NREL
Transforming ENERGY

HPC at NREL: **FY 2019**

HPC at NREL: The Year in Perspective

The high-performance computing (HPC) and related capabilities at NREL's Energy Systems Integration Facility (ESIF) are the primary HPC resources for the U.S. Department of Energy's (DOE) Office of Energy Efficiency and Renewable Energy (EERE). EERE-funded research and development projects are eligible to request computation time on the HPC system. Our computational resources support the breadth of EERE's mission to accelerate the advancement of renewable energy and energy efficiency technologies by providing:

- Robust HPC capability
- Domain-relevant expertise in modeling, simulation, machine learning, computational science, applied mathematics, and analysis at large scales
- Data management, scientific visualization, storage, and related services.

During Fiscal Year (FY) 2019, the NREL HPC User Facility supported 182 modeling and simulation projects advancing the mission across the spectrum of energy efficiency and renewable energy technologies. See pages 12–23 of this brochure for highlights from those projects.

Our big news in FY19 was the delivery and installation of our new HPC system, Eagle. Eagle was delivered in September 2018 and put into production on January 2, 2019, and users began transitioning their project work to the new system. Peregrine was decommissioned on July 31, 2019.

Peregrine paved the way as NREL's flagship compute system and the world's largest supercomputer dedicated to energy efficiency and renewable energy. With Eagle's robust 8 petaflops of peak performance, NREL's HPC capability in support of EERE has more than tripled. During the month of December 2018, as part of an Early Science effort on Eagle, a handful of projects were given dedicated time on the new system to help test the new capability to see what could be accomplished on Eagle that could not be accomplished on Peregrine. See pages 10–11 of this brochure for highlights from those projects.

In addition, the innovative liquid-cooling approach used by Eagle and its predecessor has led, in part, to two recent honors for the ESIF HPC Data Center: a 2018 Federal Energy and Water Management Award and the prestigious Data Center Dynamics 2018 Data Center Eco-Sustainability Award. The global recognition our data center is receiving cements its position as the most energy-efficient data center in the world. And now, with Eagle up and running, we're poised to deliver more scientific insights than ever before to advance our nation's energy transformation.

Lastly, there is no rest in the HPC world. Even though Eagle was put into production in January 2019, we will be kicking off the ESIF-HPC-3 project in January 2020 to gather requirements and develop specifications to be used as we look to acquire a new HPC system that will replace Eagle, to be delivered in the spring of 2022.

Steve Hammond

Director, Computational Science Center

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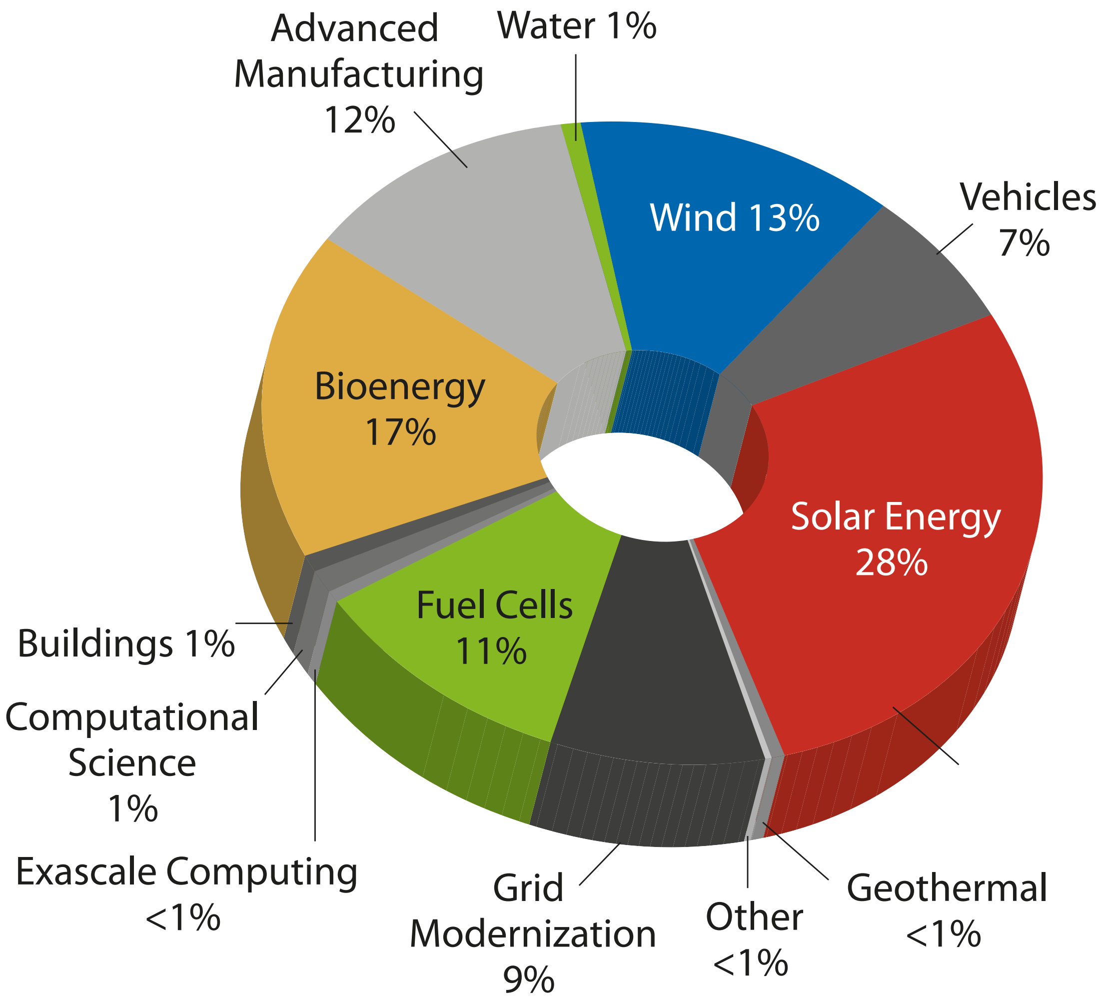
Partners from Hewlett Packard Enterprise (HPE) joined NREL and DOE January 8, 2019, to celebrate NREL's new 8.0 petaflop supercomputer Eagle, capable of carrying out 8 million-billion calculations per second. *Photo by Dennis Schroeder, NREL*

