NREL
Transforming ENERGY

ADVANCED COMPUTING
ANNUAL REPORT 2023

Director's Letter

In 2023, advanced computing saw the arrival of Kestrel, the National Renewable Energy Laboratory's (NREL's) newest high-performance computing (HPC) system. Kestrel will accelerate clean energy research at a pace and scale more than five times greater than Eagle, with approximately 44 petaflops of computing power. Kestrel's heterogeneous architecture—which includes both CPU-only and GPU-accelerated nodes—is designed to bring a much greater GPU capacity to EERE workloads compared to Eagle, enabling rapidly advancing applications in artificial intelligence and expanding research in new directions for computing.

In Fiscal Year (FY) 2023, 333 projects utilized NREL's HPC system, advancing the U.S. Department of Energy's (DOE's) Office of Energy Efficiency and Renewable Energy (EERE) mission across 13 funding areas.

Cross-disciplinary collaboration among researchers yielded more than 800 technical outputs, including 177 peer-reviewed journal articles in FY 2023. All this great work continues to advance the science of energy efficiency and renewable energy.

A major upgrade in FY 2023 was the completion of the 3D visualization capability in the Energy Systems Integration Facility (ESIF) Insight Center—with a fourfold increase in resolution, researchers now have the ability to process and display data with exceptional clarity. The 2D upgrades completed in FY 2022 are now becoming a critical and highly sought-after capability across many research projects, enabling new methods of analyzing huge and complex data sets to arrive at results and insights not previously possible.

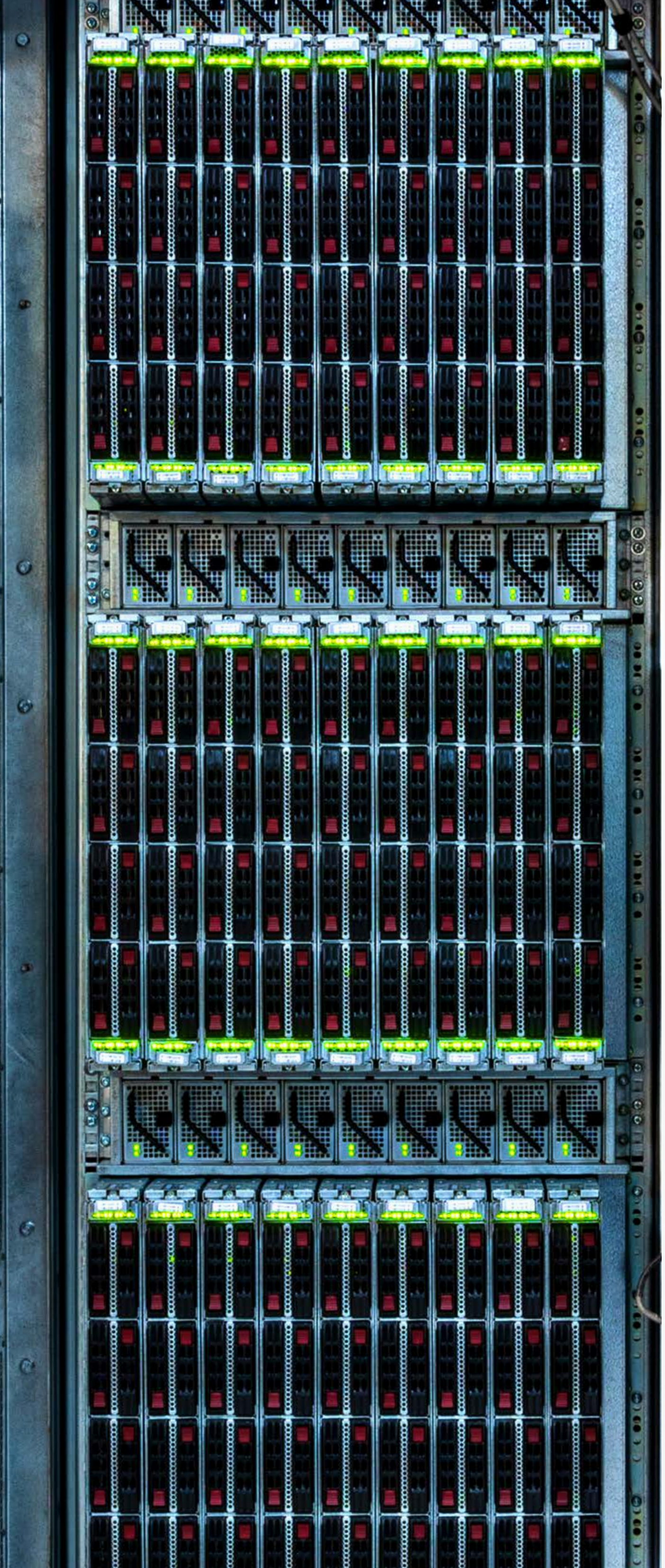
NREL continues to push the boundaries of efficient data center operation, with warm water cooling, optimization, and waste heat recovery enabling the facility to end the year with an average power usage effectiveness rating of 1.031. The ESIF HPC Data Center is nearing completion of a 2.5-megawatt power and corresponding cooling upgrade to support Kestrel, bringing the data center to a new capacity of 7 megawatts. 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.

Looking to the future, NREL—with Sandia National Laboratories and Georgia Tech—is leading the testing protocols and testing capability for Cooling Operations Optimized for Leaps in Energy, Reliability, and Carbon Hyperefficiency for Information Processing Systems, an Advanced Research Projects Agency-Energy program focused on driving supply temperatures much higher, enabling transformational, highly efficient, and reliable cooling technologies for data centers. Participants will use a new testing facility within the ESIF to test and validate new cooling approaches at the rack and modular data center level.

We will highlight many exciting developments in the following pages, and we expect many more to come.

Ray Grout,
Director, Computational Science Center

Kris Munch,
Laboratory Program Manager, Advanced Computing



CONTENTS

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 crosscutting capabilities that provide the critical foundation upon which rapid-breakthrough science is built. Advanced visualization technology helps researchers explore and interact with data in new ways that accelerate understanding and innovation. With the arrival of Kestrel this year, NREL researchers have access to even greater computing power to tackle the research challenges of a renewable and sustainable future.

Supercomputing Supports Early Career Award-Winning Research From Office of Science
New research investigating wurtzite-based nitride ferroelectric materials garnered an Office of Science Early Career Award from DOE.

Read more on **page 27**

HPC-Powered Energy Transmission and Distribution Simulation Platform Selected for R&D 100 Award
NREL's Simulation and Emulation for Advanced Systems (SEAS) simulates and validates energy transmission and distribution solutions across the buildings, transportation, and renewables sectors and the grid.

Read more on **page 9**

KEY PERFORMANCE INDICATORS

619 Total users

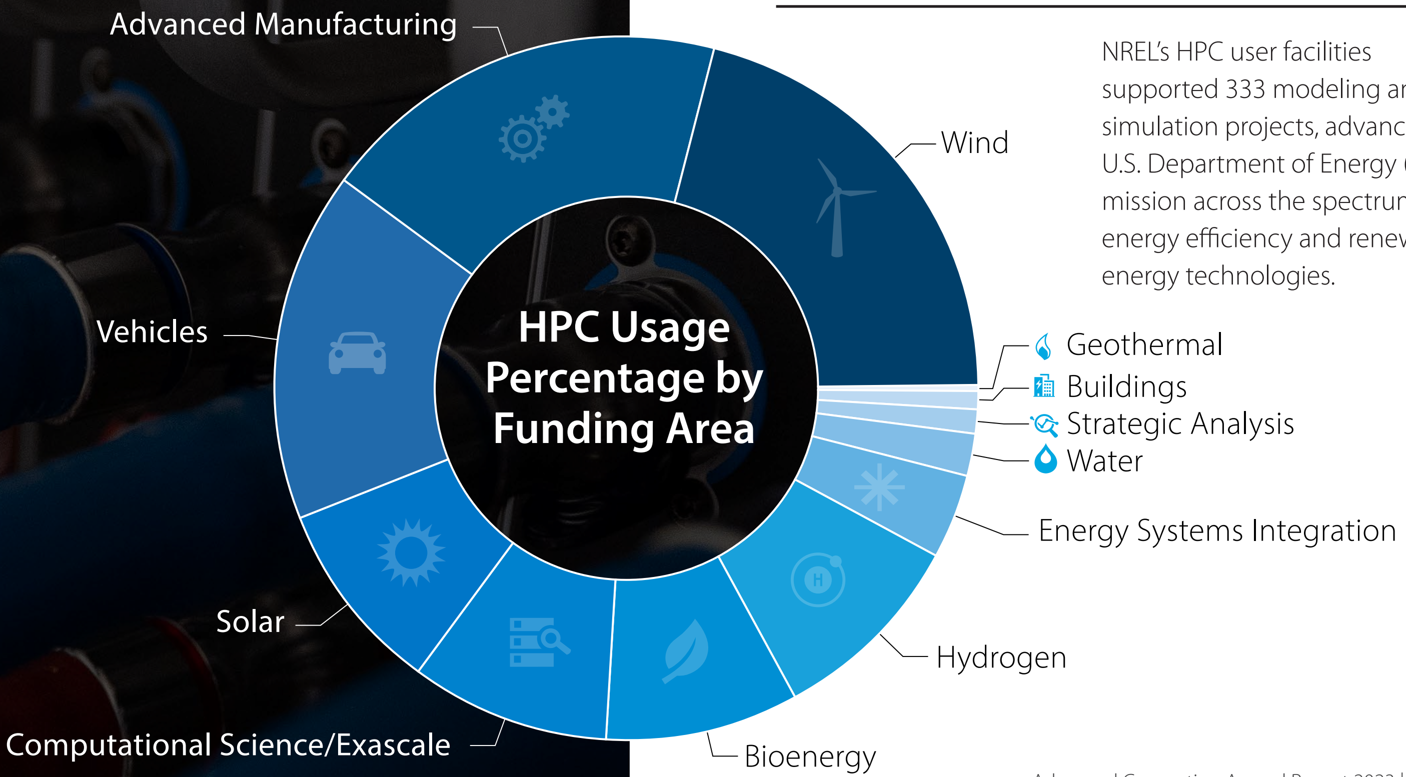
95% HPC availability

95% HPC utilization

333 Modeling and simulation projects

MODELING AND SIMULATION PROJECTS

NREL's HPC user facilities supported 333 modeling and simulation projects, advancing the U.S. Department of Energy (DOE) mission across the spectrum of energy efficiency and renewable energy technologies.



Supercomputer Kestrel Takes Flight With Substantial Increase in Computing Power

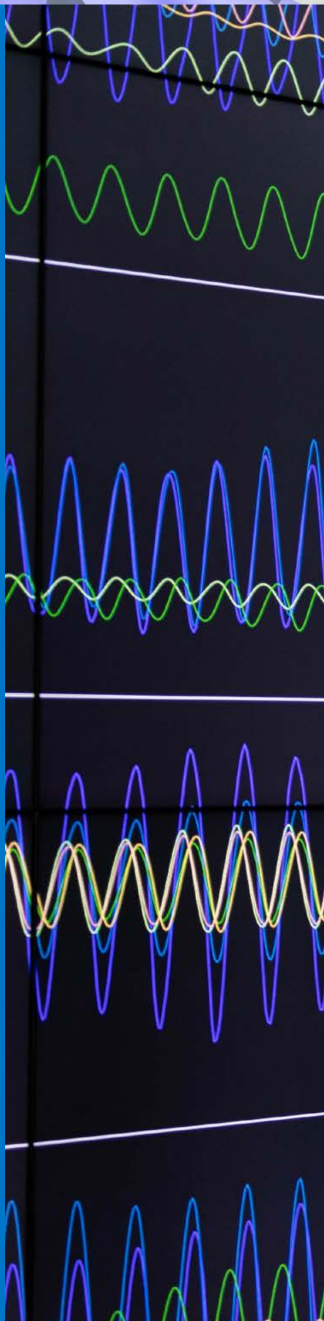
Spring and summer were a busy time in ESIF's Data Center, as the NREL and Hewlett Packard Enterprise teams installed and tested Kestrel, NREL's third-generation supercomputer dedicated to driving advancements in energy efficiency, sustainable transportation, renewable power, and energy systems integration research. The first phase of Kestrel, consisting of Intel Sapphire Rapids central processing unit-based nodes, was fully operational for the start of the fiscal year in October. In its final configuration with added graphics processing unit capability coming in winter 2024, Kestrel will provide more than five times the computing power of its predecessor, Eagle. Kestrel will play a critical role in computing for computational materials, continuum mechanics, and large-scale simulation and planning for future energy systems. Rapidly advancing applications and technologies in artificial intelligence and machine learning are fostering innovation and expansion of research into new directions for computing. These workflows drive complementary physics and data-driven approaches by fusing simulation with new sensor data sources. Kestrel's heterogeneous architecture—which includes both central processing unit--only and graphics processing unit-accelerated nodes—is designed to enable these emerging workflows, providing partners with the ability to tackle the energy challenges for moving into a renewable and sustainable future.

