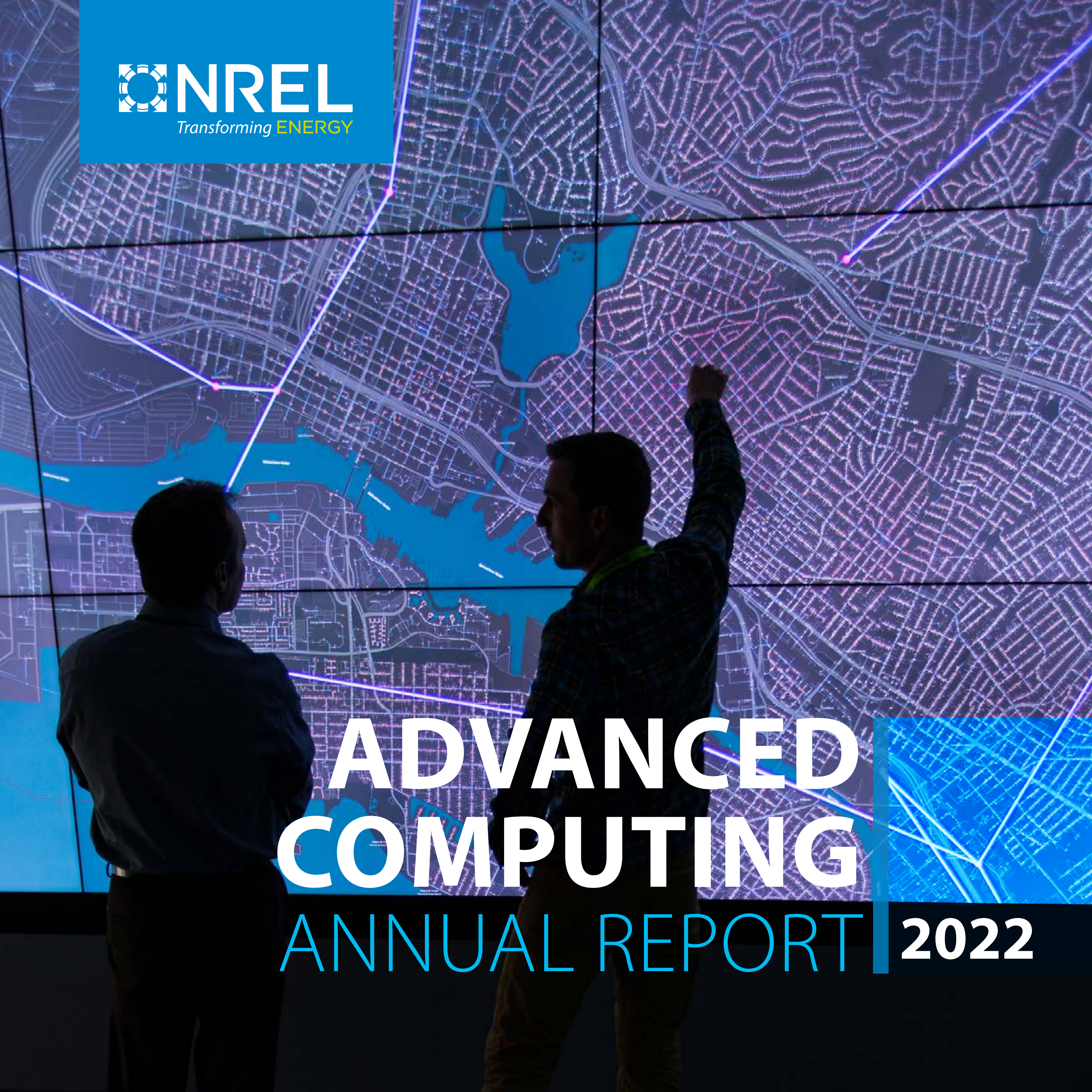

NREL
Transforming ENERGY

ADVANCED COMPUTING

ANNUAL REPORT 2022

Director's Letter

Advanced computing at the National Renewable Energy Laboratory (NREL) had an exciting 2022. For the second consecutive year, more than 300 projects advanced the U.S. Department of Energy's (DOE's) Office of Energy Efficiency and Renewable Energy (EERE) mission across 12 funding areas.

Cross-disciplinary collaboration among NREL researchers yielded more than 800 technical outputs in Fiscal Year 2022 (FY 2022). All this great work continues to advance the science of energy efficiency and renewable energy.

As the dedicated computing facility for EERE, NREL plays a critical role across the research portfolio. To stay at the cutting edge of the latest advancements in high-performance computing (HPC) technology, we are preparing for the installation of our next-generation HPC system in our Energy Systems Integration Facility (ESIF) data center. The new supercomputer, Kestrel—named for a falcon with keen eyesight and intelligence—will complement the laboratory's current supercomputer, Eagle, during the transition. When completed in fall of 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 1.031. Looking to the future, a 2.5-MW power and corresponding cooling upgrade is underway to support Kestrel, bringing the data center to a new capacity of 7 MW. 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. NREL's 2D tools now offer a multisurface, multi-user space to interact with data. In FY 2022, the team installed a 100-megapixel display that is at the forefront of high-resolution displays within DOE, as well as sophisticated touch surfaces, which has revolutionized the environment with extremely high-fidelity interactive analysis. Updates to NREL's 3D immersive room ("the cave") more than doubled the resolution and now enable multiple users to be immersed at once, exploring the virtual reality simultaneously from their own perspectives. These new, advanced technologies, including high-resolution displays and state-of-the-art interactive touch capabilities, bring complex data to life for researchers.

Many exciting developments are 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 for rapid-breakthrough science. 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

555 HPC USERS

93% HPC AVAILABILITY

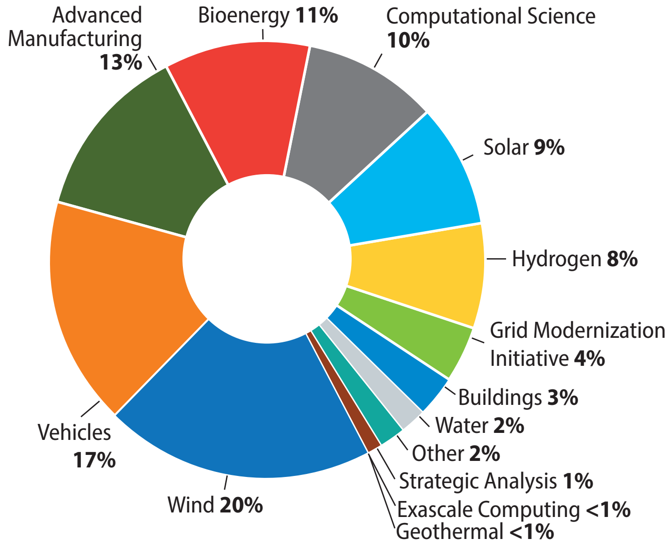
92% HPC UTILIZATION

FY 2022 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.

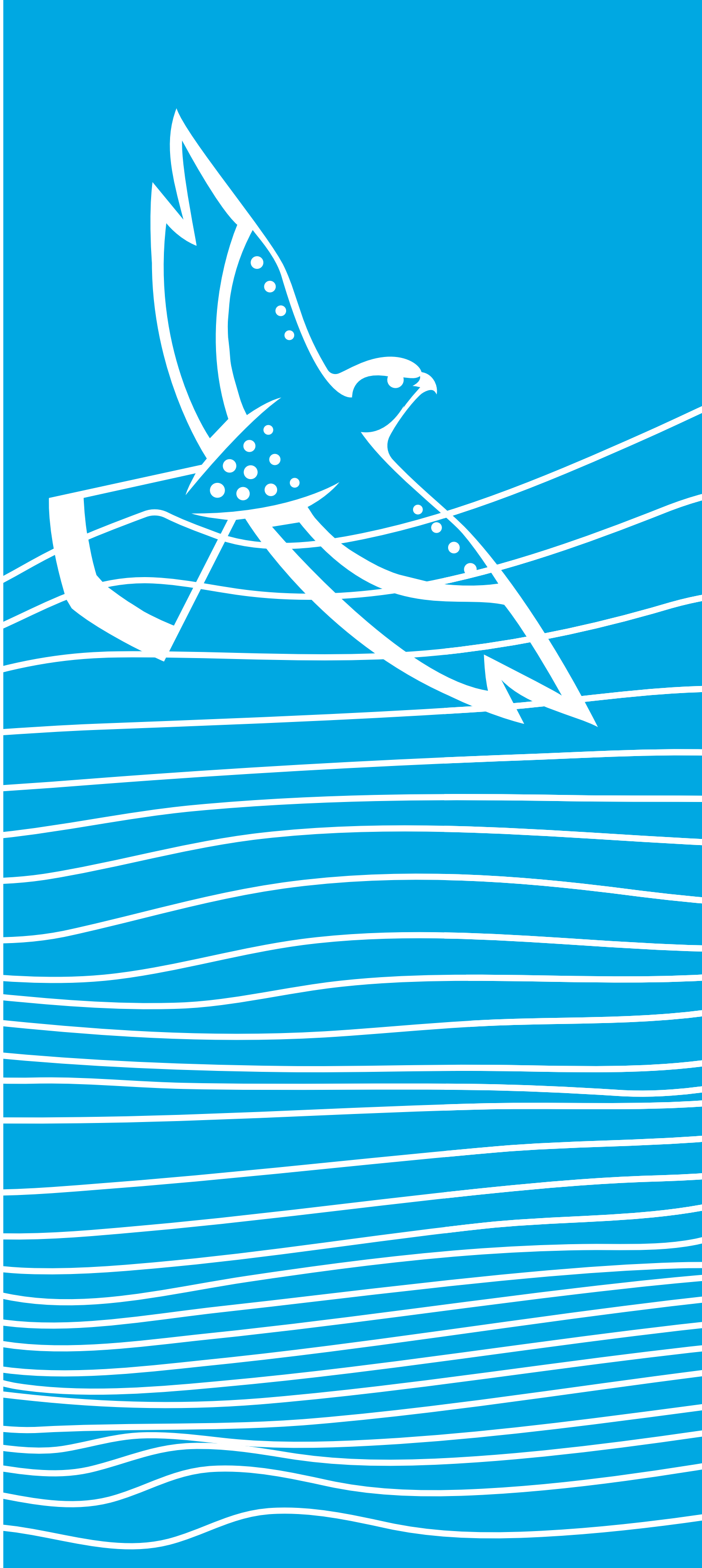
Funding Area	# of FY 2022 Projects
Advanced Manufacturing Office	29
Bioenergy Technologies Office	24
Building Technologies Office	12
Computational Science/Industry/LDRD	57
Grid Modernization Initiative	35
Geothermal Technologies Office	1
Hydrogen and Fuel Cell Technologies Office	14
Solar Energy Technologies Office	29
Strategic Analysis	21
Vehicle Technologies Office	44
Wind Energy Technologies Office	40
Water Power Technologies Office	10
Total	**316**

Percentage of HPC Usage in FY 2022 by Research Area



Kestrel Takes Flight

NREL's third-generation, high-performance computing system—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. Rapidly advancing applications and technologies in artificial intelligence (AI) and machine learning (ML) 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 (CPU)-only and graphics processing unit (GPU)-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 Visualization Capabilities Drive Discovery, Decision-Making, and Reasoning

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 NREL's 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 FY 2022, NREL developed a visual analytics capability that takes full advantage of the Insight Center's new 100-million-pixel display. This advanced visual analytics framework supports both geographic and abstract time-series visualizations. Geographic visualizations support cross-domain data explorations, for example, at the interfaces of transmission and distribution electric systems, communications assets, and other geographic data sets. Abstract visualization capabilities support multi-user, interactive analysis of high-dimension systems with multivariate timeseries, for example, in understanding power grid phenomena and their corresponding system-wide dynamics. These high-resolution capabilities are providing new views of data that are not possible on laptops—especially with increasing size and complexity of energy systems data—leading to new insights, knowledge discovery, and collaborative stakeholder analyses needed for decision-making in energy system transformation.

Building Trust in Artificial Intelligence To Ensure Equitable Solutions

Researchers at NREL see an urgent alarm in the convergence of known and unknown biases in AI. Our vision—a clean energy future for the world—is impossible if we do not address this problem. If we want everyone to have access to clean energy, that means we must plan for equity and ensure solutions do not create inequitable outcomes. And because AI and machine learning play a major part in our clean energy solutions, we need to address the potential for bias throughout the innovation process. Bias can actively derail our progress, as well as create problems that are costly or impossible to address in the later stages. NREL's computational scientists are discovering AI and ML applications to help deliver clean energy solutions to communities across the country and around the world. "We have had great success applying AI and ML breakthroughs to clean energy deployment and scale, but one grand challenge in the greater AI field at large is ensuring equitable outcomes. We at NREL see this as an opportunity to be bold and lead the way to more equitable solutions," said Ray Grout, director of NREL's Computational Science Center. In the research and development life cycle, that equitable AI process begins with our research methodologies. NREL researchers are working to quantify how bias gets introduced in modeling, simulation, and other scientific or analytic processes; identify methodologies to address the bias particularly in scenarios where the availability of data is sparse; and develop foundational AI techniques to prevent bias in outcomes.

