NREL
Transforming ENERGY

ADVANCED COMPUTING
ANNUAL REPORT
2021

Director's Letter

Advanced computing at the National Renewable Energy Laboratory (NREL) had an exciting 2021. More than 300 projects advanced the U.S. Department of Energy's (DOE's) Office of Energy Efficiency and Renewable Energy (EERE) mission. This is the most conducted in a single year to date. NREL researchers collaborated across disciplines to publish more than 600 technical outputs. All this great work continues to advance the science of energy efficiency and renewable energy.

As the dedicated computing facility for EERE, NREL computing plays a critical role across the research portfolio. To stay at the cutting edge of the latest advancements in high-performance computing (HPC) technology, NREL finalized the contract to acquire its next-generation HPC system, named Kestrel. Installation of the new system will begin in the fall of 2022 in NREL's Energy Systems Integration Facility (ESIF) data center. Kestrel will complement the laboratory's current supercomputer, Eagle, during the transition. When completed—in early 2023—Kestrel will accelerate energy efficiency and renewable energy research at a pace and scale more than five times greater than Eagle, with approximately 44 petaflops of computing power.

NREL continues to push the boundaries of efficient data center operation, with warm water cooling, optimization, and waste heat recovery enabling the facility to end the year with an average power usage effectiveness rating of 1.028. Looking to the future, a 4-MW power and corresponding cooling upgrade is underway to support Kestrel. The addition of Kestrel with higher return temperatures and greater heat output enables further advances in demonstrating the effective use of waste heat recovery at scale.

Another major capability advancement this year was in the ESIF Insight Center—the visualization labs for scientific computing. New, advanced technologies, including high-resolution displays and state-of-the-art interactive touch capabilities, will bring complex data to life for researchers.

HPC resources are being leveraged to scale up geospatial resolution in support of NREL's winning 2021 R&D 100 award for dGen™, an open-source software that simulates customer adoption of distributed energy resources through 2050. In addition, HPC is enabling large-scale simulations of wave energy converters to support the use of the Wave Energy Converter Simulator, another NREL R&D 100 award winner in 2021.

Many exciting developments will be highlighted in the following pages, and we expect many more to come.

Ray Grout,
Director, Computational Science Center

Kris Munch,
Laboratory Program Manager, Advanced Computing

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CAPABILITIES & PROJECTS AT A GLANCE

NREL hosts supercomputing systems and visualization capabilities, providing EERE researchers and industry partners with the necessary technology, tools, and expertise to tackle today's toughest energy challenges.

In collaboration with scientists and engineers, NREL HPC experts develop cross-cutting capabilities that provide the critical foundation upon which rapid-breakthrough science is made possible. Advanced visualization technology helps researchers explore and interact with data in new ways that accelerate understanding and innovation.

Key Performance Indicators

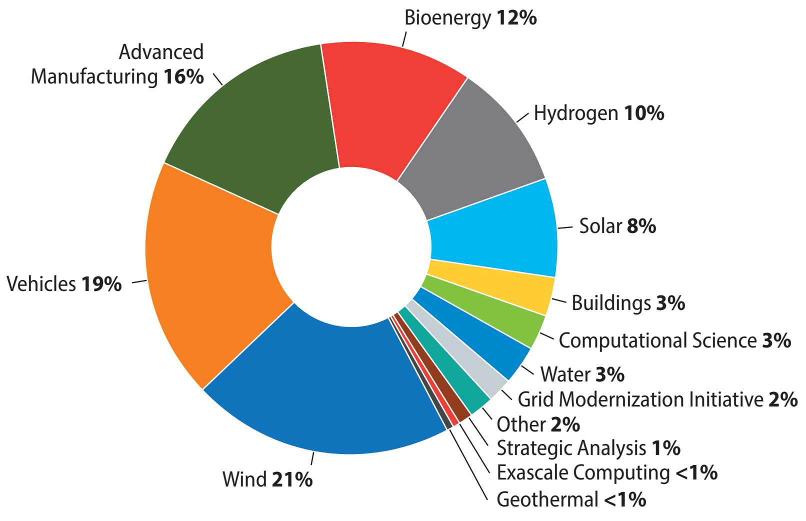
HPC Data Center Usage

- 535 users
- 95% HPC availability
- 90% HPC utilization

FY 2021 HPC Usage

NREL's HPC user facilities supported more than 300 modeling and simulation projects, advancing the DOE mission across the spectrum of energy efficiency and renewable energy technologies in FY21.

EERE Office	# of FY 2021 projects
Advanced Manufacturing Office	22
Bioenergy Technologies Office	23
Building Technologies Office	20
Computational Science/Industry/LDRD	48
Grid Modernization Initiative	30
Geothermal Technologies Office	1
Hydrogen and Fuel Cell Technologies Office	19
Solar Energy Technologies Office	31
Strategic Analysis	22
Vehicle Technologies Office	41
Wind Energy Technologies Office	34
Water Power Technologies Office	11
Total	**302**



Percentage of computing resources used across technology areas

Expanding HPC Capacity With Kestrel Procurement

NREL has selected its third-generation HPC system, called Kestrel, to rapidly advance DOE's energy research and development efforts and deliver transformative energy solutions to the entire United States. As the dedicated HPC system for EERE, Kestrel will play a critical role in computing across the research portfolio, advancing research in computational materials, continuum mechanics, and large-scale simulation and planning for future energy systems. Rapid advancements in artificial intelligence (AI) and machine learning (ML) are driving complementary physics and data-driven workflows—for instance, by fusing simulation with new sensor data sources—and fostering innovation and expansion of computing approaches for energy research. Kestrel's heterogeneous architecture, which includes both CPU-only and GPU-accelerated nodes, is designed to enable these emerging workflows, providing EERE and industry partners with the ability to tackle the challenges of moving to a renewable and sustainable energy future.

With the Kestrel HPC system on the horizon, NREL remains poised to deliver critical energy efficiency and renewable energy advancements with its HPC-supported capabilities.

Data Center Power and Cooling Upgrade

To prepare for ESIF's next supercomputer, we are adding 4 MW of power and equivalent cooling capacity. These efforts will continue the legacy of world-class energy efficiency demonstrated by the data center over the last decade. Design work started in FY21 and will be completed in FY22. Construction efforts will commence shortly after the design work is finished, and will be completed in FY23.

Vehicle Technologies Office Invests in Swift

EERE's Vehicle Technologies Office (VTO) has procured a new HPC resource, called Swift, to provide additional computing capability to complement Eagle and support unprecedented computing demand across the VTO portfolio. The Swift cluster became operational in FY21 as a 440-node cluster with 28,160 compute cores and 2 petabytes of storage. Co-location of the Swift cluster within the HPC data center facility interlaces operations with EERE-centric computational science and enables rapid data movement and economies of shared expertise and support infrastructure. In FY22 and beyond, the combination of Eagle (or Kestrel, starting in FY23) and Swift will provide robust support for the VTO portfolio.

Read more about activities within this EERE user facility at NREL

- ESIF Annual Report
- Advanced Research on Integrated Energy Systems (ARIES) Annual Report

Advancements in Scientific Visualization

As we expand our ability to generate numerical data through continued investments in HPC and experimental platforms, one of our greatest challenges is to effectively understand and make use of these data. Visualization is one of the most important tools in this regard, as it supports the human capacity to understand and reason about large, complex data. We are bringing new technologies and interactive visuals to bear on the energy research landscape.

The Insight Center, EERE's state-of-the-art scientific visualization facility, combines visualization and collaboration tools to promote knowledge discovery in energy systems. Located adjacent to the HPC data center in the ESIF, the Insight Center uses advanced visualization technology to provide on-site and remote viewing of experimental data, high-resolution visual imagery, and large-scale simulation data.

During FY21, NREL implemented major upgrades to the Insight Center, including the successful completion of two-dimensional visualization capabilities, with a 10x update in the high-resolution display wall and new interconnected tactile displays. The new large-scale, high-resolution display wall leverages visual acuity at various scales, supporting users' peripheral vision and spatial memory. The new touch interfaces provide a fluid, low-friction way to interact with the high-resolution display.

This capability supports multiple high-profile, high-impact projects, including EERE core work (such as viewing large microscopy mosaics and gaining insight into wind farm operation), intersections with DOE's Office of Electricity (such as visualizing the dynamics of the North American electrical power grid), and industry engagement that promotes the EERE mission (such as the Los Angeles 100% Renewable Energy Study).

NREL and HPE Collaborate on the Data Center of the Future

A key partnership with Hewlett Packard Enterprise (HPE) adds AI to NREL's HPC data center by developing data-driven models that combine NREL's real-time data collection/aggregation/streaming system and HPE's data monitoring/management system. Continuing into its third and final year, this project, called AIOps, has developed new power usage effectiveness and cooling ramp prediction models, and has also created a real-time anomaly detection module for the HPC and data systems under control in the data center. AI and ML approaches provide the means to improve the efficiency and resiliency of the data center's energy use, operations, and management by learning historical trends and training models to operate on real-time data collected from both information technology and facilities sources. These advances are critical to HPC data centers, which increasingly need to rely on automation to keep pace with exascale growth in compute capability and to manage and optimize the data center environment and facility resources.

INTEGRATED ENERGY SYSTEMS

Smart Community Design and Control for Enhanced Efficiency and Resilience

Many cities and states across the United States have committed to ambitious energy efficiency and renewable energy goals to achieve net-zero emissions by no later than 2050. As part of this effort, communities are transitioning to pervasive distributed energy resources, such as flexible loads, photovoltaics (PV), and energy storage. NREL, with funding from the Building Technologies Office, is advancing the design and control of high-performance residential communities to improve their efficiency and resilience.

NREL's HPC capability has supported multiple simulations using the Hierarchical Engine for Large-Scale Infrastructure Co-Simulation (HELICS) software and the Object-Oriented Controllable High-Resolution Residential Energy (OCHRE) building model. Three new frameworks target load flexibility quantification, carbon-responsive control, and optimal battery sizing. NREL applied one framework to the Basalt Vista community in Colorado, providing local electric utilities with an in-depth understanding of load flexibility at the home and community levels. Researchers simulated multiple scenarios, using combinations of different seasons, flexibility intervals, flexibility operation strategies, and preconditioning measures to quantify the load flexibility. The rule-based carbon-responsive control framework regulates the set points of the thermostatically controlled loads, responding to the grid's carbon emission signals in real time. Results indicate that the carbon-responsive controllers can reduce the homes' annual carbon emissions by 6.0% to 20.5%. The optimal battery sizing framework identified the potential for residential buildings with PV and home battery systems to support building load during blackouts. NREL researchers also incorporated homeowner energy consumption behaviors—ranging from austere to wasteful—to account for variability in homeowners' energy consumption patterns. Building resilience can be maximized with optimal battery sizing and austere user behavior.

