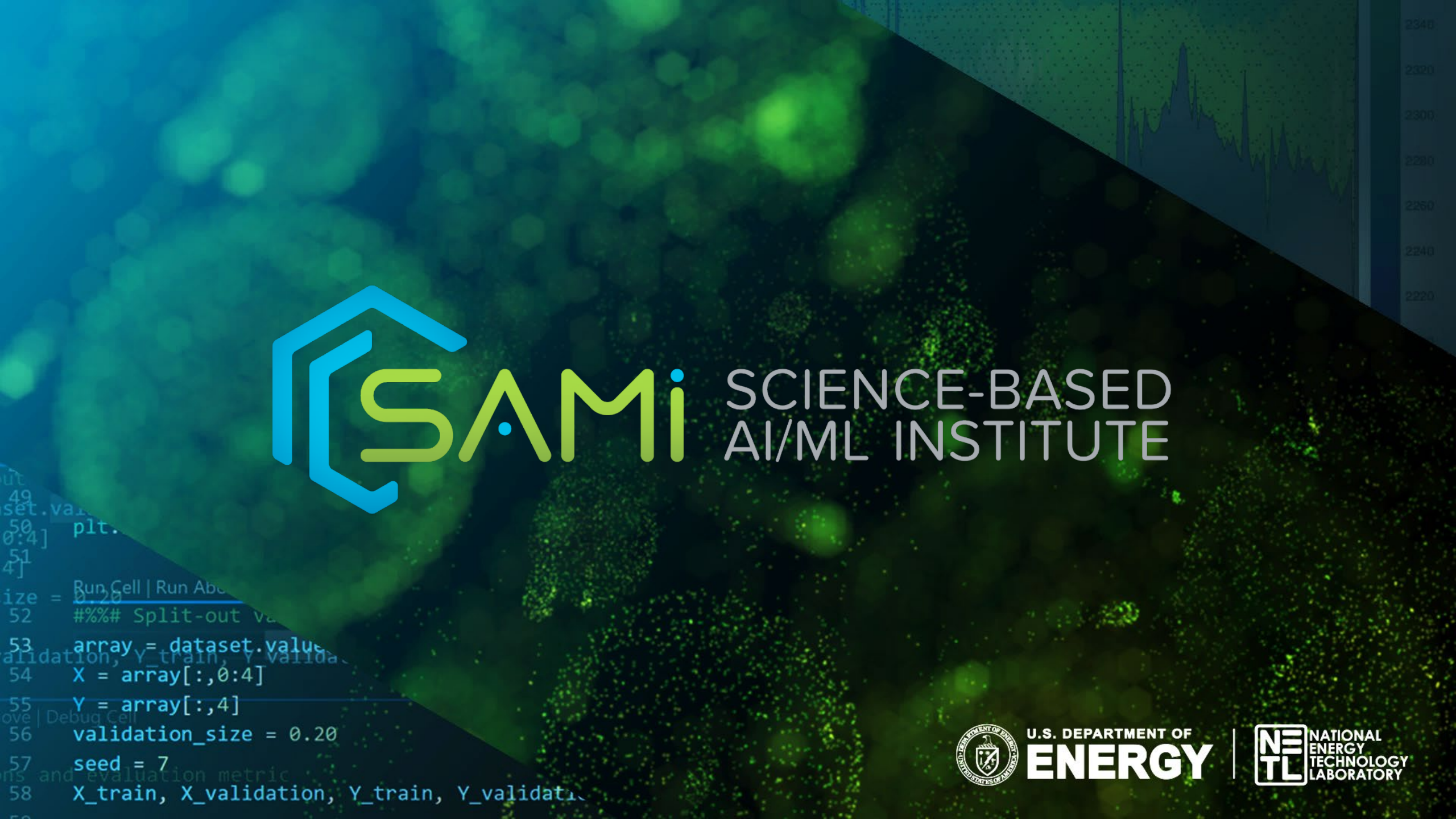
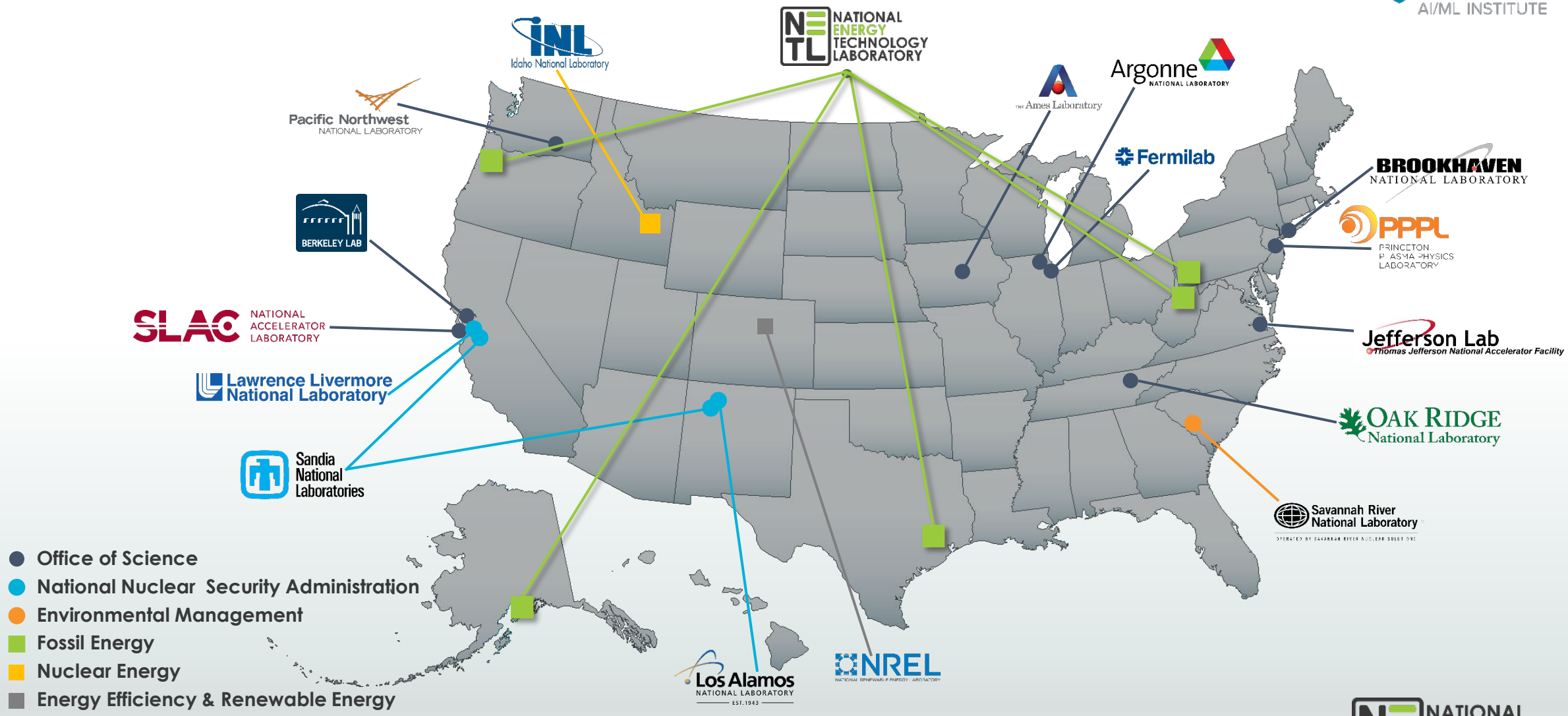