INTEGRATED ENERGY SYSTEMS

Over 200 Scenarios Explore Trade-Offs of U.S. Transmission System Buildouts

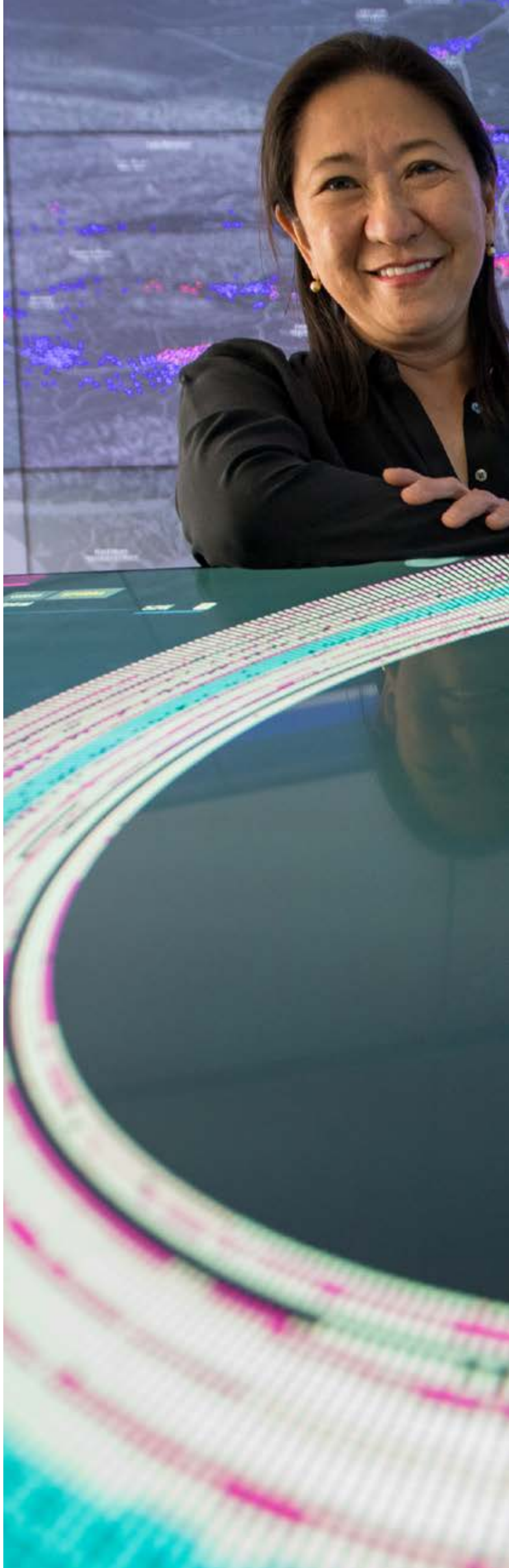
Co-leading the National Transmission Planning Study, NREL and Pacific Northwest National Laboratory (PNNL) are producing transmission expansion recommendations based on a set of planning scenarios coordinated by DOE with industry, states, and regional planning entities. The study—funded by DOE's Office of Electricity, Grid Deployment Office (GDO), and EERE Strategic Analysis Team—will articulate a national approach to upgrading the electric transmission system through scenario analysis. This year, the project set the foundation for the multiyear effort by aggregating large amounts of public and industry data related to the U.S. transmission system. The team created weather parameters from climate change models at the resolution needed for power systems models using ML techniques developed at NREL. The team also modeled more than 200 scenarios to explore trade-offs of different transmission buildouts, using NREL's publicly accessible Regional Energy Deployment System (ReEDS™) capacity planning model.

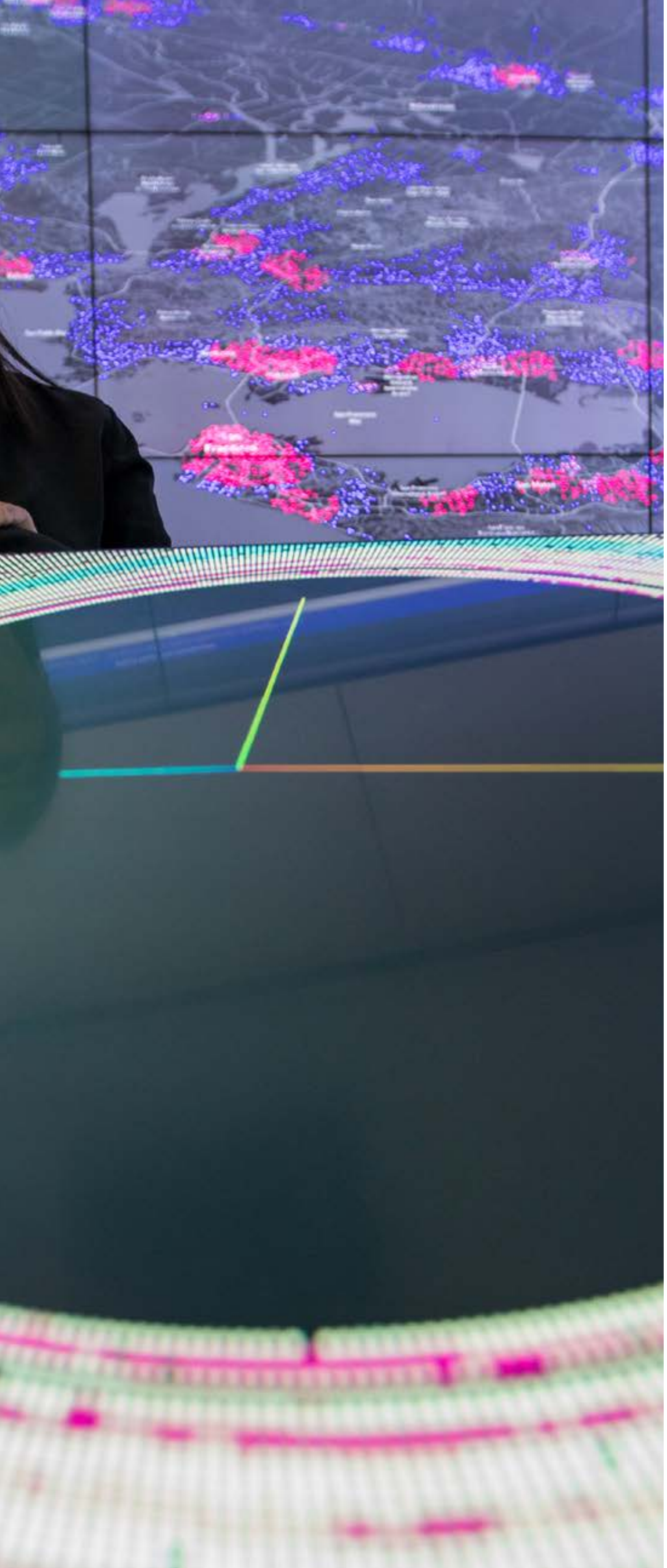
Publicly Accessible, User-Friendly Datasets Answer Buildings Energy Analysts' Questions

Evaluating the impact of deploying distributed energy resource measures—including energy efficiency, electrification, and demand flexibility—is critical to EERE's mission to equitably transition the United States to net-zero greenhouse gas emissions. Decision makers at federal, state, utility, and community levels need access to building energy usage information to accurately assess electrification's long-term impacts. They need detailed datasets to assess potential energy and cost savings for buildings after measures are implemented, to understand the impact of changing building codes, to characterize the impact of electrification measures on peak demand, and to determine the economic and market potential of heat pumps replacing other types of heating.

The successful calibration and validation of DOE's residential building stock and commercial building stock analysis tools, ResStock™ and ComStock™, respectively, supported NREL's objective to produce national datasets that empower analysts working for federal, state, utility, city, and manufacturer stakeholders to answer a broad range of analysis questions. In follow-on work, the team is currently using ResStock and ComStock to create models of a series of energy efficiency and electrification energy measure packages to calculate end-use savings—shapes that quantify the difference in energy consumption between a baseline building and that same building with the measure applied. A new dataset has been released—with all models run by Eagle—consisting of 10 residential impact measure profiles for heat pumps, envelope improvements, heat pump water heaters, and other electrical appliances at various efficiency levels for three weather-year scenarios.

The team created a variety of data access paths for the nearly 80 terabytes of 15-minute time series data, including publicly providing all individual model inputs and outputs and pre-aggregated data files at varying geographic levels, enabling users to easily download and leverage their own custom analyses using standard spreadsheet software. Additionally, a new web-based interactive data viewer enables users to easily query this large dataset and create custom aggregations.



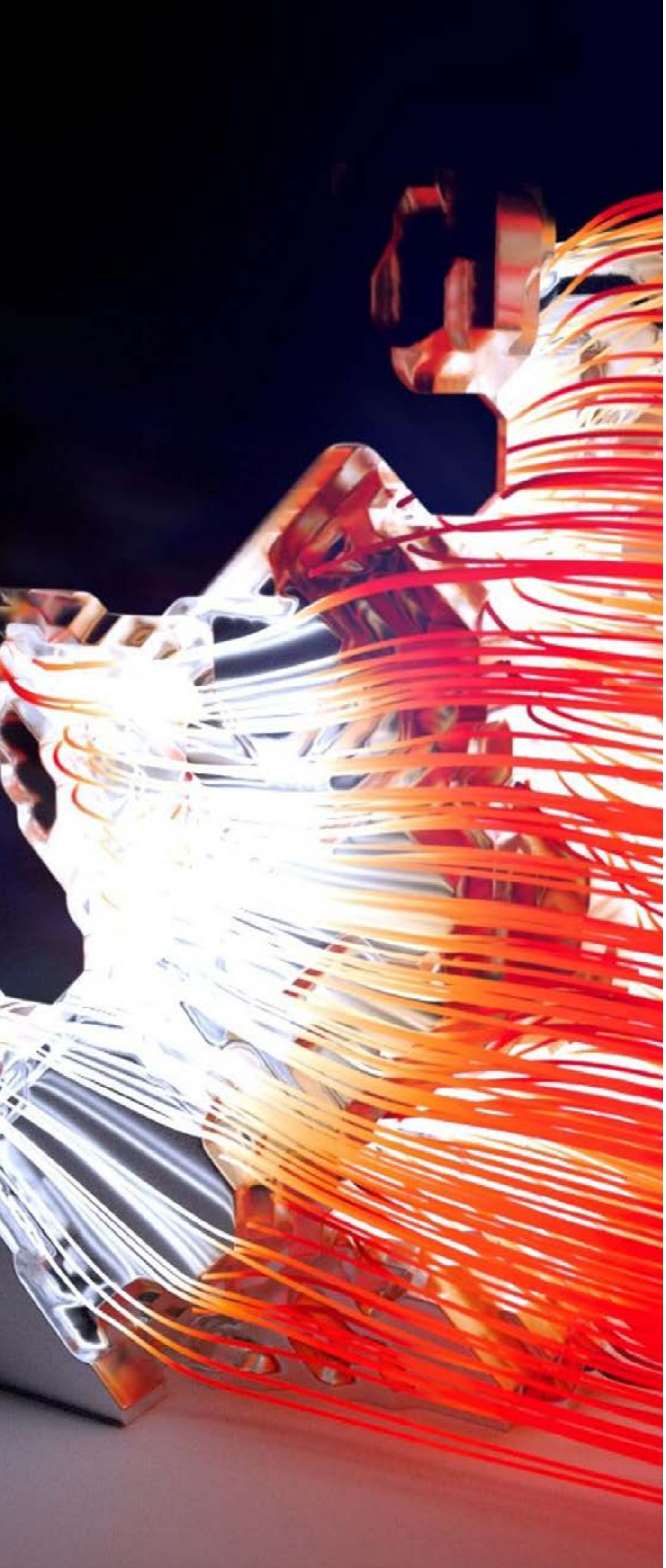


foresee™ Model's Added Emission-Responsiveness and Resilience Factors Inform Residential Community Design and Control

NREL collaborated with affordable housing developers, electric utilities, and equipment manufacturers to reduce operational carbon emissions and enhance energy resilience in residential communities. NREL developed an analysis framework to evaluate the cost-effectiveness of community microgrids and home nanogrids, inform the design of electrical infrastructure, and help developers identify the most appropriate configuration for their communities. In addition, NREL enhanced foresee's capabilities to minimize carbon emissions and prolong resilience operations during extreme weather events by including carbon emission reduction and building energy resilience as part of the model's optimization objectives. To evaluate the performance of the foresee enhancement, the team used ResStock to generate five representative models for typical residential buildings in Boston, Sacramento, and Dallas, and used OCHRE™ to simulate those buildings on Eagle. Each community simulation revealed that most homes achieved greater than 10% carbon emission reduction and cost savings. Results showed that foresee greatly enhanced the resilience of homes during extreme events, continuously operating homes for the longest duration among all scenarios while supporting all critical loads during grid outages.

