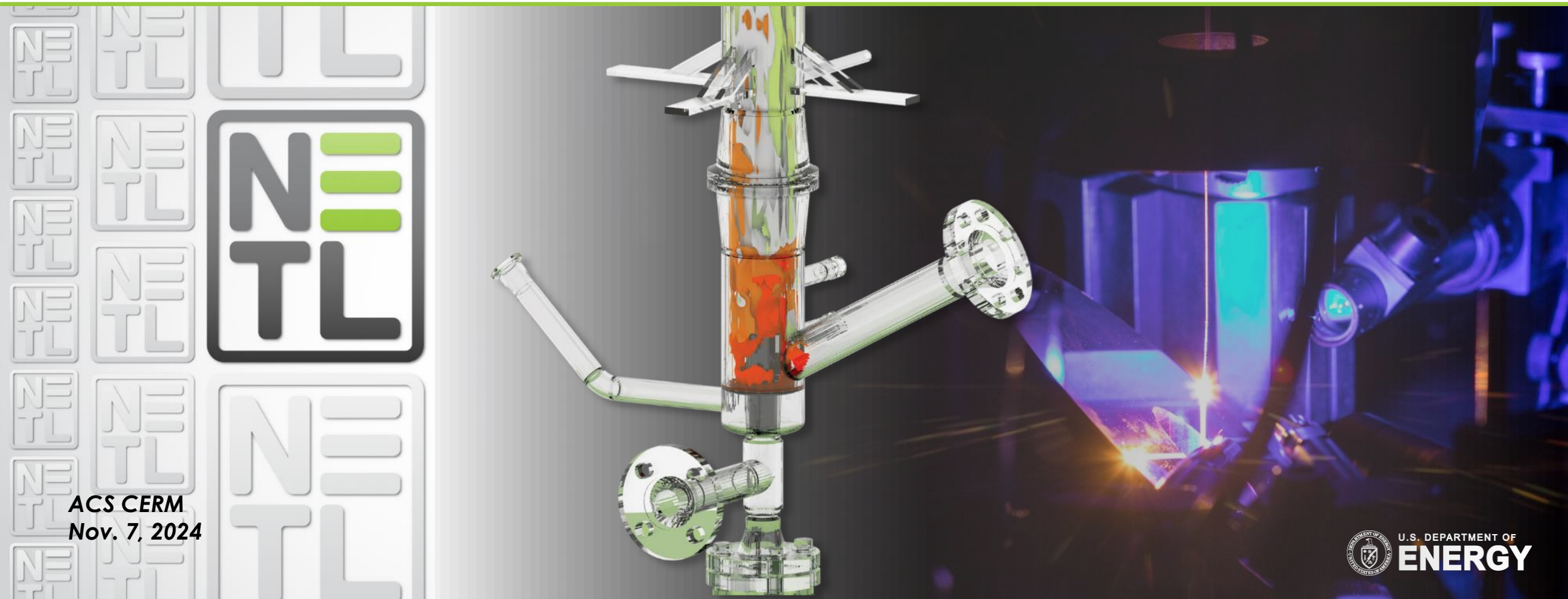
NETL & SAMI Overview

NATIONAL ENERGY TECHNOLOGY LABORATORY

Jessica Sinclair
NETL Support Contractor



ACS CERM
Nov. 7, 2024

U.S. DEPARTMENT OF ENERGY

Disclaimer

This project was funded by the United States Department of Energy, National Energy Technology Laboratory, in part, through a site support contract. Neither the United States Government nor any agency thereof, nor any of their employees, nor the support contractor, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Authors and Contact Information

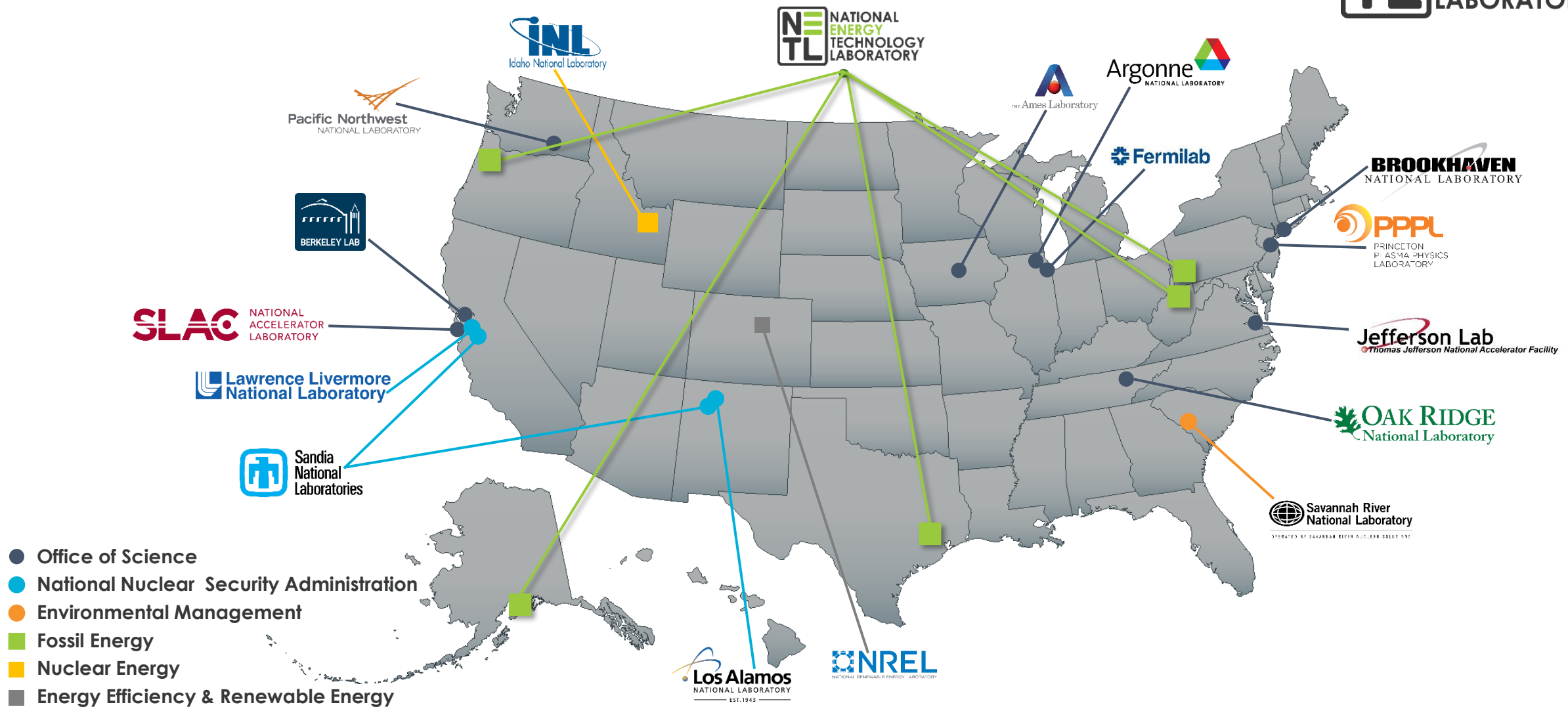
Jessica Sinclair[1,2]; Wissam Saidi[1]; Kelly Rose[3]

[1]National Energy Technology Laboratory, 626 Cochran Mill Road, Pittsburgh, PA 15236, USA

[2]NETL Support Contractor, 626 Cochran Mill Road, Pittsburgh, PA 15236, USA

[3]National Energy Technology Laboratory, 1450 Queen Avenue SW, Albany, OR 97321, USA

DOE National Laboratory System



Updated Nov 2020.