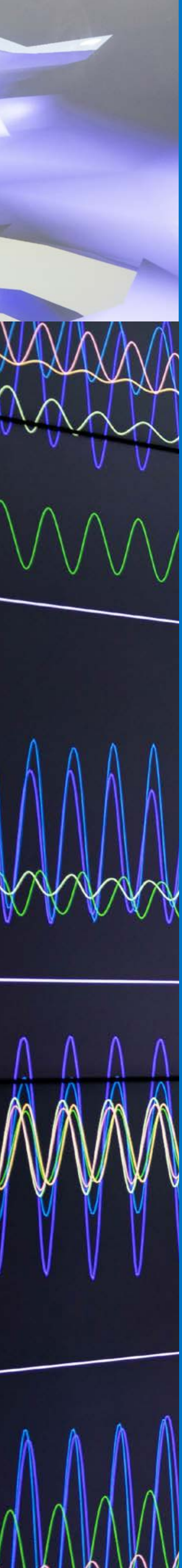
New 3D Capabilities Support Visual Analysis of 30x Larger Data

In 2023, NREL completed upgrades to the 3D capabilities of the ESIF Insight Center, bringing the Insight Center to the forefront of immersive visualization technology. This transformative upgrade provides a fourfold increase in resolution, empowering researchers to process and display data with exceptional clarity.

With higher-resolution outputs and vastly larger data sets, these capabilities increase the scale of data researchers can explore immersively. In a recent benchmark, NREL visualized data from the latest ExaWind run, representing a remarkable increase in data scale. This visualization benchmark won the 2023 Supercomputing Scientific Visualization & Data Analytics Showcase award in November.

Integrating these state-of-the-art visualization capabilities is pivotal as we transition toward supporting the Kestrel HPC infrastructure. The visualization capabilities are scaling with NREL's increase in compute power, supporting insight and knowledge discovery in our most extensive, complex data sets.





NREL's Insight Center Visualization Helps Validate Resilient Power System Controls

This year, 2D data visualization at NREL helped unravel and address oscillations triggered by a generator fault in the Kaua'i power system. The incident in question, which occurred on Nov. 21, 2021, after the disconnection of an oil power plant on the Hawaiian island, led to significant oscillatory instability in the broader system stemming from inverter-based resources (IBRs).

Analysis pinpointed the cause of the oscillations, identifying IBRs as the source. Leveraging the visualization capabilities of the Insight Center, researchers examined and tested hypotheses regarding how inverter settings influenced the system's oscillatory behavior. The high-resolution displays provided a unique vantage point, enabling power system engineers to concurrently observe the time evolution of four key state variables across six generators. This visualization also emphasized the interplay between dynamic variables, network structure, and the geographic locations of the generators. Notably, visualizations revealed how a subset of inverter-based generators drove oscillations throughout the system, uncovering dynamic nuances not readily apparent in standard time-series or geographic views. Building on these insights, researchers implemented changes to the inverter settings. When a similar fault occurred in April, the system demonstrated a smooth recovery without the previously observed oscillatory behavior. This work underscores the power of advanced visualization tools in comprehending complex power system dynamics and implementing targeted solutions for enhanced stability.

Catalyzer Leading Path to Greener Computing

The Joint Institute for Strategic Energy Analysis at NREL launched the Green Computing Catalyzer in 2022 to cultivate and scale the green computing capabilities at NREL. Now in its second year, the catalyzer is focused on bringing efficiency and accountability to computing-based research around the globe.

To better understand the magnitude and intricacies of energy usage in supercomputing, NREL researchers instrumented the lab's supercomputers, used by researchers for projects spanning the EERE technology offices as well as partner institutions, with node-level sensors that provide granular, streaming metrics of the compute system's energy and power statistics. In addition to developing approaches for more energy-efficient computing at NREL, the Green Computing Catalyzer is working to equip researchers around the world with the tools needed for energy-efficient algorithm design. In FY 2023, the team compiled a public data set of real-world algorithmic performance metrics and ran millions of computational experiments, providing data on the performance of various configurations of algorithms, input data, and hardware. The Green Computing catalyzer is now working to augment the first-of-its-kind BUTTER Empirical Deep Learning Framework data set with energy efficiency data. Making this type of data available can help researchers determine how to spend their computational energy wisely and what energy costs they might incur when training large models.

INTEGRATED ENERGY SYSTEMS

Researchers Build Virtual Communities Using SEAS To Model Clean Energy Solutions

R&D 100 2023 WINNER

Winner of a 2023 R&D 100 Award, the Simulation and Emulation for Advanced Systems (SEAS) open-source software will serve six communities that were selected to receive in-depth analysis with multistakeholder inputs. SEAS is used to build a virtual community using modeling and Advanced Research on Integrated Energy Systems (ARIES)-related hardware to validate and de-risk different clean energy solutions before implementing in the field. The software simulates and validates energy transmission and distribution solutions across buildings, transportation, and renewables sectors as well as the grid. Supporting DOE's Clean Energy to Communities (C2C) program, SEAS was deployed to support a pilot project in Fairbanks, Alaska, where it was used to plan a more reliable and affordable power system by replacing a coal plant with wind and storage. Through C2C and using SEAS, Golden Valley Electric Association worked with NREL to provide detailed, high-fidelity analysis of the generation plan and determine how wind power could be added to the grid without affecting performance. The SEAS framework can also be used to connect to ARIES assets, such as ESIF hardware, or to data analysis and visualization resources for streaming data. C2C engages with communities in multiyear projects with technical assistance collaborations aiming to bridge clean energy ambitions and real-world deployment. In 2023, C2C supported 77 communities in six-month peer-learning cohorts and provided no-cost technical assistance to 50 communities.

National Study Aims To Optimize Electrical Transmission

DOE—in partnership with Pacific Northwest National Laboratory and NREL—has directed the National Transmission Planning Study to analyze methods for optimizing electrical transmission. The work identifies the role of transmission in accelerating cost-effective decarbonization, informing regional and interregional transmission planning processes, and exploring specific high-opportunity transmission pathways.

In FY 2023, the team completed analysis of more than 200 scenarios and presented the results to the public, produced nodal transmission plans for the Eastern Interconnection electrical grid, and built a nodal production model of the whole contiguous United States. The use of HPC for this study enables NREL's grid experts to run grid simulations that are some of the largest undertaken in the world. Stakeholder engagement is also a key component of the study, and numerous meetings with system planners, regulators, operators, and others in the power system industry in the United States have helped socialize the lessons learned thus far and strengthen the study through input from across the country. The study will continue to help identify pathways for necessary large-scale transmission system build-outs that meet regional and national interests.

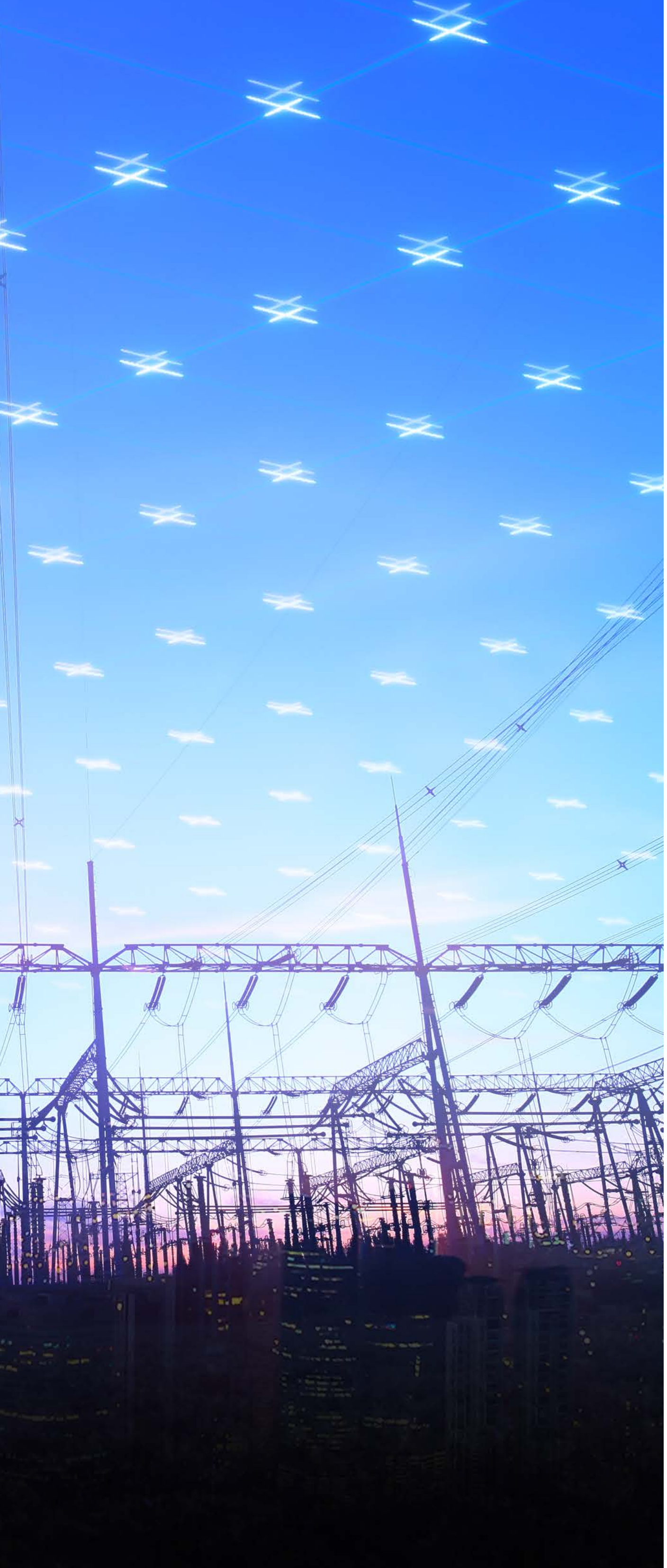
Scenarios Show Paths to Puerto Rico's Resilient, Equitable 100% Renewable Energy Goals

Unprecedented multi-laboratory collaboration on analysis of pathways to meet Puerto Rico's energy goals is concluding with the Puerto Rico Grid Resilience and Transitions to 100% Renewable Energy Study (PR100). This two-year effort—led by DOE's Grid Deployment Ofiice and funded by the Federal Emergency Management Agency —relied on an integrated analysis process (coordinated by NREL across six national laboratories) to identify pathways forward that achieve Puerto Rico's goals for renewable energy integration, resilience against extreme weather events, and energy justice. Renewable energy data sets were needed to generate scenarios that incorporated these targets. To inform comprehensive options for Puerto Rico, the team relied on HPC to develop 14-year, high-resolution historical and future projections of renewable energy resources. This included a 20-year wind resource data set that used 11 different planetary boundary layer models to capture more nuanced local and regional variations in wind resources. These resource data helped determine the technical potential of renewable resources in Puerto Rico. HPC resources allowed the PR100 team to simulate high levels of distributed solar and storage adoption across scenarios. Additionally, the PR100 team simulated the economic buildout, resource adequacy, and least-cost operation of the Puerto Rico power system of the three scenarios under different sensitivities for demand projections and land use availability. Ultimately, HPC resources allowed the PR100 team to rapidly execute the expansion and impact analysis workflows under extremely tight deadlines to help inform the Puerto Rico energy transition. The PR100 results findings were presented in a public event in February 2024 and the complete technical report will be published in March 2024.

Integrated Framework Targets Resilience of Power Systems to Cyberattacks

With cyberattack frequency growing and threatening the energy grid, the Cyber Resilient Distributed Autonomous Energy Grid project's integrated framework leverages a hybrid approach focusing on enhancing cyber resilience of the grid through design and autonomous response. The project seeks to address how to prepare, defend, and adapt power and communication systems against cyberattacks in an environment with a highly distributed attack surface and risk of cascading failures. Through Eagle's advanced computing capabilities, the research team aims to advance fundamental science and engineering approaches to cyber-resilient design and control, zero-trust architecture for autonomous grids, and autonomy to enhance cyberresilience.

Supported by the Laboratory Directed Research and Development Program at NREL, researchers this year have built a reinforcement learning framework that enables cyber-physical controls in response to cyberattacks by learning optimal policies and enabling faster system recovery. Additional work examined the use of graph neural network models for scalable modeling and analysis for power grids, enabling future cyber-physical power systems design planning to support a resilient distributed energy grid. The team has also developed a zero-trust cyberattack detection method for hierarchical power system architectures and assessed the vulnerabilities of a hierarchical control system in different types of cyberattacks. The suite of artificial intelligence/machine learning approaches developed under this effort will advance the science of cyber resilience for power grids and provide system operators with advanced tools to enable faster and accurate response and recovery of the system after a cyberattack.