HPC Usage Demographics

The NREL HPC User Facility supported **182** modeling and simulation projects advancing the DOE mission across the spectrum of energy efficiency and renewable energy technologies in FY19.



HPC Systems

NREL's HPC User Facility operates HPC systems in the ESIF HPC Data Center in support of the DOE and EERE mission. The work performed on these systems leads to increased efficiency and reduced costs for mission-critical advanced energy technology solutions, including wind and solar energy, energy storage, and the large-scale integration of renewables into the electric grid.

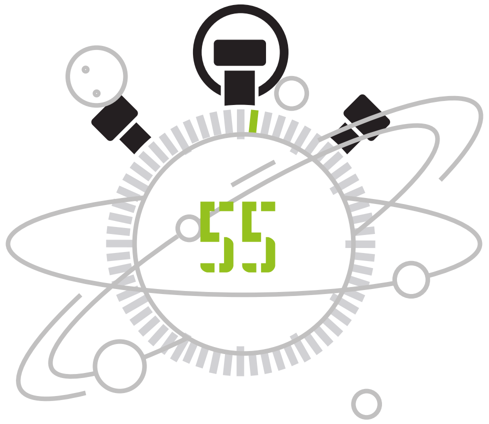
Current systems include **Eagle** (HPC cluster), **Gyrfalcon** (mass storage), **SparkPlug** (OpenStack cluster), and **Tanager** (GPU cluster).

Eagle: NREL's Newest Supercomputer Dedicated to EERE Research

As a replacement for NREL's prior supercomputer, Peregrine, Eagle was put into production use in January 2019. Like Peregrine, Eagle was designed and built by Hewlett Packard Enterprise (HPE) and has an innovative warm water liquid-cooling system that allows waste heat to be captured for reuse.

The system is a Linux cluster that uses a fast InfiniBand network. It is composed of 2,114 interconnected "compute nodes" with 4,228 Intel Skylake processors and a total of 76,104 cores—along with 14 petabytes of high-speed data storage. The peak performance of Eagle is approximately 8 petaflops, or 8 million billion floating point (mathematical) operations per second.

PEAK PERFORMANCE



In just under a minute (54.4 seconds), Eagle can do as many calculations as there have been **seconds in the universe** (4.352e17 seconds).

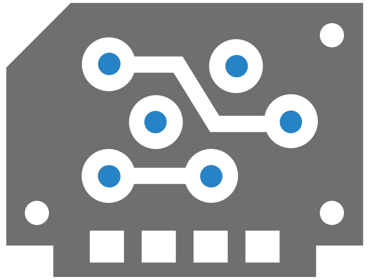
HIGH-SPEED DATA STORAGE

Where information is saved.

To match the same amount of (high-speed data) storage, you'd need 28,000 500-GB laptops—which would stack **1,423 feet, or 433.8 meters, high.**

Random Access Memory or RAM

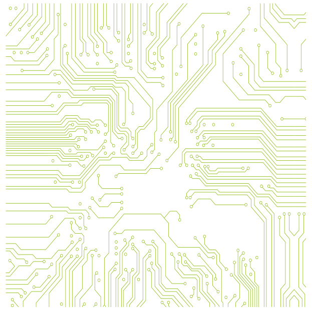
More RAM means more applications can run simultaneously.



A typical web browser tab uses 50–200 MB of RAM. Assuming an average RAM usage per tab of 125 MB (a typical YouTube video), a computer with Eagle's system memory could have **2,368,000 loaded tabs open** at the same time.

PROCESSORS

Modern laptops have an average of at least 4–8 cores. So, Eagle has **as many cores as 19,000 cutting-edge laptops combined.**



Learn more about Eagle and NREL's HPC systems at www.nrel.gov/hpc

Gyrfalcon: Mass Storage System

Gyrfalcon is the mass storage system NREL installed in early 2013 and upgraded in 2018 to 14 petabytes capacity. It provides tiered long-term storage for the ESIF HPC environment. The system is based on Oracle's platform and software; ZFS appliances; SAM-QFS; SL3000 tape library; and T10000D tape drives. It uses SAM-QFS policies to provide two copies of all data, which eliminates the requirement for external backups and moves seldom-used data to economical tape storage.

