Resilience for Building Control Systems	U.S. Department of Energy	Pacific Northwest National Laboratory	Deep learning models are used for predicting the operation of building energy systems, and detecting and diagnosing the health state or cyber attack presence, and for optimizing the building energy system response to provide resilient operation and sustained energy efficiency.		2020-03-30		Draguna Vrabie	draguna.vrabie@pnnl.gov	In-house			Simulated data generated by this project based on building simulations, and open-sourced by PNNL	Yes
Elucidating Genetic and Environmental Risk Factors for Antipsychotic-induced Metabolic Adverse Effects Using AI	U.S. Department of Energy	Pacific Northwest National Laboratory	Develop AI methids to find phenotypes that capture complex interation between human genome, chronic diseases and a drug's chemical signature to predict adverse side-effects of a mental health drug on human population		2023-02-01		Khushbu Agarwal	khushbu.agarwal@pnnl.gov	In-house			Government Dataset	Yes
APT Analytics	U.S. Department of Energy	Pacific Northwest National Laboratory	Development of AI/ML for automated analysis of APT data.		2021-10-01		Nicole LaHaye	nicole.lahaye@pnnl.gov	In-house			Generated for this project	Yes

AI used for predictive modeling and real time control of traffic systems	U.S. Department of Energy	Pacific Northwest National Laboratory	Domain aware deep learning models are used for predictive modeling of traffic. Deep learning based predictive controllers are trained from simulated data to optimize the traffic signaling and coordination for improved traffic flow and reduced energy consumption and GHG emissions		2022-09-28		Sonja Glavaski	sonja.glavaski@pnnl.gov	In-house			Open source, simulated data from digital twins	Yes
Laboratory Automation	U.S. Department of Energy	Pacific Northwest National Laboratory	Employing machine learning to identify regions of interest in SEM and TEM data. Automating data acquisition to improve efficiencies.		2022-10-10		Nicole LaHaye	nicole.lahaye@pnnl.gov	In-house			Generated for this project	Yes
Scalable, Efficient and Accelerated Causal Reasoning Operators, Graphs and Spikes for Earth and Embedded Systems (SEA-CROGS)	U.S. Department of Energy	Pacific Northwest National Laboratory	Establish a center for scalable and efficient physics-informed machine learning for science and engineering that will accelerate modeling, inference, causal reasoning, etiology and pathway discovery for earth systems and embedded systems. Advances will lead to a higher level of abstraction of operator regression to be implemented in next generation neuromorphic computers.		2022-09-15		George Karniadakis	george_karniadakis@brown.edu	In-house			Open-source, created by simulations	Yes
Physics-Informed Learning Machines for Multiscale and Multiphysics Problems (PhILMs)	U.S. Department of Energy	Pacific Northwest National Laboratory	PhILMs investigators are developing physics-informed learning machines by encoding physics knowledge into deep learning networks		2018-10-09		George Karniadakis	george_karniadakis@brown.edu	In-house			Open-source, created by simulations	Yes
Managing curb allocation in cities	U.S. Department of Energy	Pacific Northwest National Laboratory	This project's goal is to develop a city-scale dynamic curb use simulation tool and an open-source curb management platform that address the challenge of increased demand for curb-side parking.		2020-09-02		Nawaf Nazir	nawaf.nazir@pnnl.gov	In-house			City of Seattle, Port of Seattle	Yes
Regional waste feedstock conversion to biofuels	U.S. Department of Energy	Pacific Northwest National Laboratory	Unsupervised ML is used sequentially to group waste sources into different regions. Calibrated game theoretic models are used to assess the behavior and economic viability of different waste-to-energy pathways within a region.		2022-10-01		Chenlin Li	chenlin.li@ee.doe.gov	In-house			For questions please contact timothy.seiple@pnnl.gov	Yes
AI techniques for identification of suitable delivery parking spaces in an urban scenario	U.S. Department of Energy	Pacific Northwest National Laboratory	We are using AI (Graph Neural Network) to determine importance of parking spaces in a city network for curb management to promote adoption of electric vehicles for freight delivery		2023-01-02		Vinay Amatya	Vinay.amatya@pnnl.gov	In-house			Open source	Yes
Surrogate models for probabilistic Bayesian inference	U.S. Department of Energy	Pacific Northwest National Laboratory	We are using AI/ML to build surrogate models of the observable response of complex physical systems. These surrogate models will be used for probabilistic model inversion of these systems with the goal of estimating unknown model parameters from indirect observations.			2022-10-01	David Barajas-Solano	david.barajas-solano@pnnl.gov	In-house			Synthetically generated by the research team by querying existing physics solvers	Yes
Universal MCEG	U.S. Department of Energy	Thomas Jefferson Laboratory	R&D on ML based MC event generator that serves as data compatification utility.				Malachi Schram	schram@jlab.org	Other Non-Commercial Sources			Data not available at this time. Additional information from Data Science personnel and will be provided as soon as possible.	Yes
FIMS - Invoice BOT - Employee Reimbursements FIMS - Invoice BOT - Purchase Power	U.S. Department of Energy	Western Area Power Administration	PROCESS - Invoices are sent to the RPA Invoice Intake email box (RPAInvoiceIntake@WAPA.GOV). Once a day, unattended bot will extract information from PDF invoices. The invoice is classified to determine whether the invoice is an Employee Reimbursement or a Purchase Power Invoice. The information extracted from the invoice is then review/validated by the Accounts Payable Technician. After validation, the bot will load the information into the WAPA Financial Management System.	Operation and Maintenance	2021-03-01	2021-10-13	Jonathan Holstine	jholstine@wapa.gov	Contracted		Artificial Intelligence, Document Understanding	Financial System Database	Yes