Computational Speedup of Simulations Could Help Future Power System Reliability

The Intelligent Phasor-EMT Partitioning project, funded by the EERE Solar Energy Technologies Office, aims to improve the modeling accuracy and computational speed when simulating transient dynamics of power grids with extensive IBRs. As power systems move toward high levels of IBRs, conventional phasor-domain dynamic modeling may miss IBR-related interactions that can destabilize systems. In FY 2023, the project team worked toward developing and validating the individual components of an advanced systematic, HPC-compatible framework for hybrid electromechanical-electromagnetic transient (EMT) simulation intended for large-scale power grids, including up to 100,000 transmission- and distribution-connected IBRs. The NREL-led team includes the University of Texas at San Antonio; the University of Tennessee, Knoxville; Pacific Northwest National Laboratory; the Electric Power Research Institute; and Arizona State University. Using Eagle, they demonstrated 25x computational speedup of EMT simulations with large penetrations of IBRs for a 10,000-bus power system. The project additionally includes development of hybrid phasor-EMT simulations combining Grid PACK, a phasor domain simulator, and NREL's ParaEMT, an EMT simulator, via Hierarchical Engine for Large-scale Infrastructure Co-Simulation. This research will enable grid operators and planners to capture the complex transient dynamics of large, IBR-dominated power systems in tractable simulation times, which will maintain reliability of the renewable power system of the future. ParaEMT, developed under this project, is the world's first publicly available open-source tool for power system EMT simulation.

MATERIALS SCIENCE

Simulation Framework Predicts Performance of Commercial-Scale Reactors To Reduce Energy Inputs and Emissions

Ethylene and propylene are petrochemical compounds needed to create the most widely used plastics in the world: polypropylene and polyethylene. Their versatility makes them valuable commodities, but producing them creates approximately 220 megatons of greenhouse gas emissions annually. To support the decarbonization objectives of the DOE Industrial Efficiency and Decarbonization Office's Chemical Manufacturing program, NREL and industry partners Clariant and Bechtel are developing catalytic systems that reduce the energy inputs and carbon dioxide emissions for these two chemical products. This year, the research team made a landmark achievement in its catalytic systems modeling by developing a multiscale simulation framework that can predict the performance of commercial-scale reactors for timescales surpassing one year. Understanding the long-term performance of commercial-scale reactors helps industry understand sustainability and efficiency of its chemical production processes and predict how these might change as new catalysts and processes are developed. Additionally, the team developed new, atomic-scale simulation tools that are being used to guide more precise material development for efficient inductive catalytic systems. This project leveraged NREL's Eagle supercomputer, as well as chemical conversion data from Savannah River National Laboratory and Idaho National Laboratory, catalyst synthesis capabilities of University of South Carolina, and kinetic model development by Georgia Institute of Technology and the University of Houston.

New Multiscale Modeling Method Helps Industry De-Risk and Deploy Emerging Bioenergy Technologies

As the industrial sector seeks to decarbonize and become more energy efficient, transitioning to biomass conversion and catalytic upgrading processes is a viable solution. The performance of biomass conversion and catalytic upgrading processes must be optimized to reduce the cost, time, and risk associated with this transition. The outcome of these processes is determined by an interplay of chemical and physical phenomena that occur across many scales (e.g., length and time); this requires a robust, multiscale computational framework. Working with EERE's Bioenergy Technologies Office, the NREL research team used the Eagle supercomputer to develop new fast-solving methods to simulate these phenomena simultaneously through mesoscale (particle-scale) and reactor-scale simulations. This new multiscale coupling method captures microscale, intraparticle transport phenomena in macroscale reactor simulations, enabling simultaneous optimization of feedstock attributes, catalyst characteristics, and reactor operating conditions. These methods are being used to help ExxonMobil scale up and deploy biomass pyrolysis, a process related to bioenergy and biofuel production.

Dynamic Modeling of Polyester Decrystallization for Polymer Upcycling Strategies

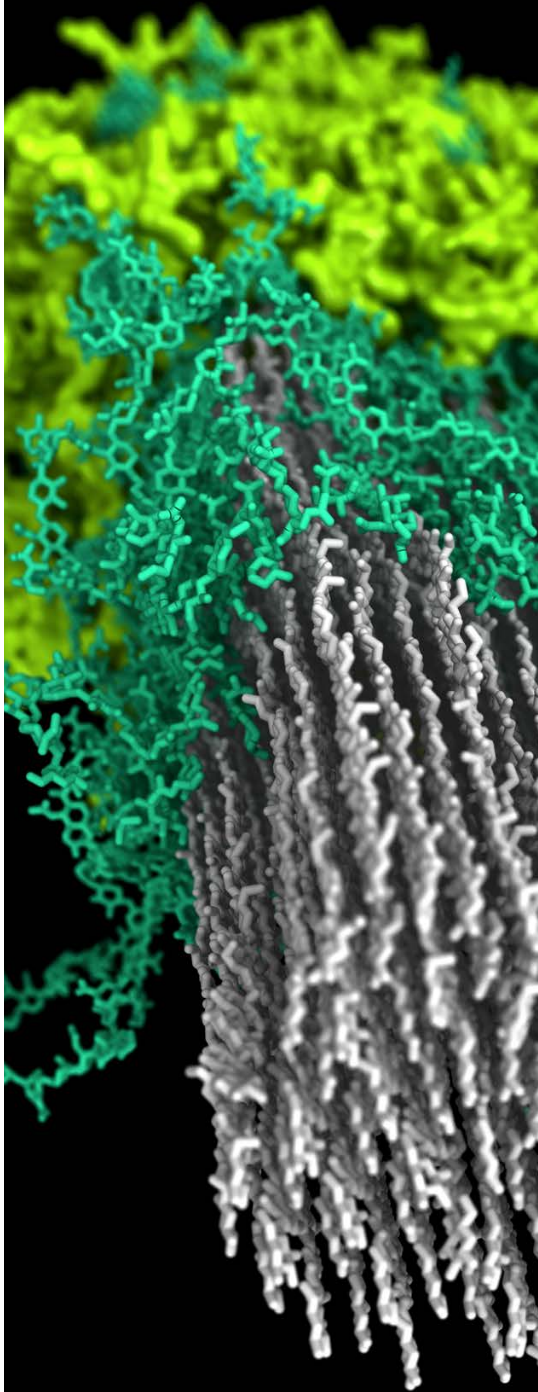
The Biochemical Process Modeling and Simulation project, supported by the Bioenergy Technologies Office, deploys modeling and simulation tools at length scales ranging from atomic to reactor, with an overarching objective to streamline experimental and engineering efforts to reduce the cost of bioderived materials and products by addressing process bottlenecks.

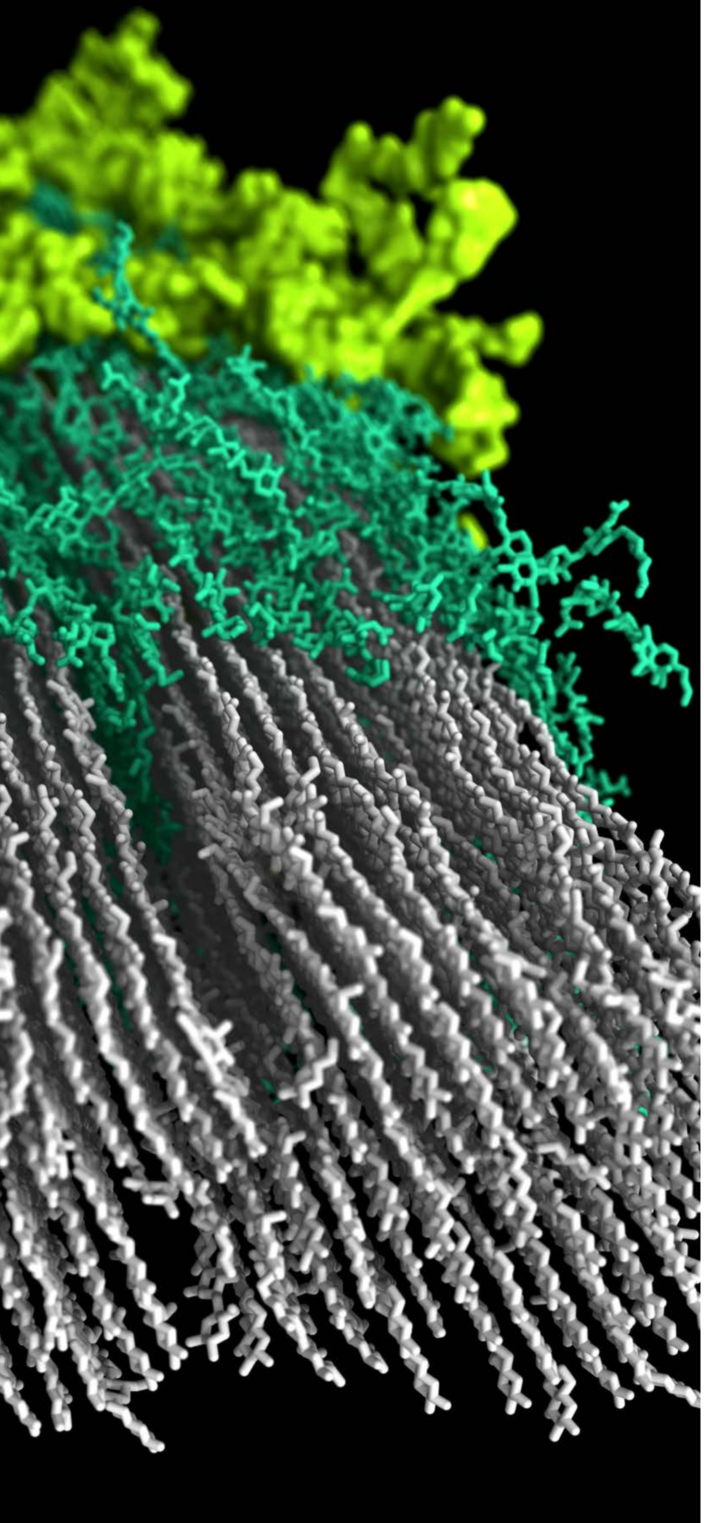
NREL researchers are successfully deploying a computational approach to tackle plastic waste, using molecular dynamics simulations to study decrystallization in widely used synthetic polyesters. Recently, the team has developed crystalline molecular models of five widely used polyesters, including polyethylene terephthalate (PET), the world's most consumed polyester, and other high-volume synthetic polyesters (polybutylene terephthalate, polytrimethylene terephthalate, polyethylene naphthalate, polyethylene furanoate). These simulations help quantify the free energy required to remove a single polymer chain from its crystalline structure, providing valuable insight into the energy barriers that need to be overcome during the decrystallization process. This knowledge offers a direction to experimental scientists for the development of more efficient plastic recycling strategies such as introducing catalysts that lower these energy barriers, fine-tuning conditions during the recycling process, guiding enzyme and chemical selections, and designing new materials.

Unveiling Molecular Insights of Plant Structure Can Yield More Efficient, Sustainable Bioenergy and Biofuel Production

Plant secondary cell walls are significant carbon and energy repositories. Their material and energy are stored as a composite of three major biopolymers: cellulose, hemicellulose, and lignin. A better understanding of the interactions between—and assembly of—these biopolymers in the architecture of the secondary cell wall is crucial for the development of more efficient and sustainable processes for bioenergy and biomaterial production, as well as biotechnological efforts to improve biomass yield and resistance to pests and pathogens. However, details regarding specific intermolecular interactions and higher-order architecture of the secondary cell wall have remained elusive. Guided and validated by solid-state nuclear magnetic resonance spectroscopy experiments, molecular modeling and dynamics simulations of representative atomistic secondary cell wall models were built and analyzed using NREL's Eagle supercomputer. The solid-state nuclear magnetic resonance experiments enabled quantitative validations of the atomistic models as they provided refined details about the structural configuration, intermolecular interactions, and relative proximity of all three major biopolymers. The study revealed that a priori knowledge of biopolymer placement relative to each other is key for building accurate atomistic models of plant cell walls. This study lays the foundation for creating more detailed models of plant cell walls with different compositions and arrangements, which could be subjected to further physics-based simulations to gain insight into the complex relationship between biomass composition, its architecture, and its ultimate material properties.

This is the second year of NREL's projects supporting the Center for Bioenergy Innovation (funded by the DOE Office of Science's Biological and Environmental Research program).