National Energy Technology Laboratory

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

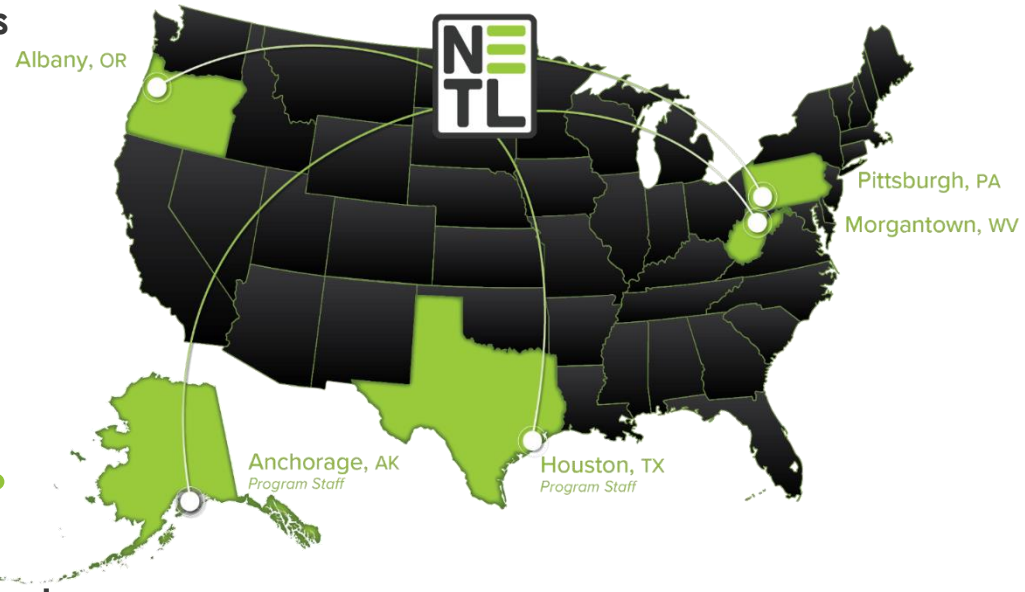
MISSION

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.



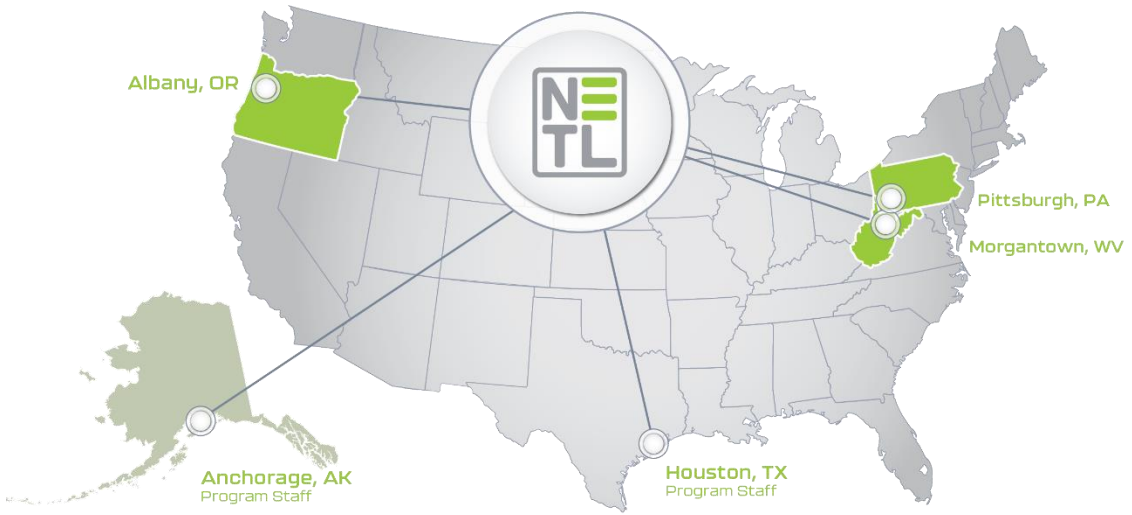
- NETL has **three research laboratories**
- **Two field office locations**
- Only national lab **dedicated to carbon management research**
- Government owned & operated
- **One of three applied research** national labs
- Leader in cutting-edge research in **conversion** to higher value products
- Flexible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

National Energy Technology Laboratory

Organization Snapshot

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

1000+ R&D projects in 50 states

$5.0B total award value

$1.3B FY23 budget

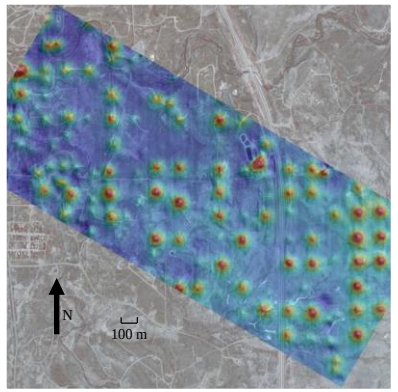
IMPLEMENTS R&D PROJECTS FOR DOE'S OFFICES OF:

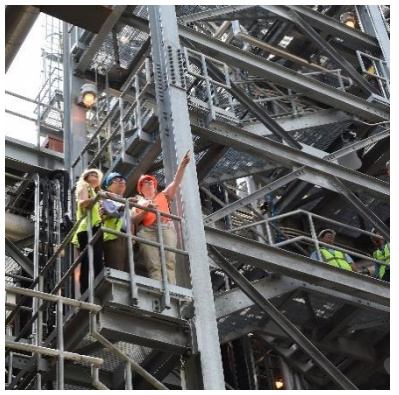
- Fossil Energy & Carbon Management
- Energy Efficiency Renewable Energy
- Electricity
- Cybersecurity, Energy Security, & Emergency Response
- Manufacturing, & Energy Supply Chains
- Grid Deployment
- Clean Energy Demonstrations