SparkPlug: Testbed for OpenStack

NREL hosts a distributed analytics compute cluster, Sparkplug, for storing, analyzing, and mining massive operational wind and transportation datasets. SparkPlug is a testbed for OpenStack and supports rapid deployment of Hadoop environments for data-intensive computing. SparkPlug has been used in the transportation research space for the analysis of commercial trucking data to produce summary features for categorizing drive cycles, and for the visualization of road network usage using billions of rows of GPS sensor data, as well as exploratory work into map-matching GPS data to road networks. With operational wind data, NREL researchers have analyzed high-resolution operational data for research on waking, turbine reliability, and wind plant performance.

Tanager: GPU Cluster for Visualization

Tanager is a graphics processing unit (GPU) cluster used for projects in advanced visualization with GPU codes, image processing, and bioinformatics. Tanager has 8 nodes with dual 10-core Intel Xeon E5-2640 v4 Broadwell processors, 512 GB 2133 DDR4, 120 GB SSD, and NVidia K80 GPU.

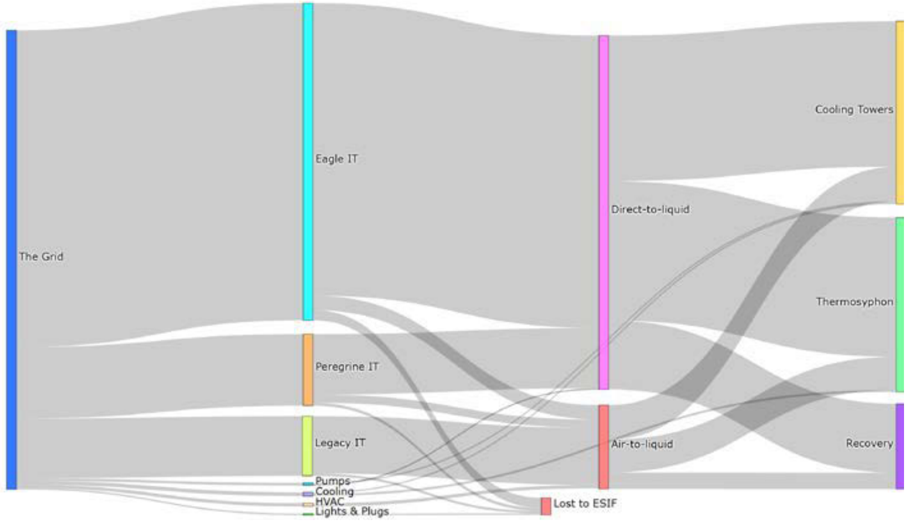
HPC Data Center

Using best-in-class technologies, NREL's ESIF HPC Data Center serves as a showcase facility for demonstrating data center energy efficiency. The data center has achieved a world-leading annualized average power usage effectiveness (PUE) rating of 1.036.

FY19 Highlight: Sensor Data Analytics

The ESIF HPC Data Center's world-leading energy efficiency was previously communicated solely through PUE, the preferred metric in the industry for measuring energy efficiency of the data center infrastructure. Although widely used throughout the industry, loose measurement standards allow for a range of interpretations when calculating this metric.

In order to encourage the industry to take a comprehensive approach to energy efficiency, NREL has leveraged sensor data collected within the data center infrastructure to produce a Sankey diagram that depicts the usage and flow of energy from input to dissipation. The height of the nodes and connections in the diagram is proportional to the quantity of energy. This method of visualization allows for better understanding of our energy usage, and comparing monthly diagrams shows seasonal trends and how outdoor weather affects our three different methods of waste heat rejection (recovery/reuse, thermosyphon cooling, and cooling towers).



FY19 Highlight: Hydrogen Fuel Cell Power Demonstration

Envisioning a future where data centers will be supplied 24/7 by renewable energy, NREL and its industry partners—HPE, Daimler, and Power Innovations—implemented a prototype carbon-free data center concept, based on automotive-scale hydrogen fuel cells within the ESIF HPC Data Center. When electricity generated from renewables (e.g., from solar and wind) exceeds the electrical power demands of the IT equipment, that excess energy is converted to hydrogen using electrolysis, and stored. When energy supply is below IT demand, a hydrogen fuel cell converts hydrogen into electricity to provide continuous power through intermittent sources.

In FY19, the project team retrofitted a retired rack of the Peregrine HPC system to provide a much higher working load compared to the original IT equipment test configuration. This change provided a much more extensive testing environment for the fuel cell. The project partners also agreed to extend the project into 2020, allowing for longer test runs to be conducted under varying operational conditions.

Data, Analysis, and Visualization

NREL's data management, data analysis, and scientific visualization capabilities help move the needle on high-impact projects dealing with complex, large-scale data. Capabilities include tools and expertise in scientific visualization; data analysis; data-focused predictive modeling using statistical, machine-learning/deep-learning algorithms; and advanced data management methods that support NREL researchers and the ESIF User Facility community in the capture, mining, and investigation of data-driven research problems to address scientific and technical goals.

The Insight Center at the ESIF combines state-of-the-art visualization and collaboration tools to promote knowledge discovery in energy systems. Located adjacent to the ESIF HPC Data Center, 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.