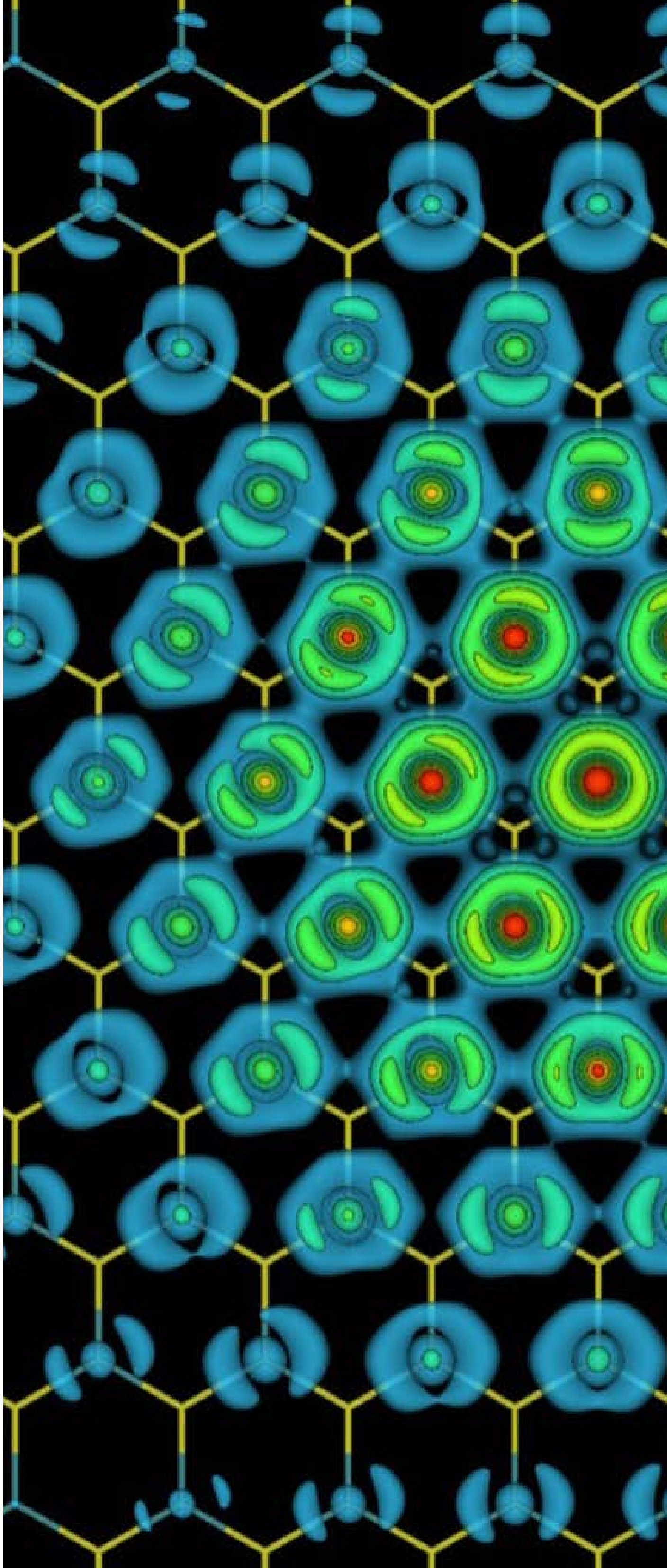


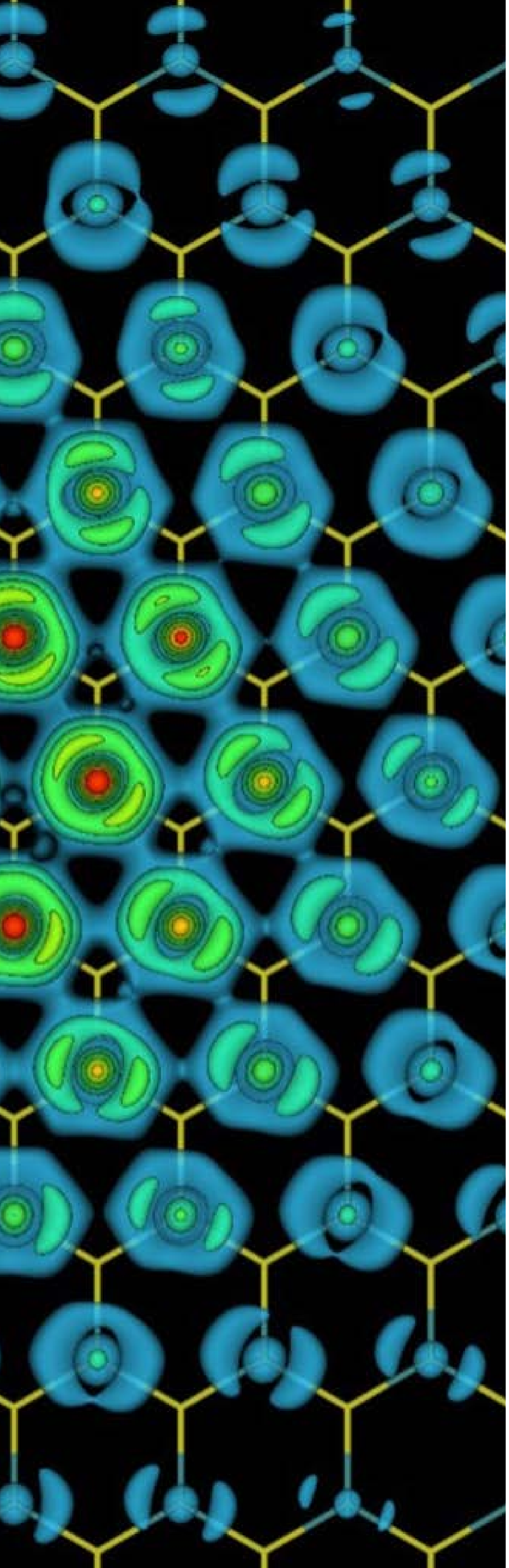
Molecular Dynamic Simulations for Efficient, Stable, and High-Performing Inverted Perovskite Solar Cells

Perovskite solar cells with an inverted structure (the p–i–n architecture) are attractive for future commercialization due to their easily scalable fabrication, reliable operation, and compatibility with a wide range of perovskite-based tandem device architectures. However, the power conversion efficiency can still be improved to make the largest impact on commercial applications. Further improvement in power conversion efficiency will help commercialize the perovskite solar cell technology. Given the remarkable advances in perovskite bulk materials optimization over the past decade, interface engineering has become the most important strategy to push perovskite solar cell performance to its limit. A team of researchers from NREL, University of Toledo, University of California San Diego, and University of Colorado Boulder found a reactive surface engineering approach based on a simple postgrowth treatment of 3-(aminomethyl) pyridine on top of a perovskite thin film. With this reactive surface engineering, the resulting p–i–n perovskite solar cells obtained a power conversion efficiency of over 25%, along with retaining 87% of the initial power conversion efficiency after more than 2,400 hours of 1-sun operation at about 55°C in air. This work was supported by NREL's Eagle and the Center for Hybrid Organic Inorganic Semiconductors for Energy, an Energy Frontier Research Center funded by the DOE Office of Science's Basic Energy Science's program.

New Chemical Simulation Code for High-Fidelity Theory Attracts Experimental Groups Worldwide

Quantum chemical simulation codes rely on HPC to solve the underlying equations and simulate chemical processes and phenomena without reference to models. Most of today's chemical simulation codes use accurate but inefficient algorithms, creating a need to modify or replace them. Using grant funding from the DOE Office of Science program in Basic Energy Sciences in Computational Chemical Sciences, NREL is adapting Questaal—an electronic structure software package—to create a chemical code, Questchem, for research on molecular systems and materials used in solar photochemistry. The first principles theoretical method employed in Questchem is uniquely suited to investigating and predicting novel behavior and response of many-atoms systems efficiently and with high-fidelity. Moreover, it is designed to take advantage of emerging leadership-class computing platforms. A new quasi-1D system—chromium sulfur bromine—has been found to combine many advantages of popular 2D systems owing to unusual properties deriving from its effective one-dimensional nature. NREL's high-fidelity theory was uniquely able to describe several key experimental phenomena—especially how excitons respond to light—and the observed angle-resolved photoemission spectroscopy spectrum. This unique ability has attracted the attention of some of the world's leading experimental groups seeking interpretation of their data.





Material Defect Discovery, Properties, and Interactions Improve Candidate Screening for Water-Splitting Technologies

FY 2023 saw the HydroGEN theory team advancing the theoretical and computational underpinnings for solar thermochemical hydrogen production. The EERE Hydrogen and Fuel Cell Technologies Office funded development of advanced methodologies for materials discovery and targeted materials-specific studies to assess potential and limitations of candidate materials. It is difficult to computationally study materials with defects because it requires extensive calculations for each individual defect site. After building a training model consisting of approximately 200 host oxide compounds and 1,500 unique defects, the NREL-led team developed a model that can predict the impact of defects on a material's properties directly from the ideal crystal structure, eliminating the need for constructing and analyzing large supercells for each defect.

This graph neural network can predict the defect properties of ideal, defect-free structures, enabling high-throughput screening of redox-active oxides. The project also introduced an approach based on density functional theory–supported sampling of defect configurations to create an equation describing defect interaction. The team demonstrated the capability and utility of the approach by simulating the water–splitting redox processes for $Sr1-xCexMnO3-\delta$ alloys: a family of complex oxide materials composed of strontium (Sr), cerium (Ce), manganese (Mn), and oxygen (O). These alloys are of interest for applications like solid oxide fuel cells, oxygen separation membranes, and catalysis, where they are used in processes like water splitting for hydrogen production and other energy-related applications. Solar thermochemical hydrogen production can provide a promising solar energy storage pathway.

High-Fidelity Calculations Yield Nanoscale Insights for Cost-Competitive Fuel Cell Electrocatalysts

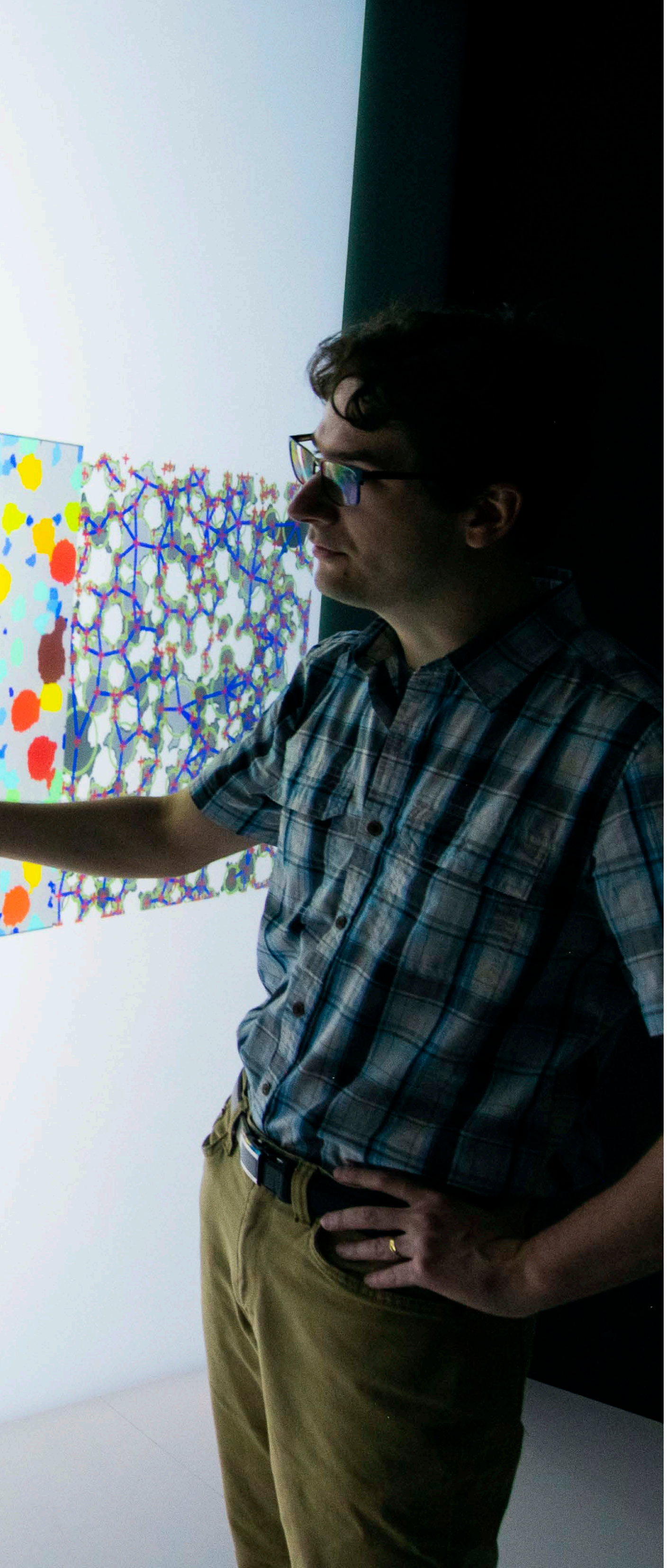
Precious metal electrocatalysts used in fuel cell and electrolyzer systems are expensive and present a material barrier to cost-competitive deployment. To explore viable catalyst design alternatives, NREL is developing state-of-the-art computational techniques for electrochemical modeling as a part of the ElectroCat Consortium: a collaboration among researchers at NREL, Argonne National Laboratory, Los Alamos National Laboratory, and Oak Ridge National Laboratory aiming to increase U.S. competitiveness in manufacturing fuel cells and hydrogen production water electrolyzers. The inability to capture the intricacies of electrochemical reactions in catalysts has historically led to discrepancies between computational predictions and real-world experimental outcomes. Popular computational techniques commonly ignore critical factors like applied potential (i.e., the influence of externally applied voltages on the electrochemical processes). To address this, NREL is adding realism to atomistic electrocatalyst models, evaluating the impacts of beyond-density functional theory methods on these catalysts, and developing techniques that will enable general multi-scale models of electrochemical systems. The core techniques include grand canonical density functional theory, beyond-density functional theory GW/random-phase approximation method, *ab initio* molecular dynamics, classical molecular dynamics, and machine learning. With funding from the Hydrogen and Fuel Cell Technologies Office, NREL achievements this year include quantifying the effects of applied potential on a promising electrocatalyst (and why NREL's approach results in predictions different from the historical approach). In addition, two studies have been carried out on bulk polymer electrolytes and the polymer electrocatalyst interface. The interface region has not been previously investigated using high-fidelity computational methods.