SAMi
SCIENCE-BASED
AI/ML INSTITUTE
plt.
Run Cell | Run Abo
#%%# Split-out va
array = dataset.value
X = array[:,0:4]
Y = array[:,4]
validation_size = 0.20
seed = 7
X_train, X_validation, Y_train, Y_validati
U.S. DEPARTMENT OF
ENERGY
NATIONAL
ENERGY
TECHNOLOGY
LABORATORY

DOE National Laboratory System



https://edx.netl.doe.gov/sites/sami

Updated Nov 2020

National Energy Technology Laboratory (NETL)

SAMi SCIENCE-BASED AI/ML INSTITUTE

One of 17 U.S. Department of Energy (DOE) national laboratories; producing technological solutions to America's energy challenges.

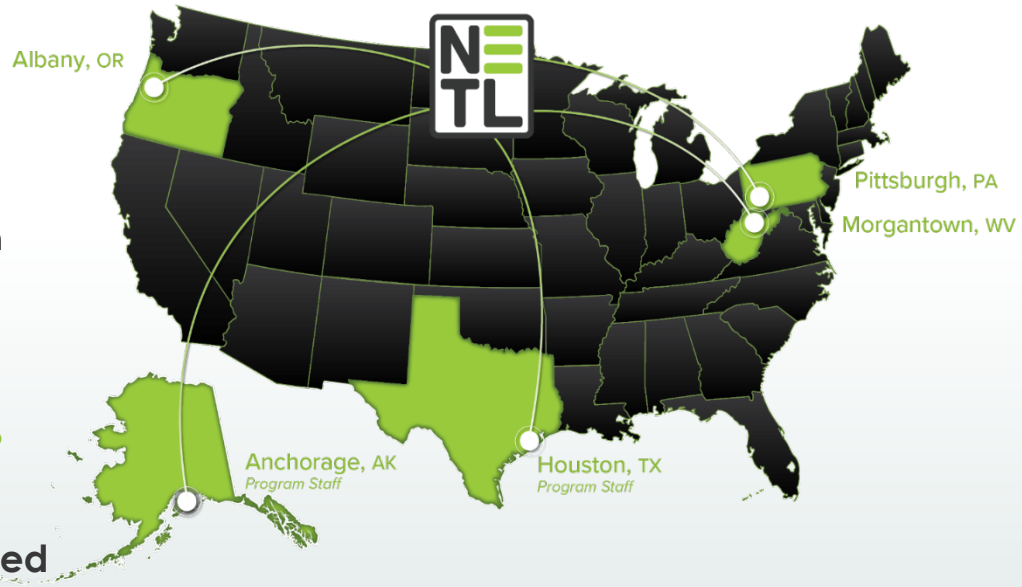
MISSION

Driving innovation and delivering solutions for an environmentally sustainable and prosperous energy future:

- Ensuring affordable, abundant and reliable energy that drives a robust economy and national security, while
- Developing technologies to manage carbon across the full life cycle, and
- Enabling environmental sustainability for all Americans.

VISION

To be the nation's premier energy technology laboratory, delivering integrated solutions to enable transformation to a sustainable energy future.



- NETL has **three research laboratories**
- **Two field office locations**
- Only National Lab **dedicated to carbon management research**
- Government owned & operated
- **One of three applied** national labs
- Leader in cutting-edge research in **conversion** to higher value products
- Flexible **Intellectual Property**

NETL NATIONAL ENERGY TECHNOLOGY LABORATORY

https://edx.netl.doe.gov/sites/sami

National Energy Technology Laboratory (NETL)

Organization Snapshot

SAMI SCIENCE-BASED AI/ML INSTITUTE

MISSION

Driving innovation and delivering solutions for an environmentally sustainable and prosperous energy future:

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VISION

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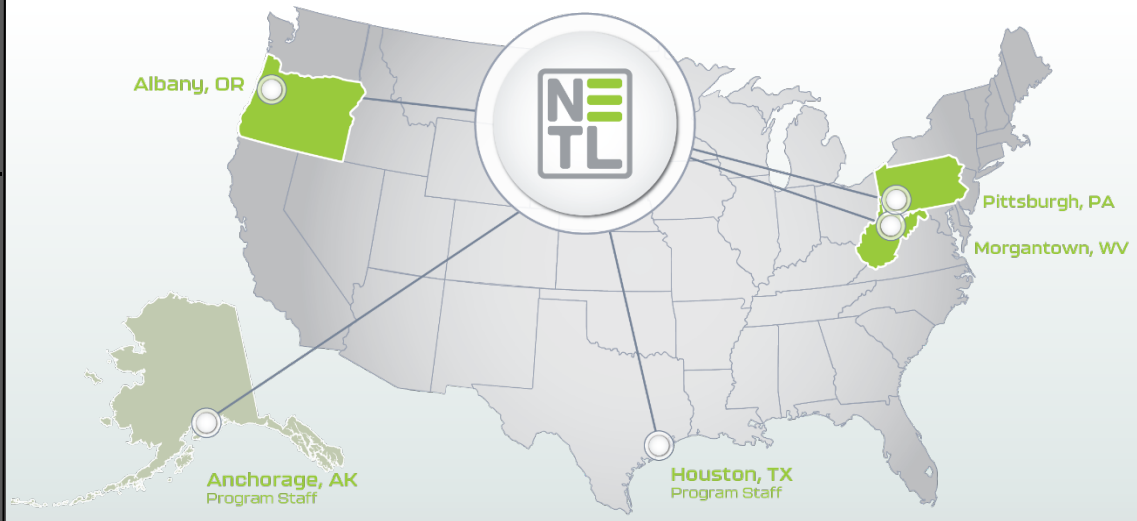
MAJOR INITIATIVES

- **Decarbonization & Carbon Management**
- **Environmentally Sustainable Supply Chains**
- **Integrated Energy & Industrial Systems**
- **Advanced Data & Computing Solutions for Applied Energy Challenges**

3 RESEARCH LABS & 2 STRATEGIC OFFICES



- One of 17 DOE national laboratories
- One of three applied research national labs
- Government owned & operated
- **1000+** R&D projects in 50 states
- **$5.0B** total award value
- **$1.3B** FY23 budget

IMPLEMENTS R&D PROJECTS FOR DOE'S OFFICES OF:

- Fossil Energy & Carbon Management
- Energy Efficiency Renewable Energy
- Electricity
- Cybersecurity, Energy Security, & Emergency Response
- Manufacturing, & Energy Supply Chains
- Grid Deployment
- Clean Energy Demonstrations

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NETL NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL Core Competencies