NETL Core Competencies

NATIONAL ENERGY TECHNOLOGY LABORATORY

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		

NETL Research: Capabilities and Technologies

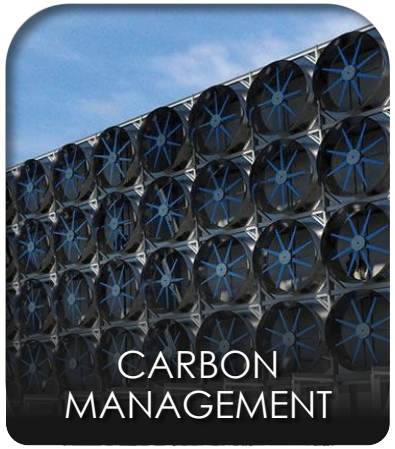
- Subsurface Research, Analysis and Characterization
- Data Analytics/Machine Learning/Decision Science
- Next Generation Materials for Harsh Environments
  - Advanced alloys, superalloys, high-entropy alloys, etc.
- Advanced Manufacturing
  - Additive manufacturing/3D printing, smart manufacturing, modular chemical process intensification, composites, etc.
- CO_2 Capture with Membranes, Solvents, and Sorbents
- Advanced Sensors and Controls for Harsh Environments
- Catalysts to Convert CO_2 into High-Value Products
- Coal to High-Value Products/Rare Earth Elements
- Carbon Capture Utilization & Storage (CCUS)
- Direct Air Capture and Negative Emissions Technologies

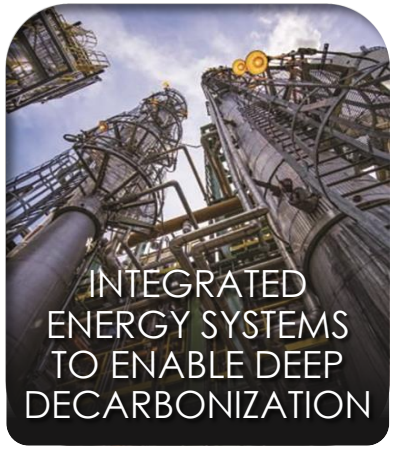
- Hydrogen Technologies (Production, Storage, Transportation, etc.)
- Microwave Reaction Technologies
- Reaction Activation and Chemical Transformation
- Integrated Energy Systems to Enable Deep Decarbonization
- Solid Oxide Fuel Cells and Hybrid Energy Systems
- Computational Materials Engineering & Molecular Science
- Multi-Scale Modeling, Simulation & Optimization
- Process Systems Engineering and Analysis
- Grid Modeling and Analysis/Grid Modernization
- Institute for the Design of Advanced Energy Systems
- Multiphase Computational Fluid Dynamics Modeling
- Customized Analyses, Assessments and Studies
- High Pressure Combustion/Advanced Cooling Technology