3D Model Identifies Stress Points in Solar Power Thermal Energy Storage Tanks

Failures in molten nitrate salts thermal energy storage tanks—which boast long storage times at low cost—present consistent issues in concentrating solar power plants. The thermal energy storage technology is still in its infancy, and in-service tanks are usually designed using standards for tanks for the oil and gas industry that operate at lower temperatures. NREL researchers—supported by the Solar Energy Technologies Office—recruited Eagle to develop and validate a 3D model of a representative molten salt thermal energy storage tank design that uses typical concentrating solar power plant operation conditions to determine the temperature and stress distribution in the tank. The model identifies critical thermal gradients in the tank floor and shell, and high-stress areas in the tank that are potential failure points. Understanding failure mechanics is critical for providing accurate guidance for future tank designs, fabrication methodology, and safe operating conditions. The model enables researchers to pinpoint the critical operating conditions that lead to excessive stress and provides the necessary guidance on how to mitigate failures in current tanks and build more reliable tanks in the future. The model is an effective tool to address reliability issues in current thermal energy storage tanks, which is fundamental for the survivability of the concentrating solar power industry and the transition toward the decarbonization of multiple industrial thermal processes.

New Cathode Coating Designs Stabilize Lithium-Ion Battery Performance

Lithium-ion batteries play a significant role in electric vehicles and renewable energy systems. However, the instability of their electrode surfaces and interfaces—which facilitate the storage and release of electrical energy—hinders the development of safe, high-energy, long life cycle and low-cost batteries. With support from the EERE Vehicle Technologies Office's Battery Materials Research Program, NREL used the Eagle and Swift HPC clusters to develop materials design principles for amorphous cathode coating selections to improve stability. In addition to four experimentally confirmed cathode coatings, the team identified three new promising cathode coatings as well as guidelines for selecting amorphous cathode coatings. The team also found a correlation between the diffusion of lithium ions and oxygen ions, presenting a formidable challenge in controlling the spread of oxygen ions (which impacts battery stability and performance). The discovery of the coatings provides potential options to stabilize surfaces and interfaces in lithium-ion battery electrodes, which will extend the lifetime and safety of current and future high-voltage Li-ion batteries.



A Database of Computed Molecular Properties Enables Explorations of Battery Reactivity and Next-Generation Machine Learning

Data science tools are a powerful way to accelerate chemical studies, but they can only be applied when large data sets are available. To date, most computational chemistry data sets are heavily biased toward stable, neutral molecules, which limits data science studies in technologically important applications like electrochemical energy storage. With funding support from the Vehicle Technologies Office, researchers sought to address this challenge. They applied density functional theory to construct a database containing more than 170,000 molecules and more than 2 million molecular properties, focusing on reactive charged molecules. This database is incorporated in the Materials Project, a multi-institution computational research effort centered at Lawrence Berkeley National Laboratory. This new database is already driving scientific discovery. Researchers are leveraging the available data to construct chemical reaction networks—exploring electrolyte decomposition to improve Li-ion battery lifetime—and to train machine learning models to rapidly predict reaction properties. Eagle's and Swift's power enabled the efficient, high-throughput deployment of thousands of single-node jobs needed for this project; the team also utilized Lawrence Berkeley National Laboratory's Lawrencium cluster and the National Energy Research Scientific Computing Center's Cori and Perlmutter supercomputers. This effort will serve as a community resource, enabling researchers around the world to explore molecules without performing costly calculations.

MANUFACTURING

Computational Insights Yield Path Forward for Nitride Synthesis

An ongoing challenge in materials science is the discovery and synthesis of inorganic solid-state materials with novel compositions, structures, and properties. Researchers predict that some ternary nitride materials can boast a broad range of properties that are relevant to energy applications such as more efficient light-emitting diodes to better ferroelectrics. Required high temperatures or extreme reaction conditions make the synthesis of nitrides difficult. With funding from an Office of Science Early Career Award, NREL researchers recruited Eagle to create first-principles high-throughput computations and machine learning to discover novel wurtzite-based nitride ferroelectric materials and predict their synthesis feasibility, in collaboration with a National Science Foundation–funded Designing Materials to Revolutionize and Engineer our Future program. The team's modeling provides key insights that will be useful for future development and deployment of wurtzite-type nitride devices.

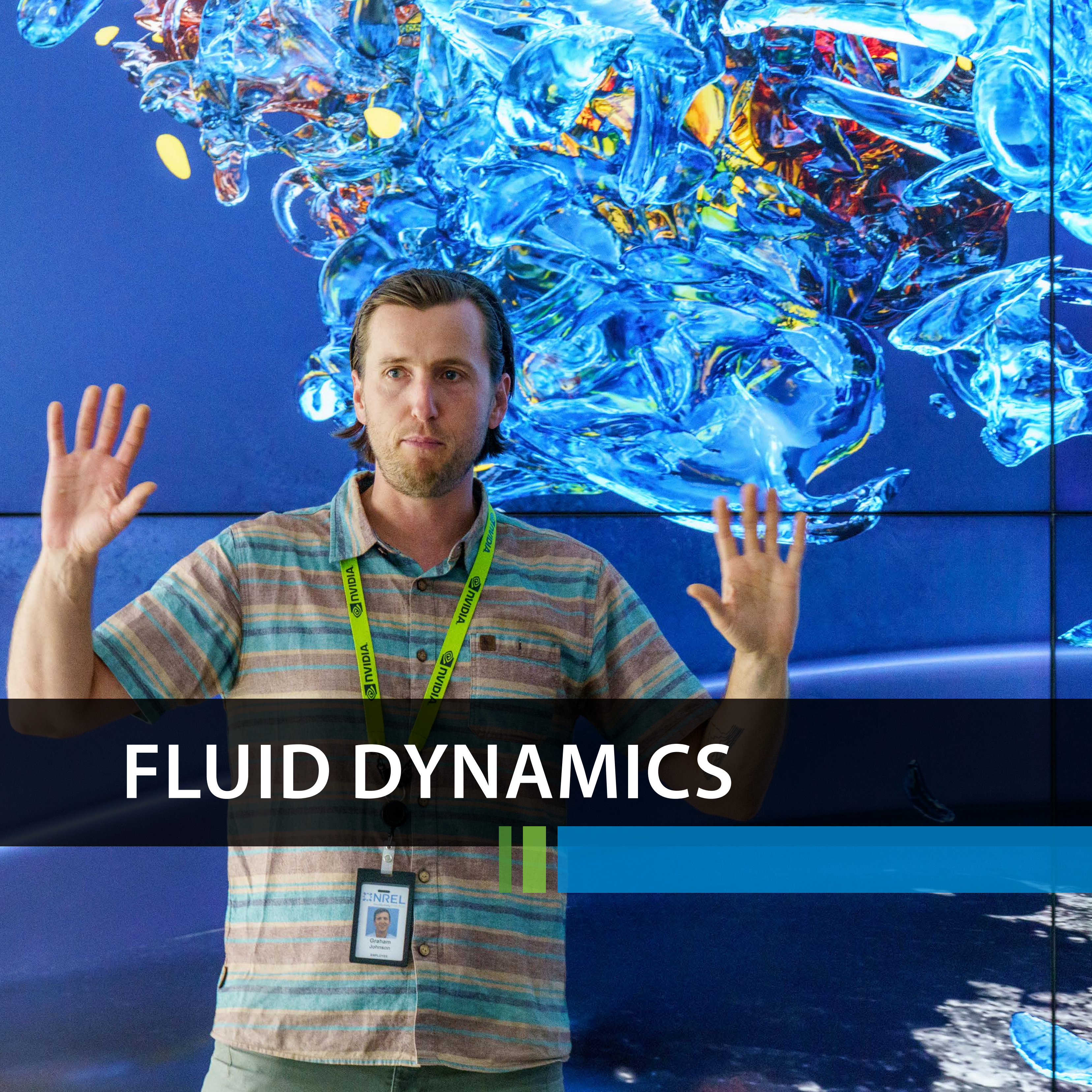
Model Shows Promising New Mechanism for Water Transport in RO Membranes

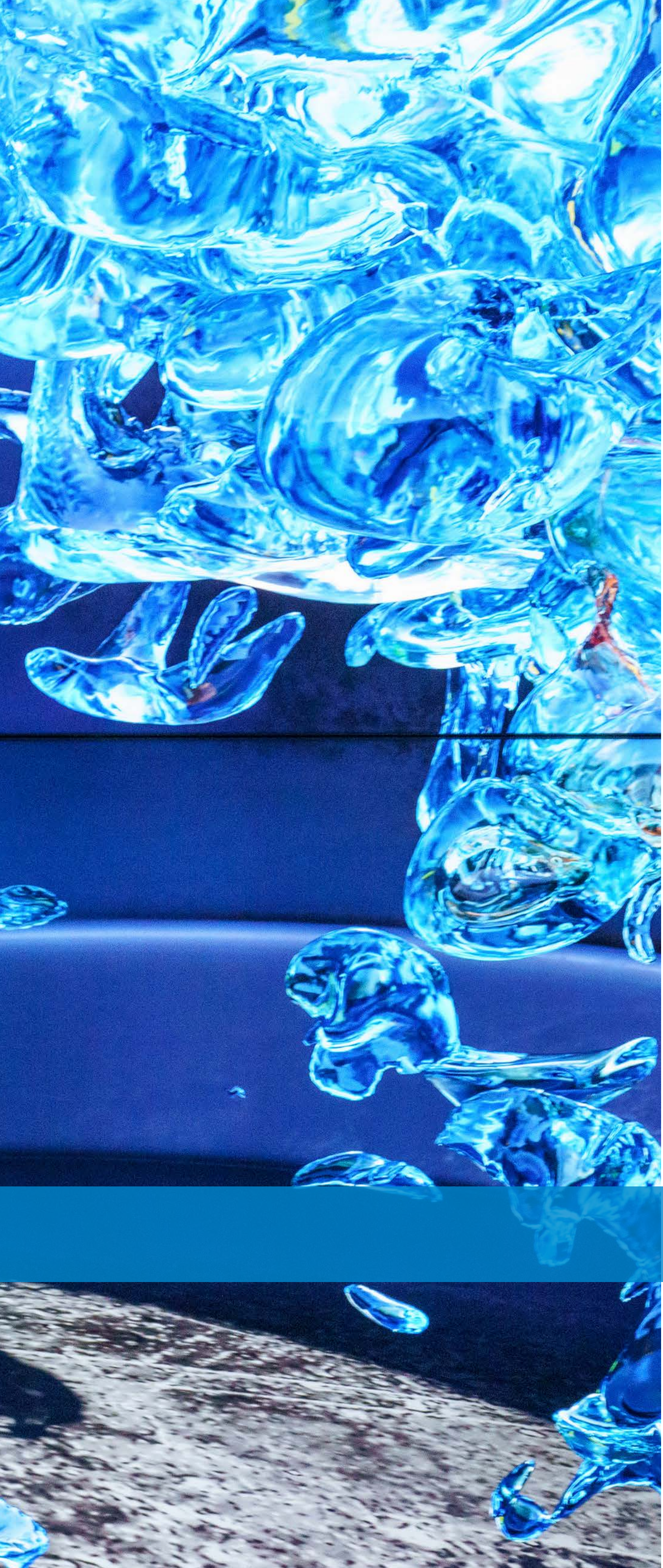
Reverse osmosis (RO) is the dominant desalination technology for augmentation of the world's water supply, especially crucial for water-scarce regions. Semipermeable desalination membranes are the center of RO technology, but little is understood about how they function. Using Eagle, in *silico* approaches have been developed to simulate transport in RO membranes under multiple projects funded under DOE's Industrial Efficiency and Decarbonization Office. In one project focused on customization of membranes for RO and nanofiltration, a model helped predict which polymer precursors can be used to create membranes with tailored selectivity and permeance. The model also showed how various manufacturing methods can impact membrane microstructure. In another project related to high-pressure RO, a model elucidated compaction mechanisms for dense polymer membranes at high pressure. This has led to further collaborations with Yale University, where the model was used to challenge the long-held beliefs that RO operates by a transport process known as solution diffusion. Key findings reveal that water transport could be driven by a pressure gradient within the membranes and not by a water concentration gradient, as has been previously reported. If true, such a finding would upend 50 years of precedent in the membrane science community.