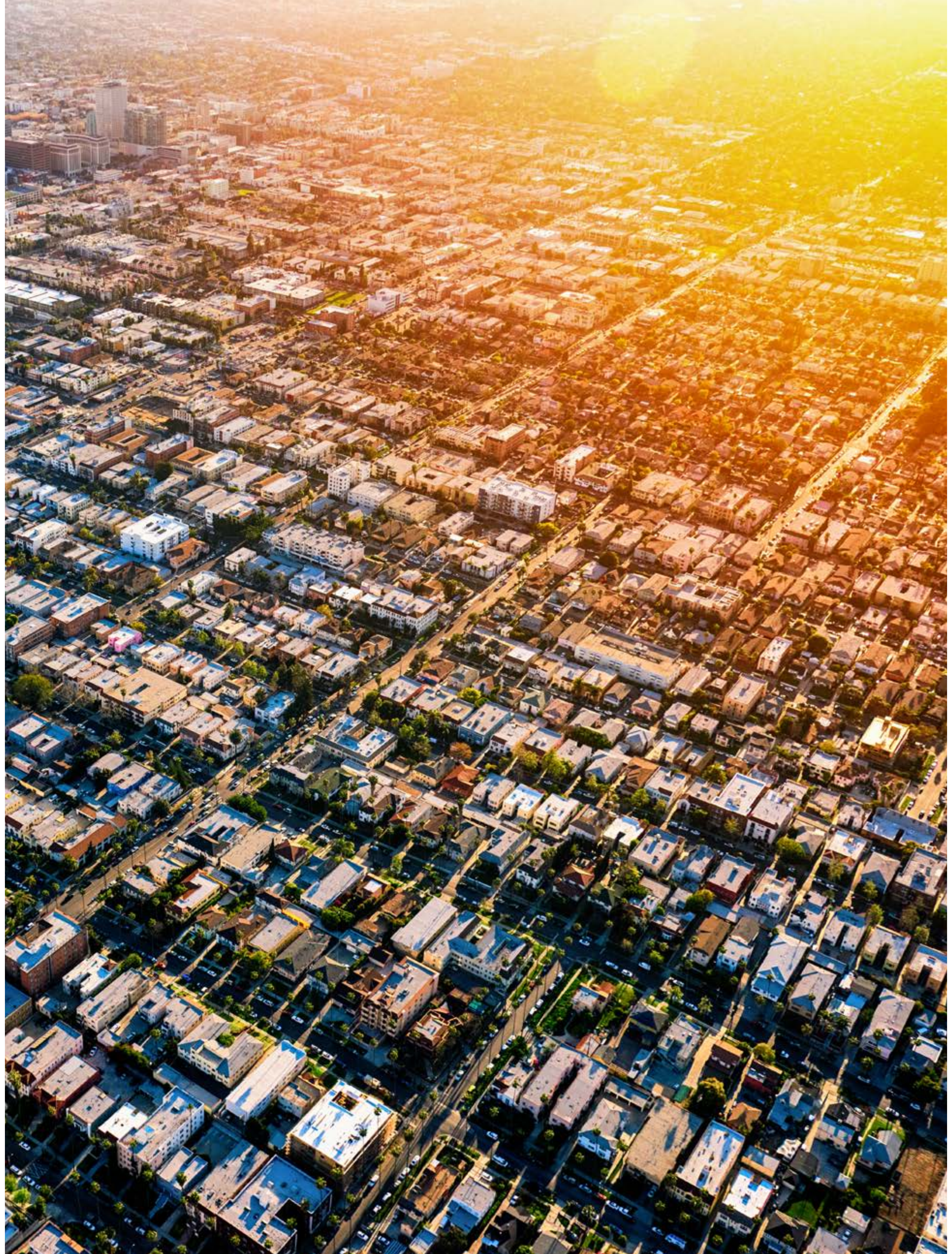
Los Angeles Can Achieve Reliable, 100% Renewable Energy

In a first-of-its-kind, objective, rigorous, and science-based power systems analysis funded by the Los Angeles Department of Water and Power—the Los Angeles 100% Renewable Energy Study (LA100)—NREL explored how the second-largest city in the nation could achieve a 100% clean energy future by 2045, or as soon as 2035. With world-class research partners from the University of Southern California, Colorado State University, and Kearns & West, NREL analyzed the Los Angeles Department of Water and Power's existing generation, transmission, and distribution assets to determine the renewable resource mix and system upgrades required to achieve a 100% renewable power system for the city while maintaining a high degree of reliability.

NREL used the Eagle supercomputer to integrate dozens of modeling tools and methods, incorporate input data from multiple sources, run more than 100 million simulations, and provide detailed results—pushing existing tool sets to new levels of sophistication. The landmark LA100 study demonstrated the importance of a robust community role in energy transition planning, identified a methodology for multi-tool integration to better capture the complexity of the energy transition and related community impacts, and demonstrated how a 100% renewable energy system can operate reliably. It also serves as an example for other cities and regions pursuing pathways to clean energy systems.

Solar Uncertainty Management and Mitigation for Exceptional Reliability in Grid Operations

NREL is creating one-year data sets of time-coincident load, wind, and solar actuals and probabilistic forecasts for U.S. power system regional transmission organizations. The data sets include site-, zonal-, and balancing-area-level resolutions. The actual solar data is generated by the Renewable Energy Potential (reV) model using resource data from



the National Solar Radiation Database. The actual wind data is simulated using the Weather Research and Forecasting model and the reV model. Probabilistic forecasts are generated by Bayesian model averaging combined with ML techniques, using data from the European Centre for Medium-Range Weather Forecasts. Some of these data sets will be provided to the research community to support future research.

Using HPC to draw from multiple data sources, researchers validated new operational algorithms that use probabilistic solar forecasts to reduce cost and maintain reliability on a large-scale test system of the Electric Reliability Council of Texas service territory. NREL processed and evaluated these probabilistic behind-the-meter solar generation forecasts in the context of the forecast generation milestones of the Solar Uncertainty Management and Mitigation for Exceptional Reliability in Grid Operations (SUMMER-GO) project, funded by DOE's Solar Energy Technologies Office (SETO).

Valuation of Solar Plus Storage

NREL, with funding from SETO, is analyzing the capacity credit (i.e., the amount of conventional power that can be replaced by renewables while maintaining the same reliability) of PV energy paired with storage. NREL aims to understand the interaction between PV and storage, and how these resources contribute to the firm capacity—and therefore reliability—of power systems. Additionally, NREL is evaluating the ability of PV and storage to mitigate curtailment events, or output reductions due to supply, demand, or transmission constraints that result in potential energy loss.

The team employed NREL's Probabilistic Resource Adequacy Suite (PRAS) model to simulate 100,000 samples of simplified system operations. The rigorous risk assessment by PRAS considered aggregated generator dispatch, storage charging and discharging, and interregional load balancing in hourly simulations under varying, randomly sampled generator outage conditions. The PRAS model outputs included a variety of reliability metrics, including the expected loss of load, expected unserved energy, and capacity credit of marginal resources. These results will help utilities and system operators maximize the value of PV-generated electricity. The results will also allow system operators to appropriately value PV with storage and enable developers to be compensated for this value.

Real-Time Signal Algorithm Optimizes Regional Mobility

NREL's digital twin of traffic flows in Chattanooga, Tennessee—funded by VTO—supports traffic situational awareness and helps minimize congestion and improve mobility energy efficiency in the Tennessee-Georgia region. In partnership with Oak Ridge National Laboratory, the Chattanooga Department of Transportation, and Siemens, NREL developed a regional control approach using AI and HPC to achieve substantial energy savings across city streets and freeways. NREL scaled up and deployed real-time traffic signal model predictive control (MPC) algorithms for the Shallowford Road corridor in Chattanooga, Tennessee, changing traffic signal settings according to real-time traffic states. Results showed that MPC real-time control decreased the corridor's average vehicle delay by 30% and its vehicle energy consumption by 4%, with up to a 30% reduction in vehicle energy consumption on some of the corridor's road segments. Traffic states were derived from real-time data pulled from GridSmart cameras installed on intersections, as well as probe data from the TomTom traffic company.

Modeling Energy Storage on the Future Grid

Energy storage is poised to be a significant part of the evolving U.S. power system, with declining costs, improved technologies, and increasing deployment. Understanding the value of storage, though, is an inherently complex modeling challenge. To investigate the potential role and impact of storage on the grid, NREL has been leading the Storage Futures Study (SFS)—a multiyear research project within DOE's Energy

Storage Grand Challenge that is accelerating the development, commercialization, and utilization of next-generation energy storage technologies.

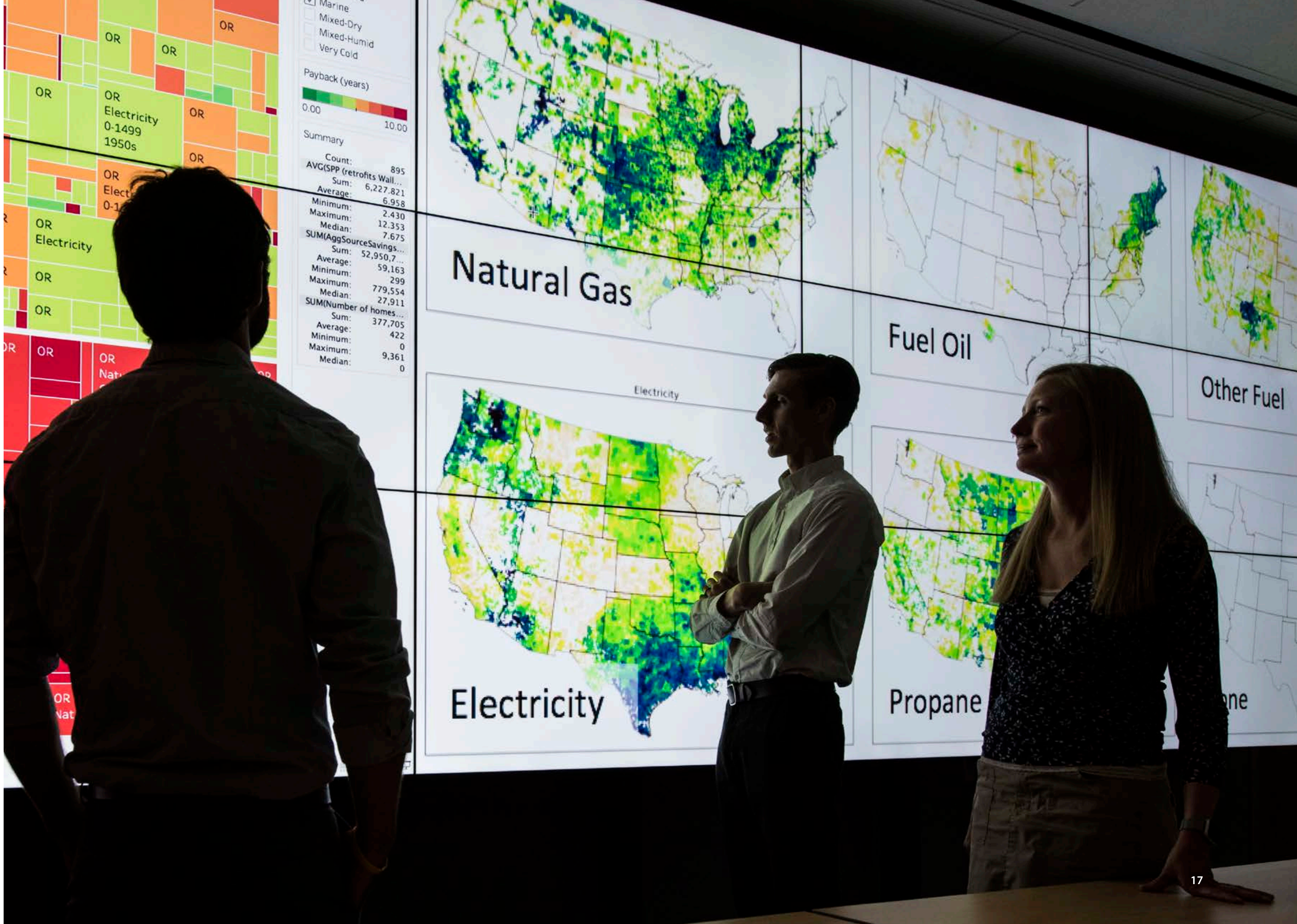
For the study, NREL added new battery capabilities to its Regional Energy Deployment System and Distributed Generation Market Demand models and used the Eagle supercomputer to simulate future high-storage power system scenarios. In one phase of the SFS, NREL modeled the cost-effectiveness and customer adoption of PV-plus-battery-storage systems—the first published estimates of distributed battery storage deployment. Across all modeled scenarios, NREL found significant economic potential for behind-the-meter battery storage, with lower battery costs and the high value of backup power driving deployment. In another phase of the SFS, NREL modeled hourly grid operations of high-storage power systems, finding that power systems operate more efficiently with lots of storage.