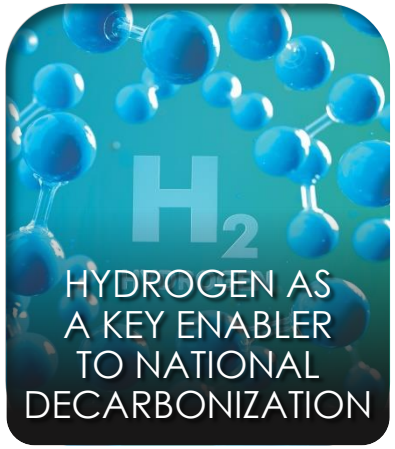
NETL Initiatives

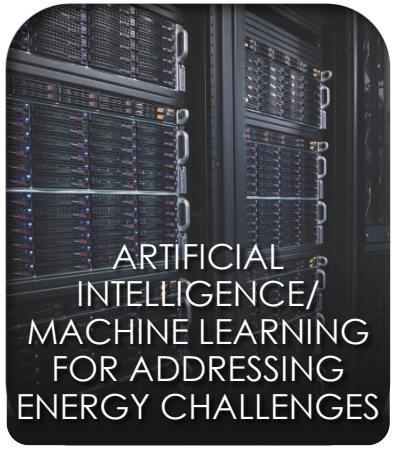
NATIONAL ENERGY TECHNOLOGY LABORATORY

STRATEGIC INITIATIVES

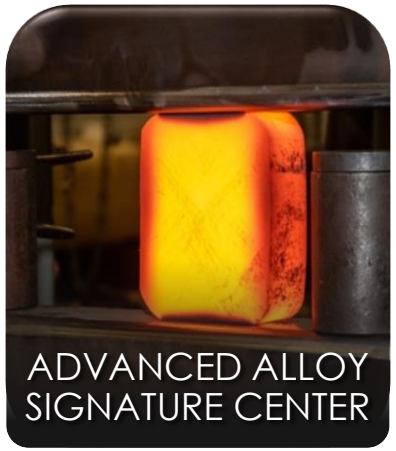


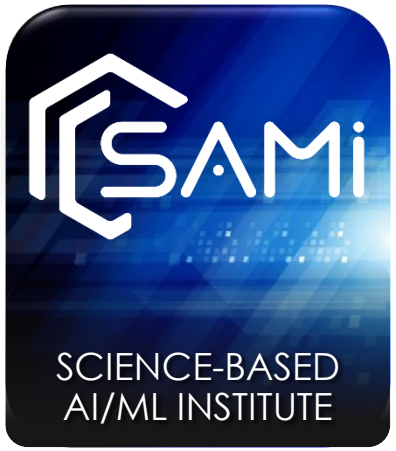


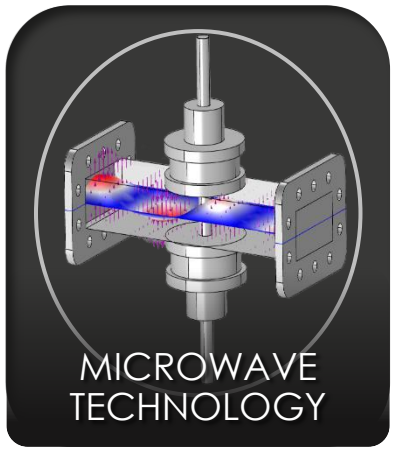


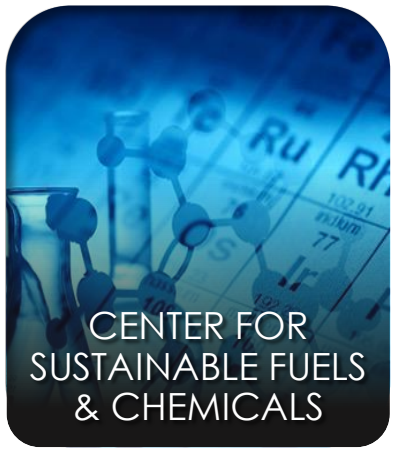


KEY LAB INITIATIVES









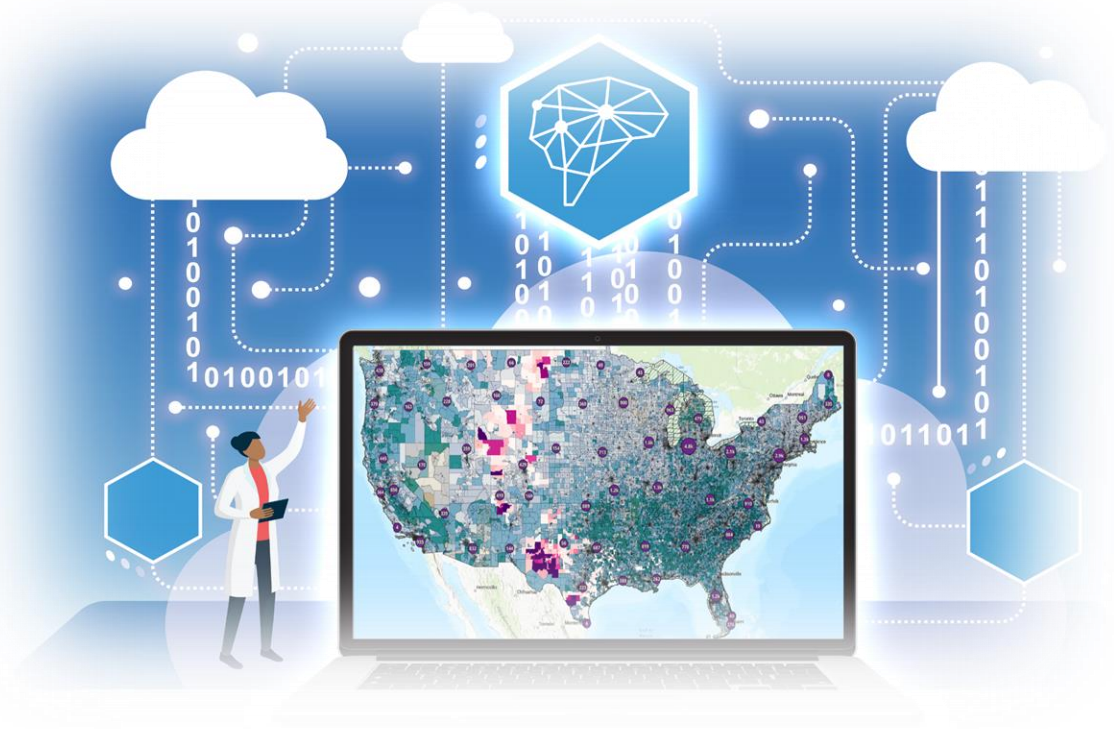
Innovating science-based, AI/ML solutions for applied energy challenges

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

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 Fossil Energy and Carbon Management (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



Science-Based AI/ML Institute's (SAMI) Mission

NATIONAL ENERGY TECHNOLOGY LABORATORY

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

- Executing mission through five key areas
- For more information:
  - Website
    - edx.netl.doe.gov/sites/sami
  - AI4AE Update email
    - Register through the website
  - Email us at SAMI@netl.doe.gov

SAMI
SCIENCE-BASED AI/ML INSTITUTE

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.

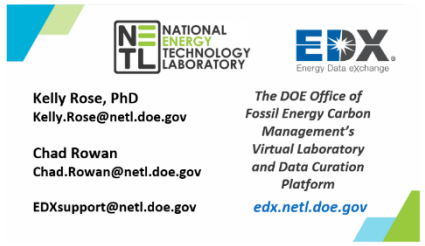
INFORM GOVERNANCE & STANDARDS
Ensure the use and development of safe and trustworthy AI.

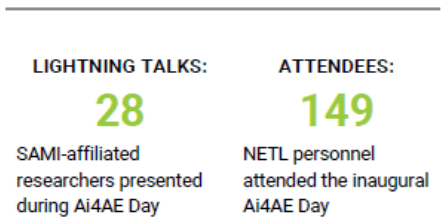
ACCELERATE AI INNOVATION
Enable NETL to push the frontiers of AI technology and create the next generation architectures, tools and approaches

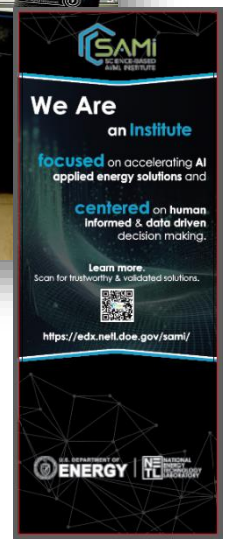
Advance AI Workforce

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 multi-cloud training
- AI/ML & data science topics







SAMI Tech Team

SAMI TECH TEAM

Jeremy Harris

- Supervised and unsupervised learning
- Time series modeling
- Image segmentation
- Predictive analytics
- Containerization

Michael Sabbatino

- Supervised and unsupervised learning
- Science-based learning
- Object detection/ computer vision
- Natural language and large language model research
- Data collection and pre-processing for ML

Chad Rowan

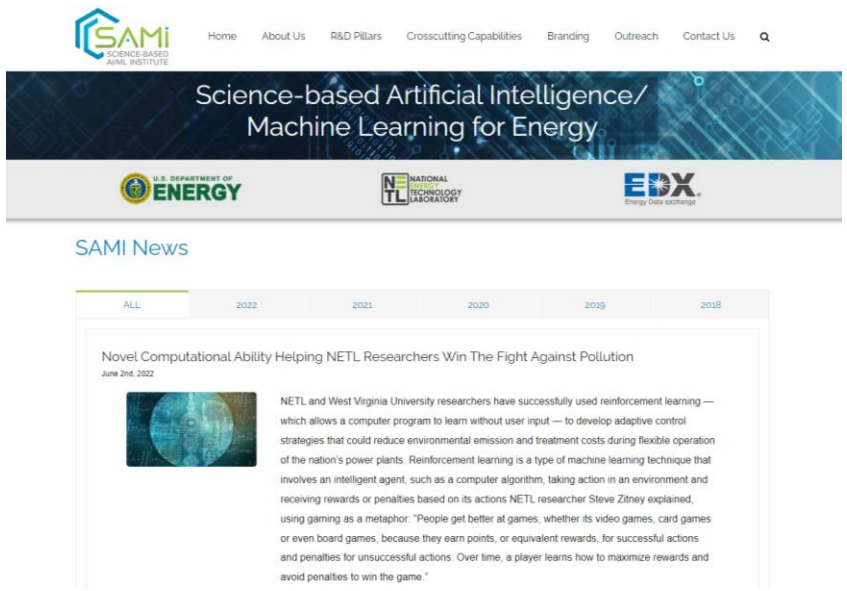
- Research data life-cycle management
- Data governance, ethics, and compliance
- Spatial data science and analysis
- Science-based learning
- Workflow process improvement