New Capabilities

NREL's latest data analysis and visualization capabilities include:

- A new spatial augmented reality framework that combines measured and modeled data with physical 3D printed models, providing the unique capability to demonstrate the impact of climate hazards on infrastructure and assets. The tool provides an economic and transportable method to communicate complicated datasets in a visually compelling and straightforward manner.
- An Apache Spark module for the Eagle HPC system, which is a popular software framework for big data analytics on parallel computing resources. This capability will enable seamless migration of data analysis workflows between the cloud and on-premise HPC resources in the ESIF HPC Data Center.
- A new open-source package for real-time data relay and visualization from lab-facing grid simulations to the Insight Center for visualization. The data pipeline consists of a desktop data streaming application and a data conditioning application to process and filter high data rates in real time for visualization applications and data storage tools.
- A new Data Streaming Platform that allows ESIF labs and projects to stream data between lab equipment, Eagle, and any other origin or destination (e.g., files, database, cloud services) for real-time analytics and visualization.

Early Science on Eagle

During the month of December 2018, a handful of projects were given dedicated time on the new Eagle HPC system to see what could be accomplished that was not possible on Peregrine. Notable results from these Early Science projects are highlighted here.

Computational Design of Disordered Chalcogenides for Solid-State Battery Electrolytes

Simulation of ion transport in disordered multinary chalcogenides using Pylada-defects code tracked stability and transport properties across 31 different phases that co-exist in these materials. For the first time, point defect energetics in disordered solid-state electrolytes were modeled explicitly, opening the doors for new families of materials to facilitate fast ion transport.

Impact: Cell makers will use these results to rationally design disordered solid-state electrolytes for flexible, safer, durable, low-cost battery architectures

ResStock™ Model

Using NREL's ResStock™ residential building portfolio energy simulation software, researchers utilized Eagle to evaluate 23 additional energy retrofit scenarios across residential buildings in the United States to identify the energy savings potential of energy efficiency. The expanded computational resources on Eagle allowed researchers to analyze the simulation data on a sub-hourly level instead of the previously available total annual energy use. Understanding these aggregate time series of building load profiles is critical to achieving higher penetration of renewable energy on the grid.

Impact: Actionable information for homeowners and policymakers to meet primary energy reduction targets

Biomass Deconstruction Enzymes

Using the molecular dynamics engine NAMD, NREL researchers determined the detailed dissociation mechanism for the cellulose-degrading enzyme TrCel7A. Eagle's scale provided for the first time a platform to directly compare competing hypothesized mechanisms.

Impact: Detailed knowledge that enables rational enzyme engineering to lower the cost of biomass deconstruction for upgrading to fuels and chemicals

Full-Resolution Wind Resource Data

To date, only a small portion (50 of 400 terabytes) of the WIND Toolkit dataset has been available for use by NREL's analysts on the HPC. The significantly larger capacity of Eagle will finally enable the extraction of the full U.S. WIND Toolkit data as well as data for the Canada and Mexico additions produced under NREL's North American Renewable Integration Study.

Impact: Enable advancements in production cost modeling by providing sub-hourly wind resource data for large-scale power system analyses

Optical Absorption in Defected WS_2

New high-fidelity, quantum-mechanical calculations using the BerkeleyGW code accurately described the light absorption of sulfur-defected WS_2, an exciting two-dimensional material under intense development for optoelectronic and catalytic applications. The ability to treat systems with defects and heavy elements like tungsten allows for microscopic insight into novel and exciting energy materials.

Impact: Realistic features of often messy optoelectronic and catalytic systems can be considered for materials discovery, development, and design

Extreme-Scale Autonomous Energy Systems Simulation

Researchers performed integrated transmission-distribution-control co-simulation at 20 times larger scale than previously simulated at NREL. This enables the in-depth analysis of complex control schemes to support "self-driving" autonomous energy systems with millions of devices and full physical grid simulation.

Impact: Enable grid and advanced controls developers to evaluate multi-energy systems at scale to enhance resiliency with grid modernization, renewables, and high electrification

Tree Decomposition of Power Grids

Real-time control and optimization of large-scale power networks is a challenging task, but it is also crucial for power system resiliency. Computing tree decomposition of power networks simplifies the required computation for real-time control and optimization.

Impact: Tree decomposition for multiple IEEE benchmark systems with thousands of buses, which benefits the development of real-time control and optimization algorithms

Research Highlights

NREL's HPC User Facility provides computing capabilities to scientists and engineers working on solving complex computational and data analysis problems related to energy efficiency and renewable energy technologies.

This section presents a selection of research highlights from FY19 based on computations and simulations run on NREL's HPC systems, illustrating the breadth of science supported by the lab in support of DOE's mission.

TRANSPORTATION

Implementing Co-Development as Means to Help Reduce Per-Vehicle Petroleum Use by 30% Beyond 2030

On-highway transportation uses over 10 million barrels of fuel per day, matching the volume of U.S. oil imports and contributing 28% of U.S. greenhouse gas (GHG) emissions. There is a long lead time for technological innovation to have an impact: advanced vehicle technologies traditionally deploy slowly, with a 10–12 year development cycle typical in the auto industry.

In FY19, NREL's HPC capabilities were instrumental in helping researchers reach a 30% reduction in per-vehicle petroleum consumption beyond the 2030 gains achieved through business-as-usual evolutionary, regulatory-driven improvements through the Co-Optimization of Fuels and Engines (Co-Optima) project. Co-Optima is pursuing the co-development of fuels and engines, which has proven successful for controlling criteria pollutants and provides great promise for reducing GHG emissions. By establishing a link early in the R&D cycle of both fuels and engines, a complete systems-based approach to create optimized solutions can be realized.

