Transforming ENERGY Through Computational Excellence

Kenny Gruchalla from NREL (left) and Brian McAdoo from Duke University's Nicholas School for the Environment brainstorm disaster recovery visualization strategies using NREL's 3D visualization lab. *Photo by Eliza Hotchkiss, NREL.*

National Renewable Energy Laboratory Supports the U.S. Department of Energy Artificial Intelligence Strategy

The U.S. Department of Energy (DOE) leads the way in seizing the promise and managing the risks of artificial intelligence (AI), largely through its national laboratories. The National Renewable Energy Laboratory (NREL) is developing and using AI to advance work and productivity across the DOE mission space: science, energy, and security.

Leading AI/ML Research to Accelerate Energy Innovation

AI advances science in a range of ways: identifying meaningful trends in large datasets, predicting outcomes based on data, and simulating complex scenarios. For decades, NREL has been using machine learning (ML) and AI to advance our clean energy mission. AI moves research beyond experimental problem-solving to address open-world challenges characterized by fluid and novel situations. We have completed hundreds of studies leveraging AI/ML as well as reinforcement learning (RL) and deep learning across research, development, demonstration, and deployment. This research has—and continues to—spur breakthroughs and advancements in energy efficiency and renewable energy, including connecting climate simulations to renewable energy resource assessments, enabling new control strategies for wind turbines, and providing new control options for grid-interactive buildings.

Through advanced computing, NREL pushes the frontier of discovery and accelerates the development of new materials that **de-risk and drive down the costs** for clean energy deployment and advances the science base for our translational research efforts.

Developing the Science of AI

AI systems can work through mountains of data, highlighting anomalies and detecting patterns that human researchers cannot spot.

AI is a force multiplier that increases the productivity of core research, development, demonstration, and deployment investments by working together with humans through interactive visualization, creating AI guides for experimental design, bridging simulation and experiments, and bringing high-end computing into the research process. As **ethics** are a key component of AI development, NREL's principles for AI development include human agency and oversight; scientific and technical robustness; suitability and sustainability; transparency and explainability; and fairness, equity, and justice. When we perform research and use technologies responsibly—address the potential for bias; assess and rigorously test effectiveness and harden the security of the models; and more—we can proceed with confidence.

Partnering for Impact

Across our mission space, NREL supports the gamut of basic science to applied energy. Partnerships with industry and academia are essential to our AI development, as the capabilities and technology developed by partners help ensure our efforts are complementary to the private sector's capabilities. Some examples include:

- Within the high-performance computing data center, NREL and Hewlett Packard Enterprise codeveloped the award-winning HP Apollo system with liquid-cooling capabilities—resulting in Hewlett Packard Enterprise's delivery of a product to market about two years sooner than originally anticipated—and pioneered AI-driven operations to optimize data center performance.
- Winner of a 2023 R&D 100 Award, NREL's Simulation and Emulation for Advanced Systems (SEAS) open-source software provides in-depth analysis with multistakeholder inputs. Simulation and Emulation for Advanced Systems builds virtual communities—simulating energy transmission and distribution across transportation, buildings, and renewables as well as the grid—to validate and de-risk energy solutions before implementing.
- NREL's AI-based "Athena" digital twin of Dallas Fort Worth International Airport informs decisions that reduce energy use and operational costs and improve long-term investments at major transportation hubs.

Stewarding Components of AI for Energy

Over the last ten-plus years, NREL has stewarded the components essential to the development of AI for energy applications.

Through sustained investments, and strong codesign and co-development partnerships with industry, NREL has empowered **cutting-edge high-performance computing hardware** advances that are enabling today's modern AI capabilities. In 2023, the arrival of the Kestrel supercomputer at NREL increased computing pace and scale by more than five times. Kestrel's heterogeneous architecture, including central processing unit-only and graphics processing unit-accelerated nodes, is designed to better enable AI and ML workflows.

NREL's **user facilities** and associated user allocation programs make the advanced computers, software, and expertise for AI research and development freely accessible to scientific users and strategic partners with the best ideas at other labs, academic institutions, and industries across the country and around the world.

Computational science and applied math research at NREL is underscored by a **workforce** that includes more than 60 computational scientists with advanced training in applied mathematics as well as computer and data sciences. NREL's AI tech-focused research activities attract the talent we need to advance the energy transformation. A hallmark of NREL's computational science capability is that research scientists stand ready to respond to any and all needs, concerns, and opportunities that may result from AI in energy. With crosscutting links to the applied energy application domains, NREL staff curate core datasets—many designed with next-generation foundation models and specialized AI models for science and engineering.

Research at NREL generates hundreds of petabytes of **scientific data** from more than 20 scientific domains. Simulation and experimental datasets are combined with 'on demand' data from energy conversion hardware to feed a realistic—but safe—training environment for AI-based control systems.

Prioritizing Secure AI Environments

NREL's ecosystem supports the development of safe, secure, and trustworthy AI tools for high-consequence applications, empowered by decades of investment and expertise. Cutting-edge facilities enable NREL development, testing, and deployment of security measures and tools.

NREL researchers work collaboratively across cybersecurity and AI, focusing on energy security, to strengthen the grid against evolving threats.