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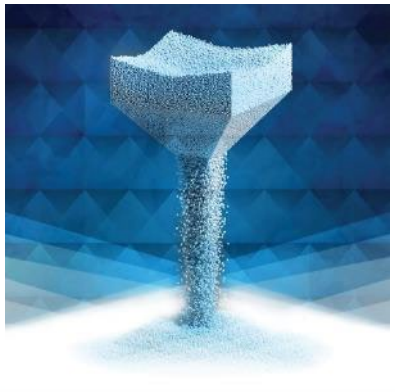
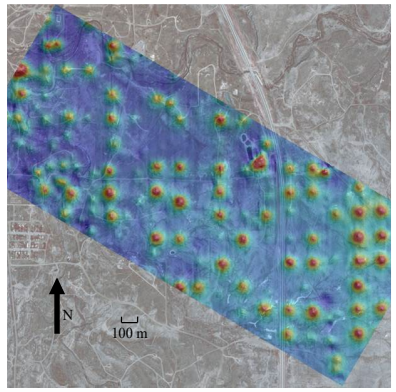
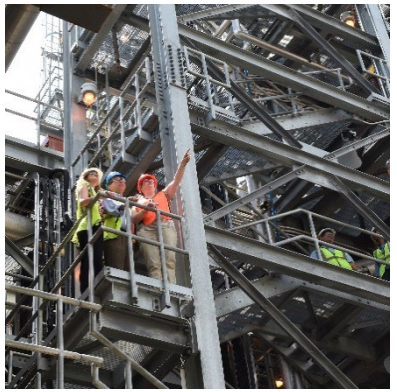
EFFECTIVE RESOURCE DEVELOPMENT • EFFICIENT ENERGY CONVERSION • ENVIRONMENTAL SUSTAINABILITY







COMPUTATIONAL SCIENCE & ENGINEERING	MATERIALS ENGINEERING & MANUFACTURING	GEOLOGICAL & ENVIRONMENTAL SYSTEMS	ENERGY CONVERSION ENGINEERING	STRATEGIC SYSTEMS ANALYSIS & ENGINEERING	PROGRAM EXECUTION & INTEGRATION
High Performance Computing	Structural & Functional Materials	Geo-Analysis & Monitoring	Reaction Engineering	Energy Process & System Engineering	Technical Project Management
Multi-Scale Modeling Atomistic to Device	Design, Synthesis, & Performance	Reservoir Engineering	Design & Validation	Multi-scale Modeling, Simulations & Optimization	
Artificial Intelligence & Machine Learning	Characterization	Geochemistry	Thermal Sciences	Energy Markets Analysis	
			Advanced System Engineering		

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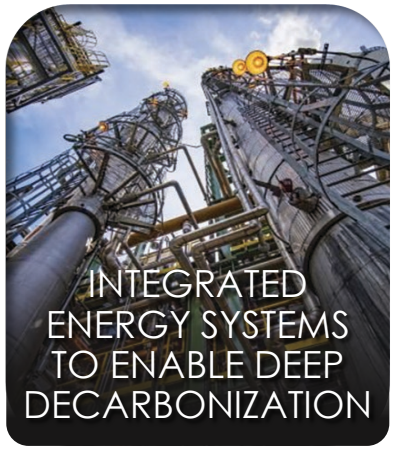
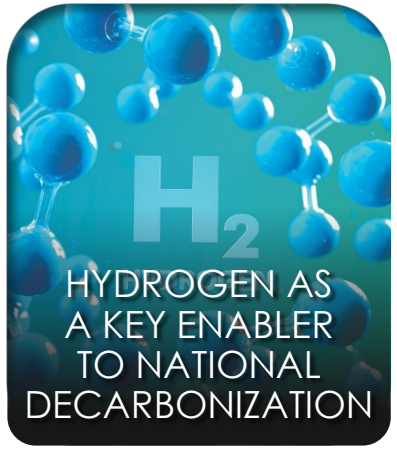
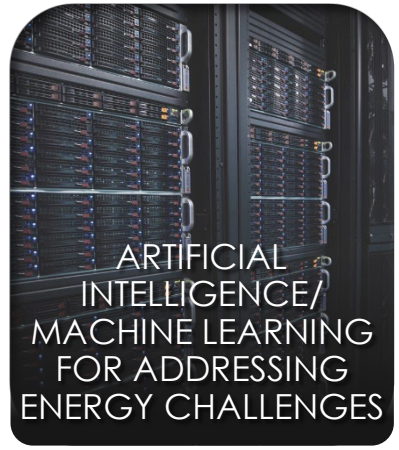
NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL Initiatives