Modeled Insights Could Make Wind Energy More Competitive and Open New Markets

The Spatial Analysis for Wind Technology Development project develops cutting-edge methods and modeling techniques and performs analysis to inform DOE's Wind Energy Technologies Office (WETO) and stakeholders regarding applied research questions. The multidisciplinary project operates at the cross-section of social, environmental, technical (e.g., radar), and regulatory (e.g., setbacks) siting considerations. Insights enable WETO to expand into new markets, as well as reduce undue risk to both the wind industry and impacted ecology or society. Data and analytical outcomes from this project are leveraged by private companies, utilities, and other federal agencies, including the Bureau of Land Management, Energy Information Agency, EPA, State Department, and the U.S. Agency for International Development (USAID). WETO investments into the Spatial Analysis project have resulted in the development of the Renewable Energy Potential (reV) model, an open-source geospatial techno-economic platform deployed primarily on Eagle. reV was used to quantify interactions between wind potential and plausible siting barriers to deployment, with results integrated into NREL's ReEDS, a capacity expansion model, which evaluated today's constraints and their impact on the power system of the future—revealing that stringent siting restrictions could reduce the pace and scale of wind power's deployment.



Analysis Identifies How To Improve Wind Plant Performance and Reduce Costs

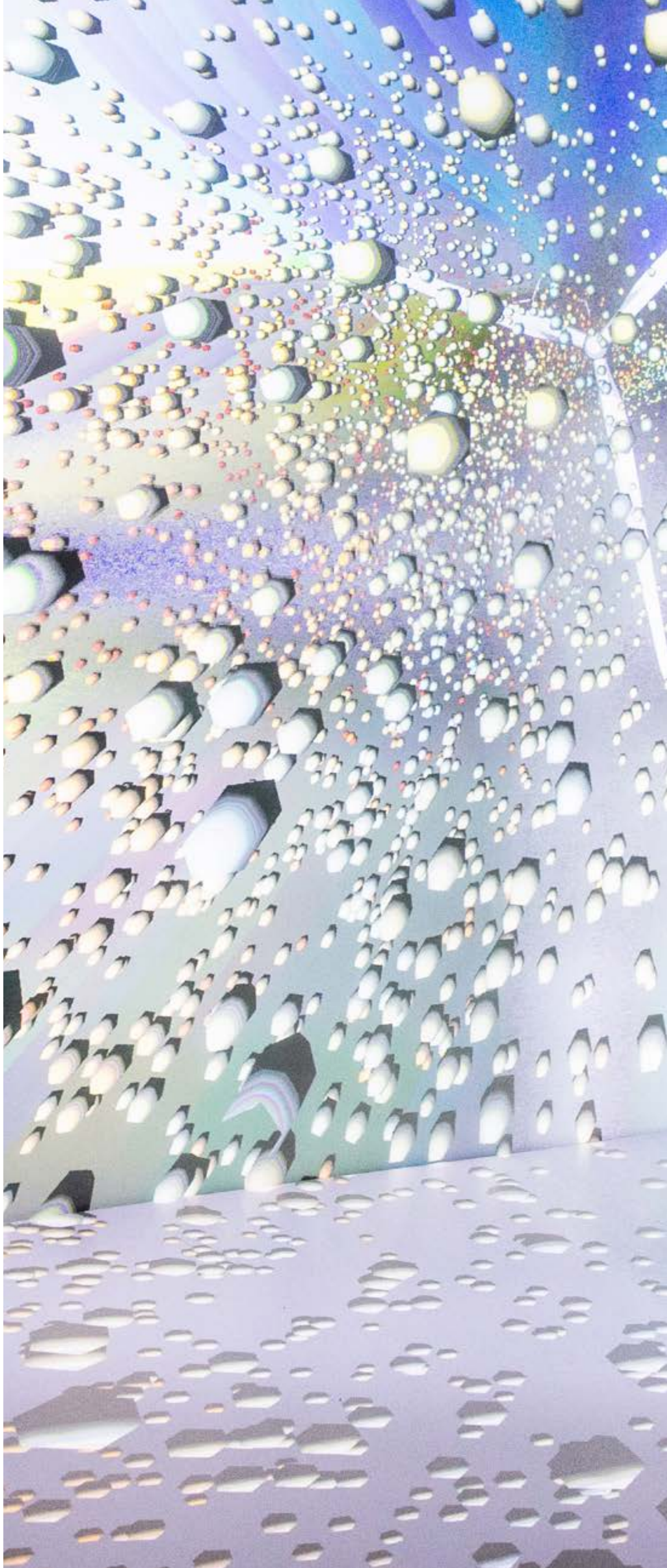
The Integrated Systems Design and Engineering project funded by WETO incorporates advances in computational algorithms, simulation methods, physics-based improvements, and cost and performance modules to assess new technology opportunities and advance the state of the art and best practices in multidisciplinary design analysis and optimization for wind energy applications. In FY 2022, NREL researchers developed a novel method to estimate wind turbine loads without running time-consuming simulations. The approach uses incoming wind velocity profiles to estimate the forces acting on the turbine components. NREL researchers simulated a large ensemble of inflow conditions and array layouts on Eagle to capture the spectrum of possible inflow conditions and generate the load estimates. ML methods were combined with physics-first principles to arrive at the surrogate models for turbine loading. This method could also potentially be applied to any turbine in any position in any type of array layout configuration, a task that typically requires significant modeling fidelity and resolution. Combining this method with simple wake models, such as those used in the wind power plant optimization tool FLORIS, could better account for extreme and fatigue load profiles in turbine control and array layout design studies in a more efficient manner—which could reduce levelized cost of electricity and add value to onshore and offshore wind systems within the greater electricity system.

Resilience Quantification Helps Boost Performance and Prevent Major Power Outages

Funded by DOE's Solar Energy Technologies Office (SETO), a new resilience quantification framework developed at NREL investigates distribution power system resilience. The Eagle HPC system was used to solve different combinations of power system states in parallel—and develop a new set of quantitative metrics with clear physical interpretation to comprehensively evaluate power system resilience.

The NREL team developed both an event-based corrective scheduling model to investigate the optimal restoration solution and help microgrid operators prepare to respond to similar events, and an online predictive control model to provide online decision-making support for operators to handle ongoing outages in the most resilient manner. The framework was tested on power system models based on real-world distribution feeders experiencing faults and extreme events. Simulation results from Eagle have been used to justify the effectiveness and superiority of the proposed quantitative resilience metrics and the resilience enhancement models compared to the state of the art.

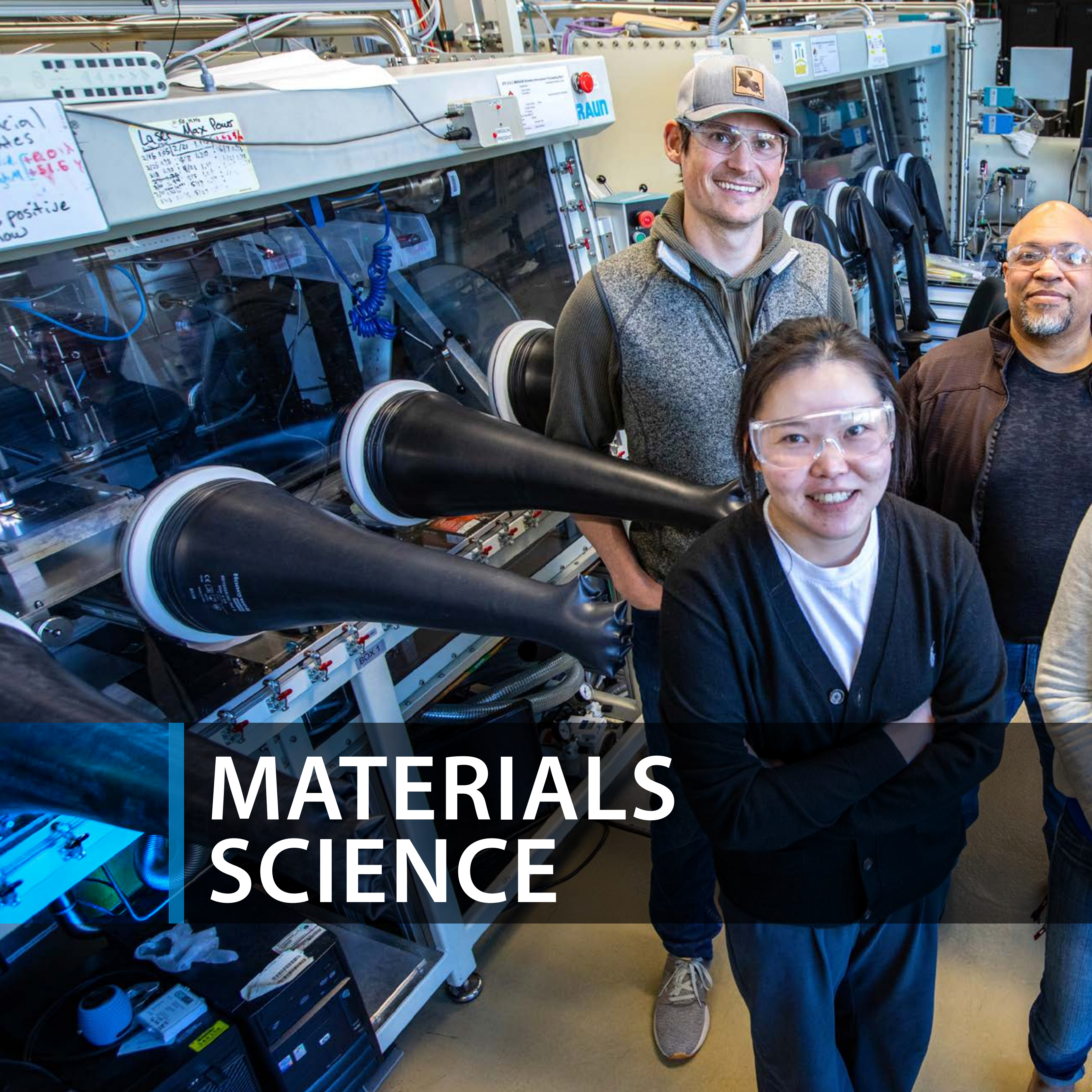
This framework will help the power industry evaluate and compare resilience and, eventually, boost the application of resilience in real-world systems to deal with the increasing threats of extreme events and prevent major power outages. Additionally, this work expanded fundamental research in adaptive power system protection for distribution systems with large-scale integration of distributed energy resources.



HPC-Powered Data Sets Provide Sophisticated Hourly Views of Future Power System Scenarios

With funding from DOE's Strategic Analysis Team, NREL used HPC to model the expansion of the U.S. bulk power system, drawing from NREL's Standard Scenarios. The resulting Cambium data sets are publicly available and contain hourly emission, cost, and operational data for modeled futures of the U.S. electric sector, with metrics designed to be useful for long-term decision-making. New features include the addition of methane, nitrous oxide, and precombustion process emissions; scenarios for 95% decarbonization nationwide by 2035 and 2050; technologies—like bioenergy—with carbon capture and storage and direct air capture; small modular reactors for nuclear; hybrid photovoltaics; battery generators; and renewable combustion turbines.

The new data release builds on the previously available hourly and annual data and now contains month-hour and time-of-day data aggregations. Working groups within the American Society of Heating, Refrigerating, and Air-Conditioning Engineers, Residential Energy Services Network, and Leadership in Energy and Environmental Design are engaging with the emissions data and assembling proposals to incorporate said data into their codes and standards. This projection of the U.S. electric sector's evolution enables sophisticated forward-looking research and decision-making—a major departure from traditional retrospective decision-making.