Researchers developed a numerical approach based on multidimensional computational fluid dynamics to predict knocking combustion in an engine, which is a major impediment to achieving higher efficiency in spark-ignition engines. Researchers performed Advanced Fuel Ignition Delay Analyzer simulations to understand the behavior of the apparatus used to measure the ignition characteristics of fuels. Compared to traditional methods, this simulation can significantly reduce the operating cost and time to characterize a fuel, providing highly repeatable data with fully automated sampling.

HPC IMPACT

Faster and lower-cost simulations to achieve higher efficiency in spark-ignition engines

Wisdom to Guide Energy Transformations at U.S. Ports

Airports are complex transportation hubs that coordinate the movement of passengers, goods, and services from the surrounding urban area. They need decision support and actionable insight to reduce uncertainty and mitigate risk for long-term planning. There are significant challenges in adapting complex transportation networks to rapidly evolving technology megatrends—and poor planning or execution may result in increased energy use, costs, and system inefficiencies.

Athena is a collaborative effort funded by the DOE Vehicle Technologies Office and industry and led by NREL in partnership with Oak Ridge National Laboratory (ORNL) and Dallas-Fort Worth International (DFW) Airport. NREL and ORNL experts are leveraging the powerful scientific computing capabilities at the labs to develop sophisticated models of current and future behaviors based on expanded mobility choices to and from transportation hubs, increased freight volume, and anticipated dynamics of airport access.

The Athena team is developing a "digital twin" model of DFW Airport with data from individuals, traffic, freight routes, flight schedules, autonomous vehicles, and other sources. Using data-driven statistical modeling and artificial intelligence, this model can simulate the impacts of future capacity expansion scenarios. It will also identify options that maximize the value of passenger and freight mobility per unit of energy and/or cost.

HPC IMPACT

Data to inform transportation hubs in integrating transformative technologies and achieving ambitious energy goals

WIND

Improving Load Predictions to Better Understand Offshore Wind Systems Physics

NREL is working on an international research project focused on validating the modeling tools used to design offshore wind systems. The goal is to improve load predictions from engineering-level models through comparison to measurement data and higher-fidelity simulations using computational fluid dynamics (CFD).

Previous work showed a persistent under-prediction (about 20% on average) of motion and structural loads across a variety of conditions, and similar levels of under-prediction have been observed by other floating wind developers.

In FY19, NREL performed simulations with the system in a fixed condition for multiple regular wave scenarios. The system was also forced to oscillate in the surge direction for different frequencies and amplitudes. The goal was to break down the individual components of the hydrodynamic loads on the offshore wind platform. This simpler structure was used as a starting point to understand the methodology and needs when performing CFD simulations of offshore wind structures.

One of these simulations can take weeks to run even on an HPC system, so this research would not be possible without HPC. NREL's access to Eagle allows the lab to drive research in floating wind analysis internationally.

HPC IMPACT

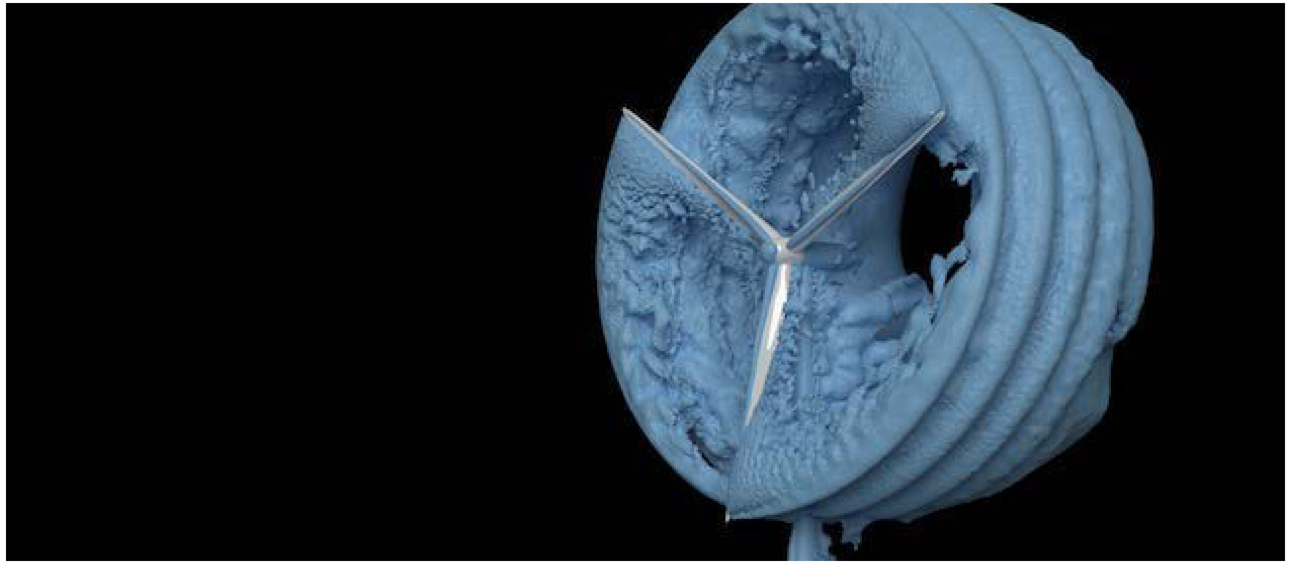
Improved understanding of how to model the physics of offshore wind systems and identify weaknesses in the modeling solutions

Developing a Next-Generation Capability for Simulating Modern Wind Turbines

NREL is developing Nalu-Wind, a next-generation wind-plant fluid flow solver, with funding from both the U.S. Department of Energy Wind Energy Technologies Office and the Office of Science's Exascale Computing Project. The objective of these projects is to instill in Nalu-Wind the highest-quality physics models for wind-plant simulation with the end goal of providing predictive simulations, and to then make the code scalable on the next-generation leadership-class exascale computing platforms, which will most likely have hybrid architectures.