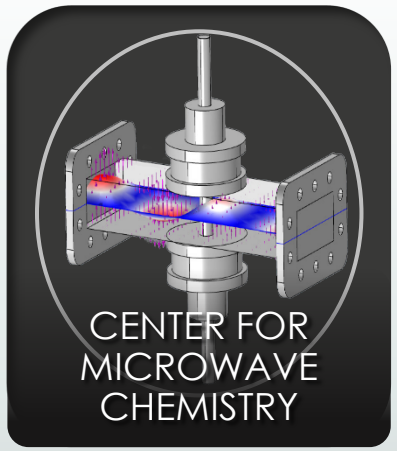
STRATEGIC INITIATIVES

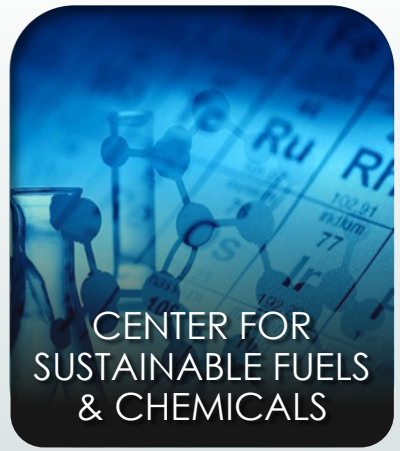






KEY LAB INITIATIVES



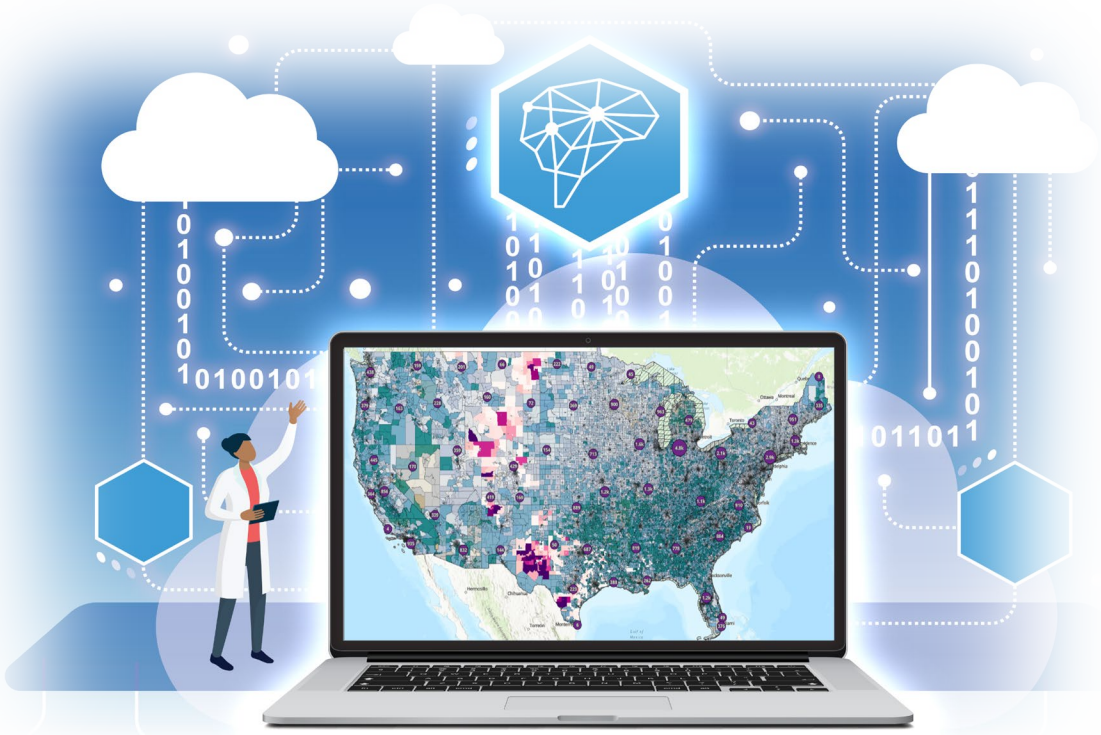


https://edx.netl.doe.gov/sites/sami

Science-based AI/ML Institute (SAMI)

An NETL Key Laboratory Initiative (KLI)

- NETL **established** SAMI, a joint institute for AI and ML, **in 2020**
- SAMI is a ***catalyzer of AI- and ML-driven solutions***, to support the acceleration of FECM technologies across the NETL R&D mission space
- Working to address **crosscutting** needs, capabilities, and resources to unlock FECM/NETL's AI technology future and **drive mutual benefits**
- **SAMI is an Institute within the Research & Innovation Center (RIC)**
  - Supports discipline-based research, across discipline boundaries



SAMI Mission

Enabling AI-driven solutions and support to applied energy science, addressing the nation's environmental, economic and social challenges.

Accelerating AI at NETL through SAMI

Meeting our Mission through Five Key Emphasis Areas

ADVANCE AI WORKFORCE
Foster multi-disciplinary AI research and cross-cutting collaborations to cultivate NETL's AI-ready workforce.

CATALYZE PARTNERSHIPS & COLLABORATIONS
Strengthen collaborations in research focus areas, within NETL and with external stakeholders to hasten the development of innovative applied-energy AI solutions.

MAKE DATA ACCESSIBLE
Support the entire lifecycle of data with secure, private, collaborative workspaces for research projects.

INFORM GOVERNANCE & STANDARDS
Ensure the use and development of safe and trustworthy AI.

ACCELERATE AI INNOVATION
Enable NETL to push the frontiers of AI technology and create the next generation architectures, tools and approaches

https://edx.netl.doe.gov/sites/sami/

ADVANCE AI WORKFORCE

Foster multi-disciplinary AI research and cross-cutting collaborations to cultivate NETL's AI-ready workforce.

- AI4AE Day
- Panel discussions (e.g., ChatGPT)
- Media stories on AI/ML research at NETL
- SAMI Tech Talks
  SAMI Tech Tutorials
- SAMI Spotlight Series (speakers sourced externally)
- EDX training

LIGHTNING TALKS:	ATTENDEES:
28	149
SAMI-affiliated researchers presented during Ai4AE Day	NETL personnel attended the inaugural Ai4AE Day

SAMI SCIENCE-BASED AI/ML INSTITUTE

"I just want to let you know that the SAMI workshop was absolutely amazing. I learned so much."

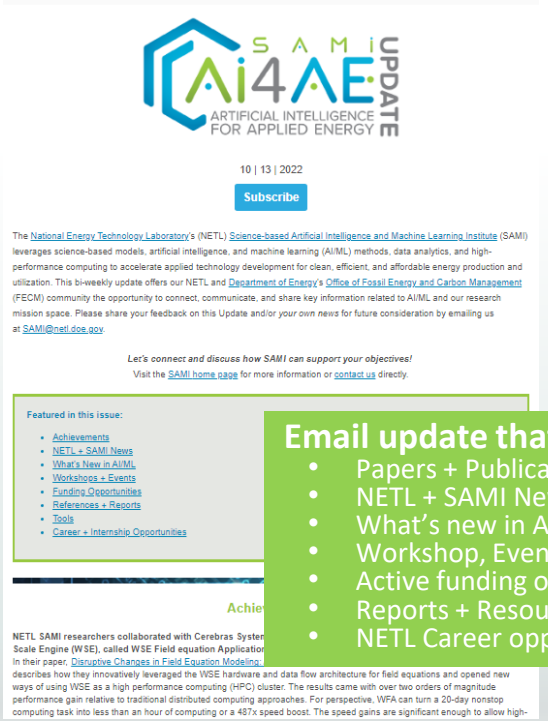
https://edx.netl.doe.gov/sites/sami/

SAMI is Making AI/ML Information Available

SAMI Website: NETL's current research and accomplishments in AI/ML and learn more about SAMI:

Sign up for our AI4AE Update email here:

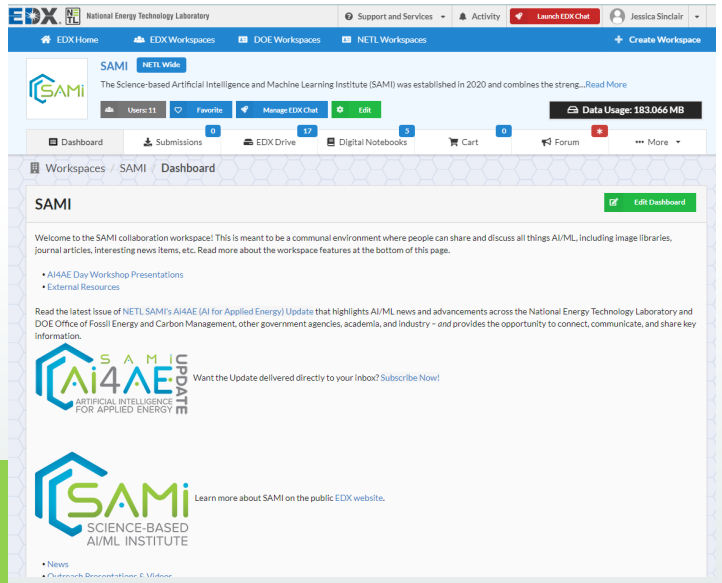
AI4AE Update monthly email learn about applied energy AI at NETL and AI innovations, policy, etc.:



Email update that includes:

- Papers + Publications
- NETL + SAMI News
- What's new in AI/ML
- Workshop, Events + Conferences
- Active funding opportunities
- Reports + Resources
- NETL Career opportunities

EDX Workspace: Access information on AI/ML, proposal text, data management plan:



https://edx.netl.doe.gov/sites/sami

NATIONAL ENERGY TECHNOLOGY LABORATORY

CATALYZE PARTNERSHIPS & COLLABORATIONS

Strengthen collaborations in research focus areas, within NETL and with external stakeholders to hasten the development of innovative applied-energy AI solutions.