MATERIALS SCIENCE

Dataset Yields Mediators for Solar Thermochemical Hydrogen Production

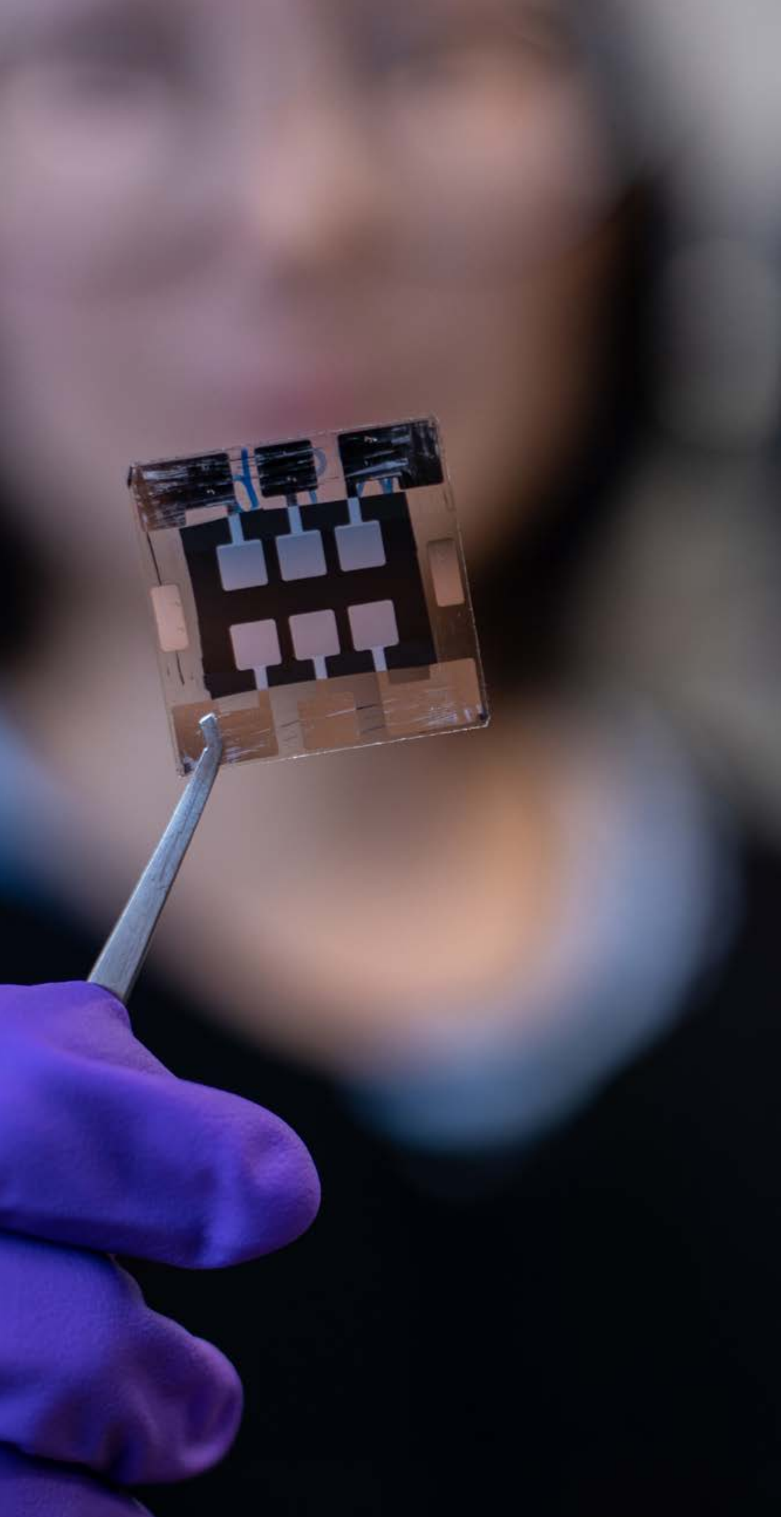
Funded by EERE's Hydrogen and Fuel Cell Technologies Office, and specifically the HydroGEN Advanced Water Splitting Materials Consortium, and in partnership with Sandia National Laboratories, NREL used HPC to predict the properties and accelerate the discovery of novel solar thermochemical hydrogen (STCH) active redox mediators. A promising method for generating carbon-neutral fuels from water using concentrated solar energy, STCH production is currently limited by the efficiency of known redox-mediating materials. Using high-throughput, density-functional theory (DFT) calculations, the team explored the promising perovskite oxide material class to identify superior water-splitting redox mediators. The team computationally investigated the bulk structures and stabilities of nearly 65,000 theoretical perovskite oxides and generated the largest-known computational dataset of these materials. By extending this framework from 83 identified gadolinium-containing STCH candidates to the manganese-containing perovskite oxides, the team rediscovered two previously known STCH redox mediators and discovered three novel STCH-active perovskites. Future work will look at tuning the composition of redox mediators identified from this dataset to maximize the STCH activity of these compounds.

Optimized Band Offset Enables Efficient and Stable Perovskite Solar Cells

With funding from DOE's Office of Science, NREL and collaborators from University of Toledo used DFT calculations to confirm a design strategy for perovskite solar cells (PSCs). The use of 2D perovskite as the interfacial modification layer has shown great potential for improving PSC performance. Using Eagle, researchers achieved computationally demanding hybrid functional DFT calculations while searching for different configurations of metastable 2D polymorphs and the corresponding electronic band offsets. The new design strategy maximizes charge transport using a metastable 2D structure through tuning of hydrogen bonding configurations based on asymmetric organic molecules. The metastable 2D polymorph reduces the energy barrier for charge transport and significantly improves the out-of-plane transport. Efficient and stable PSCs were achieved by using the metastable 2D perovskite surface layer with optimized band offsets between the inorganic planes and the organic cation layers. Improving the PSC device stability could improve viability for commercialization.

Graph Neural Network Accelerates Design of New, Stable Solid-State Battery Materials

A critical barrier to the development of solid-state batteries (SSBs) is the thermodynamic instability of electrode-electrolyte interfaces. Improved SSB design requires new materials that are stable at suitable reduction and oxidation potentials. Discovering new stable materials in unexplored chemical spaces necessitates quick and accurate prediction of thermodynamic stability and efficient search strategies. NREL set out—in alignment with DOE's Energy Storage Grand Challenge 2020—to computationally design new solid-state battery materials using a combination of generalized ML, reinforcement learning, and graph neural networks. Using Eagle, the NREL team developed a new approach to finding stable and functional crystal structures by using a graph neural network (GNN) to predict an upper bound to the fully relaxed energy obtained from DFT. New structures were generated via substitution of known prototypes, and a GNN was trained on a new database of close to 128,000 DFT calculations. Many DFT-validated material candidates were found to be stable and exhibit desired functional properties such as a large electrochemical stability window and suitable reduction and oxidation potentials. This coupling of recent advances in GNNs with reinforcement learning is expected to improve prediction accuracy and structure validity over emerging methods by 8x and 25x, respectively, while reducing computational costs by 100x over exhaustive approaches. The framework will be applicable to a wide range of design challenges in materials science.



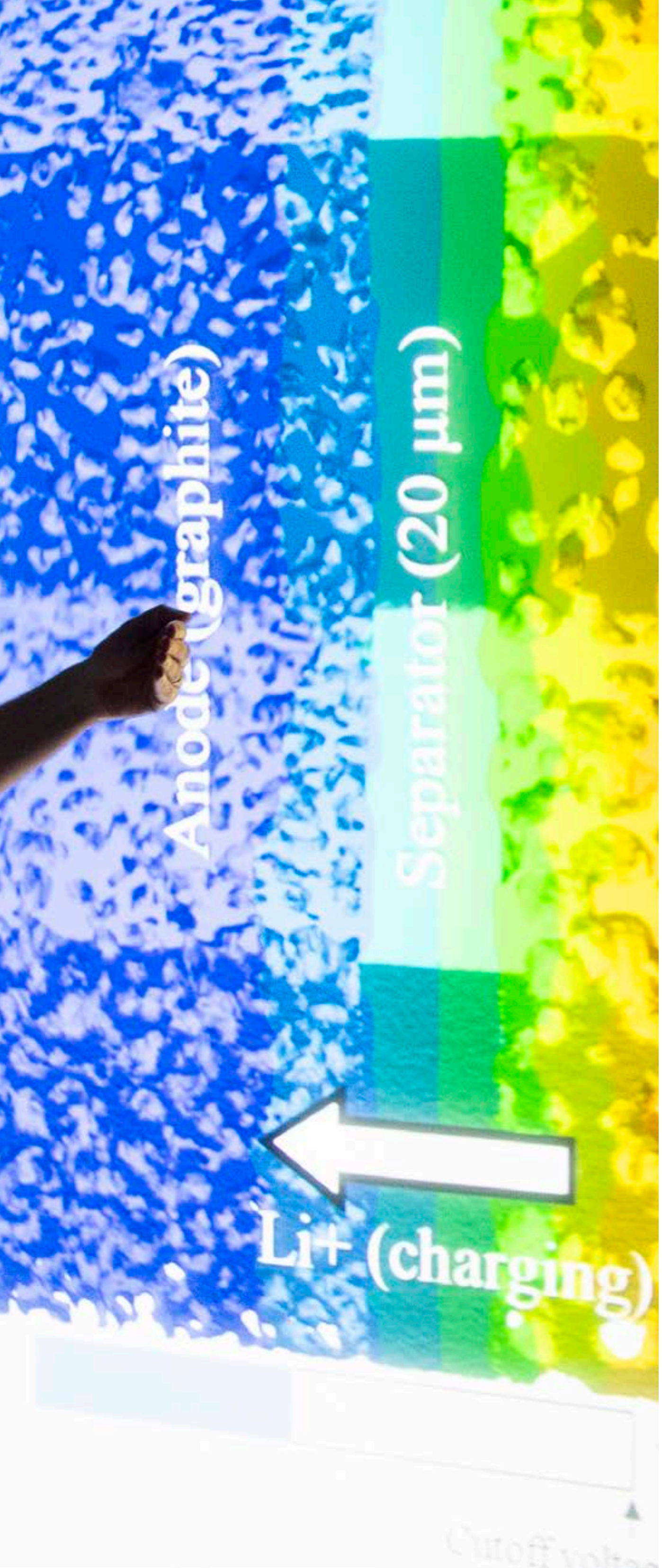
Zero-Strain Li-Ion Cathodes Can Expedite Battery Industry Growth

Funded by DOE's Vehicle Technologies Office (VTO), and with the help of Eagle and Swift computing resources, the NREL, Lawrence Berkeley National Laboratory, and UC-Berkeley team performed simulations to investigate charge-induced volume changes in lithium (Li)-ion cathodes and established general guidelines for designing zero-strain cathode materials (materials that undergo little to no volumetric changes during electrochemical cycling) created without scarce and expensive cobalt and nickel. First-principles methods were used to identify factors that control the volume change upon Li extraction, including composition, ionic ordering, and metal coordination. This resulted in the design of zero-strain cathodes that not only optimize cycling performance but also serve as promising candidates for potential all-solid-state battery applications. All-solid-state batteries offer improved operational safety and the potential for greater storage density and increased reliability, among other benefits. In the next fiscal year, this project at NREL will continue efforts to accelerate the design of earth-abundant disordered rocksalt Li-excess cathode materials with optimal electrochemical performance.

Multiscale Modeling Framework Predicts Structural Characteristics for High-Performance Li-Ion Batteries

With funding from VTO, researchers from Lawrence Livermore National Lab (LLNL) used HPC—including NREL's Eagle—to generate ML potentials to simulate performance deterioration of solid-state electrolytes—useful alternatives to liquid electrolytes found in Li batteries. The team used the ML potentials as a foundation for constructing and validating an integrated multiscale modeling framework to simulate crystalline, disordered, and amorphous lithium lanthanum zirconium oxide (LLZO) systems across a wide range of conditions. The model was based on a neural network algorithm and trained using ab initio data, and represents the first of its kind specifically optimized to capture the complex atomic disorder present at interfaces and boundary regions. Performance tests prove that the developed ML potential can predict accurate structural and vibrational characteristics, elastic properties, and Li diffusivity of LLZO comparable to ab initio simulations.

As a demonstration of its applicability to larger systems, the team showed that the potential can correctly capture grain boundary effects on diffusivity—proposed as key performance bottlenecks—as well as the thermal transition behavior of LLZO. These examples show that the ML potential enables simulations of disordered structures with quantum-level accuracy at speeds thousands of times faster than ab initio methods. Results obtained from these atomistic simulations are now being incorporated into the MesoMicro continuum code, which can evaluate the additional impacts of grain structure and other microstructural features on transport and chemo-mechanical failure modes coupling effects under realistic battery cycling conditions.



Atomic-Scale 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 enable and accelerate the development of new catalyst materials and optimize conversion processes to produce fuels and chemicals from biomass and waste resources. Now in its tenth year performing atomic-scale simulations powered by NREL HPC, in FY 2022 this project provided insight into the structure and composition of active sites on multicomponent catalysts important for the development of carbon dioxide, biomass, and waste conversion processes. Specifically, NREL's Eagle supercomputer enabled the discovery of the particle surface structure and composition of low-cost molybdenum carbide catalysts needed to advance diverse reaction applications, including carbon dioxide hydrogenation (which can renewably produce multiple important C1 feedstocks, including formic acid, carbon monoxide, methane, and methanol), and Fischer-Tropsch synthesis and hydrodeoxygenation for the conversion of biomass to hydrocarbons. In addition, this project worked in collaboration with the Chemical Catalysis for Bioenergy (ChemCatBio) DataHub project to develop a high-throughput framework for evaluating catalyst deactivation via impurity adsorption trends across metal and metal-oxide catalyst materials. Data will be uploaded to the ChemCatBio Catalyst Property Database—an online library of catalyst property data that aims to make it faster and cheaper to identify the right catalyst formula for targeted biomass and waste conversion processes.

Inverse Polymer Design Identifies Performance-Advantaged, Bio-Based PET Replacements

In search of a sustainable replacement for polyethylene terephthalate (PET)—a nonbiodegradable, crude oil-based polymer—NREL's Inverse Bioproduct Design team, with support from DOE's Bioenergy Technologies Office, combined ML and molecular simulation to narrow the candidate pool of materials that have the highest probability of achieving desired performance. Using Eagle, and in collaboration with experimental work performed by the Performance-Advantaged Bioproducts experimental counterparts team, the Inverse Polymer Design project used a data-driven approach to identify and validate a bio-based polyester replacement. Their molecular simulations provided design principles for recycle-by-design polymers, which could not be determined through analytical techniques. An AI-based tool developed by the team, PolyIDTM, enabled computational screening of more than one million bio-based polymers so experimental efforts could focus on polymers with the greatest performance. The impact of this project is being realized within five partnered projects, including DOE's multi-organizational BOTTLE Consortium. Two of these projects include industrial partners that are using the tools developed within this project, including computational predictions.

