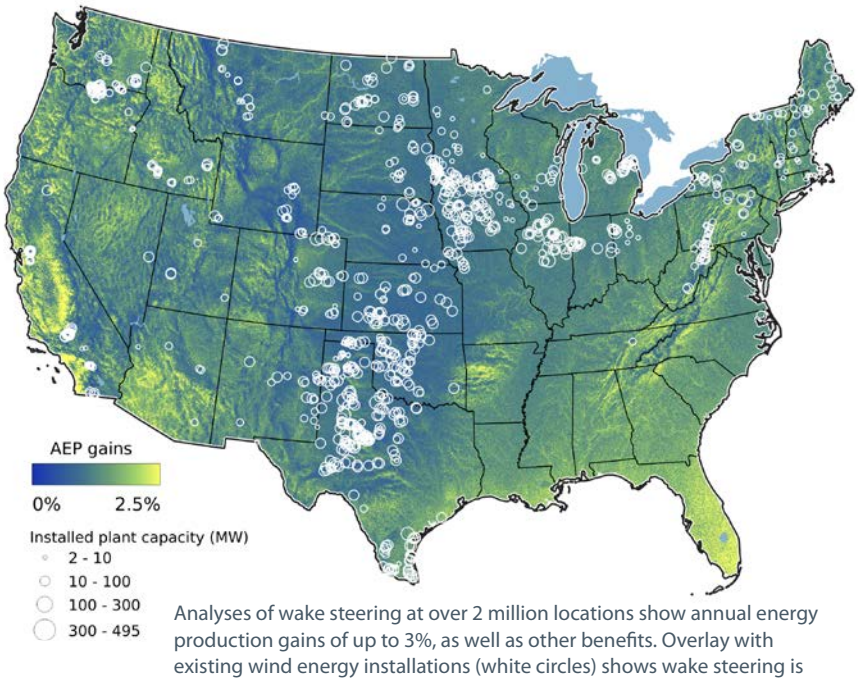
NREL
Transforming ENERGY

Transforming **ENERGY** Through Computational Excellence

Artificial Intelligence and Machine Learning

The National Renewable Energy Laboratory's (NREL's) expertise accelerates a decarbonized energy economy through the most advanced computational techniques, including artificial intelligence (AI) and machine learning (ML). AI is the simulation of human intelligence processes by machines, while ML encompasses the study of computer algorithms to imitate the way humans learn.

NREL's high-performance computing (HPC) system is the flagship capability serving the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy community. Our computational scientists employ AI to analyze data sets unique to NREL, including approaches to network training and hyperparameter optimization to efficiently tackle complex data streams, and embedding physical constraints for stability outside training bounds when modeling real-world processes.



Analyses of wake steering at over 2 million locations show annual energy production gains of up to 3%, as well as other benefits. Overlay with existing wind energy installations (white circles) shows wake steering is most effective in regions with low to moderate wind resources where wind deployment was previously uneconomical. *Figure by Dylan Harrison-Atlas, NREL*

From Planning to Reality With System-Level Research

NREL creates virtual replicas—digital twins—of existing transportation and mobility systems. Stakeholders can manipulate data points and insert the "what ifs?" to see a variety of options play out. Industry partners optimize passenger and freight mobility to minimize cost and energy use. ML and AI are used for time series forecasting to predict future traffic demand using data from individuals, traffic, freight routes, flight schedules, autonomous vehicles, and other sources.

Core Competencies and Capabilities

Applied Predictive and Explanatory Modeling

AI and ML use existing data to predict a future state of a system or unknown quantity, for example through digital twins.

Example: Predicting Wind Plant Performance and Wake Steering Outcomes

The ability to predict wind plant performance over a range of layout designs, technology innovations, and spatial locations is increasingly important for policy and investment decisions. NREL developed **state-of-the-art AI surrogate models** to illuminate divergent geographic and design outcomes for the United States, including assessment of the impact

of plant control strategies and plant layout decisions. These **predictive models of wind plant performance** demonstrate how wake steering technology can address a trifecta of operational, economic, and land-use related challenges commonly identified as barriers to large-scale deployment and integration of wind power.

Surrogates and Data-Driven Adaptation

AI and ML empower prediction of properties for not-yet-measured materials and molecules, allowing for high throughput screening of candidates for synthesis.

Example: The High Throughput Experimental Materials (HTEM) Database

The HTEM Database—the **world's largest materials database**—contains more than 140,000 data sample entries collected by NREL scientists investigating inorganic materials for use in advanced energy applications, such as thin-film solar cells. This collaboration with commercial partners, other research organizations, and universities promises continued expansion of the breadth and depth of this key materials data resource.

Inverse Design

AI and ML are used to identify optimal molecular makeup—in contrast to conventional approaches focused on manipulating molecular structures to achieve preferred behaviors.

Example: Binary Compound Semiconductor

A new semiconductor—antimony nitride—was recently predicted and synthesized for the first time, using AI. This Department of Energy-funded collaboration is accelerating discovery of experimentally accessible materials such as heterostructural alloys and crystal structure prediction, and the discovery of novel nitrides.

Control Problems

AI and ML anticipate rapidly changing conditions, such as load distribution among grids, and adapt in real time.

Example: KRoad

This two-dimensional, lightweight simulator uses 3D vehicle driving model considerations and enables the driver to make control decisions with less computation time and programmer effort required than full-fidelity 3D simulators. Fully compatible with OpenAI gym, KRoad contains a factored framework for composing gyms from various components including process, reward and observation functions, and termination conditions.

Operational Efficiency

Based on learnings from historical trends and real-time systems and facilities data, AI and ML train models to operate data centers more efficiently.

NREL's high-performance computing system, Eagle. *Photo by Dennis Schroeder, NREL 53840*

Example: Energy-Intensive HPC Data Centers

NREL is partnering on a research effort: adding AI to NREL's existing real-time data collection, aggregation, and streaming system, and to Hewlett Packard Enterprise's data monitoring and management system. This approach could improve the operational efficiency of the data center through analytics on data from information technology systems and facilities operations.

Cloud-Enabled Workflows

The cloud enables AI and ML workflows that are more difficult or even impossible using solely on-premise computing.

Example: NREL Hybrid Advanced Computing

Emerging workflows at NREL fuse data streams, modeling and simulation, and ML. Detailed consideration of each task in a workflow empowers alignment of optimal capability, data, and user intent with the right resources: edge, cloud, or HPC. To provide flexible data-centric capabilities, NREL makes cloud services accessible to a lab-based scientific community on commercial offerings and on-premise cloud resources.

Industry and academia are collaborating with NREL to leverage breakthrough advancements in advanced computing. Learn more at https://www.nrel.gov/computational-science/artificial-intelligence.html.

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