- NREL deploys red teaming to assess flaws and vulnerabilities of AI models and improve the security of such systems to address cybersecurity threats.
- NREL's Advanced Research on Integrated Energy Systems (ARIES) platform provides unique simulation and emulation capabilities—including interfaces with real devices and infrastructure—to generate cyber physical data at scale. The ARIES Cyber Range also provides emulation and virtualization capabilities for red teaming AI models in a safe and isolated environment.

Join Our Quest

A track record of successful AI applications tells the story of NREL's AI expertise, and our culture of responsibility at NREL leads to a commitment to and support for AI ethics.

Contact us to piggyback on the research and investment foundation. **Ray.Grout@NREL.gov**

National Renewable Energy Laboratory
15013 Denver West Parkway, Golden, CO 80401
303-275-3000 • www.nrel.gov

NREL/FS-2C00-89401 • November 2024

Transforming ENERGY Through Computational Excellence

Widely Referenced AI Publications

Recent peer-reviewed journal articles:

- Artificial Intelligence-Aided Wind Plant Optimization for Nationwide Evaluation of Land Use and Economic Benefits of Wake Steering. *Nature Energy*, 2024. https://doi.org/10.1038/s41560-024-01516-8
- High-Resolution Meteorology With Climate Change Impacts From Global Climate Model Data Using Generative Machine Learning. *Nature Energy*, 2024. https://doi.org/10.1038/s41560-024-01507-9
- "Adversarial sampling of unknown and high-dimensional conditional distributions." *Journal of Computational Physics*, 2022. Generative adversarial networks can train competing neural networks to produce a network that effectively generates samples from a training set distribution. https://doi.org/10.1016/j.jcp.2021.110853
- "Artificial Intelligence and Critical Systems: From Hype to Reality." *Computer 53,* 2020. AI use in systems that affect public health, safety, and welfare helps these systems better utilize scarce resources, prevent disasters, and increase safety, reliability, comfort, and convenience. https://nrel.primo.exlibrisgroup.com/permalink/01NREL_INST/1e90bo2/alma991001010562303216
- "Artificial Intelligence for Power Electronics in Electric Vehicles: Challenges and Opportunities." *Journal of Electronic Packaging, Transactions of the ASME*, 2023. AI can help make power electronics more compact and reliable. https://nrel.primo.exlibrisgroup.com/permalink/01NREL_INST/1e90bo2/alma991001105265303216
- "Bridging Nano- and Microscale X-Ray Tomography for Battery Research by Leveraging Artificial Intelligence." *Nature Nanotechnology,* 2022. Modeling complex interactions in batteries, creating new possibilities for predicting and optimizing battery design and performance. https://doi.org/10.1038/s41565-022-01081-9
- "Two-Stage Reinforcement Learning Policy Search for Grid-Interactive Building Control." *IEEE Transactions on Smart Grid*, 2022. Intelligent controllers can optimize building operation during normal hours and demand response events. https://www.osti.gov/servlets/purl/1841140
- "Invertible Neural Networks for Airfoil Design." *AIAA Journal*, 2022. https://doi.org/10.2514/1.J060866

Recent NREL publications:

- PINN Surrogate of Li-Ion Battery Models for Parameter Inference, Part I: Implementation and Multi-Fidelity Hierarchies for the Single-Particle Model. *Journal of Energy Storage*, 2024. https://doi.org/10.1016/j.est.2024.113103
- PINN Surrogate of Li-Ion Battery Models for Parameter Inference, Part II: Regularization and Application of the Pseudo-2D Model. *Journal of Energy Storage,* 2024. https://doi.org/10.1016/j.est.2024.113104
- "PolyID: Artificial Intelligence for Discovering Performance-Advantaged and Sustainable Polymers." *Macromolecules,* 2023. Reducing material development timelines by predicting material properties and screening millions of possible polymer designs down to a short list with advanced performance and greater sustainability. https://doi.org/10.1021/acs.macromol.3c00994
- "Scaling Wind Power Innovation Assessment for Rapid Energy Transition with Artificial Intelligence." *NREL presentation*, 2022. Use of a surrogate model to conduct fleet-wide wind plant layout optimizations shows how wake steering technology can address barriers to large-scale wind power deployment and integration. https://www.nrel.gov/docs/fy23osti/84403.pdf

From the FY 2023 NREL Advanced Computing Annual Report:

- Material Defect Discovery, Properties, and Interactions Improve Candidate Screening for Water-Splitting Technologies: AI/ML predicts the impact of defects on a material, eliminating the need for constructing and analyzing large supercells for each defect.
- High-Fidelity Calculations Yield Nanoscale Insights for Cost-Competitive Fuel Cell Electrocatalysts: Precious metal electrocatalysts present a material barrier to cost-competitive deployment. NREL's computational techniques explore viable catalyst design alternatives for electrochemical modeling as a part of the ElectroCat consortium.
- New Cathode Coating Designs Stabilize Lithium-Ion Battery Performance: With support from the VTO's Battery Materials Research program, NREL uses high-throughput computations to develop materials design principles to improve lithium-ion battery stability.

NREL Transforming ENERGY

National Renewable Energy Laboratory
15013 Denver West Parkway, Golden, CO 80401
303-275-3000 • www.nrel.gov

NREL prints on paper that contains recycled content.

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency and Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC

NREL/FS-2C00-89401 • November 2024