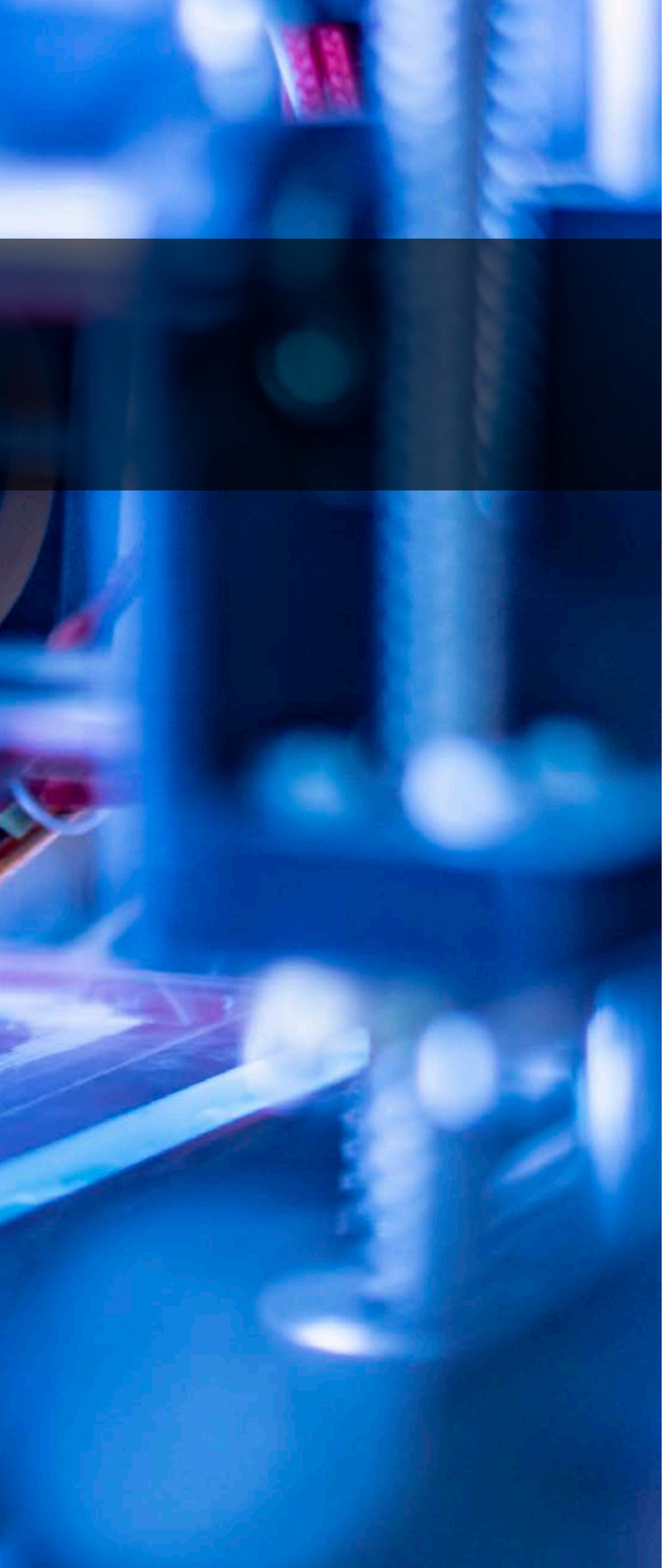
Modeling Defect-Free Interface for CdTe Thin-Film Solar Cells

Interface recombination is one of the limiting factors affecting the performance of cadmium telluride (CdTe)-based thin-film solar cells—an alternative to silicon-based cells that can be manufactured quickly and inexpensively. Advancing these technologies increasingly requires control and design of interfaces between dissimilar materials. The direct interface between CdTe and stannic oxide (SnO2) is highly defective because the two crystal structures do not match well. Using an interface structure prediction algorithm called Kinetically Limited Minimization, in conjunction with DFT calculations, NREL researchers used Eagle to model the interface between CdTe and SnO2, discovering a unique, atomically thin 2D interlayer structure of cadmium chloride that facilitates a seamless lattice transition and removes defect-states from the band gap. Subsequent device simulations based on the predicted interface properties demonstrated the theoretical feasibility of bufferless oxide-CdTe heterojunction solar cells approaching the theoretical efficiency limit. Results will inform approaches to cost-effective manufacturing of efficient CdTe-based thin-film solar cells.

Discovery of Novel Contact Materials for CdTe Thin-Film Solar Cells

Funded by First Solar Inc.—one of the leading producers of thin-film CdTe solar cells—and with support from SETO, NREL performed a computational search for a new p-type back contact for CdTe solar cells in order to minimize absorber-contact interface recombination and thus improve their lifetime and efficiency. NREL used first-principles DFT calculations in combination with models to predict the various materials properties that are needed for a back contact. With extensive use of the NREL Materials Database, NREL computed and assessed the thermodynamic bulk and interface stability, carrier mobility, band gap, band alignment with CdTe, and dopability of a set of approximately 300 semiconductors. Through this effort, NREL identified seven new potential candidates for CdTe back contacts. Additionally, NREL found that binary alloys of some of these candidates offer the flexibility to tune band-edge positions that will likely suppress the deleterious interface barrier effects.

MANUFACTURING



Thermal Energy Storage Simulations Offer Product Design Optimization for Industrial Heat Processes

Funded by DOE's Advanced Manufacturing Office (AMO) and in partnership with LLNL's HPC4Energy Innovation Program, NREL used Eagle to advance thermal energy storage (TES) product design using a high-fidelity HPC model validated by experimental data. Applying NREL experience in complex fluids and ML design, the team modeled heat transfer to optimize sulfur TES designs by validating various modeling approaches to deal with challenging property variation with temperature and transient simulations. TES that increases the utilization of waste and renewable heat could provide significant energy savings and reliable heat sources, decrease emissions, and increase U.S. manufacturing competitiveness through reductions in fuel consumption. This work was performed for Element 16 Technologies, Inc., which seeks to develop and commercialize low-cost and high-impact molten sulfur TES for dispatchable industrial process heating. The NREL team has been successfully achieving the project goals in supporting Element 16's product development and accelerating its technology to market. Two papers from the collaboration have been submitted for publications, with ML code being published for public use.

Modeling High-Pressure Membranes for Water Desalination via Reverse Osmosis

To facilitate the development of innovative manufacturing processes for desalination, researchers must understand the influence of existing membrane manufacturing techniques on polyamide membrane properties, microstructure, and morphology at high-pressure reverse osmosis. Using Eagle for high-accuracy molecular dynamics simulations, the NREL team compared polyamide reverse osmosis membranes fabricated via industry-leading techniques: molecular layer-by-layer deposition, interfacial polymerization, and 3D-printing techniques. Membranes fabricated with 3D printing have similar performances to those manufactured using molecular layer-by-layer deposition, showing impermanent open-closed pores that enable water to jump through membranes. Membranes formed with interfacial polymerization exhibit faster water transport, lower rejection, worse structural integrity, and more inhomogeneous network pores. Water movement across membranes formed with interfacial polymerization provides a continuous transport channel at high pressure, with more significant compaction features at high pressure than for membranes formed with 3D printing or molecular layer-by-layer deposition.

The multiscale model connects manufacturing methods to membrane chemistry, structure, and function. Results will guide the manufacturing of high-pressure reverse osmosis membranes to replace energy-intensive thermal desalination—ultimately reducing the energy consumption of brine concentration. Financial support comes from the National Alliance for Water Innovation (NAWI), funded by AMO.

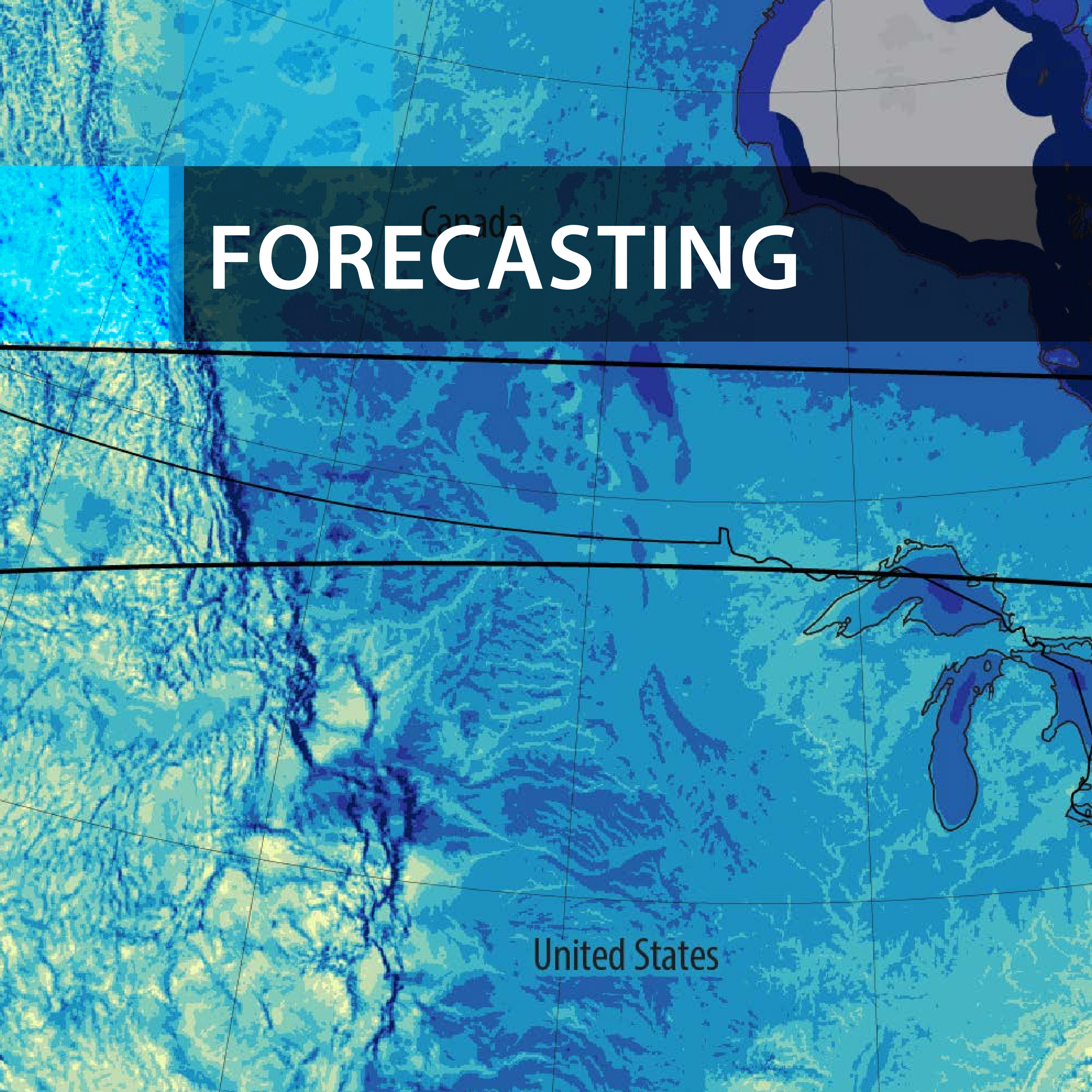
Optimizing Water-Supply Pathways Under Climate Uncertainty

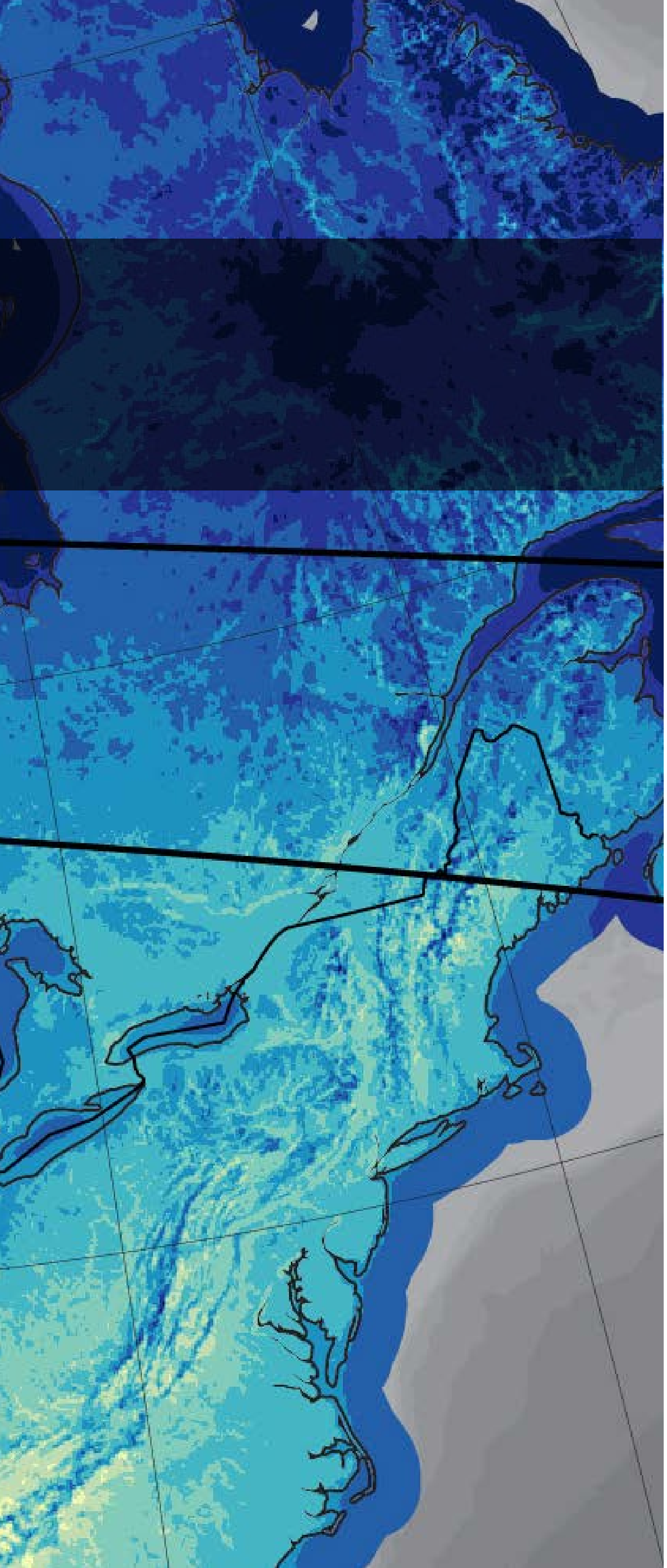
Increasingly frequent droughts strain municipal water resources and challenge urban drought planning. Novel decision-support tools are needed to assess the interactions between climate uncertainty, hydrological variability, and technology attributes. In 2022, the Drought Resilient Inter-scale Portfolio Planning (DRIPP) model was introduced to generate flexible pathways of water supply portfolio expansion under climate uncertainty at high spatial, temporal, and technological resolution.