SAMI SCIENCE-BASED AI/ML INSTITUTE

- Create collaborative opportunities within NETL across all core competencies/RIC directorates
- Work with external stakeholders to further development of AI-driven solutions for applied energy
  - Introducing new technologies
  - Collaborative research
- Collaborate on AI strategy discussions within DOE
- Communications & outreach

https://edx.netl.doe.gov/sites/sami/

MAKE DATA ACCESSIBLE

Support the entire lifecycle of data with secure, private, collaborative workspaces for research projects.

EDX Energy Data eXchange

SAMI SCIENCE-BASED AI/ML INSTITUTE

Energy Data eXchange®++: For 14 years EDX has served as a data curation and collaboration platform for applied energy RD. Multi-cloud hosted system which:

- enables accelerated development, application and testing of carbon management and fossil energy resiliency models, tools, and data
- supports computing both in the cloud and for authorized users via NETL's on-premise advanced computing clusters, accelerating AI research, validation, and benchmarking for a wide array of applied energy and environmental needs.
- https://edx.netl.doe.gov/about

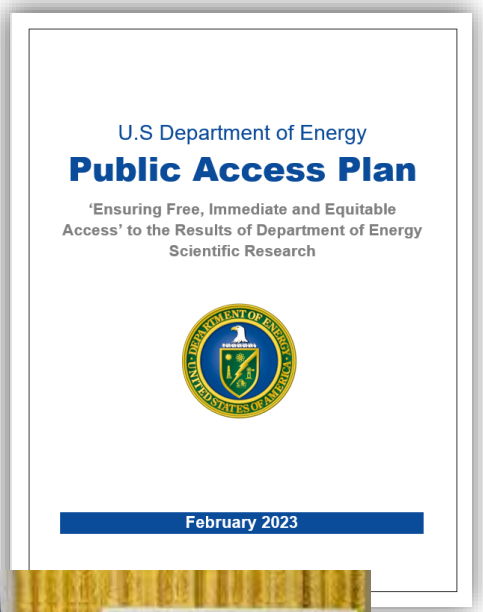
https://edx.netl.doe.gov/sites/sami/

INFORM GOVERNANCE & STANDARDS

Ensure the use and development of safe and trustworthy AI.

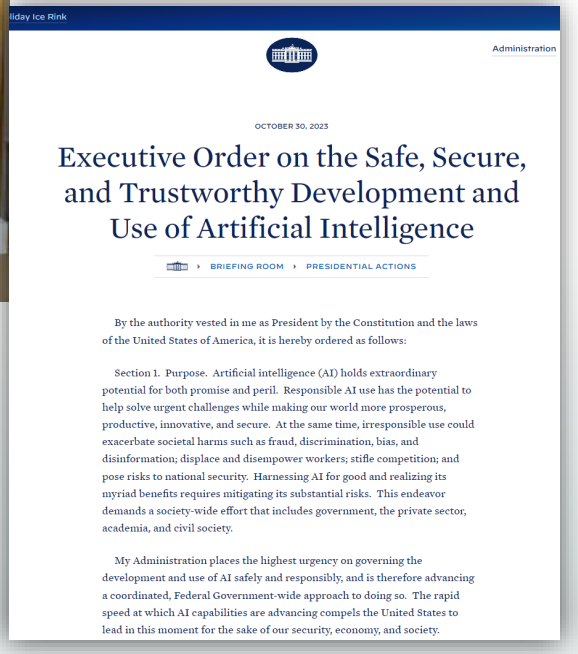
Inform compliance with federal orders, supporting our mission in a rapidly changing world, for example:

- DOE Public Access Plan
- Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence
  - Date signed: October 30, 2023
  - To govern the development and use of AI safely and responsibly, through a coordinated, Federal Government-wide approach to doing so.



SAMI SCIENCE-BASED AI/ML INSTITUTE

Source: www.forbes.com



Administration

OCTOBER 30, 2023

Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence

BRIEFING ROOM › PRESIDENTIAL ACTIONS

By the authority vested in me as President by the Constitution and the laws of the United States of America, it is hereby ordered as follows:

Section 1. Purpose. Artificial intelligence (AI) holds extraordinary potential for both promise and peril. Responsible AI use has the potential to help solve urgent challenges while making our world more prosperous, productive, innovative, and secure. At the same time, irresponsible use could exacerbate societal harms such as fraud, discrimination, bias, and disinformation; displace and disempower workers; stifle competition; and pose risks to national security. Harnessing AI for good and realizing its myriad benefits requires mitigating its substantial risks. This endeavor demands a society-wide effort that includes government, the private sector, academia, and civil society.

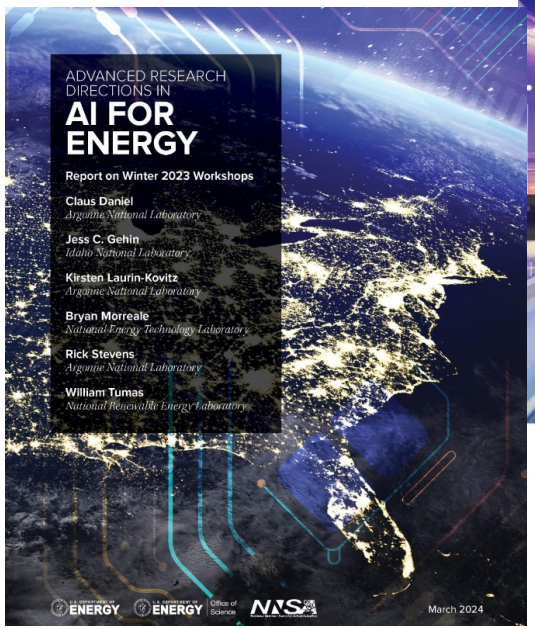
My Administration places the highest urgency on governing the development and use of AI safely and responsibly, and is therefore advancing a coordinated, Federal Government-wide approach to doing so. The rapid speed at which AI capabilities are advancing compels the United States to lead in this moment for the sake of our security, economy, and society.

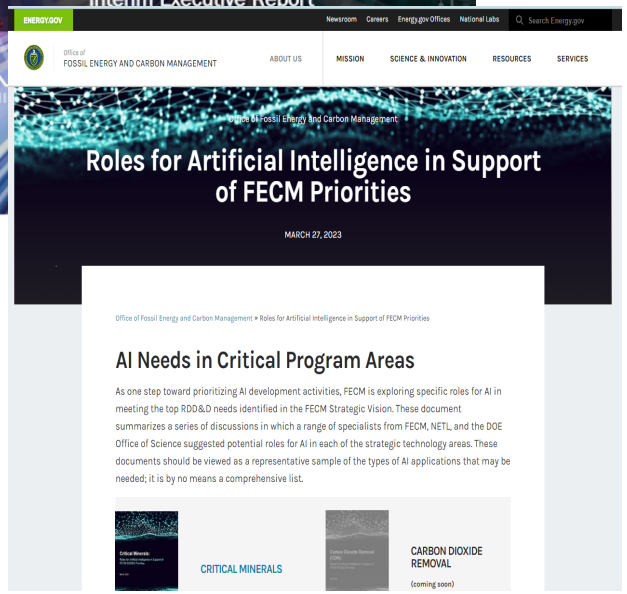
https://edx.netl.doe.gov/sites/sami/

ACCELERATE AI INNOVATION

Enable NETL to push the frontiers of AI technology and create the next generation architectures, tools and approaches