Simulations Seek Optimal Component Grain Structure

Additive manufacturing is an attractive processing route for many aerospace components made of titanium alloys because it offers the ability to manufacture component geometries that are not readily possible by other conventional thermal and mechanical processes. This advantage—coupled with the economies of near-net-shape processing and elimination of post-process heat treatment—could result in significant savings in energy and cost. However, the chemical composition of alloys used in additive manufacturing must be tailored to withstand the extreme thermal conditions that are experienced during additive manufacturing as well as exploit these thermal conditions to produce mechanical properties that can equal or even surpass those of existing alloys used in conventional processing. With support from Lawrence Livermore National Laboratory's High Performance Computing for Energy Innovation Program, this work was focused on developing a new titanium alloy composition that could potentially replace the alloy that is commonly used in many aerospace components. Modeling with accurate capture of the physics involved in processing-properties relationships resulted in the identification of a new alloy composition. In conjunction with the new computational tool and HPC along with Raytheon's capabilities in additive manufacturing, the work will open a new paradigm in alloy design for additive manufacturing of aerospace alloys.

FLUID DYNAMICS





Computational Fluid Dynamics Models Enable Rapid Prototyping of High-Pressure, Low-Temperature Electrolysis Cells

Low-temperature electrolysis is a promising technique for producing green hydrogen by splitting water into hydrogen and oxygen using electrical energy. This project, funded by the Hydrogen and Fuel Cell Technologies Office and H2NEW consortium, focused on rapid prototyping to guide designs of flow fields (i.e., channels that carry gases and/or liquids) to maximize performance and efficiency of low-temperature electrolysis cells, which can be used in both water electrolysis and carbon dioxide electrolysis. Eagle was used to create computational fluid dynamics models that simulate the fluid flow through the high-pressure low-temperature electrolysis cell and assess key performance metrics such as pressure drop and uniform velocity distribution.

This HPC project enabled the development of an open-source high-pressure, low-temperature electrolysis hardware design that was made available to the general public. The project was also used to inform cell hardware and architecture choices from industry partners for larger-scale designs. Planned future work related to this project will study more novel flow field architectures and focus on the multiphase transport aspects.

Simulations Show Which Sustainable Aviation Fuel Could Be an Alternative to Conventional Fuels

Use of sustainable fuels in aviation supports a path to achieve zero net carbon dioxide emissions by 2050. Drop-in sustainable aviation fuels—those that can be used in existing aircraft engines and infrastructure without requiring modifications—for commercial aviation engines are a critical component in reducing aviation's carbon footprint. This project, funded by the Vehicle Technologies Office, studies the effect of 100% drop-in sustainable aviation fuels on aviation combustor performance. Powered by the Eagle supercomputer, numerical simulations of fuel-air mixing properties downstream of a lean direct-injection combustor indicate that 100% Hydroprocessed Esters and Fatty Acids sustainable aviation fuel has quicker evaporation properties (due to its thermophysical and transport properties) when compared to alcohol-to-jet sustainable aviation fuel and petroleum-based Jet A fuel. Quicker evaporation properties can be advantageous for efficient combustion depending on engine design. These predictive numerical simulations, coupled with property measurements being performed at NREL, act as virtual engine tests. These virtual engine tests pave the way to de-risk and reduce costs associated with introducing newer sustainable aviation fuels to decarbonize commercial aviation.

AWAKEN Reduces Unexpected Power and Financial Losses Using Control Strategies for Neighbor-Induced Wake Losses

The American WAKE experimeNt (AWAKEN) is an international, multi-institutional effort to understand how individual wind turbines interact with one another and with the atmosphere in a wind farm. Wake interactions (i.e., the behavior of slower or disturbed air flows trailing behind turbines) are among the least understood physical phenomena in wind plants today, leading to unexpected power and financial losses. More accurate wind plant models can improve farm layout and optimize operations, ultimately leading to lower wind energy costs. In FY 2023, the research team relied on Eagle to power large-eddy simulation models to investigate wind farm-atmosphere interactions, wind turbine wake losses, and wind plant performance optimization at a range of scales and fidelities. The simulations of a 50-turbine cluster yielded a detailed description of its internal aerodynamics, making it valuable for calibrating lower-fidelity computational models. Controls and optimization-focused engineering models are focused on mitigating wind turbine wake losses between neighboring turbines and nearby wind plants. The team was able to quantify neighbor-induced wake losses and evaluate controls strategies to stabilize power supply and lower operating costs. Funded by the EERE Wind Energy Technologies Office, AWAKEN is part of DOE's larger Atmosphere to Electrons effort to improve the efficiency of wind power plants.

The Next-Generation of Land-Based Wind Turbines: Predictive Modeling and Promising Innovations

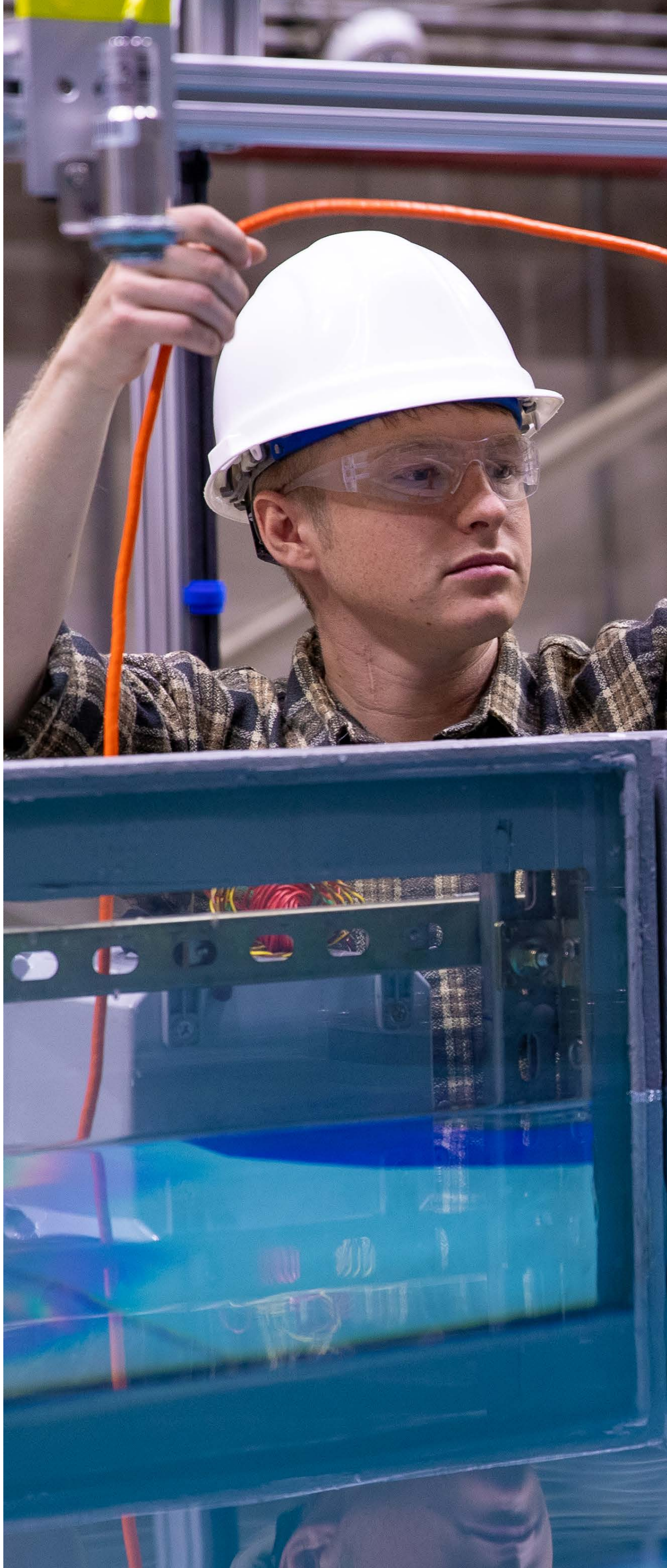
The Big Adaptive Rotor project is funded by the Wind Energy Technologies Office to find promising technologies for the next generation of land-based wind turbines. The Big Adaptive Rotor project focuses on turbines with rotors that stretch 206 meters in diameter, increasing capacity factors by 10% or more over a typical land-based turbine. Now in its second phase, the project leveraged Eagle to run hundreds of wind farm simulations and thousands of aero-servo-elastic simulations (i.e., coupled interactions among aerodynamics, structural dynamics, and control systems) to investigate the performance and dynamic behavior of very flexible wind turbines. The computational work on Eagle resulted in more accurate numerical models that are leveraged to accurately predict the dynamic behavior and the performance of wind turbines in the field. The new models investigate the potential of new concepts, such as new automated wind turbine optimization techniques based on full aero-servo-elastic models and the potential of trailing edge flaps (i.e., movable sections or surfaces of a blade edge), which are used to dynamically control and optimize the aerodynamic performance of the blade during different wind conditions. Another example is the investigation of wind farms made of turbines flying downwind rotors (rotors that sit behind, and not in front of, the tower), which have the potential to maximize the power performance of very large wind farms. The Big Adaptive Rotor team works with a variety of industrial partners exchanging data, models, and improvements. The entirety of this work provides a foundation for numerous design studies to innovate the world of land-based wind energy.

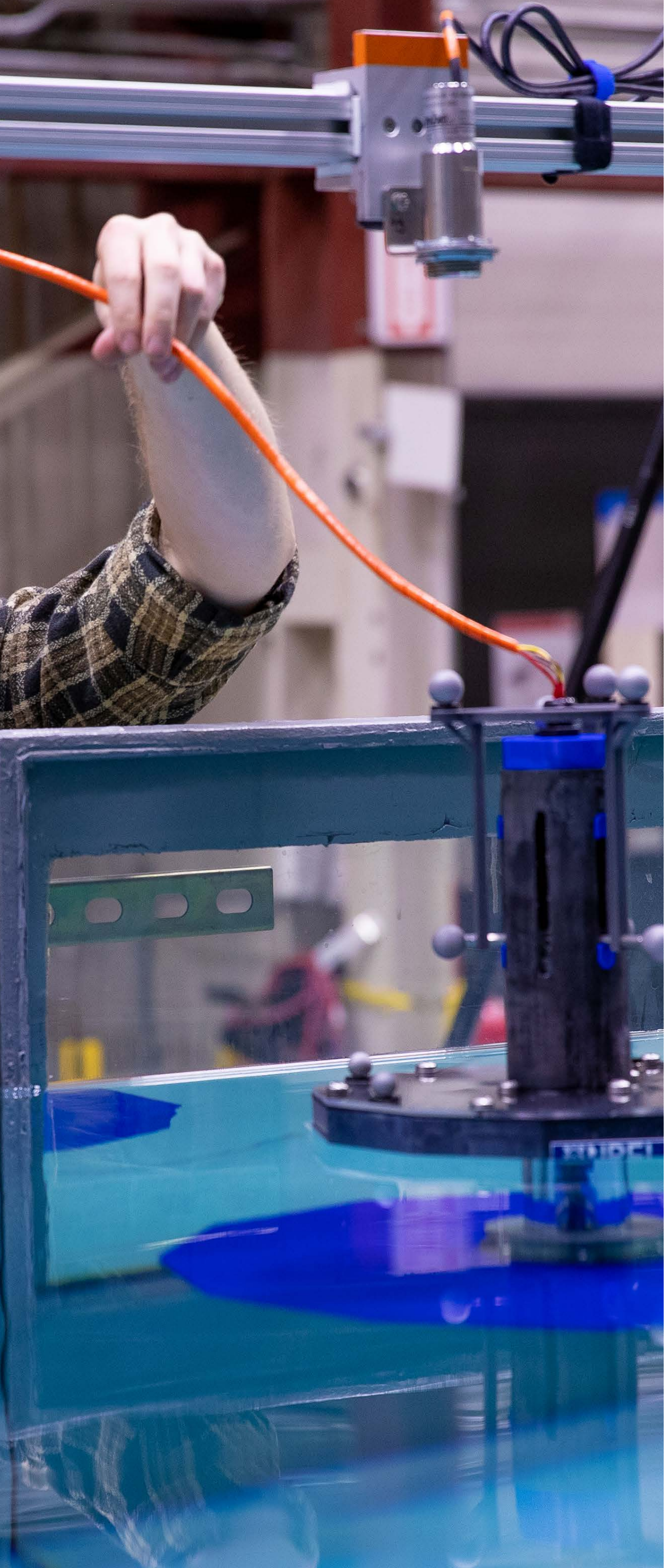
Modeling Offshore Wind Speeds Over Long Term Improves Wind Project Planning

The Wind Integration National Dataset Toolkit is the largest publicly available U.S. wind resource data set in the world. NOW-23 (2023 National Offshore Wind data set)—NREL's new 21-year data set—now replaces the Toolkit's offshore wind component, leveraging state-of-the-art advancements in the Weather Research and Forecasting modeling for wind speed not previously available. These long-term data sets are critical for wind energy stakeholders to perform more accurate energy production estimates, capacity expansion studies, and levelized cost of energy analyses. In fact, studies show that a small uncertainty change in the modeled mean wind speed translates into almost double the uncertainty for the long-term prediction of the annual energy production of a wind plant, which is associated with significantly higher interest rates for new wind project financing. Thus, the NOW-23 data set will be invaluable to offshore wind energy stakeholders, including developers, owner/operators, consultants, financiers, utilities, and researchers. With funding from the National Offshore Research and Development Consortium managed by the New York State Energy Research and Development Authority, the Bureau of Ocean Energy Management, and DOE, NREL's latest data set also incorporates wind speed uncertainty quantification for selected U.S. offshore regions, and it is available at no cost to the public.