Veronika Vasylkivska

- Mathematics and statistics
- Software development
- Data analysis
- Numerical modeling and analysis
- Supervised and unsupervised learning

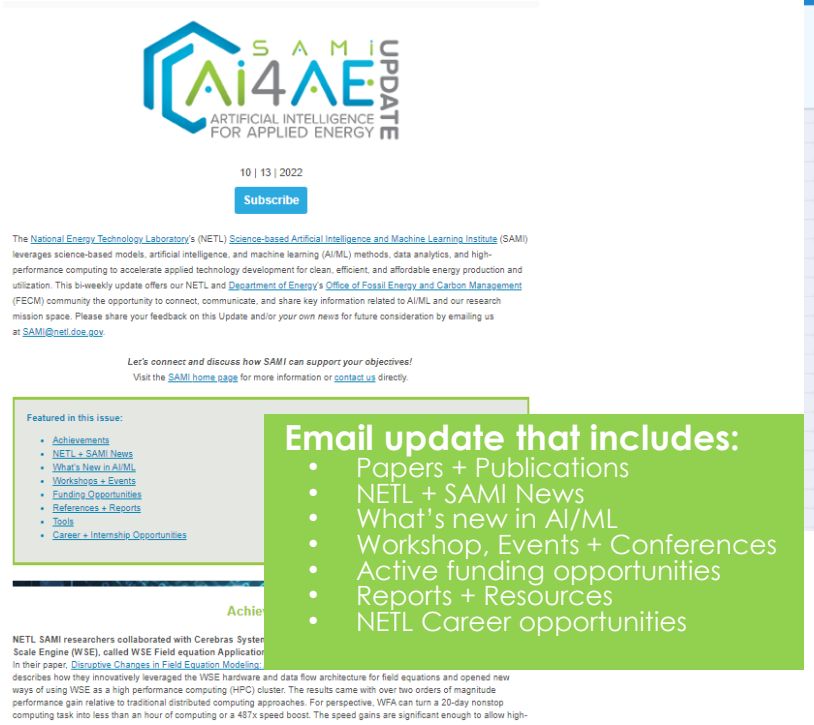
SAMI is Making AI/ML Information Available

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



Sign up for our AI4AE Update email here:

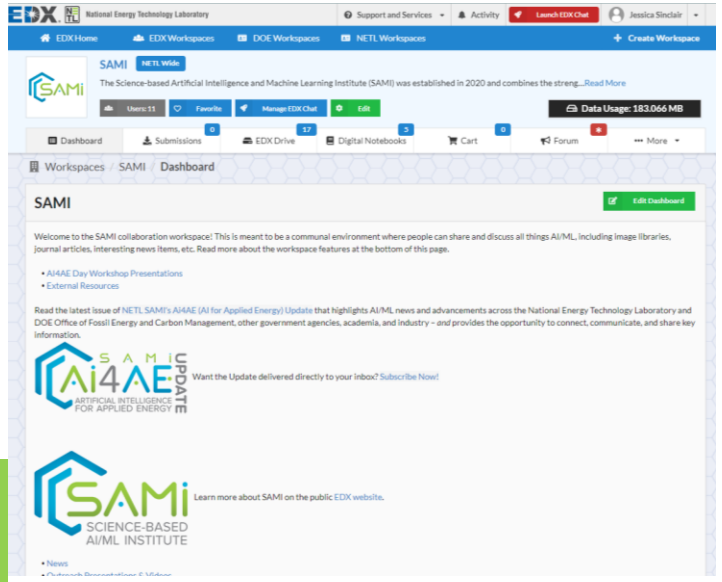
AI4AE Update: Monthly email to learn about applied energy AI at NETL and AI innovations, policy, etc.



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



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.

- Create collaborative opportunities within NETL
- 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

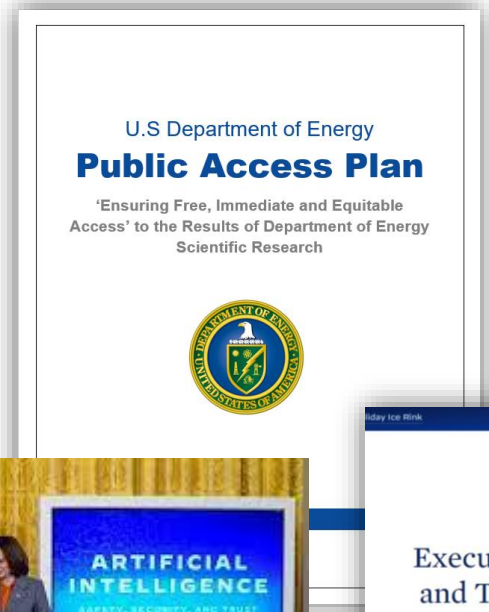
Inform Governance & Standards

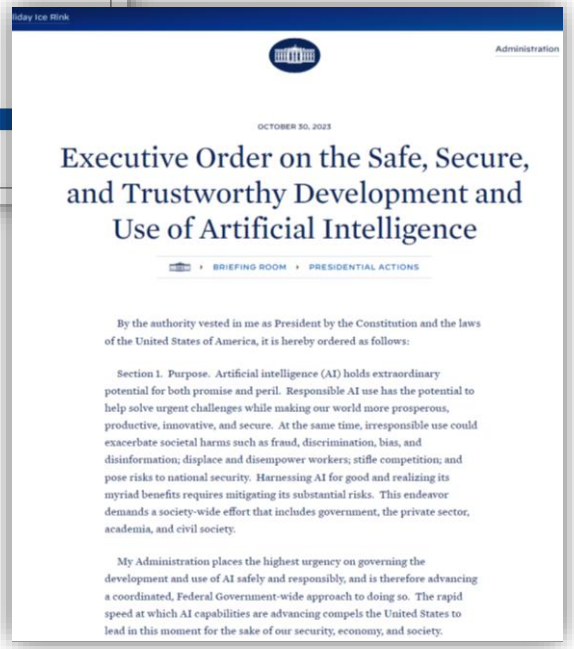
Ensure the use and development of safe and trustworthy AI.