The inclusion of storage capabilities in the NREL models opens the door to further research on the evolution of energy storage on the grid.

Chicago Energy Efficiency Planning and Analysis

Led by Elevate and in partnership with the city of Chicago and Commonwealth Edison (ComEd), NREL conducted technical analysis using its ResStock™ tool to develop a roadmap for deep residential energy efficiency in Chicago, Illinois. Powered by NREL supercomputing, the ResStock model has run more than 20 million building energy simulations across a variety of projects based on a statistical model of housing stock characteristics. With this data, researchers have uncovered $49 billion in potential annual utility bill savings that could be achieved through cost-effective energy efficiency improvements. To support Elevate, NREL calibrated ResStock using Chicago-specific data and used the tool to assess the potential of reducing the energy consumption of the existing housing stock by 50%. NREL then used the simulation results to develop recommendations for the City of Chicago and its utilities—ComEd and Peoples Gas.

ResStock simulated a wide range of building energy retrofits, from which NREL curated a portfolio of efficiency measures that Elevate will validate in real Chicago homes. NREL and Elevate also provided the City of Chicago with a tailored, actionable, city-scale analysis on the impacts that retrofits have on utility bill savings, cost-effectiveness, carbon emissions, and energy equity. This work can inform municipal policy decisions by demonstrating which energy efficiency interventions are low-cost, energy-saving, and scalable. This work also places NREL among the few in the published building energy space to have conducted city-scale energy analyses using a bottom-up, detailed simulation model that leverages local partnership and place-based data. The ability to perform detailed, large-scale building stock simulations was key to the success of this project.

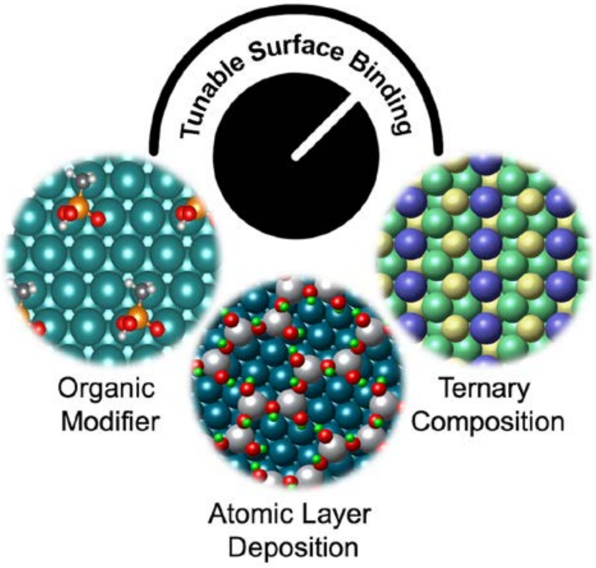


MATERIALS SCIENCE

Modeling To Reduce Energy and Carbon Intensity of Biomass and Waste Conversion

The Consortium for Computational Physics and Chemistry's Atomic-Scale Modeling project, supported by DOE's Bioenergy Technologies Office, utilizes computational modeling to inform the design and synthesis of more active and selective catalyst materials that can reduce the overall energy and carbon intensity of biomass and waste conversion processes.

NREL applied quantum mechanical simulation tools to provide atomic-scale insight—which cannot be obtained using solely experimental tools—into the structure-function relationships of diverse tailored catalyst materials. Working in collaboration with experimental partners in academia, industry, and other national labs, as well as the Chemical Catalysis for Bioenergy Consortium, NREL HPC enabled the discovery of strategies to improve the hydrogenation activity of palladium catalysts through the addition of organic or inorganic overlayers, which operate through distinct mechanisms. In addition, the research team established a ternary transition metal phosphide platform for understanding the composition-dependent activity of these tunable materials in the electrochemical hydrogen evolution reaction.



Simulations Drive Bioenergy Innovations

The Center for Bioenergy Innovation (CBI) accelerates the domestication of bioenergy-relevant, non-model plants and microbes to produce anaerobically derived biofuels with proven fuel value. Funded by DOE's Office of Science Biological and Environmental Research program and in collaboration with CBI researchers at multiple institutions, NREL researchers are providing HPC-facilitated molecular dynamics simulations to identify the most promising targets for enzyme variants, to guide enzyme engineering for biomass synthesis and deconstruction, and to identify candidate specialty fuels with supply-chain-compatible properties.

Simulation-guided engineering of alcohol dehydrogenase and aldehyde dehydrogenase enzymes are critical to consolidated bioprocessing approaches for converting biomass to four-carbon alcohol fuels. Some organisms assemble these enzymes into higher-order structures called spirosomes (spiral structures that consist of dozens of enzymes or more). Understanding the mechanisms of formation, compaction, and extension of these spirosomes is key to conducting more informed engineering and improving the performance of four-carbon alcohol production.

Additionally, NREL's HPC-generated, molecular-level views into the enzyme-substrate interactions in plant biosynthetic enzymes and the successful modulation of acetylation are laying the foundation for enzyme engineering strategies that can precisely modulate and produce biomass with tuned properties using natural plant pathways.

Improving Biofuels and Plastic Upcycling Through Biochemical Process Modeling and Simulation

NREL's molecular-scale modeling and simulation capabilities have identified mechanisms for enzymatic plastic degradation and enzyme engineering for thermal stability. In addition, NREL's powerful computational workflows have analyzed the depolymerization of lignin—an abundant, organic polymer in plants that, when reduced, can improve the production efficiency of fuels and products. NREL's LigninWrangler program, which analyzes mass spectroscopy data from lignin products, was expanded to improve mass accuracies and to quickly reduce the size of raw mass spectroscopy output files significantly, thereby aiding file moving, sharing, and processing (which often requires hundreds of terabytes for a single study).

To reduce the cost of biofuels, separating high-value co-products from crude pyrolysis oil—a synthetic fuel under investigation to replace petroleum—is key. Centrifugal partition chromatography is a promising separation technology, but it requires tremendous experimental effort to measure numerous compounds in a variety of solvent combinations. Funded by DOE's Bioenergy Technologies Office and with the aid of HPC, NREL's computational tool enabled in silico high-throughput screening of numerous solvent systems, which will substantially benefit the experimental research.

For metabolic modeling at the cellular scale, NREL's Eagle GPU hardware built ML models that link enzyme sequence and structure to function. These models guide pathway engineering for enhanced microbial biotransformations. Continuum modeling of mass-transfer and transport processes leverages computational fluid dynamics models to determine the best design parameters at production scales, de-risking scale-up. Ongoing work on simulations of butanediol synthesis will enable efficient production of butanediol at scale, which will be an important intermediate step for producing sustainable aviation fuels.

Center for Hybrid Organic-Inorganic Semiconductors for Energy (CHOISE)

DOE's Center for Hybrid Organic-Inorganic Semiconductors for Energy (CHOISE) accelerates discovery and elucidates design principles of molecular structure-property-function relationships to achieve unprecedented control over spin, charge, and light-matter interactions, leading to advanced energy-efficient technologies.

Funded by DOE's Office of Science Basic Energy Sciences program, partners in industry, academia, and national laboratories across the United States utilized NREL's Eagle HPC to perform first-principles calculations to investigate the carrier dynamics and luminescent properties of hybrid organic-inorganic metal halide perovskites (HOIPs). Understanding the exciton-phonon interaction is critical to the design of efficient HOIP-based optoelectronic devices that source and control light, like semiconductors. Researchers calculated the intrinsic quantum efficiency of HOIPs and identified potential strategies to improve their efficiency. For instance, by introducing defects, self-trapped excitons (STEs) can be bounded to defect sites, contributing to solid-state lighting. These defect-bound STEs could produce fast and efficient scintillators, i.e., materials that can convert high-energy radiation into visible light. The study revealed the mechanism and design rules for future high-performance scintillators. With the calculated quantum efficiency, the luminescent properties can be fully controlled, ultimately providing theoretical guidance for future search and design of solid-state optoelectronics with the desired properties and improved performance.

Optimizing Battery Materials and Molecules

Developing high-performance energy generation and storage materials currently requires costly experimentation and computation to identify optimal structures and properties, and the new technologies that

follow often take decades to reach commercial viability. Even with computational screening tools, the vast landscape of possible molecular or crystal structures exceeds current computational capacity, over 1,060 possible organic molecules with appropriate molecular weight are hypothesized to exist. However, ML approaches have demonstrated best-in-class performance to address this problem. NREL researchers have developed a generalized ML approach for optimizing targeted and complex functional properties across possible material structures, enabling faster identification of promising candidates.

NREL, in partnership with the Colorado School of Mines and Colorado State University, used Eagle to demonstrate design application tasks for short- and long-term energy storage, respectively; these include the design of solid-state ion conductors (for solid-state batteries) and the design of organic redox-active materials (for polymer flow batteries). By coupling recent advances in graph neural networks with reinforcement learning-based structure generation, the team improved prediction accuracy and structure validity over emerging methods by 8x and 25x, respectively, while reducing computational costs by more than a factor of 100 compared to other, more exhaustive approaches.

The Surprising Chemistry Behind a Self-Improving Photocathode for Hydrogen Production

HydroGEN, a member of DOE's Energy Materials Network consortium, is addressing water-splitting materials challenges by making world-class national lab capabilities—in photoelectrochemical, solar thermochemical, and low- and high-temperature electrolytic water splitting—more accessible to academia, industry, and other national labs.