- Through strategic discussions
  - DOE AI R&D Strategic Plan
  - AI for Science, Energy & Security Workshops
  - AI for Energy
  - AI-related Data Calls
  - FECM AI Strategy & advisory team
  - The Inter-agency AI Community of Practice (CoP)
  - DOE AI Community of Interest
  - AI for Operations Committee
- SAMI Tech Team
  - Data Science projects, research, training, or advisory
- Research





https://www.energy.gov/fecm/articles/roles-artificial-intelligence-support-fecm-priorities

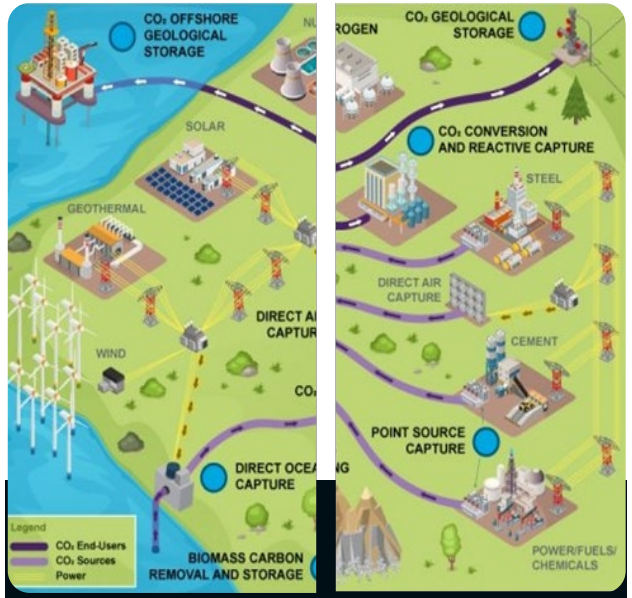
https://edx.netl.doe.gov/sites/sami/

NATIONAL ENERGY TECHNOLOGY LABORATORY

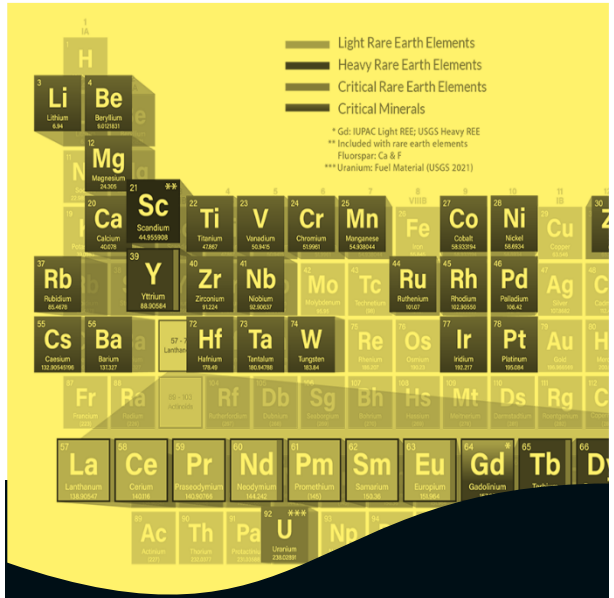
ACCELERATE AI INNOVATION

Enable NETL to push the frontiers of AI technology and create the next generation architectures, tools and approaches

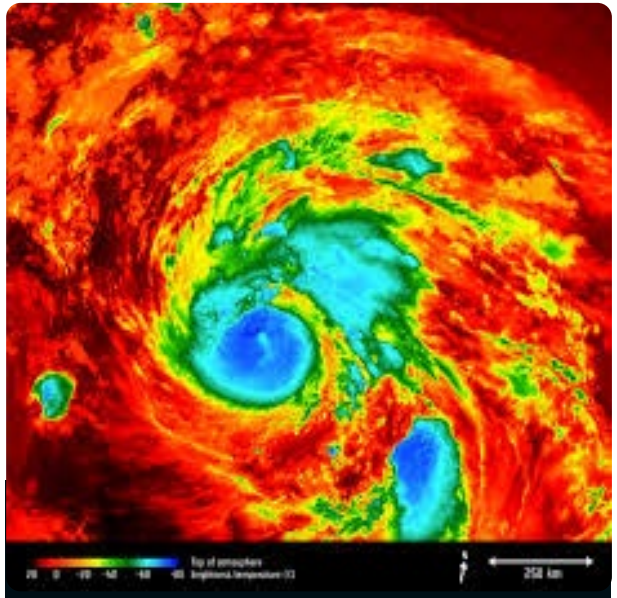
SAMI
SCIENCE-BASED AI/ML INSTITUTE



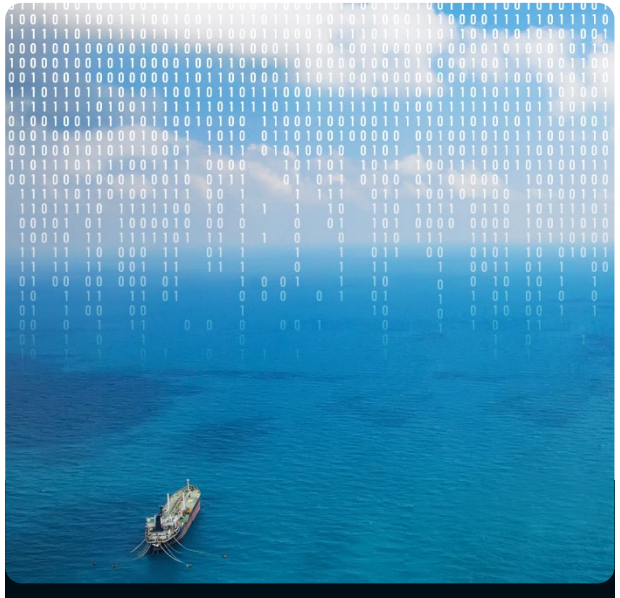
CARBON MANAGEMENT



RESOURCES AND MATERIALS



INFRASTRUCTURE & ENVIRONMENTAL RESILIENCY



BIG DATA, FOUNDATIONAL DATA & A.I. SOLUTIONS

The following slides contain examples of research innovations in these areas but are not comprehensive of all AI/ML research at NETL.