The Stanford team created a decision-support tool to help partners address urban water insecurity. The tool—run on Eagle—and findings were shared with research partners in the City of Santa Barbara, who informed the framing and research questions and provided data. In Santa Barbara and similar coastal cities, drought intensity, not duration or frequency, is the main driver of planning cost, risk of incurring water shortage, and regret associated with planning for the wrong drought type. Results for Santa Barbara show that higher climate resilience can be achieved through a diversified portfolio of water augmentation measures that includes modular, rapidly deployed technology, such as technology for distributed water reuse. The generalized design of Stanford's tool encourages adoption by other cities, and findings on water conservation policies will maximize the benefits of water efficiency investments. Future work will include development of climate-specific research and development targets for new water technologies by identifying cost-optimal technological attributes for enduring droughts of varying duration and severity.

This work is supported by NAWI, and funded by AMO and the California Department of Water Resources.

FORECASTING



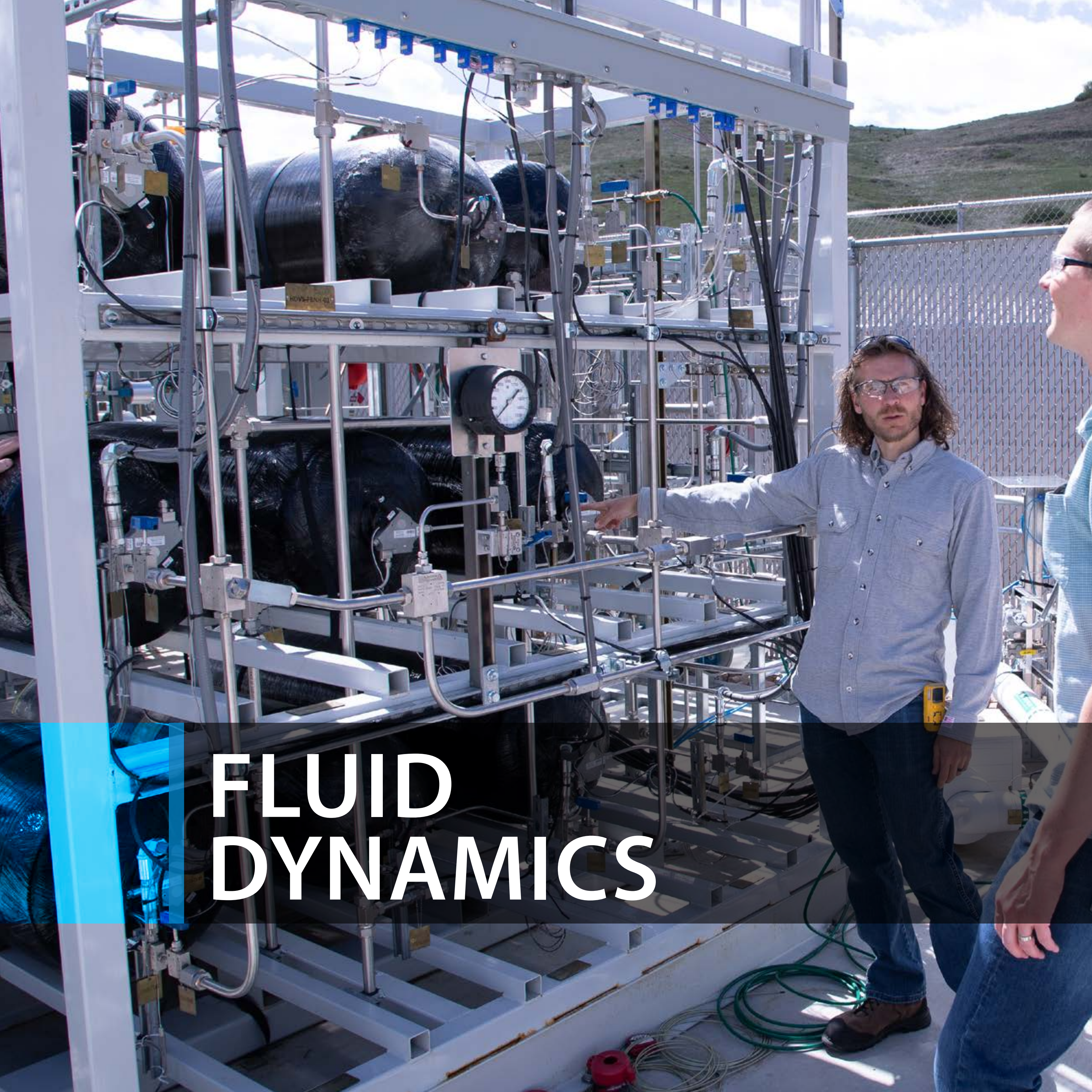


Producing Uniform Solar and Wind Forecasts Across CONUS

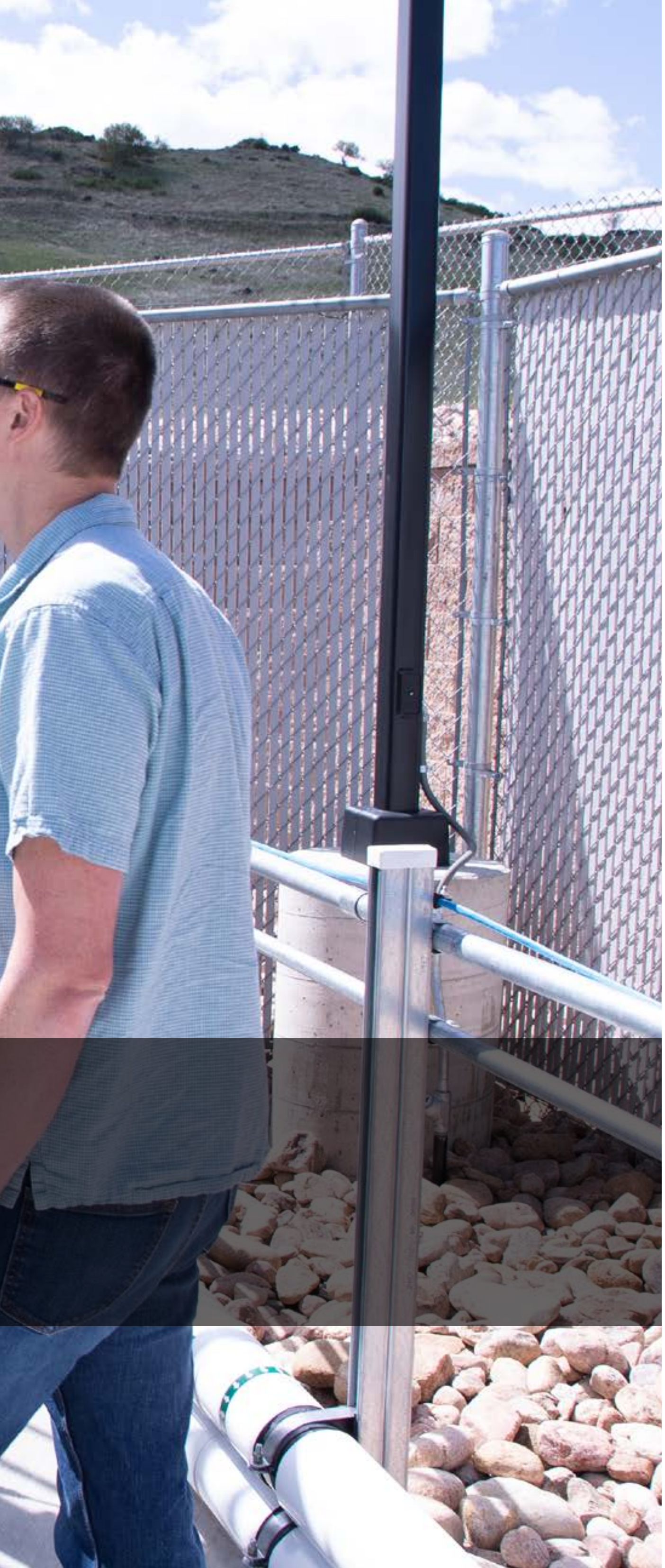
To address the lack of uniform power data points among multitudinous resource data sets, the North American Energy Resilience Model team developed a combined wind and solar power forecasting service using NREL's Eagle. Researchers created a system framework that integrates weather prediction data and time series data processing, converting disparate resource data points into uniform power data points. The numerical weather prediction forecasts are combined with Energy Information Administration (EIA) generator metadata to convert wind and solar resource data into power data, ultimately providing site-specific, day-ahead forecasts for all known installed wind and solar generators across the continental United States (CONUS). Eagle was used in conjunction with the High-Resolution Rapid Refresh model archive, which is supported by the University of Utah and produced by the National Center for Environmental Prediction. This is the only tool that can generate accurate day-ahead forecasts for all EIA-860 solar and wind plants in CONUS, and these forecasts are pushed to the cloud for use by other DOE laboratories to simulate day-to-day operations and perform resilience and reliability analyses.

Data Sets Inform Scenarios for Puerto Rico's Path to 100% Renewable Energy

Evaluating 100% renewable energy pathways through an integrated analysis process will support Puerto Rico in reaching its renewable energy goals, help ensure energy system resilience against future extreme weather events, and advance energy justice. An important part of generating scenarios for the Puerto Rico Grid Resilience and Transitions to 100% Renewable Energy Study (PR100) is the development of solar, wind, and hydropower data sets. These datasets allow determination of the resource potential, capacity factor, technical potential, and supply curves for wind, solar, and hydroelectric sources of generation. For example, high-quality, user-friendly, gridded wind resource datasets for all of Puerto Rico will enable users to estimate wind energy development costs. Also run on Eagle for PR100 are dGen™ modeling of distributed rooftop solar and storage adoption, the Engage model, and grid operations analysis—critical to confirming reliability. The project, led by GDO and funded by the Federal Emergency Management Agency, developed new simulation parameters that enable accurate simulation of wind speed; the team then generated 20 years (2001–2020) of deterministic and ensemble data sets and postprocessed these outputs using NREL's WIND Toolkit so that they can be used easily by downstream models. The data sets generated provide the baseline for models used in scenario analyses and selection of paths forward.



FLUID DYNAMICS



First-Ever Simulations of Medium- and Heavy-Duty Hydrogen Tank Fueling Processes

DOE and four industry partners—Air Liquide, Honda, Shell, and Toyota—funded an NREL project to perform computational fluid dynamics (CFD) simulations of thermal and flow fields inside medium- and heavy-duty hydrogen vehicle tanks during fueling processes—which had not been previously demonstrated in experiment and numerical simulation prior to this work. The Eagle system's rapid CFD simulations enabled robust, accurate evaluation of thermal and flow fields inside hydrogen tanks under various fueling conditions; these in turn revealed which fill conditions cause gas temperature in the tanks to overheat. These CFD models were validated in parallel with hardware research inside ESIF's Hydrogen Infrastructure Testing and Research Facility. The hardware testing consisted of some of the first-ever fast-fill (10 kg/min transfer of 80 kg+) datasets generated in the medium- and heavy-duty fuel cell electric vehicle space.

Simulations Tune Offshore Wind System Models and Predict Hydrodynamic Performance

To improve offshore wind system design, NREL performed three validation studies using high-fidelity CFD simulations of the DeepCwind floating wind platform. The first two supported the OC6 project—an international research project run under IEA Wind focused on validating the tools used to design offshore wind systems. With funding from WETO and using Eagle, the two studies respectively validated the CFD predictions of the nonlinear, low-frequency wave loads and the free-decay motion of the platform. The third validation study was also funded by WETO and supported the Reproducible CFD Joint Industry Project for Floating Offshore Wind Application, focusing on the global performance of the platform in realistic irregular seas. NREL leveraged state-of-the-art numerical tools for coupling nonlinear potential-flow waves to CFD simulations, and predicted the nonlinear, low-frequency responses to 3-hour irregular seas through high-fidelity CFD simulations. The low-frequency responses of semisubmersible offshore wind platforms can have significant contributions to structural loads. The results of the three studies greatly increase confidence in using high-fidelity CFD simulations to accurately predict the nonlinear responses. These simulations can be used directly in the design process or to tune mid-fidelity, engineering-level models when measurements from more costly wave-basin experiments are unavailable. These results also greatly facilitate the CFD investigation of the novel TetraSpar offshore wind platform as part of OC6 Phase IV planned for FY 2023.