The development of advanced photoelectrochemical water splitting and low-temperature electrolysis for hydrogen production requires a detailed understanding of interfacial processes at electrodes. Researchers from Lawrence Livermore National Laboratory made use of NREL's Eagle supercomputer to perform first-principles simulations to understand the interfacial reactivity and stability of the gallium nitride photocathode.

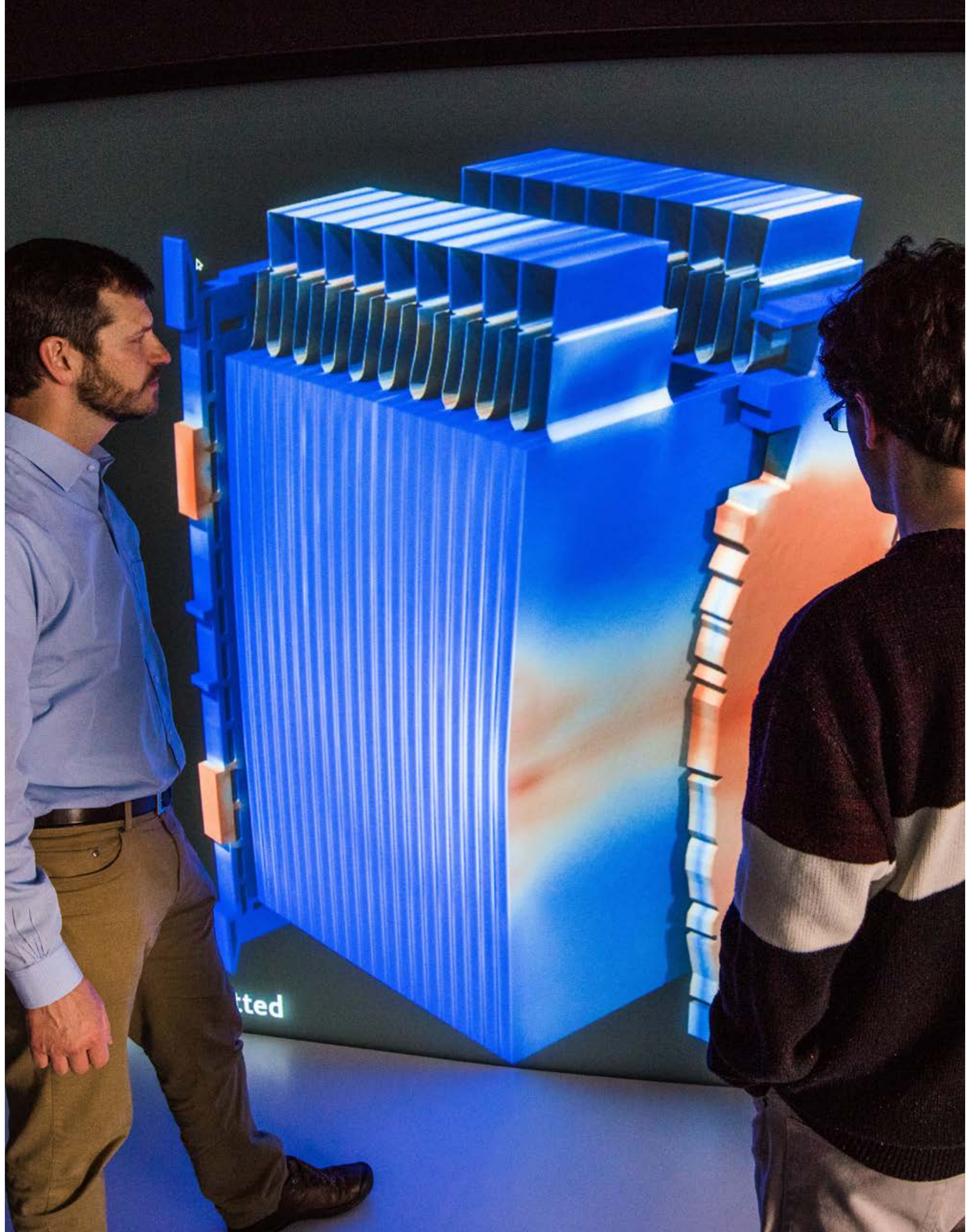
The team found an unusual self-improving behavior that contributes to highly efficient and stable performance when converting light and water into carbon-free hydrogen. By coupling first-principles calculations with spectroscopic and microscopic techniques, the team revealed that the chemical transformation of gallium nitride into gallium oxynitride leads to both sustained operation and enhanced catalytic activity.

The study shows the promise of using oxynitride layers as protective catalytic coatings for hydrogen evolution. It also demonstrates the tight integration of theory and experimentation enabled by the HydroGEN consortium, which is critical for further improving renewable hydrogen production technologies.

Liquid- and Solid-State Hydrogen Transport and Storage

Hydrogen is an excellent energy carrier, but its low ambient temperature density means that advanced methods are required to achieve higher energy density levels for long-term storage. A key focus of the DOE-EERE Hydrogen Storage Materials Advanced Research Consortium (HyMARC) is accelerating the discovery of solid- and liquid-phase materials that meet industry requirements for hydrogen storage onboard vehicles and in stationary grid applications, or that can be used as carriers to transport hydrogen from production to city gate or industrial sites.

HyMARC's computational work, funded by DOE's Hydrogen and Fuel Cell Technologies Office in partnership with Sandia National Laboratories, Pacific Northwest National Laboratory, Lawrence Livermore National Laboratory, and Lawrence Berkeley National Laboratory, provides a foundational understanding of the thermodynamic and kinetic limitations of hydrogen storage and carriers, with a focus on developing solutions for practical applications. Simulations have led researchers to sorbents and metal hydrides for onboard vehicle application, liquid carriers for transport, and intermetallic hydrides for stationary storage. Additional multiscale simulations are assessing the impacts of contaminants, nanoscaling



and confinement, and chemical composition on hydrogen uptake properties. HyMARC researchers are also calculating complex chemical reaction pathways that remove hydrogen from solids and organic compounds. These findings will be useful for engineering the chemistry, composition, and microstructure of catalysts for liquid hydrogen carriers and materials for solid-state hydrogen storage.

Faster-Charging, Longer-Lasting Lithium-Ion Batteries

DOE's eXtreme Fast Charge Cell Evaluation of Lithium-Ion Batteries (XCEL) program seeks to develop 275-Wh/kg lithium-ion batteries that can reach 80% charge in 10 minutes while maintaining battery health (a minimum of 1,000 cycles and a 10-year lifetime) for automotive applications. Challenges include reducing electrolyte transport resistance, suppressing electrode mechanical degradation, reducing heterogeneities that lead to early degradation, reducing detrimental lithium plating effects, and optimizing thermal systems to accomplish rapid (pre-)heating followed by uniform cooling.

To facilitate the rapid development of a fast-charge cell, NREL, in partnership with Argonne National Laboratory, Idaho National Laboratory, University College London, and University of Ulm, leveraged HPC for microstructure modeling, image processing, and multiscale electrochemical-mechanical modeling (originally developed under DOE's Computer-Aided Engineering of Batteries program). One of the models that arose from this effort is NREL's microstructure-scale electrochemistry model, which has enabled full-cell simulations and provided design recommendations that eventually led to prototyping cells tailored for fast charging. In addition, the research team developed a new model to identify cathode-related mechanical failures during fast charging, such as surfaces, cracks, and secondary phases. This grain-scale model explored how cathode particle geometry affects degradation, concluding that small particles with large or single-grain internal structure have better capacity retention.

Computational Fluid Dynamics Simulations Target Efficiency and Costs of Producing Metal Powder for Additive Manufacturing

Additive manufacturing (AM), also known as three-dimensional (3D) metal printing, enables the creation of lighter, stronger parts and systems, and is revolutionizing the metals manufacturing industry. As its name implies, AM incrementally adds melted feedstock material—metal powder—to create an object. Much of this feedstock powder is made by close-coupled, inert gas-metal atomization. This process normally produces a size distribution of spherical powders that approximately satisfies the specific size range needed for each AM method, especially if screen size classification is used. Unfortunately, the current lack of size tuning capability for these atomizers means that low yields are common for specific size ranges, leading to excessive cost and material use, along with inefficient utilization of pressurized gas and melting energy.

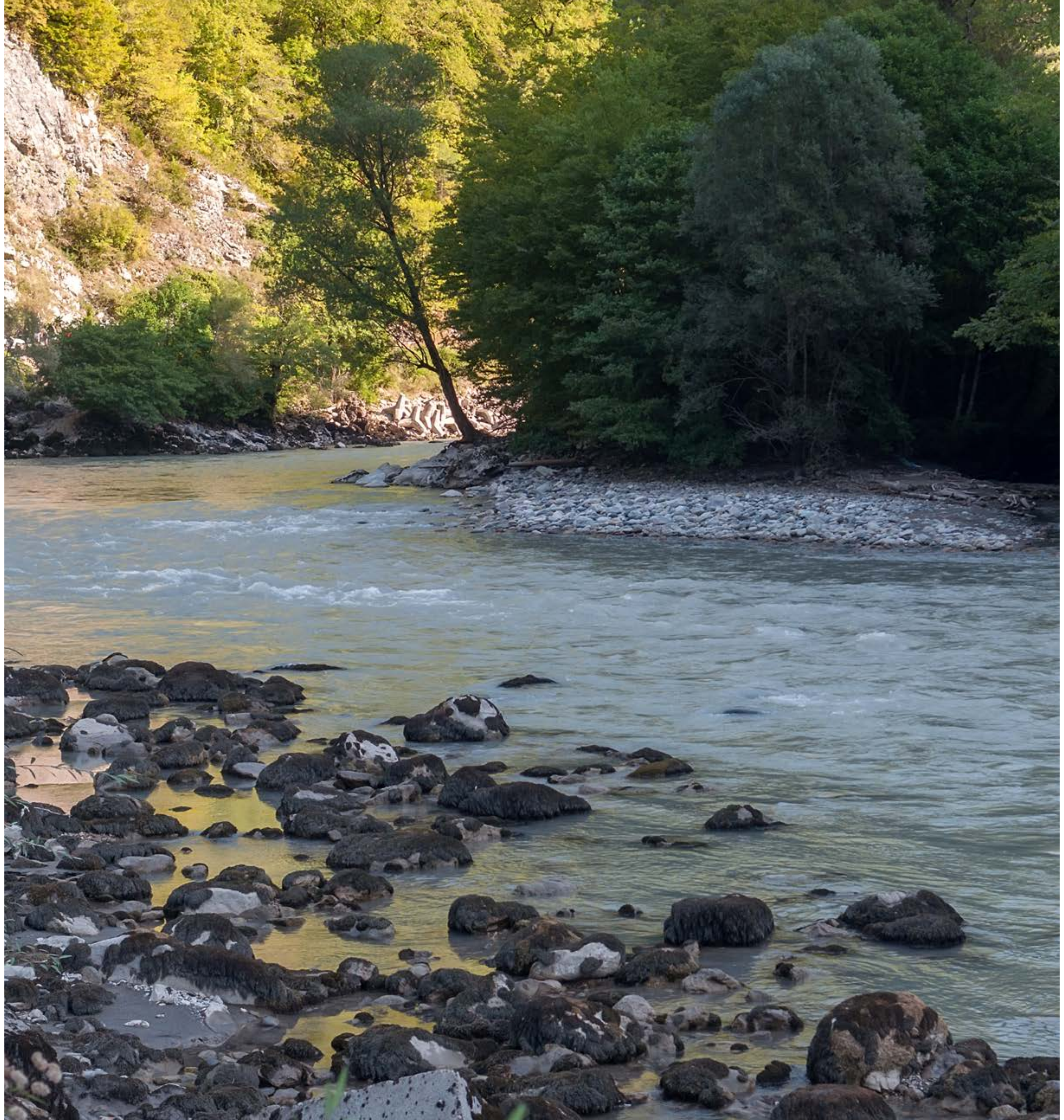
NREL and Ames Laboratory leveraged Eagle to create 3D numerical and computational fluid dynamics simulations of new geometries for atomization trials that would enhance flow efficiency, increase the rate of metal powder production, and improve gas utilization. These simulations facilitate investigation of flow mechanisms for different gas pressures, melt velocities, and atomization gas-die geometries. For the first time, researchers were able to simulate the 3D effects of process physics on the melt spray breakup and atomized particle size distributions. The study found that a smoother atomization gas-flow pathway leads to less energy loss and improved flow efficiency.