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

Source: www.forbes.com





Accelerate AI Innovation

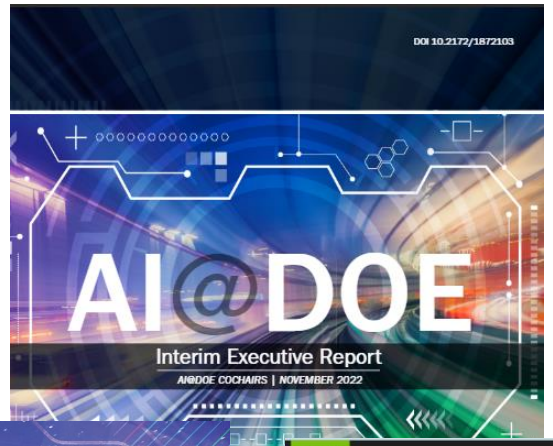
Enable NETL to push the frontiers of AI technology and create the next generation architectures, tools and approaches

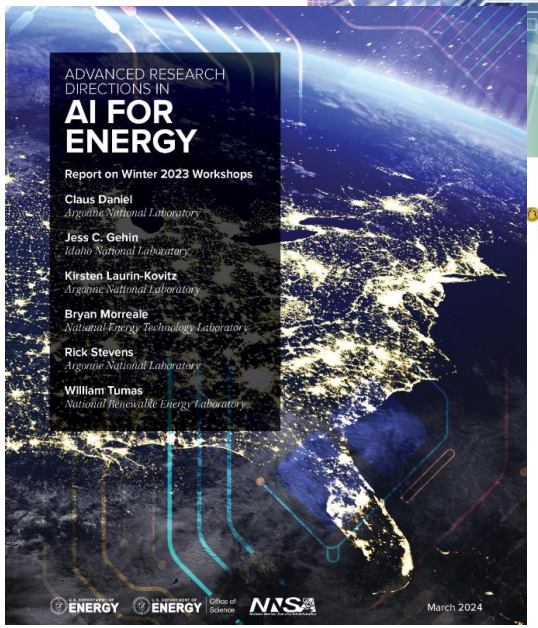
Through strategic discussions

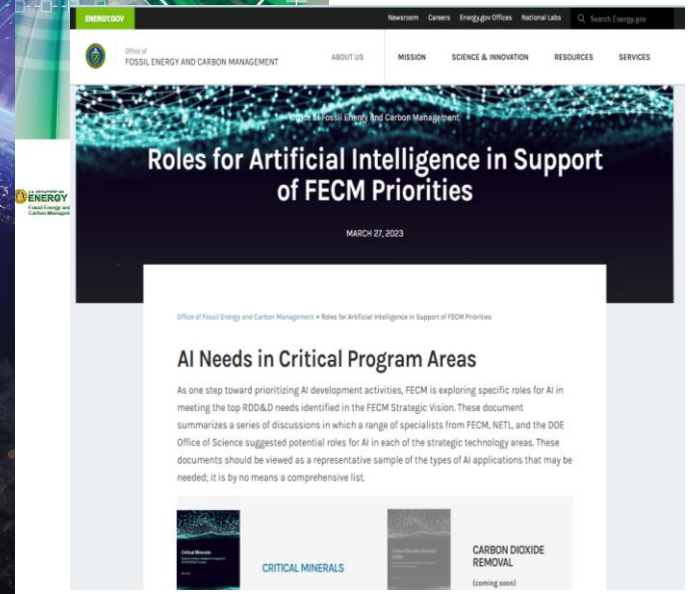
- DOE AI R&D Strategic Plan
- AI for Science, Energy & Security Workshops
- AI for Energy
- AI-related data calls
- FECM AI Strategy & Advisory Team
- The Inter-agency AI Community of Practice (CoP)
- DOE AI Community of Interest
- AI for Operations Committee

SAMI Tech Team

- Data science projects, research, training, or advisory



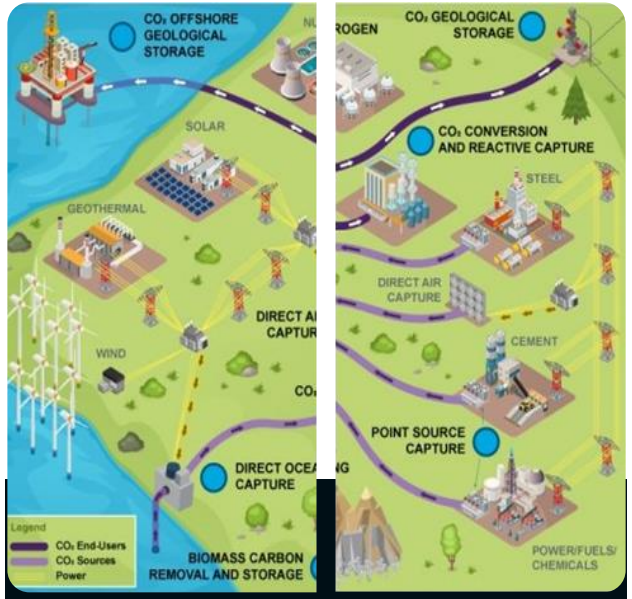




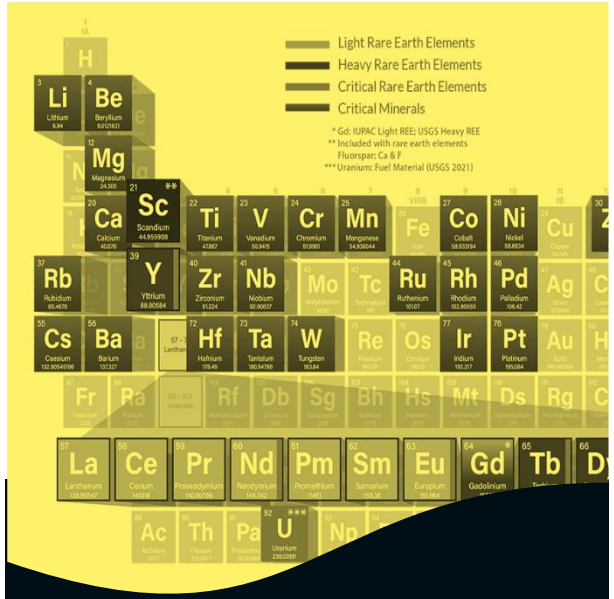
Accelerate AI Innovation

NATIONAL ENERGY TECHNOLOGY LABORATORY

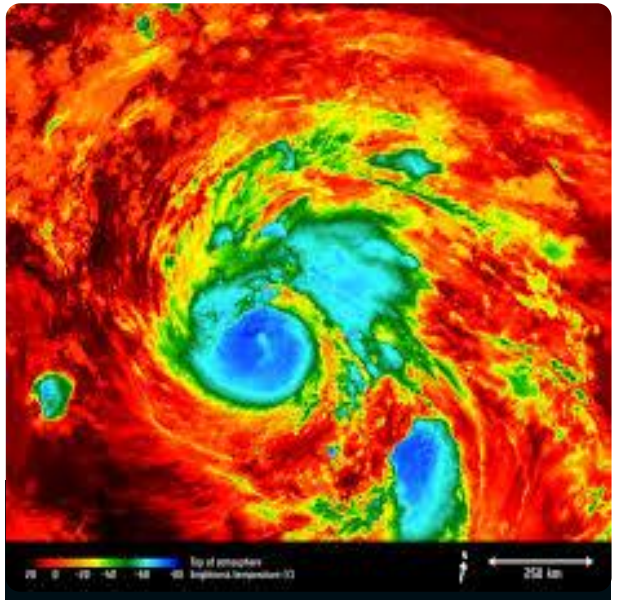
Enable NETL to push the frontiers of AI technology and create the next-generation architectures, tools, and approaches