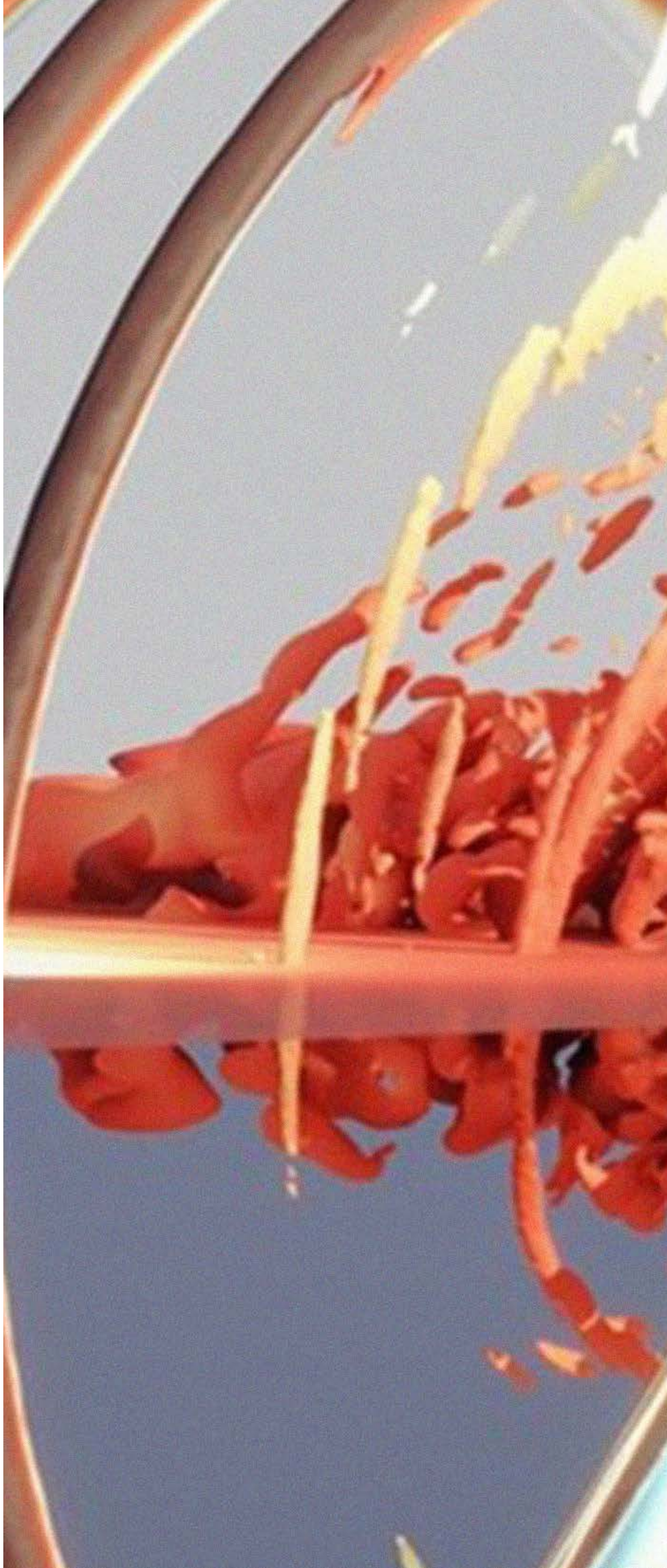
Revealing Ideal Temporal and Regional U.S. Coastal Conditions for Wave Energy Planning

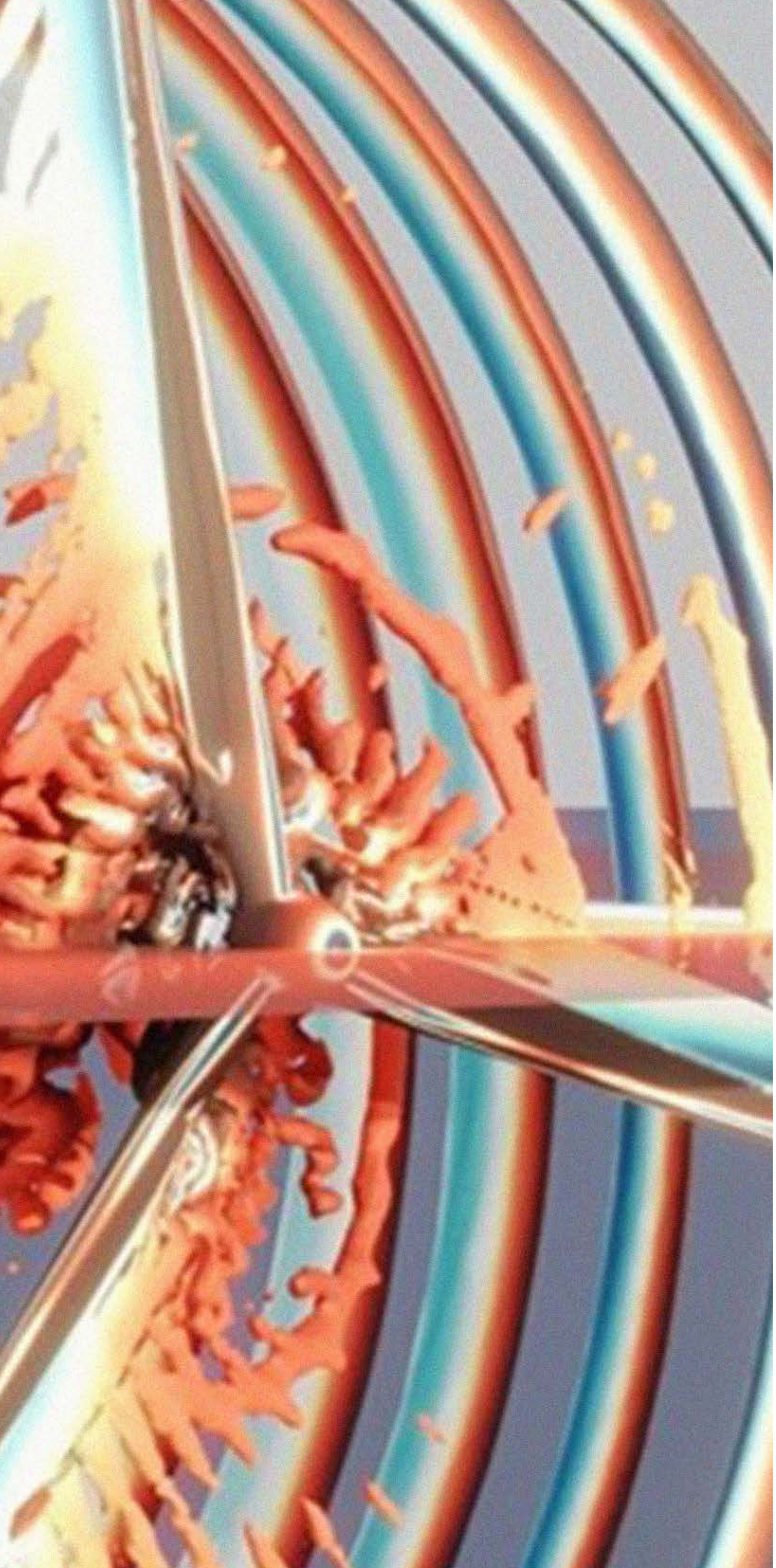
High-resolution wave hindcasts—numerical model simulations that estimate past wave conditions—are the basis for understanding how and where wave energy can contribute to the nation's energy goals. The data output from these models is critical to estimating how much energy can be generated from waves, identifying where wave energy projects should be built, and how devices should be designed. Using Eagle, the multilab team of researchers at PNNL, Sandia, and NREL simulated wave climates using an unstructured, nested-grid modeling approach and validated the results against wave buoy measurements. The hindcast reproduced the wave field over 42 years at high temporal (3 hours) and spatial (approximately 200 meters in shallow water) resolution. This approach captured the seasonal variation of the sea state: large waves that occur in the winter and early spring months, and the calmed sea state during the summer. The nested-grid modeling framework employed in this study provided a powerful and efficient modeling approach to accurately simulate wave climate over greater temporal and regional scales with sufficiently fine resolutions in the nearshore region. Results will inform the deployment of wave energy converters and other nearshore instrumentation/devices in nearshore regions, assist in prioritizing hotspots for near-term market opportunities and development, and provide wave resource assessment data and information to inform resource estimates for marine and hydrokinetic energy technologies..

Augmenting Exascale-Reacting CFD Codes

Over the past 7 years, DOE's Advanced Scientific Computing Research (ASCR) Exascale Computing Program (ECP) has supported the development of simulation tools for turbulent combustion and for wind farm analysis, both of which target massive calculations on the world's largest supercomputers, but with only a limited ability to incorporate flow in and around complex boundary geometries. However, many NREL-specific applications, such as screw auger feeder reactors and oscillating airfoils, consist of moving parts with extremely complex geometries. Researchers are taking advantage of Eagle to augment the ECP flow codes with highly robust solution algorithms that can accurately and efficiently incorporate these complex-shaped, moving simulation domains. The new capabilities dramatically expand the applicability of the ECP-developed tools.

In addition to augmenting the geometry capabilities of the ECP codes, researchers have added important physical sub-processes to expand the applicability of the tool set. In the combustion area, for example, NREL is developing the tools to improve the potential of ammonia to become a mainstream carbon-free fuel by pursuing the idea that low-temperature plasma-assisted ignition of ammonia can reduce ignition delay, improve flame stability, and reduce nitrogen oxide emissions. The team has implemented a model that captures the most important effects of a nanosecond low-temperature plasma discharge, including fast gas heating and the production of key radicals useful for enhancing the reactivity of the mixture. By incorporating such details into the ignition process, researchers now have a more complete picture of the entire combustion process and the tools to analyze and optimize the system holistically.





Largest-Ever Ultralight Downwind Turbine Rotors Yield Optimal Design and Resilience

With NREL's Eagle and funding from Advanced Research Projects Agency–Energy, the Segmented Outboard Articulating Rotor (SOAR) project investigated the techno-economic feasibility of ultralight downwind turbine rotors at the 25-MW scale—the largest ever designed. Downwind-facing rotors provide advantages over upwind rotors, including decreased mechanical loads and lower likelihood of tower strike, resulting in desirably reduced rotor mass. HPC-powered aerodynamics, structural, and control designs resulted in upscaled and redesigned models demonstrating that larger blade lengths are possible with cone-wise load alignment. The systems engineering frameworks Wind-Plant Integrated System Design & Engineering Model and Wind Energy with Integrated Servo-controls Toolset and the aeroservoelastic solver OpenFAST were used to assess these designs, revealing that blade segmentation and outboard pitching may be the key to rotor design at this large scale. SOAR is a continuation of the Ultralight Morphing Rotor project, which studied the conceptual design of two-bladed downwind turbine designs of 13.2 MW, 25 MW, and 50 MW. SOAR's results have informed DOE-funded projects such as the Big Adaptive Rotor project and the Wind Systems Engineering project.

A BROADER COMPUTING ECOSYSTEM

Chicago's Road Map to Savings via Deep-Energy Retrofits

To address the City of Chicago's goal to reduce residential energy use intensity by 50%, NREL, in collaboration with Elevate, is proposing, assessing, and field-validating deep-energy retrofits. NREL developed retrofit packages using the ResStock residential energy analysis tool, whose simulations were computed on Eagle and analyzed and post-processed using cloud computing. The ResStock simulations quantified the costs of the building retrofits, as well as their potential energy, cost, and carbon emission savings. These findings helped inform Elevate's city-scale analysis and field validation for priority building segments by proposing viable packages for the field test and providing expected energy savings for comparison. This research showcases a road map to achieving energy savings and utility bill savings via energy-efficient retrofits paired with high-efficiency air-source heat pumps in community areas that have historically been targets of disinvestment. Additionally, this research showcases the benefits of heat pumps not only for efficient heating but increasing the penetration of air conditioning in Chicago's residential homes.