The recommended designs are expected to have better performance and better melt spray formation. The designs are being tested to determine the improvements in production rates and yields, which will inform the potential energy savings and cost reductions.

Electrocatalysis for Water Purification

One of the consequences of industrial-scale agriculture is nitrate runoff pollution in local water sources, spurring a need for economical and environmentally friendly water purification techniques. Electrocatalysis provides a renewable and potentially cheaper alternative to current methods used to remove nitrates from wastewater, but this approach requires low-cost, high-activity electrocatalyst materials. Density functional theory (DFT) calculations have successfully aided in the exploration of viable electrocatalysts in the past; however, the high computational cost of such calculations makes the systematic screening of thousands of materials impractical.

In partnership with Lawrence Berkeley National Laboratory and funded by DOE's Advanced Manufacturing Office and the National Alliance for Water Innovation, NREL researchers used crystal graph convolutional neural networks to develop an efficient technique for screening large materials databases for potential electrocatalysts—reducing the number of DFT calculations required from tens of thousands to hundreds. The research team applied state-of-the-art ML to conduct high-throughput screening of over 77,000 bimetallic alloys. This screening process identified more than 100 promising electrocatalyst candidates for nitrate reduction reactions, including low-cost alloys such as iron-nickel compounds. The ML-predicted adsorption energies from over 1,000 surface morphologies of these candidate materials were validated using DFT, with computational resources provided by NREL's Eagle HPC system. Computationally validated electrocatalytic candidates are being synthesized by the experimental team to further assess their catalytic activity.



Simulations Improve Materials for Extreme Operating Environments

DOE's Advanced Manufacturing Office is seeking to increase the efficiency of energy conversion technologies and improve the performance of industrial manufacturing processes with electronics that can operate in extreme operating environments (i.e., among coupled thermal, chemical, and mechanical stresses).

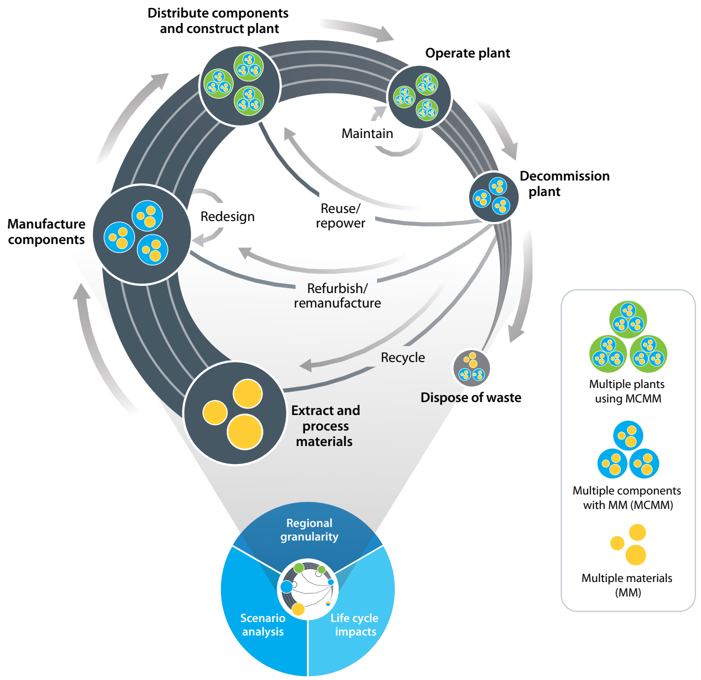
Current semiconductor technologies are either unsuitable for high-temperature operation or have not been fully validated for extreme environments. Oxides are known to operate well under ambient conditions in electronic devices and at high temperatures in ionic fuel cells. Wide-bandgap semiconductors permit devices to operate at much higher temperatures, voltages, and frequencies. Gallium oxide is desirable for use in electronic devices due to its ultrawide bandgap and the low projected cost of fabrication of large, high-quality crystals.

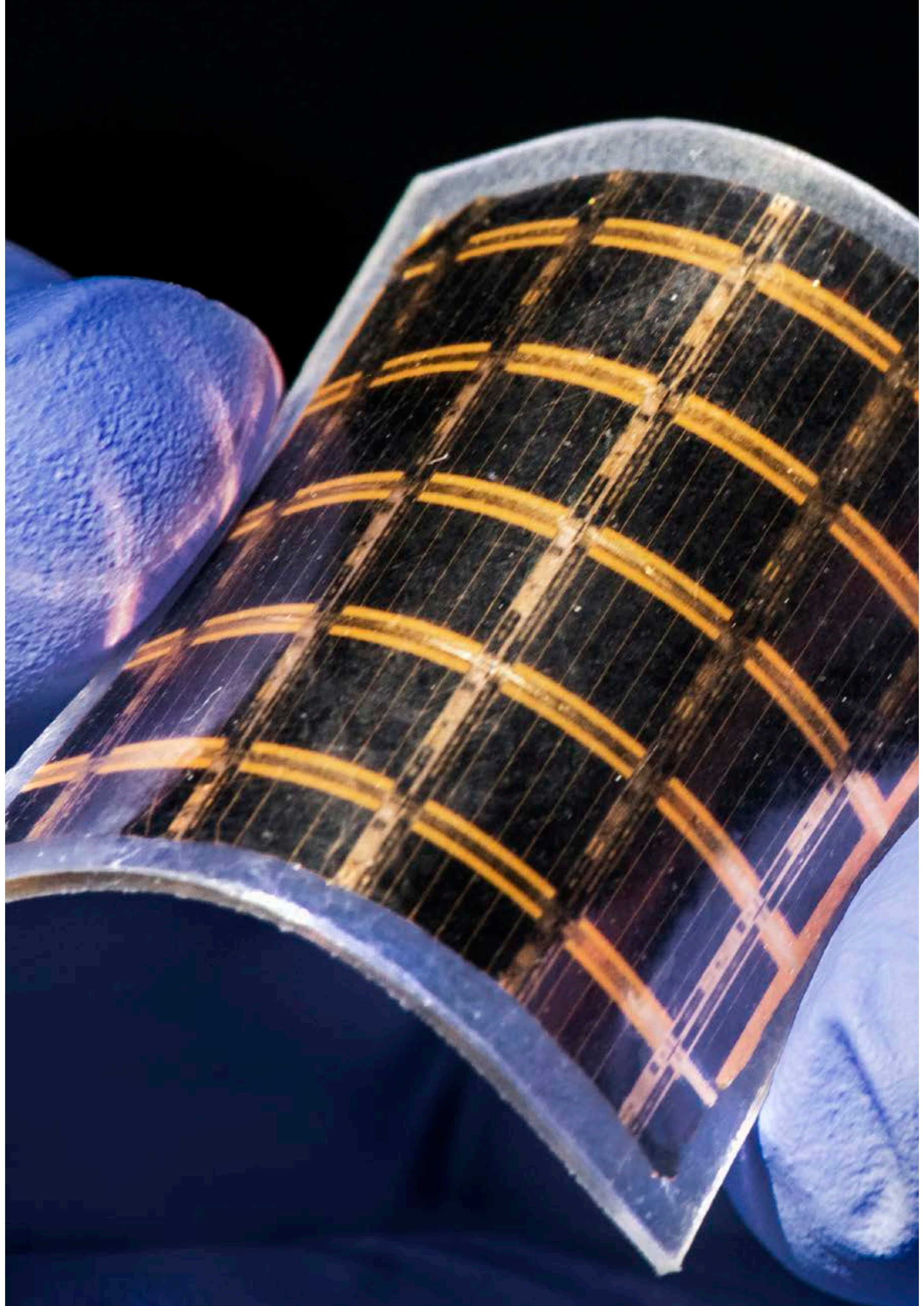
Through first-principles defect theory and defect equilibrium calculations, Colorado School of Mines researchers simulated a three-step synthesis protocol for hydrogen-assisted gallium oxide doping (i.e., introducing impurities into the semiconductor crystal) to achieve the desired conductivity. Using atomistic computational methods, the team also investigated the potential energy barrier formed by the metal–semiconductor junction of platinum and gallium oxide (i.e., its Schottky barrier), with results providing insight into improving the performance of future gallium oxide devices.

This project made extensive use of the NREL Materials Database for phase stability analysis.

Circular Economy Lifecycle Assessment and Visualization (CELAVI)

Modeling circular systems in a clean energy economy requires capabilities beyond what any single previously developed method offers. The Circular Economy Lifecycle Assessment and Visualization (CELAVI) tool, funded by NREL's Laboratory Directed Research and Development Program, models the impacts of clean energy supply chains during the transition from a linear economy to a circular one, capturing impacts at the county, state, and national levels. It is intended to support decision-making by governing bodies, corporations, and nongovernmental organizations who are working toward a circular economy at the local, regional, and national levels. CELAVI can provide insight into the circularity potential of new technologies, the level of technological learning needed for circular technologies to reach cost parity with linear technologies, and the environmental impacts of renewable energy technologies in an increasingly circular economy.





CELAVI uses a combination of material flow methods, life cycle assessment, and discrete event simulation to create a novel circular economy analysis framework for energy systems. The framework is under active development and can provide insight into the technological changes involved in a linear-to-circular transition as well as the associated environmental externalities. It captures selected energy technology supply chains using detailed, dynamic models of production, use, and circular pathways. These supply chain models are linked to background life cycle processes that may be dynamic or static, and which can be represented at several levels of aggregation, depending on how impactful each background process is relative to the overall system. CELAVI was applied to an energy system use case—wind blade circularity in Texas—and the outcomes have helped NREL frame strategic discussions about circular economy analysis work (both internally and externally).