In FY19, NREL and partners created a new blade-resolved model of a large modern wind turbine, enabling scientists and engineers to begin understanding the complex flow physics in multi-turbine wind farms that will take advantage of future exascale modeling and simulation capability. When validated by targeted experiments, these and other predictive physics-based high-fidelity computational models—and the new knowledge derived from their solutions—provide an effective path to optimizing wind plants.

With a code that can run at exascale, researchers will be able to simulate wind plant cases at unprecedented resolutions and domain extents, allowing for new scientific discovery about wind plant physics. Likewise, even future smaller HPC systems will borrow technology from these capabilities.



HPC IMPACT

Ability to model and simulate billion-cell computations of wind turbines in high fidelity to gain new insights into wind plant physics

GRID MODERNIZATION

Evaluating the Impact of Water Availability on Grid Configurations

The U.S. electric power sector relies heavily on cooling water and hydroelectric power for reliable and consistent operation. The impacts of water scarcity on power sector operations can be quantified using a variety of metrics, including total system production costs, regional energy generation, and regional energy prices, among others.

NREL is using a power systems model to evaluate the impact of water availability and grid configurations, considering region-wide impacts as well as sub-regional responses to capture regional capacity differences and realistic grid connectivity dynamics. In FY19, NREL used Eagle to capture multiple climate-forced water availability scenarios across a range of historical and future years. Researchers believe this work represents the largest set of power system simulations under climate-forced water constraints to date.

HPC is critical for this project because each of the 700 individual-year simulations takes about 2 days. The simulations are completed in 6-month chunks, taking about 24 hours each. With traditional computing, run time could take two months. Eagle allows NREL to parallelize the simulations and complete them in about a day.

HPC IMPACT

Rapidly quantify the impacts of water scarcity on power sector operations

SOLAR

Analyzing Costs and Benefits of Distributed PV Generators to Help Evaluate Solutions

To help utilities, solar developers, and distributed energy resource aggregators evaluate different solutions to integrate distributed photovoltaics (DPV) on the grid, NREL is evaluating the costs and benefits of DPV generators to distribution systems as a function of penetration level.

Researchers use a bottom-up methodology that combines power flow modeling and hosting capacity analysis with techno-economic analysis. In FY19, NREL incorporated innovative quasi-static time-series simulation in order to capture time-dependent impacts of PV as well as consider a broader set of advanced technology options for grid integration, including distributed energy management systems and flexible interconnection approaches.

Access to Eagle allows NREL to conduct this analysis for a much larger number of DPV penetration levels in order to elucidate the key drivers of costs. Without the HPC, these simulations would be much slower and, due to memory limits, researchers would not be able to collect and process as much data from each simulation. Additionally, the HPC allows for rapid prototyping development of new algorithms and tools for distribution grid integration.

HPC IMPACT

Scaling up analysis to facilitate reliable, low-cost, smart integration of distributed solar

Processing Big Data for the National Solar Radiation Database

The National Solar Radiation Database (NSRDB) is the leading public source of high-resolution solar resource data in the United States for use in energy modeling, with over 55,000 unique users and more than 245,000 pageviews annually. This database represents the state of the art in satellite-based estimation of solar resource information and uses a unique physics-based modeling approach that enables improvements in accuracy with the deployment of the next-generation geostationary satellites.

Making the highest quality, state-of-the-art, regularly updated datasets available on a reasonably timely basis for a variety of users reduces the costs of solar deployment by providing accurate information for siting studies and system output prediction, and thereby reduces levelized cost of electricity. Additionally, the NSRDB enables the integration of high amounts of solar on the grid by providing critical information about solar availability and variability that is used to enhance grid reliability and power quality.

The NSRDB is a significant big-data processing challenge with massive requirements, so the storage available on Eagle as well as the speed and memory available on the compute nodes are invaluable to the effort.

HPC IMPACT

Data-processing speed and memory to power the leading public source of solar resource data

FUEL CELLS

Demonstrating Power and Utility of High-Fidelity Computation Methods to Model Meaningful Catalytic Systems

Affordable energy storage is of paramount importance if renewables are to become a dominant contribution to the U.S. energy supply. One approach is to store the energy in the form of a liquid fuel, using either a photoelectrochemical cell or an electrolyzer hooked into an electrical source. Both approaches require insight into electrochemistry, which involves complex processes in which chemical reactions happen at the surface of a solid, with the solid acting as a catalyst or otherwise playing a principal role in the reaction. The study of such processes via theoretical means is a nascent area of study that is ripe for the insights that can be provided by advanced high-fidelity computational methods.

In FY19, NREL used a promising catalyst as a model to: demonstrate that our implementation of high-fidelity computational methods will scale to large system sizes; show that we can extend this framework into systems involving solvent screening; and incorporate additional energetic terms that account for room temperature entropic contributions in the reaction pathway. Taken together, these results demonstrate the power and utility of our techniques to model physically meaningful catalytic systems at realistic operating conditions using high-fidelity computational methods.