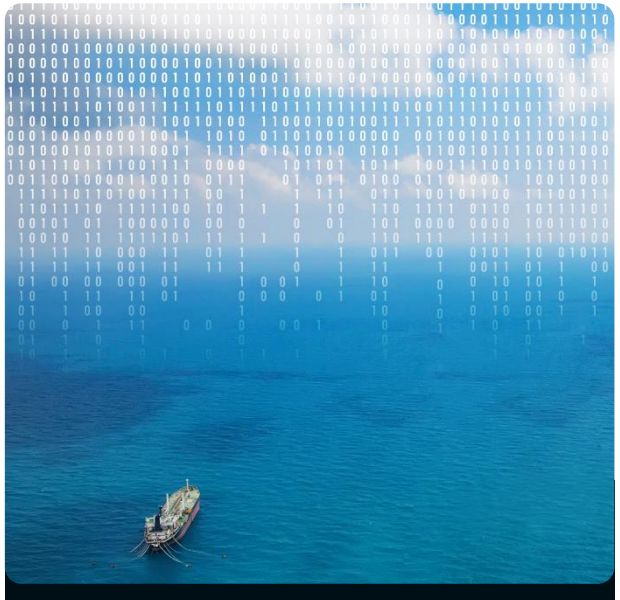
CARBON MANAGEMENT



RESOURCES AND MATERIALS



INFRASTRUCTURE & ENVIRONMENTAL RESILIENCY



BIG DATA, FOUNDATIONAL DATA & AI SOLUTIONS

Carbon Management

Applied AI for Carbon Capture and Storage Data Products

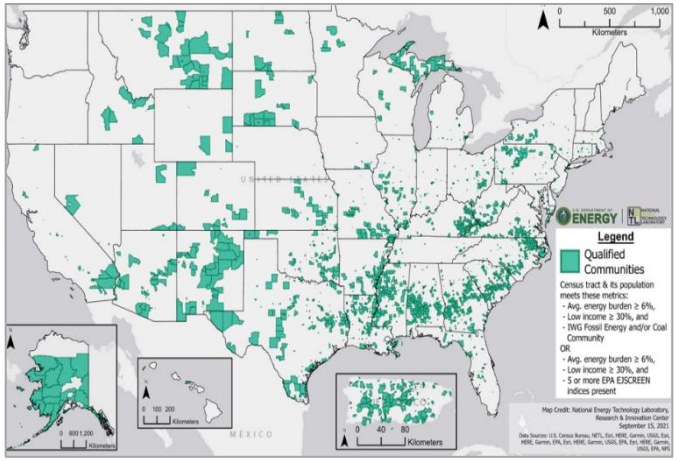
CO_2 Smart EJ/SJ Route Planning Tool

The interactive smart tool will assist in planning routes for CO_2 transport across the country considering environmental justice and social justice (EJ/SJ).

Explore the public database on EDX.

The Pipeline Route Planning Database team published research in Data in Brief in December 2023.

Researchers behind the tool met with representatives from industry on collaborative ideas.



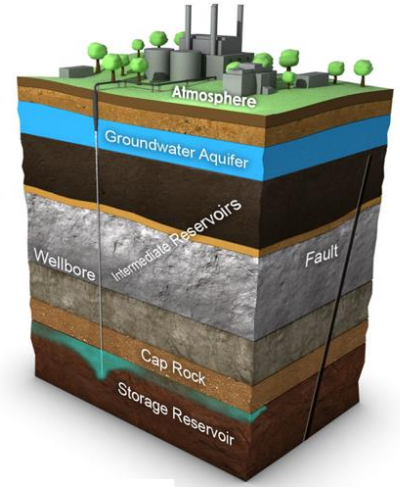
Fast Facts

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 geologic carbon sequestration 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.



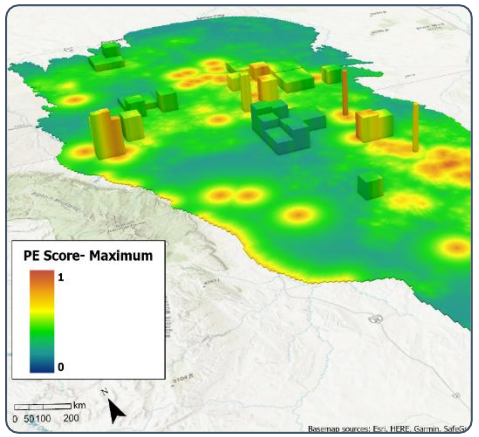
Explore the entire NRAP toolset:

Resources and Materials

Applied AI for REE/CMs and Alloy Discovery

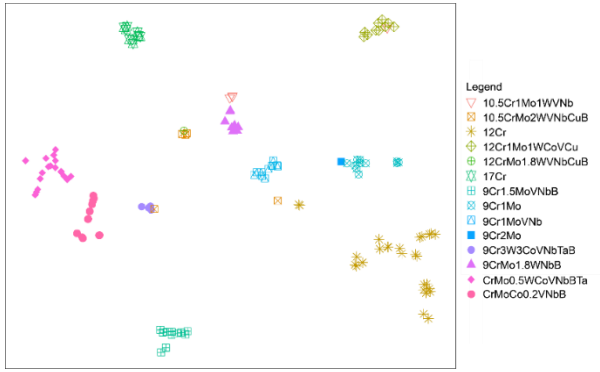
Federated-AI modeling for improving discovery of domestic critical mineral deposits

- 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 U.S.**
  - Featured in the Wall Street Journal - WSJ
  - Also featured in energy trade journal, *JPT*
- Recently, NETL has released **five, peer-reviewed, data-driven products** that help characterize unconventional critical minerals

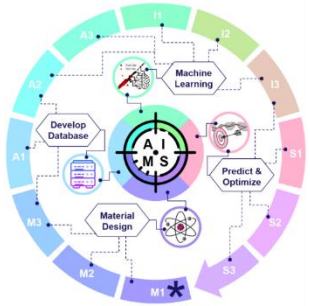


Machine learning prediction and outlier detection for alloy development and AI for alloy discovery

- 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.