Manufacturing Cost Reductions for High-Efficiency Solar Cells

Hydride vapor phase epitaxy (HVPE) is a growth technique often employed to produce semiconductors; it is a promising technology for reducing material costs of high-efficiency solar cells for space and terrestrial applications. However, recent demonstrations of ultrafast growth rates via uncracked hydrides are not well described by present growth models.

To enable fast and uniform growth, NREL, in partnership with Kyma Technologies, set out to understand the kinetics of the growth process and its coupling with transport phenomena. The team integrated a kinetic model into a computational fluid dynamics simulation of an HVPE reactor and improved an existing hydride cracking model. Numerical simulations conducted with the developed models were shown to accurately predict experimental data, showing that the developed growth model and the improved cracking model can predict experimental growth measurements. The model calibration procedure adopted was unique to this project. Typical model calibration is done with experimental measurements collected in simple systems so that performing multiple simulations of the experiments is as cheap as possible. For this project, however, simulating the experiments required 3D computational fluid dynamics runs, demonstrating NREL's ability to reliably simulate complex fluid flows under a variety of conditions.

FORECASTING

Radiation Database Estimates Solar Resources To Reduce Deployment Barriers

The National Solar Radiation Database (NSRDB) is the leading public source of high-resolution solar resource data in the United States, with over 150,000 unique users annually. This database provides satellite-based estimations of solar resources using a unique physics-based modeling approach. These high-quality, long-term solar resource data sets reduce barriers to solar deployment on the grid by allowing private companies, utilities, public entities, academic institutions, and research laboratories to accurately predict solar installation output and verify performance.

NREL's HPC capabilities provide the necessary computing and storage resources to generate solar radiation data sets for use in downstream applications, such as PVWatts® and the System Advisor Model. Recent improvements in satellite technology—which have resulted in data sets with improved spatiotemporal resolution—and the use of ML have had a demonstrable impact on NSRDB's data quality. Atmospheric data for 2020, including aerosols, water vapor, temperature, humidity, wind speed, and wind direction, were produced from lower-resolution data sets. These data, along with satellite-based cloud properties, were used to generate 2x2-km global horizontal irradiance, direct normal irradiance, and diffuse horizontal irradiance every 5–10 minutes, covering North, Central, and South America for 2020.

With 23 years of data, NSRDB enables improvement in plant output predictions, reduces the cost of solar development, enhances awareness of the grid, and enables achievement of 2030 cost goals for PV and concentrating solar power.

Geothermal Energy Generation Improved by Machine Learning

ML algorithms that are run using the Eagle supercomputer have enabled improved predictions for geothermal reservoir performance. NREL researchers—funded by DOE's Geothermal Technologies Office and working with Heateon, Ormat Technologies, and the United States Geological Survey—used reservoir simulations to train an ML model to predict reservoir performance. The model provides accurate predictions of reservoir performance in seconds for a range of scenarios, allowing optimization of the system. Integration of high-fidelity, physics-based reservoir modeling with state-of-the-art ML methods shows promise for increasing energy generation with less field testing and engineering effort.

NREL's novel approach to processing and modeling reservoir simulation data shows excellent results in terms of model accuracy and is likely to be generalizable beyond the data set studied initially. A set of ML experiments was completed for Brady Hot Springs, a geothermal production field in Nevada that has been the target of geothermal development for decades. The developed code artifacts have been shared with the company that operates the power plants at Brady.

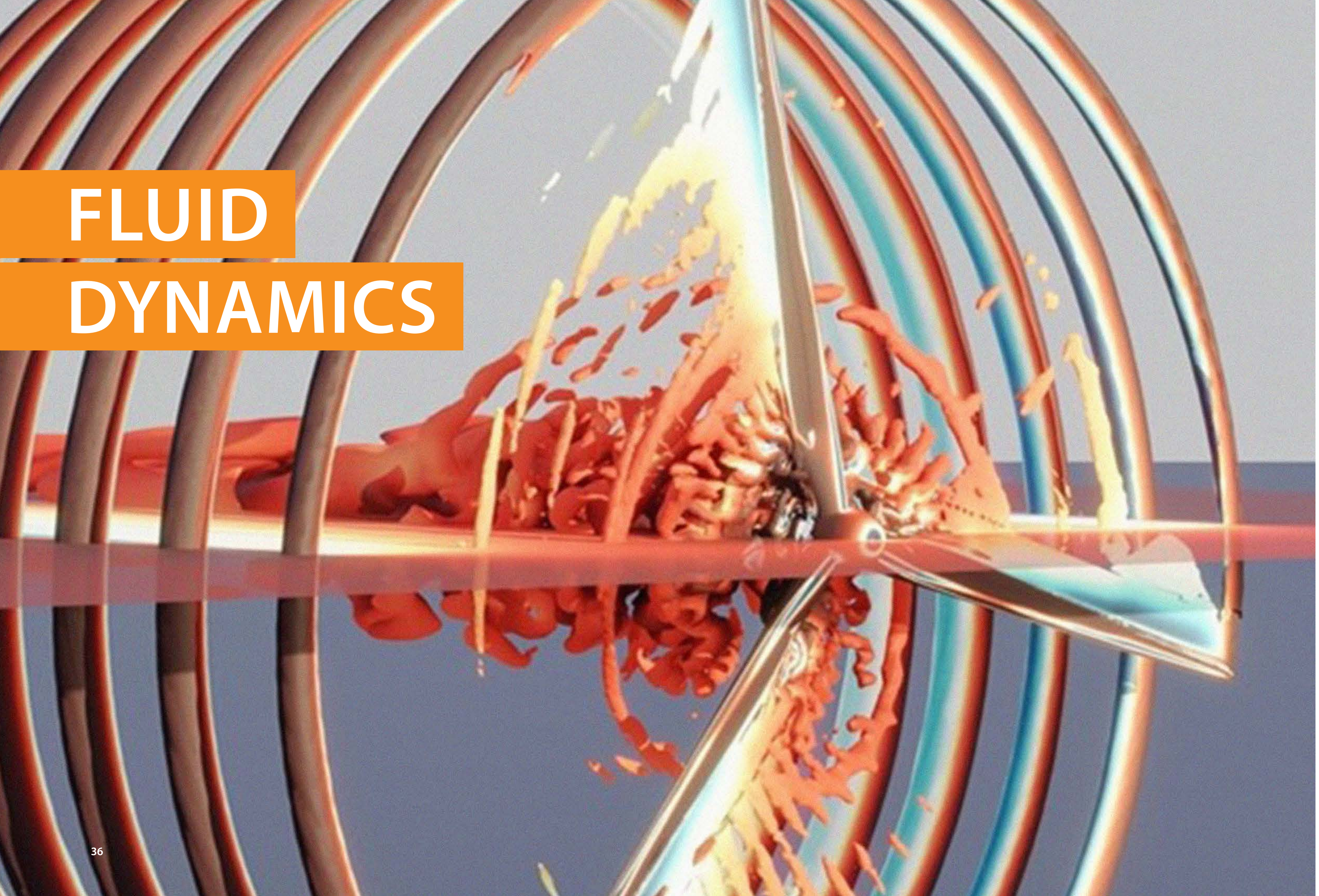
Tools for Assessing Wind Project Performance From Distributed to Airborne

NREL researchers have developed a distributed wind-specific resource data set, along with a computational framework, called Tools Assessing Performance (TAP), funded by DOE's Wind Energy Technologies Office (WETO). This new data set aims to improve wind resource assessment so that distributed wind system developers can better predict turbine performance and enable

distributed wind turbines to become a more economically viable and reliable distributed energy resource. TAP features functionality that enables project developers to quickly and cost-effectively understand the potential for, and uncertainty around, energy generation. TAP does this by providing access to high-fidelity wind resource data, enabling modeling of obstructions like buildings and trees, implementing downscaling of wind data to specific heights and locations, and allowing users to perform timely and accurate resource assessments. Brought together within a single software package that is accessible through both a web interface and an application programming interface, these core innovations will improve distributed wind resource assessment and ultimately enable better performance predictions. This new data set can also help make siting decisions for large-scale wind energy generation plants, including characterization of wind resources from the surface to 1,000 m above ground, supporting utility-scale wind turbines and the airborne wind energy community as well.

To create TAP, researchers leveraged ensemble modeling and an ML technique to combine several model simulations into one optimal predictive model. This enabled the team to map the uncertainty from multiple one-year simulations onto a single 20-year data set. NREL has completed yearlong simulations for the years 2016 to 2019, which stakeholders have immediately used. TU Delft has used the simulations to analyze wind potentials for airborne wind energy, and UC Merced has used them to support research for a zero-carbon grid in California. Mesoscale model wind resource data sets such as this are used extensively in the wind industry by a broad range of stakeholders (e.g., developers, consultants, utilities, financers, policymakers, planners, and researchers) to complete several types of analyses (e.g., energy estimates, extreme event analyses, grid integration, life-cycle cost of energy, and capacity expansion). Follow-on work will include modeling the remaining 20 years over the continental United States and Alaska.

FLUID DYNAMICS



NREL Modeling Reduces Wind Plant Energy Losses and Costs

Through its High-Fidelity Modeling (HFM) project—part of the Atmosphere to Electrons Initiative—NREL creates, verifies, and validates predictive, high-performance simulation tools for wind plants at the highest possible fidelity. The goal of this work is to better understand wake formation and propagation and help reduce wind plant energy losses and costs. HFM complements DOE's ExaWind project and predominantly uses the ExaWind simulation environment.

ExaWind includes a predictive simulation capability for turbines, which combines high-fidelity, blade-resolved simulations; a large eddy simulation of the atmospheric boundary layer (ABL); and simulations generated using NREL's aero-servo-elastic wind turbine tool, OpenFAST. NREL is adapting the computational fluid dynamics solver AMR-Wind, which is capable of running on next-generation exascale computing platforms, to model ocean waves, bodies immersed in water, and the ABL for wind energy applications.

The ExaWind environment can simulate wind energy flows across a range of length scales and was recently used to perform a validation-quality simulation of a 2-MW turbine as well as high-fidelity ABL and offshore marine ABL simulations over waves.

Future work will refine this capability to simulate, verify, and validate floating offshore turbines. HFM is funded by WETO, and work is performed in partnership with the DOE's Office of Science and National Nuclear Security Administration Exascale Computing Project.

Hindcasting: Modeling the Past Informs the Future of Wave and Tidal Energy

NREL's HPC-generated, high-resolution wave and tidal model hindcasts support in-depth wave and tidal energy resource assessment within U.S. coastal waters. These hindcasts—statistical calculations that model probable past conditions—offer insights into the highly complex marine environment that significantly lower the uncertainty and risk associated with advancing nascent wave and tidal technologies and accelerate the pace of marine energy technology development.

These new high-resolution models, which run on the HPC hardware as a collaboration between NREL, Pacific Northwest National Laboratory, and Sandia National Laboratories, and are funded by DOE's Water Power Technologies Office, are made available to the public through the Marine Energy Atlas. These data sets have proven useful to commercial developers, who have a growing need for resource data to help with project planning and device engineering. The data sets also support the International Electrotechnical Commission Technical Committee's international standards and the Marine Energy Operational Management Committee's certification development. The resource data is also critical for informing future research on project viability, technology survivability in extreme conditions, fatigue load reduction, and reduction of peak-to-average power ratios.