These calculations required many massively parallel jobs on 96 nodes for several hours to achieve high-fidelity results on our 55-atom unit cells. Smaller-sized clusters do not have the memory to run these calculations, and would slow our throughput by at least an order of magnitude, i.e., we would get results in weeks instead of days. NREL could not have achieved these results without the scale and throughput provided by Eagle .

HPC IMPACT

Large-scale demonstrations of high-fidelity computational methods for electrochemical energy storage research

BUILDINGS

Assessing the Relationship Between Energy Efficiency and Demand Response in Future Power Systems

Energy demand is increasing, grid infrastructure is aging, and wind and solar generation assets are being added throughout the United States. As such, the load flexibility provided by grid-interactive efficient buildings promises to play a key role in maintaining grid reliability, reducing the cost of electricity, and enabling the integration of more renewables. However, while demand response (DR) is reasonably well understood at the single-building level, its impacts are largely unknown at the aggregated, stock-modeling level.

NREL is using HPC to provide a realistic and detailed understanding of the relative value of and interaction between the energy efficiency (EE) and DR characteristics of building technologies in terms of power systems' time-varying costs and emissions. The project builds upon past work to tackle these challenges; research occupant requirements and preferences; and analyze the value of EE and DR in at least three regions, leveraging several NREL models. The outcome will be an analysis platform that can assess trade-offs and co-benefits between EE and DR in a variety of different power system futures.

This will be a unique capability, especially considering the scale and fidelity of the model. Having access to HPC resources allows NREL to work fairly unconstrained in terms of geospatial extent and resolution of the analysis.

HPC IMPACT

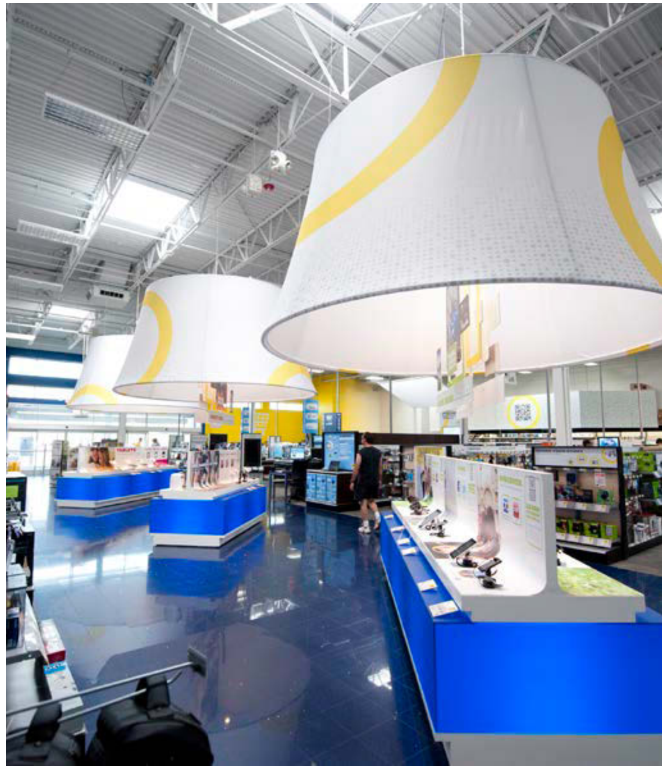
High-resolution analysis of the trade-offs and co-benefits between energy efficiency and demand response in a variety of different power system futures

Developing End-Use Load Profiles for the Entire U.S. Building Stock to Inform Stakeholders

End-use building load profiles are critically important to understanding the time-sensitive value of energy efficiency, demand response, and other distributed energy resources. NREL and partnering labs are developing a foundational dataset to help electric utilities, grid operators, manufacturers, government entities, and research organizations make critical decisions about prioritizing research and development, utility resource and distribution system planning, and state and local energy planning and regulation.

The team is using a hybrid approach that combines the best-available ground-truth data—from submetering studies, statistical disaggregation of whole-building interval meter data, and other emerging data sources—with the reach, cost-effectiveness, and granularity of data-driven and physics-based building stock modeling using the ResStock and ComStock capabilities developed by NREL for the U.S. Department of Energy.

HPC resources are essential to the success of this project, as a typical analysis at the national scale includes the simulation of 350,000 building energy models. Each of the models on average takes about 5 minutes to simulate. Running a single national-scale simulation in serial on a laptop would take approximately 3.3 years.



HPC IMPACT

Scaling up building stock simulations for the entire nation to help stakeholders make critical R&D and planning decisions

BIOENERGY

Deepening Our Understanding of Mechanisms in Biochemical Processes

NREL's Biochemical Process Modeling and Simulation project works closely with dozens of experimental projects to test hypotheses, predict research directions, and deepen understanding of mechanisms in DOE Bioenergy Technologies Office (BETO)-relevant biochemical processes.

Synthesizing experimental data into atomic-scale biomass models would be a boon to generating mechanistic insight into how biomass responds to different pretreatments. Given recent progress in modeling lignin, researchers are now uniquely positioned to combine biomass components into a complete model of cell walls. Due to the large size of these systems, estimated at over 100 million particles, the capabilities of the Eagle HPC system are critical to developing these models.

Without HPC resources, there would be insufficient sampling to draw meaningful and statistically significant conclusions in this research. Having access to Eagle also expands the scope of possible research significantly, such as by testing additional enzyme substrates or lignin stereochemistries, with degrees of freedom in simulation design that could not be probed before.