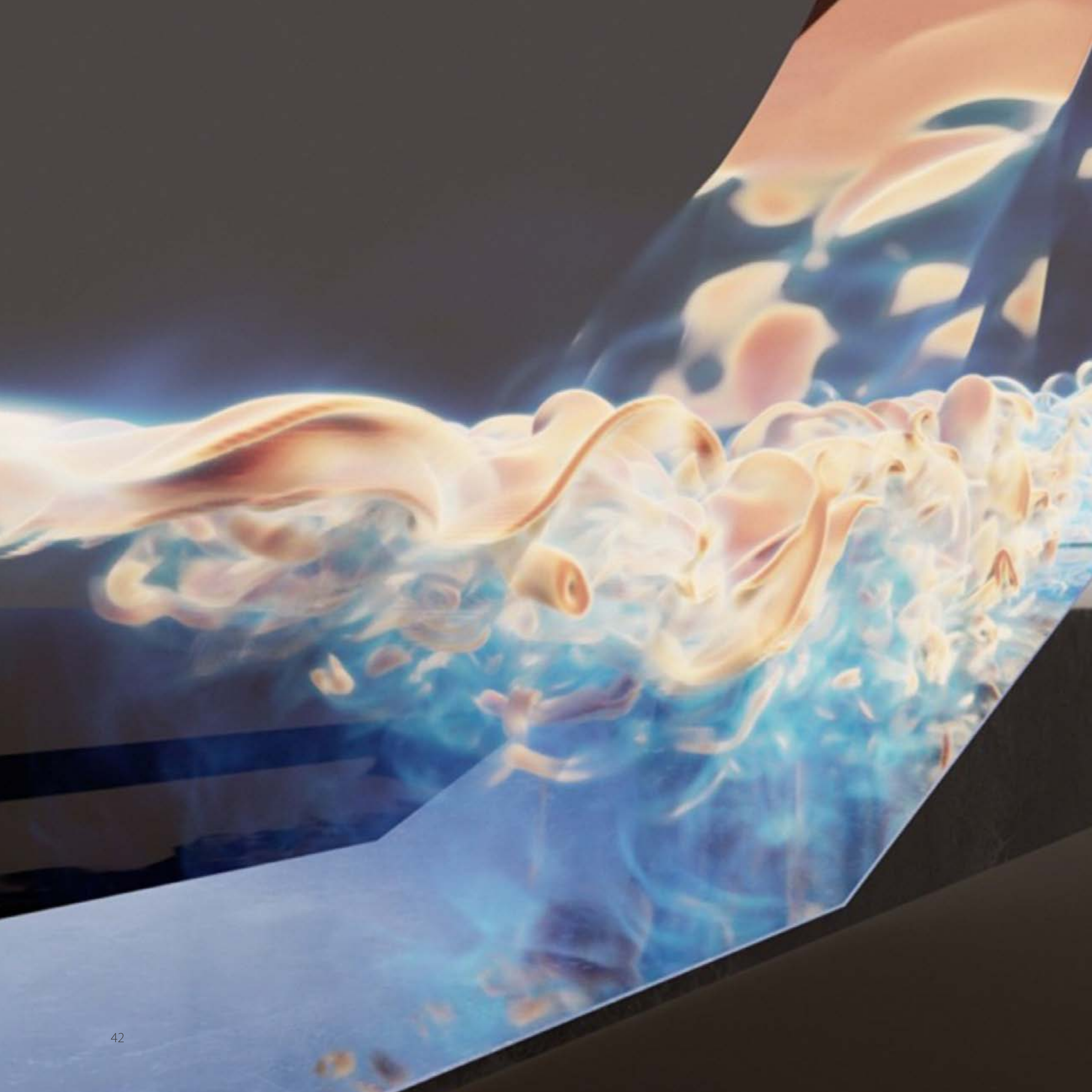
Marine Energy Atlas Advances Online Data Availability

Funded by DOE's Water Power Technologies Office (WPTO), the Marine Energy Atlas tool provides researchers and commercial entities the ability to easily visualize and download class-leading data sets, which can be used in a wide variety of project planning, device development, or marine operations tasks. Model development and validation was led by PNNL and Sandia National Laboratories with extensive collaboration from NREL. In 2022, NREL-supported cloud resources were utilized to provide public access to the tool as part of ongoing efforts within the Marine Energy Resource Characterization project. The open-access data include the WPTO Wave Hindcast Dataset, a high-resolution spatial and temporal dataset on key wave parameters that spans 40 years, which is crucial for siting marine renewable energy projects. The Capacity Factor Tool within the Atlas calculates a wave energy converter's capacity factor in a given area, helping developers estimate performance of equipment in different locations, and providing spatial data visualization of outputs. This tool sees active daily usage and its data have already been used in several projects beyond NREL and contributing partners. Availability of Atlas on the cloud has also encouraged contributions to the development team—building a significant list of requested features—and has established a baseline for future partnerships.

Expanded Access to WIND Toolkit—International and Long-Term—Enables Analysis of Wind Resource Potential and Decarbonization

With funding from WETO, NREL provided the original Wind Integration National Dataset (WIND) Toolkit, which is currently the largest publicly available U.S. wind power dataset in the world. In FY 2022, NREL's cloud services and Highly Scalable Data Service (HSDS) application enabled data download capabilities of wind resource datasets for Central Asia, India, Mexico, the Philippines, and Vietnam, as well as the offshore areas and land-based wind resources in the entire United States. Wind resource datasets for foreign countries were developed with funds from USAID or supported by the Mexican government (in the case of Mexico) to help capacity building in these countries and aid grid integration studies.

NREL also provided the newly developed WIND Toolkit Long-term Ensemble Dataset (WTK-LED) 20-year dataset, which combines continental and offshore wind datasets and includes Hawaii and Alaska, and will replace the aging hardware/tech stack with a renovated web-based delivery system powered by Amazon Web Services and the HSDS infrastructure. Access and use of WTK-LED data has included TU Delft to analyze wind potentials for airborne wind energy, UC Merced to support research for a zero-carbon grid in California, and the DOE-funded National Intra-hour Wind Power Production Database project.



Bridging to DOE Leadership Computing

Insights Into Topological Semimetal Properties Guide Development For Applications

Electronic materials, including semiconductors, have historically been a backbone of clean and sustainable energy technologies. Now, a newer class of materials called topological semimetals exhibit high electron mobilities, low phonon mean free paths, and the ability to control electron spin, making them promising materials for low-power electronics, thermoelectrics, and catalysts. Control of point defects and alloying will be critical to manipulating these properties similarly to semiconductors, but more must be understood about the defect-composition-property relationships in topological semimetals before designing them for next-generation technologies.

Funded by DOE's Office of Science Basic Energy Sciences program, NREL is using Eagle and National Energy Research Scientific Computing HPC platforms to computationally evaluate how defects and impurities influence bandstructure, carrier concentration, and potential electron scattering behavior. That information is then used to direct semimetal synthesis to tailor their properties and behavior, as well as being applied to understanding the origin of phenomena found in topological semimetals, such as linear magnetoresistance, and inspire new applications.

NREL HPC Sets Stage For Largest Wind Farm Simulations

Researchers at NREL, Sandia National Laboratories, Oak Ridge National Laboratory, and Lawrence Berkeley National Laboratory are creating the ExaWind code for predictive simulations of wind turbine and wind farm fluid dynamics and structural dynamics. NREL's Eagle supercomputer has been the principal platform for developing, implementing, and validating ExaWind physics models. ExaWind researchers used NREL's Eagle supercomputer to show that ExaWind can simulate a wind farm where eight orders of magnitude are resolved—from micron-scale boundary layers near wind turbine blades to the kilometer-scale domain. A tenet of ExaWind is that it must be performant on current HPC systems and next-generation supercomputers accelerated with GPUs. Through an ECP allocation on the Summit supercomputer, researchers have been developing and optimizing ExaWind on GPUs, showing that simulations primarily run on GPUs can be significantly faster that CPU-only simulation. Eagle and Summit simulation results were the foundation of a successful proposal for a 2022 allocation on Summit through the ASCR Leadership Computing Challenge (ALCC) program. The ALCC simulations will set the stage for simulations on the Frontier supercomputer, the fastest in the world, and are expected to be the largest, highest-fidelity wind farm simulations to date. Since 2016, funding for ExaWind has been provided by the WETO and ECP.

INNOVATIONS & PUBLICATIONS

Software Records

Title	NREL Number
RLC4CLR: Reinforcement Learning Controller for Critical Load Restoration Problems	SWR-22-27
Hybrid-RL-MPC4CLR: Hybrid Reinforcement Learning Model Predictive Control for Reserve Policy-Assisted Critical Load Restoration in Distribution Grids	SWR-22-25
MPC4CLR: Model Predictive Control for Critical Load Restoration in Power Distribution Systems	SWR-22-24
Geothermal OSR: Energy Predictor for Geothermal Open-Source Reservoir	SWR-22-23
VE: Virtual Engineering of Low-Temperature Conversion	SWR-22-19
GANISP: A GAN-Assisted Importance Splitting Probability Estimator	SWR-22-10
PowerGridworld: A Framework for Multi-Agent Reinforcement Learning in Power Systems	SWR-22-07
Graph-Env: Graph Search as a Reinforcement Learning Problem	SWR-22-37
JobQueue-PG: A Task Queue for Coordinating Varied Tasks Across Multiple HPC Resources and HPC Jobs	SWR-22-41
BUTTER: An Empirical Deep-Learning Experimental Framework	SWR-22-42
G2Aero: Separable Shape Tensors for Aerodynamic Applications	SWR-22-44
PeleLMeX: An Adaptive-Mesh Low Mach Number Hydrodynamics Code for Reacting Flows	SWR-22-48
MPRL: Multi-Pulse Reinforcement Learning	SWR-22-49
L-Marshal: Python Lightweight Marshaler	SWR-22-55
Mesoflow: A Mesoscale Modeling Tool for Heterogenous Gas-Solid Reacting Flows	SWR-22-56
BDEM: Discrete-Element Simulator for High-Solids Granular Flows	SWR-22-72
NOODLES: NREL Object-Oriented Data Layout and Exploration System	SWR-22-78
LBC: Learning Building Control	SWR 22-21
dsgrid: Demand-Side Grid Model	SWR-21-52
ParaEMT: Parallelizable Large-Scale Power System Electro-Magnetic Transient (EMT) Simulator	SWR-22-16
ML4PD: Machine Learning for High-Throughput Process Design	SWR-22-62

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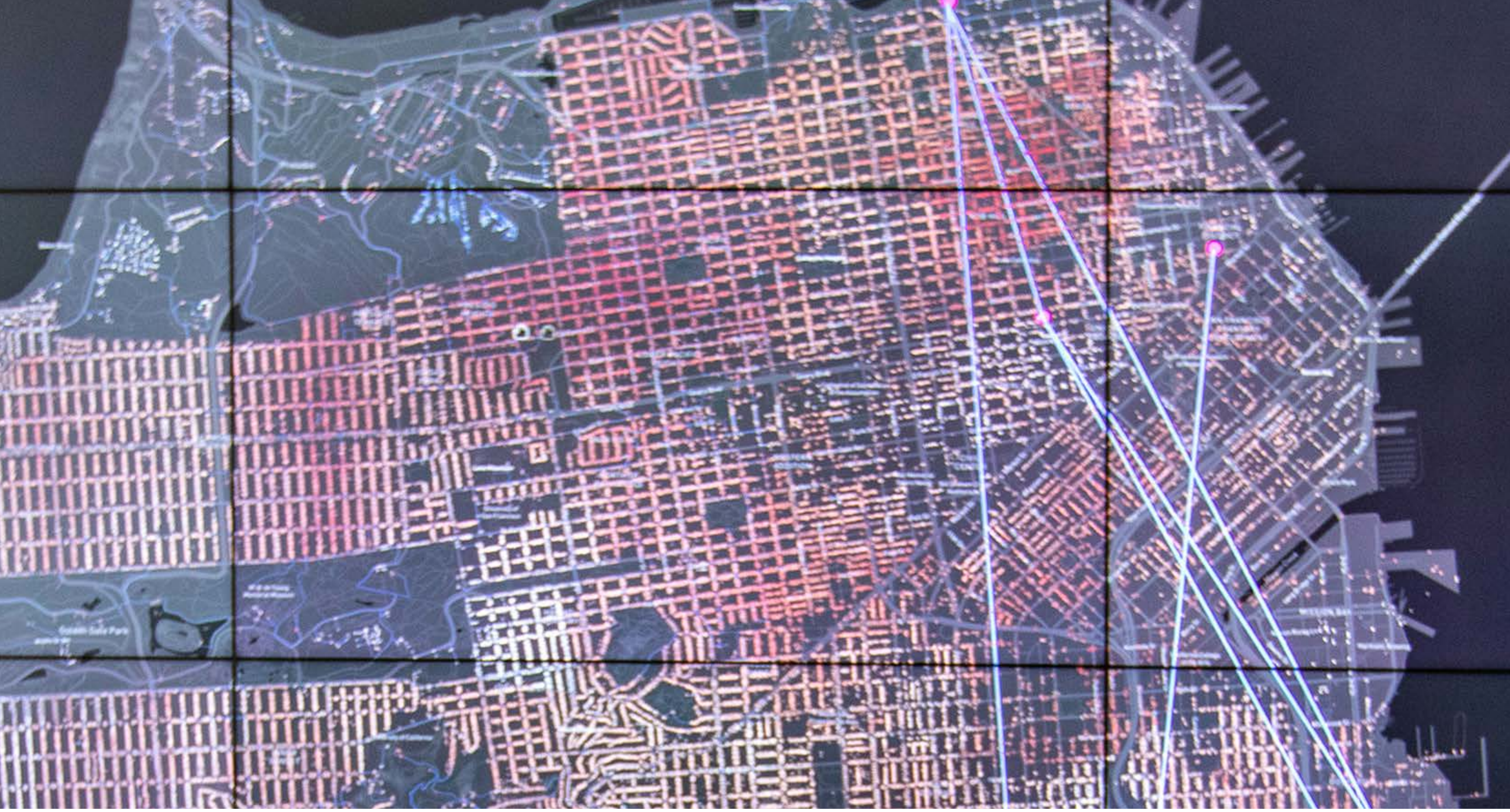

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