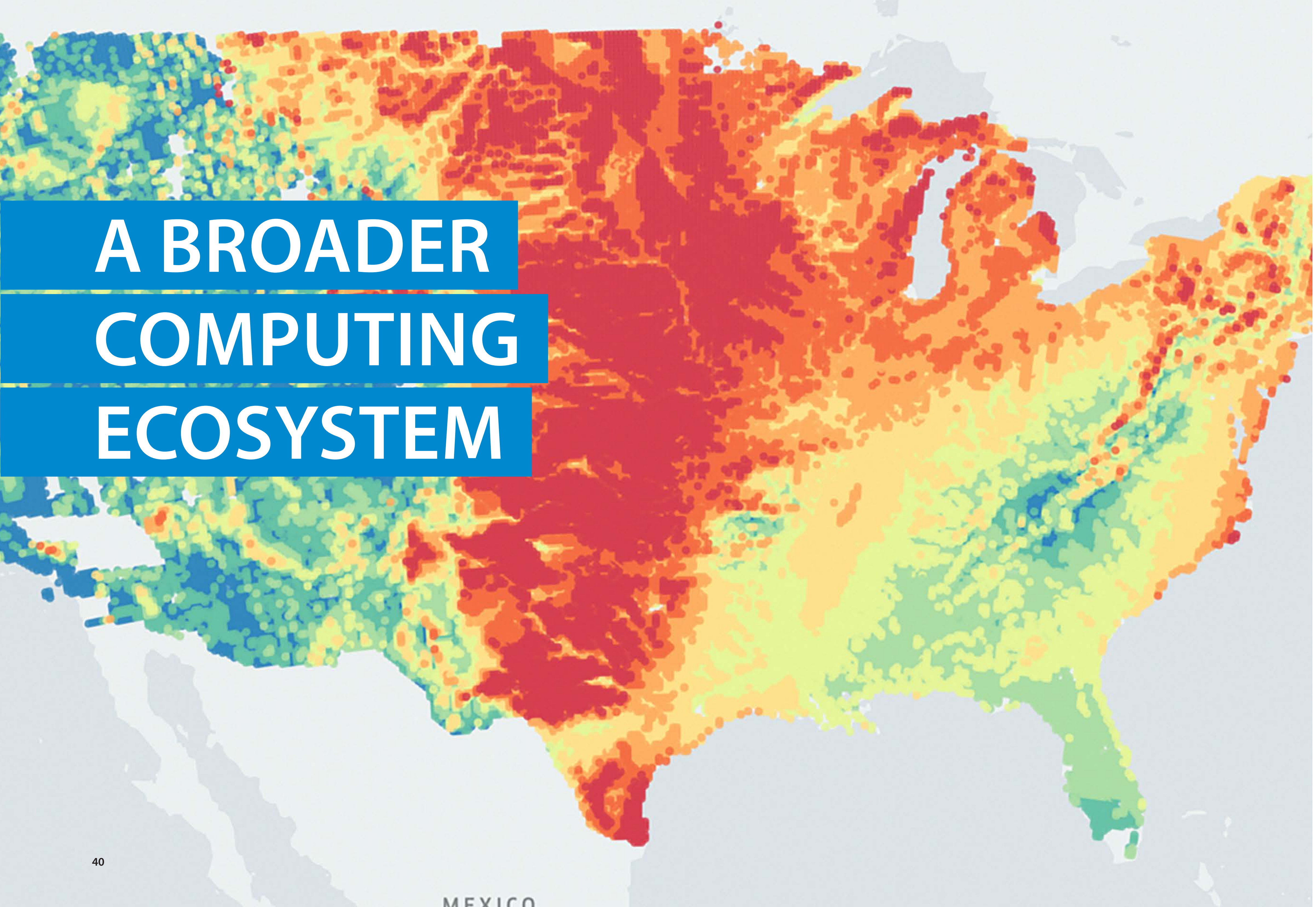
Risk Modeling Could Lead to Eagle-Smart Wind Plants

To help mitigate risks to golden eagles posed by wind turbines, NREL and industry partners are developing a golden eagle behavioral model that captures conflicts between eagles and wind turbines. The model combines atmospheric and wind farm simulations, ML, and knowledge of eagle biology and ecology to predict the likelihood of eagle interactions with wind turbines. This behavioral model forms the foundation for tools that can be used to design and operate "eagle-smart" wind plants, which protect eagles and reduce economic risks for utility companies (who could otherwise face penalties under the Migratory Bird Treaty Act).

The model, which is being developed by NREL computational and wind energy scientists, includes multiple risk assessment tools that will predict wind power plant locations and atmospheric conditions that have a high potential for eagle collision risk. The behavior modeling framework uses weather model data from the Wind Integration National Dataset Toolkit's Long-Term Ensemble Dataset, a new data product developed under DOE's WETO TAP project. In addition, high-fidelity models and techniques developed within WETO's Mesoscale-to-Microscale Coupling (MMC) project were applied to simulate turbulent updraft fields over complex terrain that are likely to be used by eagles to sustain soaring flight.

This modeling framework lays the foundation for more general avian behavior models and paves the way for future study of wind–wildlife interactions. These tools will inform future wind plant siting and operations decisions, enabling tradeoffs between energy production, cost of energy, and wildlife risk. Modeling insights from this project continue to inform WETO's MMC and other ongoing DOE projects, including the WETO HFM project.

A BROADER COMPUTING ECOSYSTEM



Visualizing Uncertainty in Energy Deployment Scenarios

NREL visualization scientists are building new ways to explore energy deployment scenarios by creating visualizations that help users make decisions on data with uncertainty. Through NREL's LDRD program, this project is addressing these challenges by developing new interactive dashboards to explore the outputs of the Renewable Energy Potential (reV) model, specifically designed for understanding how different land use policies and characteristics, as well as uncertainty in development costs, could affect future wind farm deployment. The reV model assesses renewable energy generation based on the geospatial intersection with grid infrastructure and land-use characteristics. The model can predict energy deployment scenarios that explore factors such as the effect of varying technology types and using land previously unavailable for energy usage. However, with the power of the reV model comes challenges in visualization, particularly around the uncertainty that arises when trying to understand how different factors can influence energy generation possibilities. The new visualization capabilities are enabling energy systems analysts to interactively explore and compare the output scenarios from the reV model by integrating geographic information with land characteristics and ownership, as well as supply curve levels. Users can filter the data by land type and target supply levels, which then updates the data displayed on the map. They can then toggle through different scenarios, such as high transportation costs or policy changes, for comparison. By enabling comparative exploration of the uncertainty arising from the variability across scenarios, we can see how things like policy decisions or increases in materials transportation costs can impact the feasibility of the placement of wind farms.

PV Durability and Reliability Database

Understanding field-based PV performance can offer insights into installation and improvements for PV modules. NREL's PV Durability and Reliability Database (PVDRDB) is a large-scale, cloud-based, time-series database of performance and monitoring data that is streamed and processed from many PV array sites, including NREL experimental platforms and data partners' solar installations. This database provides a means of directly monitoring the field performance of local PV systems in near real-time. Analysis of the consolidated data allows NREL to identify changes in system performance and look at long-term degradation rates. The database currently stores data from over 7.2 GW of PV installations, contained in over 27 billion measurement records.

The PVDRDB impacts three core areas of work. The first is supplying a monitoring feed for NREL's experimental PV module installations to help identify problems early on and inform changes. This data provides detailed information about new PV module and cell designs, as well as other system equipment, such as inverters, trackers, and battery storage.

Second, the database serves as an archive for data from Regional Test Center sites, allowing researchers to study outdoor PV installations in different climate areas and with different PV technology types.

The third and highest impact area is to support the PV Fleets project—a core program, supported by SETO, that gathers data from a variety of fleet owners and monitoring systems across the United States to create a benchmark of cumulative performance and degradation rates for the U.S. fleet. This large study shows that, in general, a PV site's degradation rate is different than that of the individual modules within a site. Data partners and fleet owners receive reports that include detailed information about changes in their fleets over time, information on possible causes, and a comparison to the overall U.S. PV fleet performance. Additional data, such as soiling data, operations and maintenance data, and bills of materials, are being gathered to understand the mechanisms behind degradation. Analysis of this large data set will lead to a deeper understanding of how large-scale PV systems perform over time and under a variety of conditions.

Data Set Quantifies How and When Energy Is Used Across All Major U.S. Building Types and Climate Regions

In partnership with Lawrence Berkeley National Laboratory and Argonne National Laboratory and funded by the Buildings Technology Office, researchers at NREL used a combination of cloud computing and NREL HPC resources to develop a new data set of end-use load profiles for the U.S. building stock, representing all major building types and climate regions. The data set is critical for helping utility planners, regulators, state energy offices, researchers, and building owners to understand ways to best manage energy use. End-use load profiles can identify which efficiency measures are most valuable to the grid or which energy-consuming activities can be shifted to different times of the day to reduce peak loads that drive utility costs, reduce customer bills, and use clean, renewable energy sources when available.

Researchers worked with partners such as utilities, regional energy efficiency organizations, program administrators, and a large technical advisory group to gather anonymized hourly load data from 11 utilities and more than 2.3 million electric meters. The data informed updates to hundreds of model inputs, significantly improving the models' accuracy and usefulness.

The computationally intensive workflow required for this project was enabled by cloud computing and NREL's HPC resources. Cloud computing was critical for securely collecting and aggregating the anonymous data that was then used to inform calibration of the ResStock™ and ComStock™ models, which in turn are simulated using the Eagle supercomputer. The scalable, on-demand nature of cloud computing also made it ideal for fast, parallel data aggregation to analyze the model outputs. It also allowed researchers to publish the results in an open data registry.

For utility providers, this resource can be used to estimate the value of energy efficiency, demand response, and other distributed energy resources for a wide range of timescales. Such analysis will guide utility resource and distribution system planning, research and development prioritization, and state and local energy planning and regulation. Additionally, the calibrated models can help quantify the difference in energy consumption between a baseline building and a building with an energy efficiency, electrification, or demand flexibility measure applied.

Human Metrics for Energy-Efficient Mobility Systems

There are a variety of metrics available to quantify mobility, such as Walk Score and All Transit, but there is a pressing need for an open metric that can quantify the quality of mobility options available as a result of new technologies in vehicle automation, connectivity, electrification, and a shared transportation economy. To address this need, NREL researchers developed the Mobility Energy Productivity (MEP) metric as a part of DOE's Systems and Modeling for Accelerated Research in Transportation (SMART) Mobility Consortium. MEP assesses the proximity to and energy impact of access to a variety of goods, services, employment opportunities, and other activities. The MEP metric measures existing levels of mobility and assesses how technologies, services (e.g., scooters, ride hailing, electric and automated vehicles), and infrastructure investments (e.g., bike lanes, mixed-use development) may impact mobility over time.