HPC IMPACT

Greatly expanded research scope for modeling and simulating biochemical processes

WATER

Wave Energy System Modeling to Reduce Costs and Improve Reliability

Performance and design load predictions for ocean renewable energy systems, such as wave energy converters and marine current turbines, are challenging due to the complex interaction of nonlinear wave and current forces on floating, possibly flexible, multi-body systems. This can lead to overdesigned, costly systems or a lack of reliability.

NREL is developing methodology for applying computational fluid dynamics (CFD) simulation to extreme design load analysis and improving its accuracy—which is essential for the success of future ocean renewable energy converter designs and for moving the technology forward.

Using HPC allows for an accurate evaluation of the design load cases, which enables an optimized structural design, ensures survival, and reduces overall costs. The application of HPC also makes it possible to use numerical wave tank CFD simulations for design load analysis as well as fluid structure interaction simulation.

HPC IMPACT

More accurate modeling of ocean renewable energy systems to move the technology forward

Awards and Partnerships

Read highlights of NREL's HPC awards and new partnerships in FY19.

NREL Garners Top Sustainability Honor at Data Center Dynamics Awards

In December 2018, NREL won the prestigious Data Center Dynamics (DCD) Data Center Eco-Sustainability Award, bolstering the lab's status as a world leader in data center efficiency and sustainability. Referred to as the 'Oscars' of the data center industry, the annual DCD Global Awards recognize the industry's top data center projects and people. An independent panel of data center experts selected finalists from hundreds of entries from organizations across the globe.

This award recognizes innovative and pioneering approaches to sustainability through the design or major retrofit of a data center facility. The win solidifies NREL's claim of having the most energy-efficient data center in the world, which NREL designed in partnership with SmithGroup, LLC, and Johnson Controls, Inc.

NREL Computational Science Director Steve Hammond (left) and Winthrop Engineering Business Development Director Barry Hennessy at the December 6, 2018, DCD Global Awards gala in London. Winthrop was the corporate sponsor of the DCD Eco-Sustainability award won by NREL. *Photo courtesy of DCD*

NREL's Scott Haase (left), Steve Hammond, and Rob Leland—along with HPE's Gerald Kleyn, Glen Rowe, and Bill Mannel—sign a memorandum of understanding to collaborate on the application of edge and data-centric computing to solve complex energy system challenges. *Photo by Dennis Schroeder/NREL*

HPE and NREL Expand Partnership with New Focus on Edge and Data-Centric Computing

In FY19, NREL finalized a new partnership agreement with HPE aimed at demonstrating how a thoughtful combination of sophisticated edge computing with traditional computing can enable enhanced control of advanced energy systems.

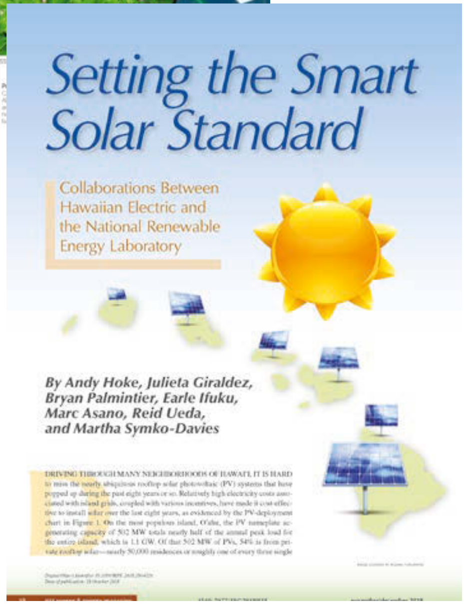
NREL and HPE will explore new market opportunities and platforms for edge and data-centric computing. NREL's scientific computing, energy analysis, and energy systems integration researchers will work with HPE to lead the research, which will span a broad range of topics, including:

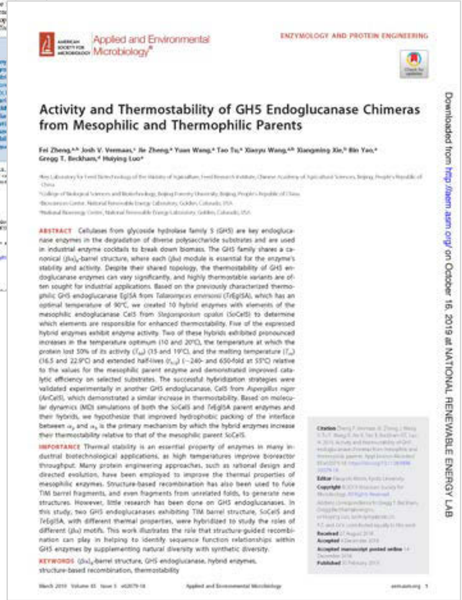
- Energy system edge computing
- Data-centric computing
- Fault-tolerant computing
- Optimization and integration of grid-edge controls and architecture
- Cybersecurity
- Energy system security and resilience.

Publications

In FY19, NREL staff reported authoring or coauthoring 142 published papers that involved NREL HPC resources. This included 63 peer-reviewed scientific journal articles, 15 conference papers, and 51 presentations, showcasing NREL's continued involvement in advancing the state of the art of computational science.

To access a comprehensive list of publications and presentations, visit www.nrel.gov/computational-science/publications.html





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

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