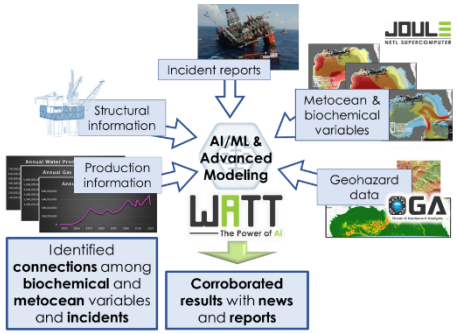
AIMS: Artificial Intelligence Materials Selection	
M1	*Literature Data Extraction*
M2	*High Throughput Synthesis*
M3	*Database Creation*
A1	*Data Preparation*
A2	*Explore and Visualize*
A3	*Data Sampling and Splitting*
I1	*Initial Model Creation*
I2	*Model Refining and Tuning*
I3	*Predict and Visualize*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

Infrastructure and Environmental Resiliency

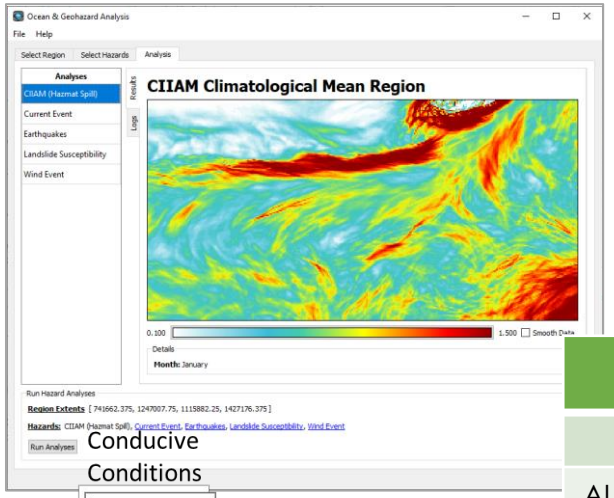
Applied AI for Extreme Climate & Infrastructure Resiliency

Award Winning AI/ML Multi-Model Forecasting Infrastructure Integrity



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



Ocean & Geohazard Analysis

Gradient Boosting Classifier
Artificial Neural Network

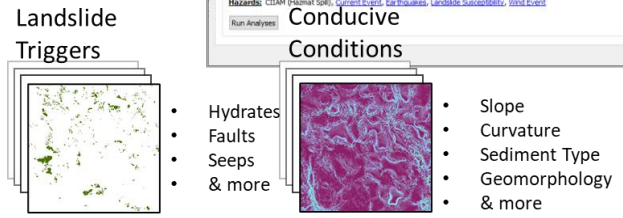
Fast Facts

AI Multi-Model Tool

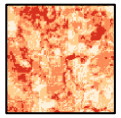
Evaluating infrastructure integrity and forecasting remaining useful lifespan and risk likelihood through applied **Machine Learning (ML) models**

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



Output Landslide Susceptibility Map



Fast Facts

Version 2 Tool

AI/ML Smart Tool

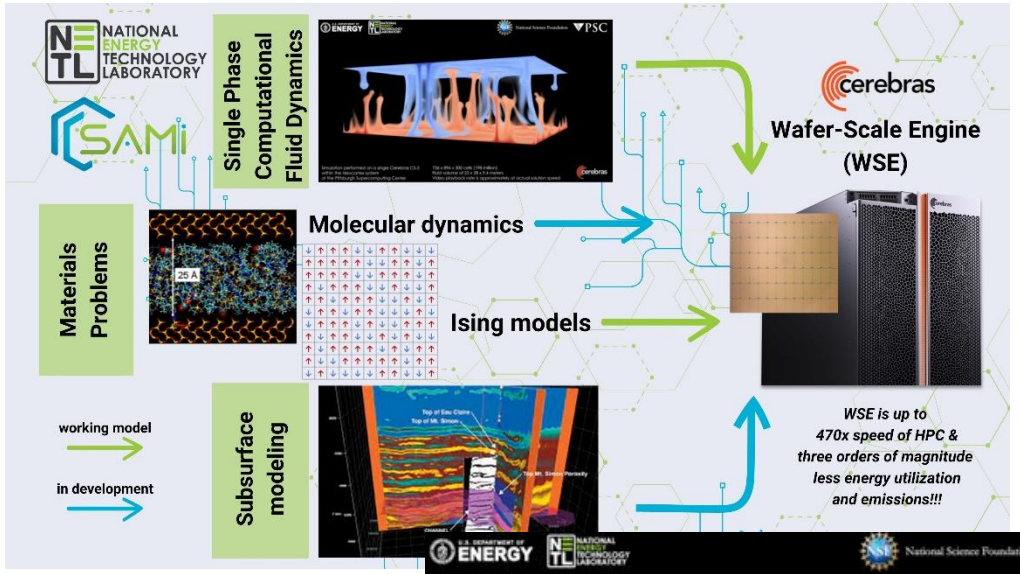
Improves characterization and forecasting of seabed and metocean hazards

Reduce risks to operations, including carbon storage activities, and the environment

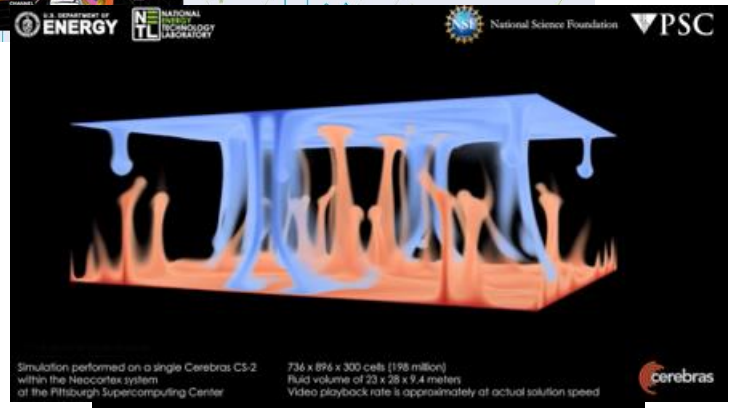
Big Data, Foundational Data, and AI Solutions

Cutting-edge, advanced AI computing and modeling to accelerate solutions to real-world challenges

- The NETL-developed WFA programming interface for the wafer-scale engine allows researchers to tackle tough AI problems
  - Materials and climate modeling
  - Computational fluid dynamics
  - Molecular dynamics
  - 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)

Make Data Accessible

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

Energy Data eXchange®++: For 14 years EDX has served as a data curation and collaboration platform for applied energy research and development.

- EDX++ couples highly scalable computing and simulation capabilities through a multi-cloud hosted system, enabling accelerated development, application, and testing of carbon management and fossil energy resiliency models, tools, and data.
- Multi-cloud solution also supports computing both in the cloud and for authorized users via NETL's on-premise advanced computing clusters (Watt and Joule), accelerating AI research, validation, and benchmarking for a wide array of applied energy and environmental needs.
- https://edx.netl.doe.gov/about

SAMI
SCIENCE-BASED AI/ML INSTITUTE

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

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

Contact Us: SAMI@netl.doe.gov

Learn more about SAMI:
https://edx.netl.doe.gov/sites/sami/

Questions?

NETL RESOURCES

VISIT US AT: **www.NETL.DOE.gov**

@NETL_DOE

@NETL_DOE

@NationalEnergyTechnologyLaboratory

CONTACT:
Jessica Sinclair
jessica.sinclair@netl.doe.gov