https://edx.netl.doe.gov/sites/sami/

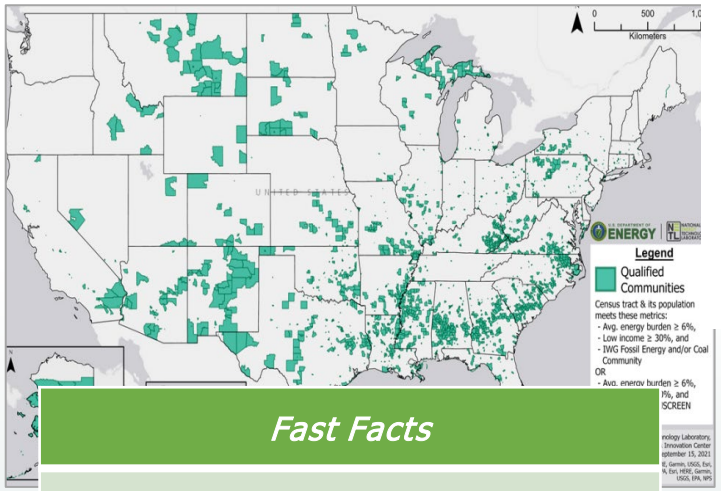
Carbon Management

Applied AI for Carbon Capture and Storage Data Products

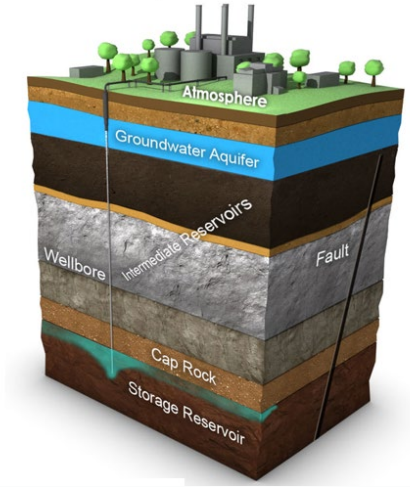
CO_2 Smart EJ/SJ Route Planning Tool

- The interactive smart tool will assist in planning routes for CO_2 transport across the country. **Explore the** [public database](). The Pipeline Route Planning Database team [published research in Data in Brief]() in December.

- Researchers behind the tool met with representatives from industry on collaborative ideas and recently presented the tool at the **FECM Interagency Carbon Transport Topic Team Meeting.**



Fast Facts
Database released 3/23; Article on NETL site
Anticipated Tool Release 2024
Interactive smart tool for CO_2 Route Planning
A **machine learning model** has been trained on multivariate data representing pipeline regulations, legislation, and best practices to **evaluate and identify safe and sustainable routes** to inform national pipeline planning efforts.



NRAP Open Source Integrated Assessment Model (OPEN-IAM)

- An [open-source software product]() that enables quantification of containment effectiveness and leakage risk at storage sites in the context of system uncertainties and variability
- The model comprises a set of reduced-order and analytical models of various components of the GCS system and is incorporating a [Machine and Deep Learning Approach]() to overcome deficiencies of the analytical multi-segmented reduced order model.
- NRAP-OPEN-IAM allows for **crosscutting functionality** with the entire NRAP toolset.

Explore the entire NRAP toolset:

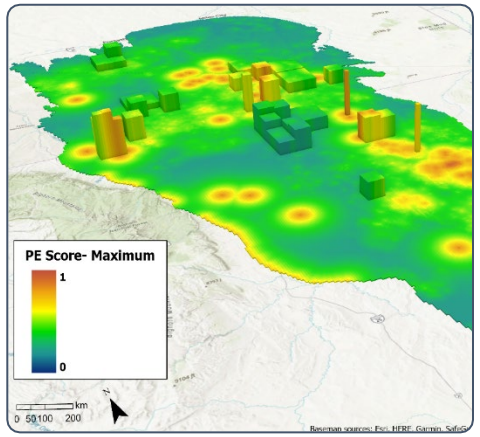
https://edx.netl.doe.gov/sites/sami

Resources & Materials

Applied AI for REE/CMs and alloy discovery

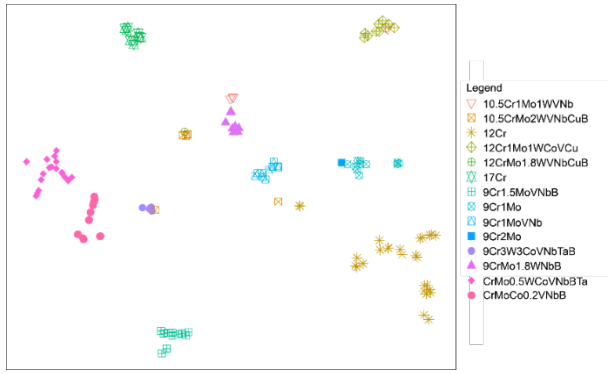
Federated-AI modeling for improving discovery of domestic critical mineral deposits

- NETL's geologic resource assessment AI Model helped uncover **the largest unconventional deposit of magnetic rare earth elements (REE) in the U.S.**
- **The AI model** was tested at a coal mine in Wyoming's Powder River Basin and revealed the **largest unconventional deposit of magnetic REEs discovered in the US.**
  - Featured in the Wall Street Journal - WSJ
  - Also featured in energy trade journal, *JPT*
- In the last year, NETL has released **five, peer-reviewed, data-driven products** that help characterize unconventional critical minerals

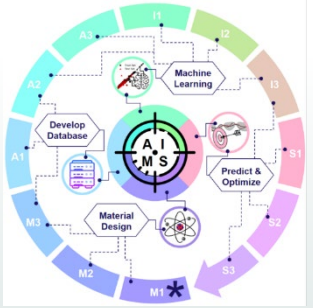


Machine learning prediction and outlier detection for alloy development and AI for alloy discovery

- Clustering: assessing trends in materials data
- Integrating domain knowledge into analysis
- Assessing outliers to the dataset



Wenzlick, M., et al. *J of Mat Eng and Perf*, 2021. https://doi.org/10.1007/s11665-020-05340-5



AIMS: Artificial Intelligence Materials Selection	
M1	*Literature Data Extraction*
M2	*High Throughput Synthesis*
M3	*Database Creation*
A1	*Data Preparation*
A2	*Explore and Visualize*
A3	*Data Sampling and Splitting*
I1	*Initial Model Creation*
I2	*Model Refining and Tuning*
I3	*Predict and Visualize*
S1	*Optimization*
S2	*Materials Selection*
S3	*Design of Experiments*

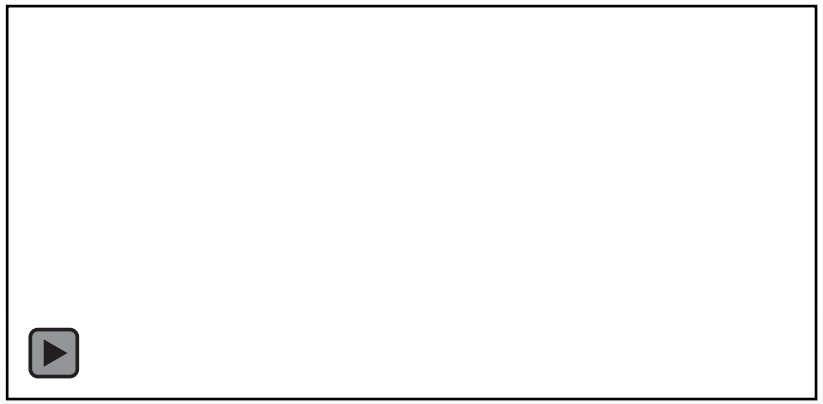
The Artificial Intelligence Materials Selection Framework is used to develop a high-quality database for compositions, processing, and test parameters for various responses of alloys, as well as predict optimized materials for multi-objective problems. https://doi.org/10.1016/j.actamat.2022.117751