Modeled Wave and Tidal Hindcasts Help Planning and Engineering

Interest in offshore wind, water, and tidal energy power generation is growing, necessitating models that can estimate wave conditions, tidal currents, and relative-risk-ratios for design. This project is a joint effort between Pacific Northwest National Laboratory, Sandia National Laboratories, and NREL. Researchers utilized the Eagle supercomputer as well as cloud computing to simulate and process wave and tidal hindcasts and expanding publicly available high-resolution data sets using the wave models WaveWatch3 and SWAN. The team further computed global extreme significant wave heights and modeled the effects of the Gulf Stream on ocean waves and wave energy. Commercial developers have shown interest in the data sets, which meet their growing need for resource estimates to help with project planning and device engineering. The research also helped determine hot spots and inform site selection for other multilaboratory research projects such as the Deployment Readiness Framework and coastal structure integrated wave energy converters. An updated user interface in the Marine Energy Atlas aims to make querying data layers and downloading bulk data more efficient.

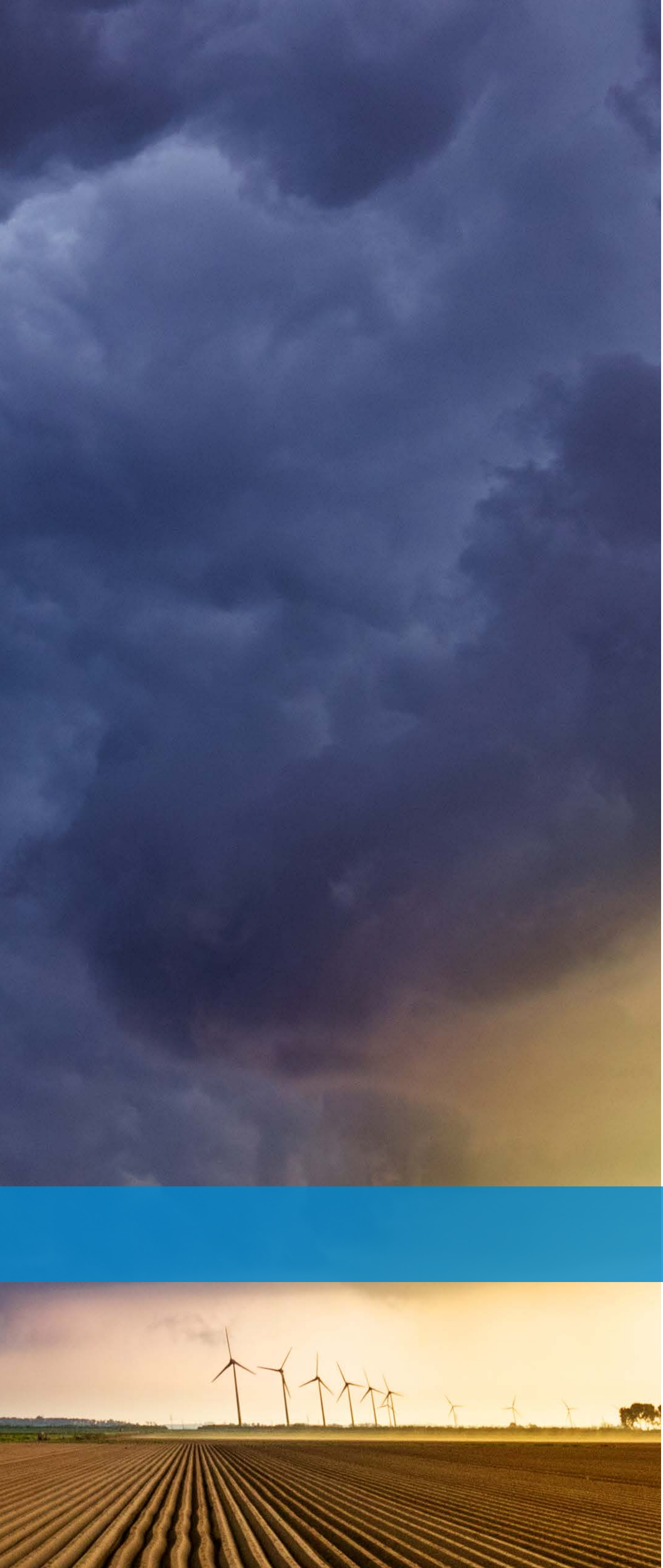




Computational Modeling Targets Wave Structural Loads for Designing Marine Energy Converters

Performance and load predictions for ocean renewable energy systems are complex—nonlinear waves and ocean current forces interact and affect floating, possibly flexible, multibody systems. Wave energy converter design methods have traditionally only considered hydrodynamic loads, so NREL researchers—funded by the EERE's Water Power Technologies Office—aim to accurately evaluate structural loads to develop cost-efficient wave energy converters. NREL's Eagle supercomputer enabled the team to quantify the accuracy of numerical tools with different fidelity (from low to high) for wave energy converters, implement computational fluid dynamics of marine energy conversion devices, and verify and validate an oscillating water column wave energy converter. Additionally, the verification and validation effort for an unsteady loading tidal turbine benchmarking study demonstrated a large data set that researchers and design engineers can test models and implementations against, helping reduce uncertainty and provide increased confidence in the engineering process. The work highlights potential guidelines to produce benchmark experimental data suitable for comparing the relative accuracy of different levels of numerical modeling. The work also enhanced wave energy converter simulation capabilities, which can accelerate marine energy converters' development through the availability of open-source tools and reduced computational requirements.

FORECASTING

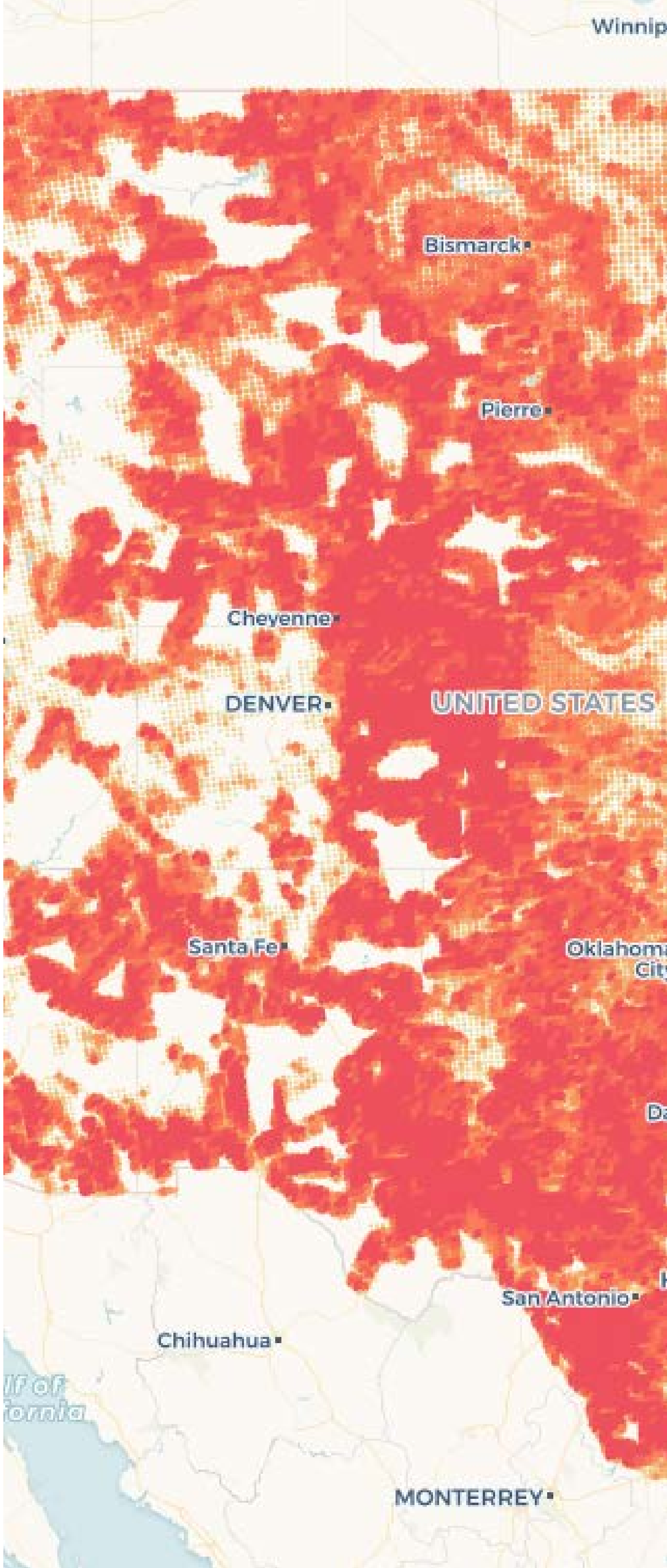


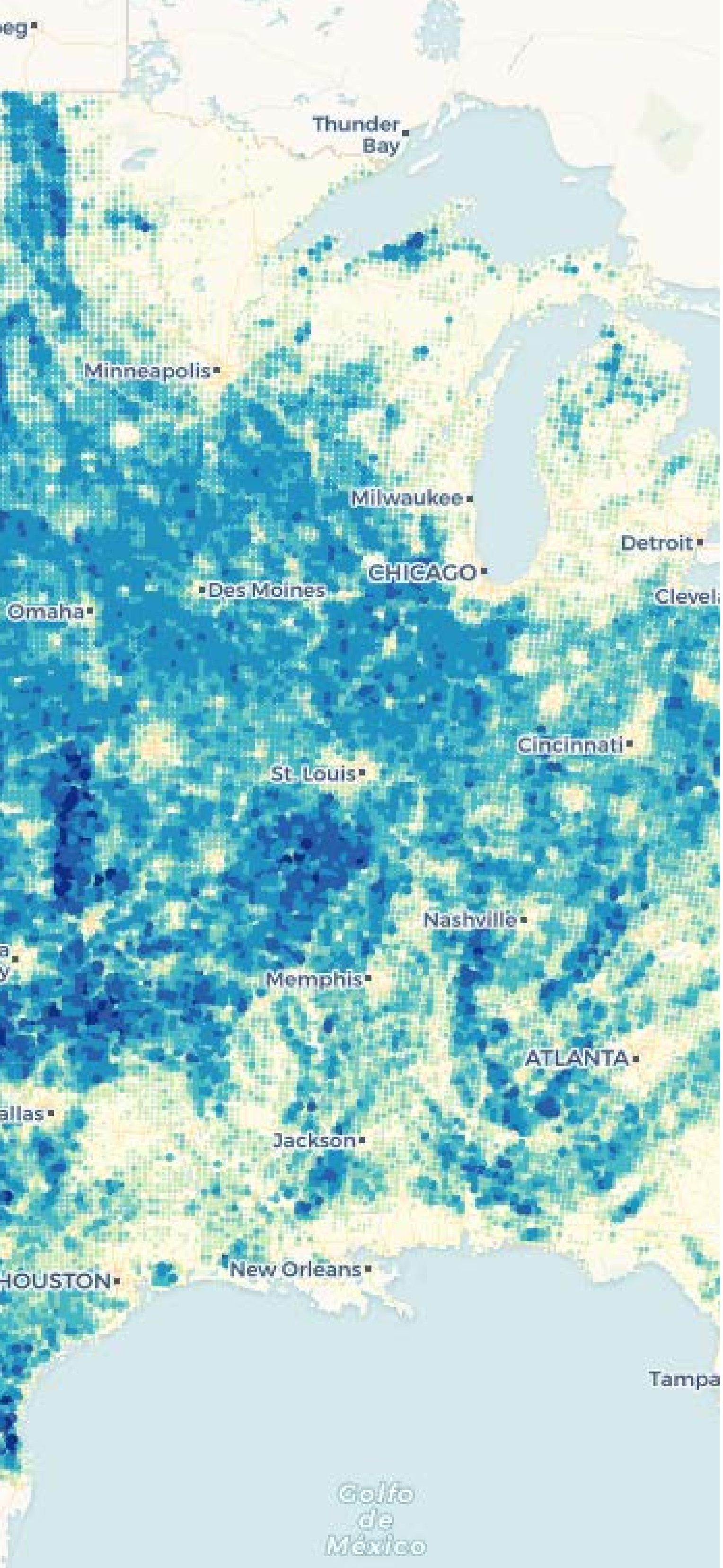
Evolving Climate Conditions and Uncertainty Are Key to Assessing Market Dynamics

To investigate the impact of wholesale electricity market mechanisms on power system reliability, operations, and prices, a team comprised of researchers from NREL, Argonne National Laboratory, Lawrence Berkeley National Laboratory, the Electric Power Research Institute, and Johns Hopkins University—and funded by the Wind Energy Technologies Office, the Office of Nuclear Energy, the Water Power Technologies Office, and the Office of Strategic Analysis—convened to tackle a broad range of market design topics. Researchers used input from U.S. independent system operator stakeholders to examine how market design—capacity markets and operating reserve demand curves, which differ in how they support resource adequacy—affect resource adequacy. The team then used these insights to explore how market structure can efficiently signal for attributes needed to ensure resource adequacy. Results indicate that capacity markets incentivize more capacity than operating reserve demand curves alone, while operating reserve demand curves better signal needed capacity commitment with a one-day outlook. Using the Eagle supercomputer, researchers demonstrated the importance of capturing evolving climate conditions and climate uncertainty when assessing wholesale market dynamics, as changes in weather patterns can significantly affect system costs and resource revenues. The project results showcase how various market rules can efficiently incentivize independent system operators to focus on attributes likely to contribute to resource adequacy on operational and investment timescales.