MEP metric capability enhancements allow researchers to answer an even wider range of questions associated with emerging transportation alternatives. In particular, MEP has been rewritten as a cloud-native application in the Amazon Web Services ecosystem, meaning that complex MEP computations can be requested as part of an automated pipeline with collaborators in the SMART Mobility Consortium. In preliminary experiments, this refactoring has led to upward of a 77% improvement in runtimes over the original implementation.

These enhancements add robustness to MEP's quantification of the impacts of evolving transportation system scenarios, and connect the impact of broader VTO vehicle technology investments to holistic mobility and energy outcomes under these scenarios. Metrics and tools will be released as open source in the future and can easily be integrated into transportation planning and evaluation processes in public and private sectors. In addition, the methodological contributions of the metric will be extended so that a wider group of stakeholders can benefit from adopting the metric. Transportation researchers and city planners have utilized the MEP metric to assess mobility, energy, and equity outcomes of new technology on existing road systems, airport infrastructure, curb fronts, parking capacities, and overall urban architecture.

Next-Generation Data Ecosystem for AI-Enabled Materials Science

Scientists at NREL are helping pave the way for the next generation of data-driven, AI-enabled materials science. Funded by NREL's Laboratory Directed Research and Development Program, the Research Data Infrastructure project is enabling materials discovery by building a modern data ecosystem to support close interaction between the computational sciences and materials sciences. Databases are the cornerstone of modern data-driven material science; they summarize crystal structures and predicted properties for tens of thousands of calculated materials. To provide access to large amounts of experimental data, NREL has opened to the public the High-Throughput Experimental Materials Database (HTEM DB), which allows researchers to discover experimental materials with useful properties. This experimental data set includes material synthesis conditions, chemical composition, crystal structure, and physical properties. The data set initially contained 140,000 samples, with more than half available to the public, and now holds more than 320,000 samples. The data infrastructure built through this project is integrated into the laboratory workflow; data collected from experiments conducted at NREL is cataloged, and processed materials data is then uploaded to a collaborative cloud-based system, providing data for scientists conducting both experiment-driven and data-driven materials research. This project showcases the immense value in building a common framework for carefully curated experimental data and metadata for materials discovery.

Bridging to DOE Leadership Computing

Developing Improved Submodels for Low-Carbon Engines

Internal combustion engines (ICEs) power more than 90% of the transportation fleet and will remain the primary source of power for the foreseeable future, as they combine unmatched power density with high versatility and low cost of operation. Emission requirements and environmental pressures have driven the need for highly efficient, low-emission ICEs that can operate on low-carbon and zero-carbon fuels.

To develop accurate submodels that industry can use in their engine design workflows, direct numerical simulations and wall-resolved large eddy simulations of ICE flows and processes were performed using the Nek5000 code on both Argonne National Laboratory's and NREL's computing facilities. Access to HPC resources across the DOE national laboratories was critical in performing these one-of-a-kind simulations. Device-level calculations requiring large numbers of computing nodes were performed on Argonne's Theta supercomputer, whereas simulations on simplified domains requiring fewer nodes were performed on NREL's Eagle system, where the shorter queue times helped with a quicker turnaround.

Led by researchers at Argonne, this project is funded by DOE's VTO Partnership for Advanced Combustion Engines (PACE) program, the recently formed DOE light-duty combustion consortium that combines unique experiments with world-class DOE computing and machine learning expertise to accelerate discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with the potential for best-in-class life cycle emissions.

Interface Atomic Structure Prediction for CdTe PV

"The interface is the device," as the saying goes. The atomic structure at the PV device interface determines the properties of the device and, accordingly, the device performance. However, it is usually known only for relatively simple atomic structures at epitaxial interfaces and is notoriously difficult to access at nonepitaxial and incoherent interfaces. NREL researchers, funded by SETO, extended first-principles methods for bulk crystal structure prediction to interface systems and predicted the atomic structures at the SnO_2/CdTe junction, which is of current interest for the American PV manufacturer First Solar. The team utilized computing on both NREL's Eagle and National Energy Research Scientific Computing Center Cori supercomputers to perform simulations with and without $CdCl_2$ treatment, and predicted the formation of an atomically thin $CdCl_2$ interlayer, showing that the interface without $CdCl_2$ has severely limited device performance, whereas the junction with the $CdCl_2$ interlayer exhibits a defect-free electronic structure and a near-ideal band offset. This study provides the first explicit atomic structure model for $CdCl_2$-treated interfaces in CdTe PV and demonstrates the potential of interface design based on first-principles computations. The ability to make use of multiple computing systems across the DOE complex accelerated the research progress by improving computer accessibility and simulation turnaround times.

Asynchronous Single-Stage Stochastic Direct Model Programming

Funded by NREL's LDRD program, this project aims to produce guidelines and automated tools for enabling more efficient and scalable machine learning (ML) approaches. Deep learning is a powerful ML technique that has been successfully applied across many energy domains; however, the total human and computer time spent applying these techniques is dominated by the optimization of the learning algorithm's hyper parameters. NREL researchers are using a Direct Model Programming approach to study the effect of neural network topology on training performance and efficiency, paving the way for new tools enabling researchers to easily, and without specialized knowledge, find and train an effective deep neural net topology at any scale or level of fidelity. Using the team's new implementation of a highly scalable work queue capable of executing many experiments in parallel across multiple computing systems, large numbers of coordinated jobs were executed across NERSC's Perlmutter and Cori, and NREL's Eagle and Vermillion. Access to NREL's Eagle supercomputer, enabling testing and development of GPU codes, coordinated with leadership-class supercomputing facilities, is critical to enabling rigorous large-scale study and refinement of emerging AI methods. GPU-accelerated systems such as Perlmutter enable the project to multiply impact by extending the experiments and findings to study complex convolutional, graph, and recurrent networks at a broader scale.

Computational Science Software Records and Records of Invention

Title	NREL Number
Athena - Shuttle Bus Optimization and Event Driven Simulator	SWR-20-105
Athena - Digital Twin for Airport Terminal Traffic	SWR-20-106
DER Communication Library for Control of Distributed Energy Resources (DERComm)	SWR-20-110
Real-Time Feedback-Based Optimization of Distributed Energy Resources for Virtual Power Plant Control Providing Grid Ancillary Services (RTOPF-VPP)	SWR-20-111
IEC61850 to DNP3 converter (IEC61850-DNP3)	SWR-21-03
Sparse Invertible Networks (SpIN)	SWR-21-28
Sparse Invertible Neural Networks for Airfoil Design	ROI-21-29
Toolset for Easily Configuring and Dispatching Experimental Runs on HPC Systems	SWR-21-29
3D Campus Power Flow Visualization Intelligent Campus (STM)	SWR-21-51
The Renewable Energy Potential Model Dashboard (reV)	SWR-21-59
Diverse Super-Resolution (diverse_SR)	SWR-21-60
ReV Supply Curve Viewer	SWR-21-66
Multi-Fidelity Economic Dispatch Dashboard (EconDispDash)	SWR-21-70
A Reinforcement Learning-Ready Mobility On Demand Simulator (RLMoD)	SWR-21-77
Stochastic Soaring Raptor Simulator (SSRS)	SWR-21-78

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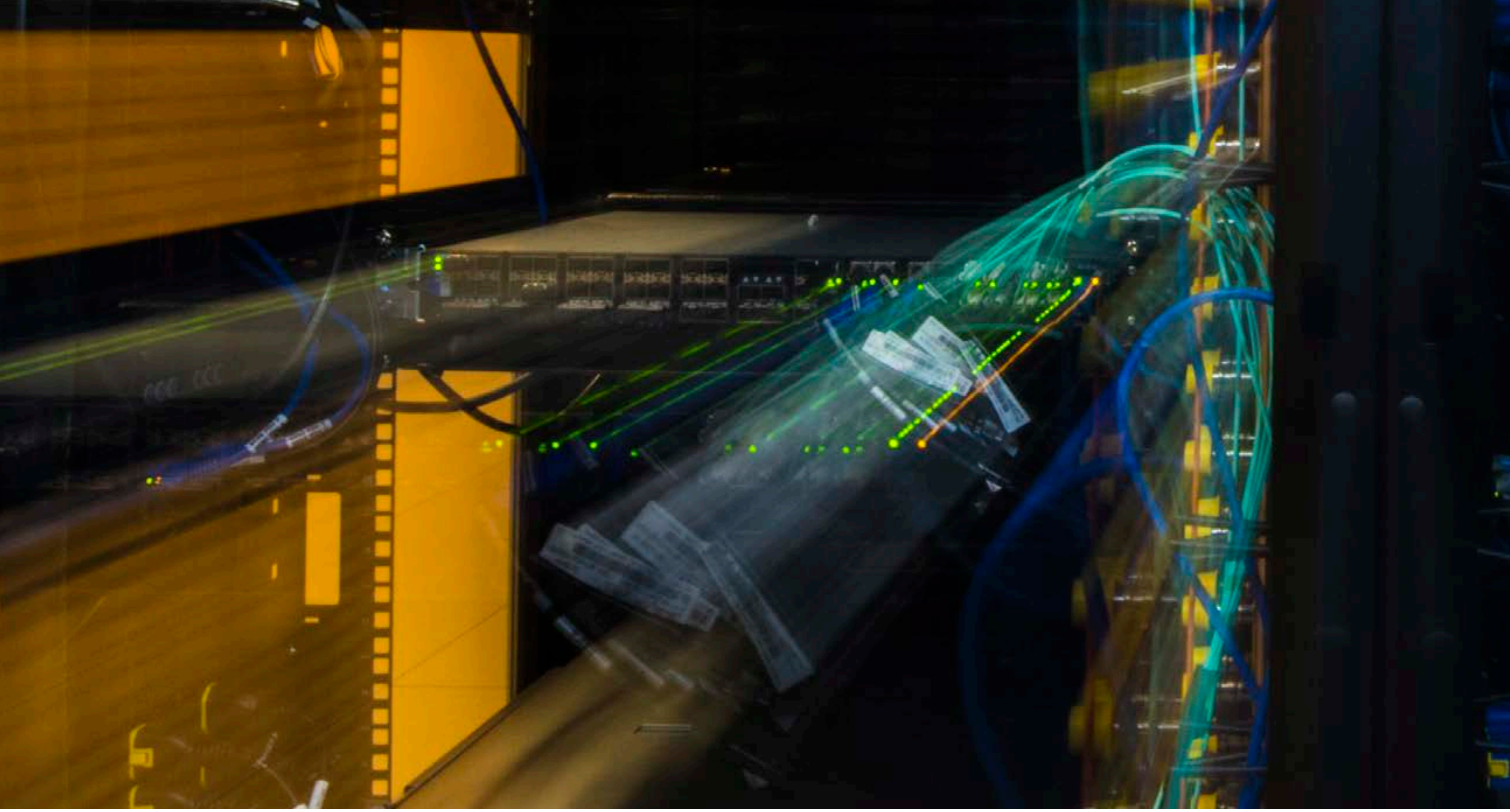

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