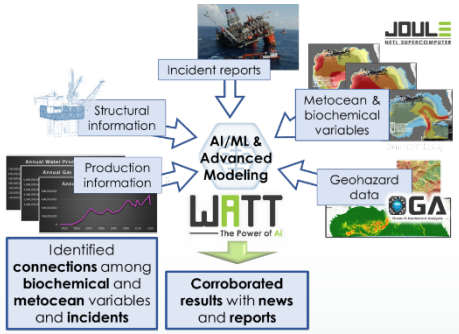
https://edx.netl.doe.gov/sites/sami/

Infrastructure and Environmental Resiliency

Applied AI for Extreme Climate & Infrastructure Resiliency

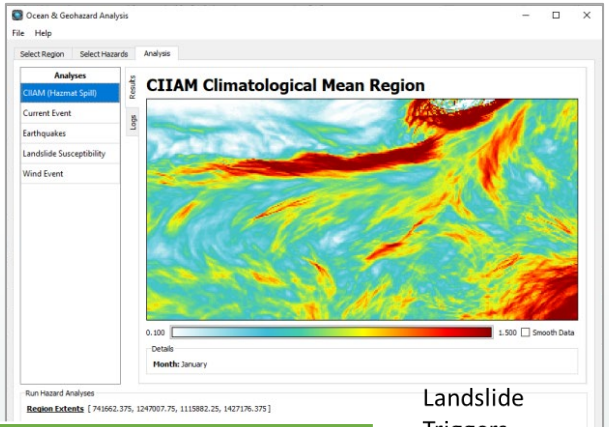
Award winning AI/ML Multi-Model Forecasting Infrastructure Integrity





Artificial Intelligence (AI) Enhanced Workflow for Natural Hazards Forecasting

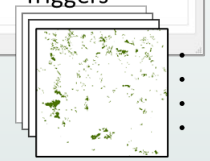
Data driven AI/ML analytical models and tools rapidly forecast and predict offshore hazards based off metocean and subsurface environments



OGA Ocean & Geohazard Analysis

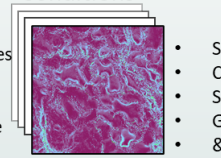
- **Gradient Boosting Classifier**
- **Artificial Neural Network**

Landslide Triggers



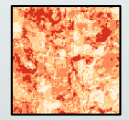
Conducive Conditions

- Hydrates
- Faults
- Seeps
- & more



- Slope
- Curvature
- Sediment Type
- Geomorphology
- & more

Output Landslide Susceptibility Map



Fast Facts

AI Multi-Model Tool - coming in 2024
Evaluating infrastructure integrity and forecasting remaining useful lifespan and risk likelihood through applied **Machine Learning (ML) models**
Multiple ML models **(two gradient boosted decision trees and one artificial neural network)** have been trained to evaluate comprehensive datasets for pipelines and platforms
Offshore infrastructure reuse potential, lifespan extension, remediation and safe-use strategies, identifies potential vulnerabilities

Fast Facts

Version 2 Tool released 3/23
AI/ML Smart Tool
Improves characterization and forecasting of seabed and metocean hazards
Reduce risks to operations, including carbon storage activities, and the environment

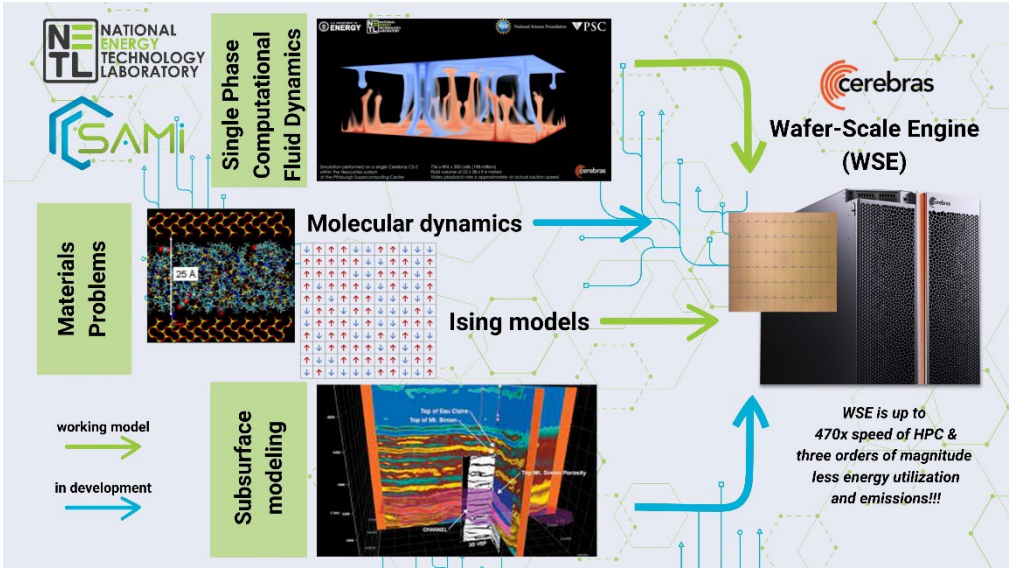
https://edx.netl.doe.gov/sites/sami

NATIONAL ENERGY TECHNOLOGY LABORATORY

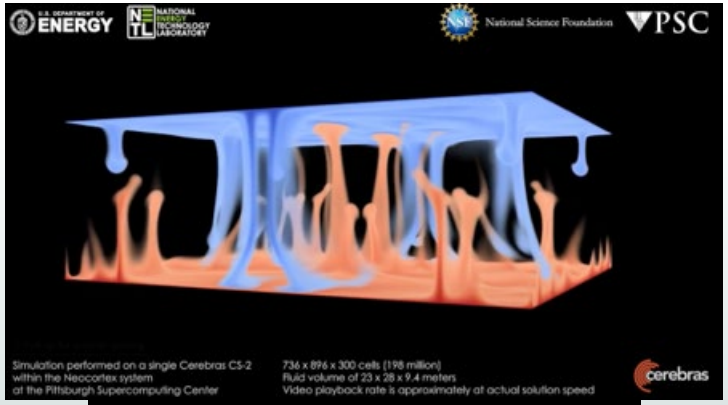
Big Data, Foundational Data, and AI Solutions

Cutting-Edge, advanced AI computing & modeling, accelerating solutions to real world challenges

- The NETL-developed WFA programming interface for the wafer-scale engine allows researchers to tackle tough AI problems from materials and climate modeling to computational fluid dynamics to molecular dynamics to AI-accelerated scientific computing.
- The wafer-scale engine has up to 470x the speed of HPC with **3 orders of magnitude** less energy usage and emissions



Woo, Mino, et al. "Disruptive Changes in Field Equation Modeling: A Simple Interface for Wafer Scale Engines." *arXiv preprint arXiv:2209.13768* (2022).
[2209.13768] Disruptive Changes in Field Equation Modeling: A Simple Interface for Wafer Scale Engines (arxiv.org)



Real-Time Computational Fluid Dynamics (youtube.com)

https://edx.netl.doe.gov/sites/sami/

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SCIENCE-BASED AI/ML INSTITUTE

Innovating science-based, AI/ML solutions for applied energy challenges

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Contact Us: SAMI@netl.doe.gov

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