More Realistic Interpretation of Solar Potential Revealed Through Local Ordinance Models

Understanding the solar energy potential of a region is one part of the equation to make decarbonization a reality. Ultimately, land siting restrictions at the county or township level influence whether solar technologies can be installed. To date, decarbonization futures research has not incorporated the many rules local communities are instituting to guide or restrict solar energy development. To address this knowledge gap, NREL researchers collected more than 800 solar ordinances at the county level—and some at the municipal level—in the contiguous United States to understand their impacts on solar potential and illuminate possible land-use conflicts. The team found that extrapolating these ordinances throughout the country can reduce solar potential by 38%, depending on the size of the setbacks applied. These results indicate the importance of capturing setback ordinances in resource assessments to avoid overstating the resource potential, especially when considering highly decarbonized futures.





Well-Designed Wholesale Electricity Market Structures Necessary To Achieve Clean Energy Targets

Electric power generators need confidence in clean energy resource adequacy to achieve clean energy targets cost-effectively across timescales in an evolving system—before they incorporate clean energy technologies into their fleets. Performance metrics are influenced by competitive wholesale electricity market structures that vary across regions. Using DOE Office of Strategic Analysis funding to run the Electricity Markets and Investment Suite agent-based simulation model, NREL investigated the influence of market designs on the deployment of different technologies over multiple years—while also accounting for risk, uncertainty, and decarbonization policies of 45%–100% clean energy by 2035. Results highlight a complexity conundrum, whereby finding the "right" market design to achieve decarbonization goals can be a highly nuanced, nonincremental challenge. A promising insight is that even one well-designed market mechanism can help power producers achieve desired clean energy targets. These results help market planners, operators, and other stakeholders understand how various market products can enable the evolution of the generator fleet to simultaneously achieve a range of decarbonization goals and resource adequacy targets.

A BROADER COMPUTING ECOSYSTEM

Improved Data Pipeline Supports Scalable Clean Energy Solutions for Communities

Underpinning community projects are big, complex integrated modeling efforts that attempt to integrate historically siloed models to answer big questions. Coordinating and managing this integration across multiple models, community data sources, researcher analytics, and visualization capabilities is challenging. This data flow—or "pipeline"—is composed of multiple steps to manage, collect, transform, analyze, and visualize data across an integrated modeling project. Inspired by this complex data management challenge, NREL created Pipeline for Integrated Projects in Energy Systems (PIPES), a project management, data management, and workflow management layer for integrated modeling teams. PIPES works to connect and synchronize modeling and data requirements across diverse modeling workflows to help manage team activities and the diverse data paradigms associated with integration; helps teams find and share data, track progress, validate models, and find errors early; and improves integration speed (by reducing coordination time). PIPES is built as a hybrid computing solution that is model- and data-agnostic. It can work with data from any model in any location, enabling critical data and analyses to flow between these assets and coordinate data sharing and dissemination of results across teams and with the community. PIPES was developed under DOE's Clean Energy to Communities (C2C) program to help scale multiyear and multilab in-depth partnership projects with many communities simultaneously.

Capturing Supply Chain Processes To Improve Sustainable Manufacturing

Current understanding of supply chain greenhouse gas emissions and energy use in the manufacturing sector is often skewed by focusing exclusively on process-level activities. To get a more comprehensive view of manufacturing activities, NREL developed the Material Flows Through Industry tool. Analyses supported by this tool provide a holistic view of the overall energy-related carbon emissions associated with the entire supply chain's activities for commodity material or technology deployment—from evaluating energy and materials inputs in the initial manufacturing stages to evaluating those of the final production stages.

Utilizing cloud computing capabilities enables the Material Flows Through Industry tool to be accessible to a broad public audience. It also enables the project team to easily add new data on novel technology pathways and commodity materials, perform scenario analyses, debug the tool, and maintain data access and privacy for the users. The Material Flows Through Industry tool has advanced research in decarbonization scenario analysis across multiple sectors, including plastics and petrochemicals, iron and steel, wind energy, glass, pulp and paper, cement, and chemicals, and is key to identifying opportunities to reduce the energy and carbon intensities of supply chains in the U.S. manufacturing sector.

BRIDGING TO DOE LEADERSHIP COMPUTING

New Energy Build-outs, Scenarios, and Contingency Data Aid Power Grid Planning

For a resilient power grid, transmission expansion planning and resilient operations tools must keep pace with evolving power generation technologies and threats to resilience. As more renewable energy is added, power grids will need updates that can handle this new generation. The Exascale Computing Project Stochastic Grid Dynamics team developed high-fidelity mathematical models and representations of uncertainty—modeling generation scenarios and security contingencies—to address these challenges. They developed a workflow that uses NREL tools—the Renewable Energy Potential Model and System Advisor Model—along with the Wind Integration National Dataset Toolkit on the Eagle supercomputer to perform build-outs of renewable energy resources on large-scale, realistic test systems. These build-outs enable the study of stochastic operations, infrastructure expansion, and the ramifications of high penetrations of renewable energy resources on existing power grids. The results from Eagle enabled the Exascale Computing Project Stochastic Grid Dynamics team to demonstrate the performance of their software stack on Frontier, the new exascale HPC system located at Oak Ridge National Laboratory.

Enhanced ExaWind Code Enables High-Fidelity Simulations of Breaking Waves for Offshore Wind Energy

Led by NREL, a multilaboratory team of researchers developed ExaWind, a high-fidelity suite of codes designed for HPC, including the first exascale-class supercomputer, Frontier. Originally designed for land-based wind turbines and plants, ExaWind—thanks to the team's recent efforts—can now produce high-fidelity simulations of the wind-wave environment, which is a key step toward simulating floating offshore wind turbines. This capability is key to achieving U.S. offshore wind energy deployment goals. In FY 2023, the AMR-Wind solver in ExaWind was enhanced to simulate breaking waves, a highly nonlinear phenomenon, which is important for modeling and understanding the dynamics and loads of offshore wind turbines. In addition to increasing our understanding of an incredibly complex system, simulations from high-fidelity models, like ExaWind, serve as the foundation for next-generation engineering models.

INNOVATIONS & PUBLICATIONS

Software Records

Title	NREL Number
ADoSPSiQS (Automated Detection of Symmetry Protected Subspaces in Quantum Simulations)	SWR-23-55
BuildingsBench (BuildingsBench: A Benchmark for Universal Building Load Forecasting)	SWR-23-51
Day-Ahead Market Price Interpretability	SWR-23-61
eagle-jobs	SWR-23-34
EvoProtGrad (Directed Evolution for Proteins with Gradients)	SWR-23-48
ExaWind-driver	SWR-23-10
MARBLES (Multi-scale Adaptively Refined Boltzmann LatticE Solver)	SWR-23-37
NMACFoam (Numerical-model for Membrane-spacer Assemblies and Configurations in OpenFOAM)	SWR-23-57
OCHRE ™ Gymnasium (ochre_gym)	SWR-23-47
PVade (PV Aerodynamic Design Engineering)	SWR-23-49
pyletid	SWR-23-40
Sulfur Thermal Energy Storage Machine Learning ML	SWR-23-02
tih_vqe (Variational Quantum Eigensolver for the Bond Dissociation of Hydride Diatomic Molecules)	SWR-23-32

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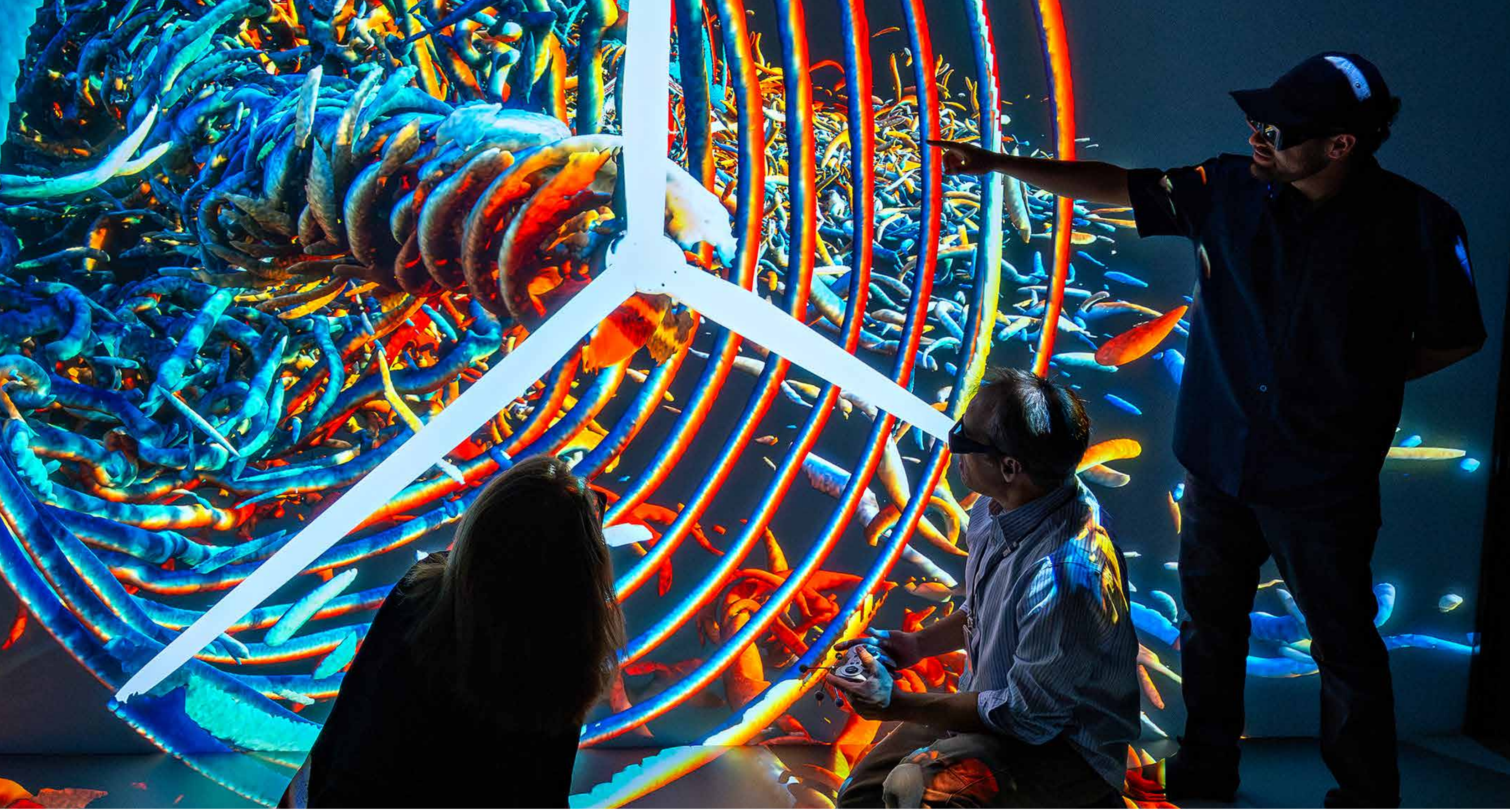

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