High-Performance Computing at the National Renewable Energy Laboratory's Energy Systems Integration Facility: **FY2018**

Computational Science Center Director's Letter

HPC at NREL: The Year in Perspective

Fiscal Year 2018 (FY 2018) was another exciting and productive one at the National Renewable Energy Laboratory's (NREL's) Energy Systems Integration Facility (ESIF). Our High-Performance Computing (HPC) User Facility supported 106 modeling and simulation projects, advancing the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) mission across the spectrum of energy efficiency and renewable energy technologies. Peregrine, our primary HPC system, provided 20 million node-hours during 12 months of production in FY 2018.

Looking ahead to the future of HPC in support of the EERE mission, we initiated the ESIF-HPC-2 project in January 2017 to acquire new HPC capabilities. Project milestones achieved include:

- Following the DOE Office of Science model, a Design Review was held July 2017
- The request for proposals was issued in September 2017
- Proposals were received in November 2017
- The Source Evaluation Team selected a system in December 2017
- The contract was awarded to Hewlett Packard Enterprise (HPE) in March 2018
- Hardware was delivered in September 2018.

The new system, named "Eagle," will be put into production use in January 2019. Eagle will have a peak performance of 8 petaflops, about 3.6 times the capability of Peregrine. Comprised of 76,104 Xeon-Gold Skylake 6154 processor cores and 100 NVIDIA Tesla V100 PCIe graphics processing units (GPUs), this new system from HPE is a Linux cluster that uses a fast InfiniBand network to connect nodes. It has 14 petabytes (PB) of shared disk space and 2.5 PB of disk distributed in nodes.

Like its predecessor, Eagle uses warm-water-liquid cooling that allows more than 97% of the waste heat to be captured for reuse, supercharging NREL's notable leadership in energy-efficient data centers.

While Peregrine has been a tremendous workhorse for carrying out the laboratory's modeling and simulation efforts over the past 4-plus years, Eagle will supersede Peregrine in January 2019, and we will start to decommission about half of Peregrine in January and work with the user community on an orderly transition to Eagle.

The ESIF HPC Data Center itself continues to be a showcase facility, generating a constant stream of visitors looking to learn from NREL about sustainable and energy efficient data centers. Our pioneering work to install a prototype BlueStream dry cooling system in the data center continues to pay dividends, as it has cut our water use in half without compromising energy efficiency. This pioneering collaboration with Johnson Controls and Sandia National Laboratories continues to reinforce our sustainability focus and is drawing interest from other DOE labs and data center operators.

Looking ahead, we are envisioning a future in which hydrogen might have a more prominent role in our energy mix. In that context, NREL is working with industry partners to explore an innovative carbon-free data center concept, based on automotive-scale hydrogen fuel cells that would provide DC power directly to server racks within the ESIF HPC Data Center.

St. W. Hammond

Steve Hammond

Director, Computational Science Center

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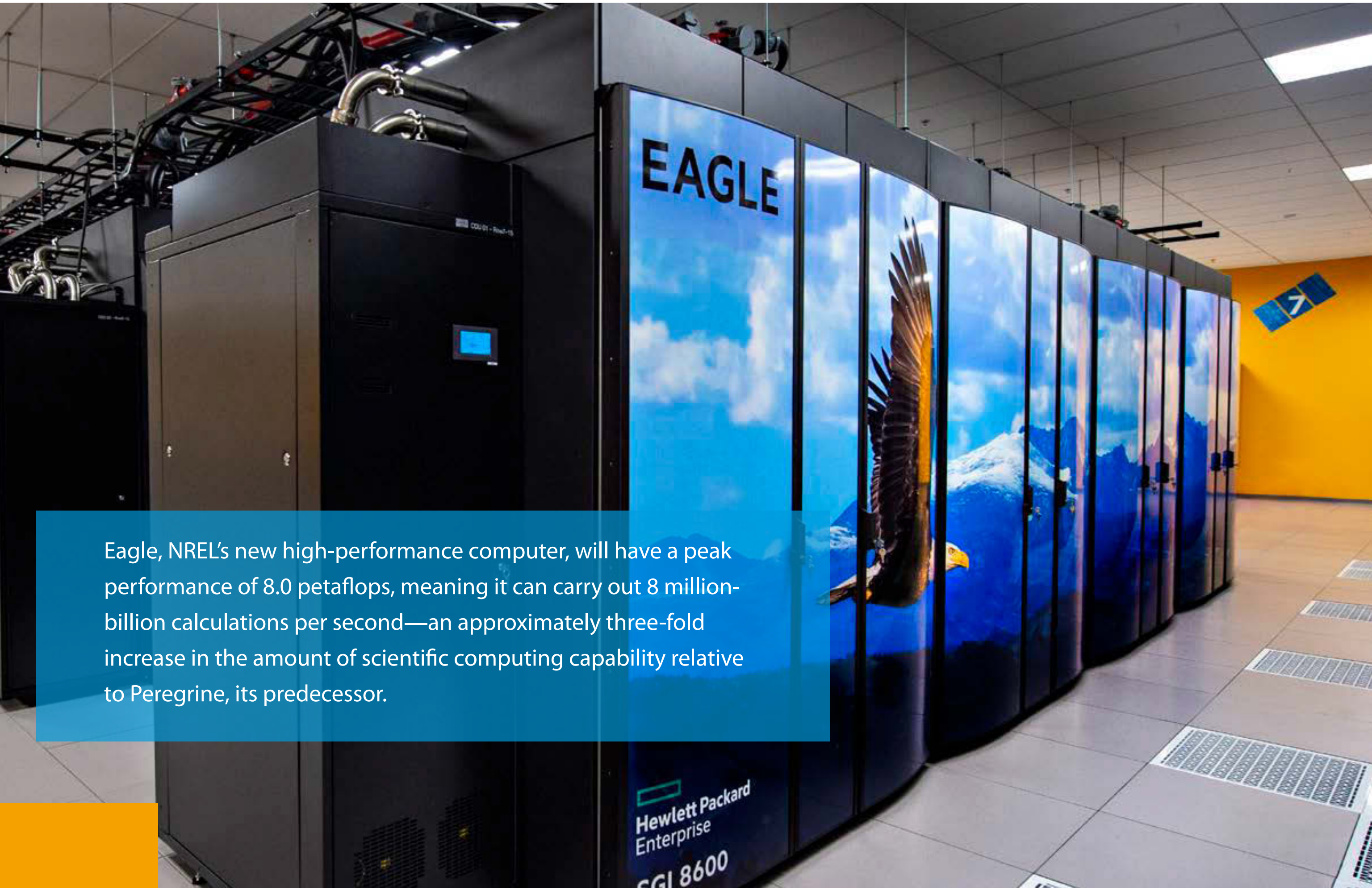
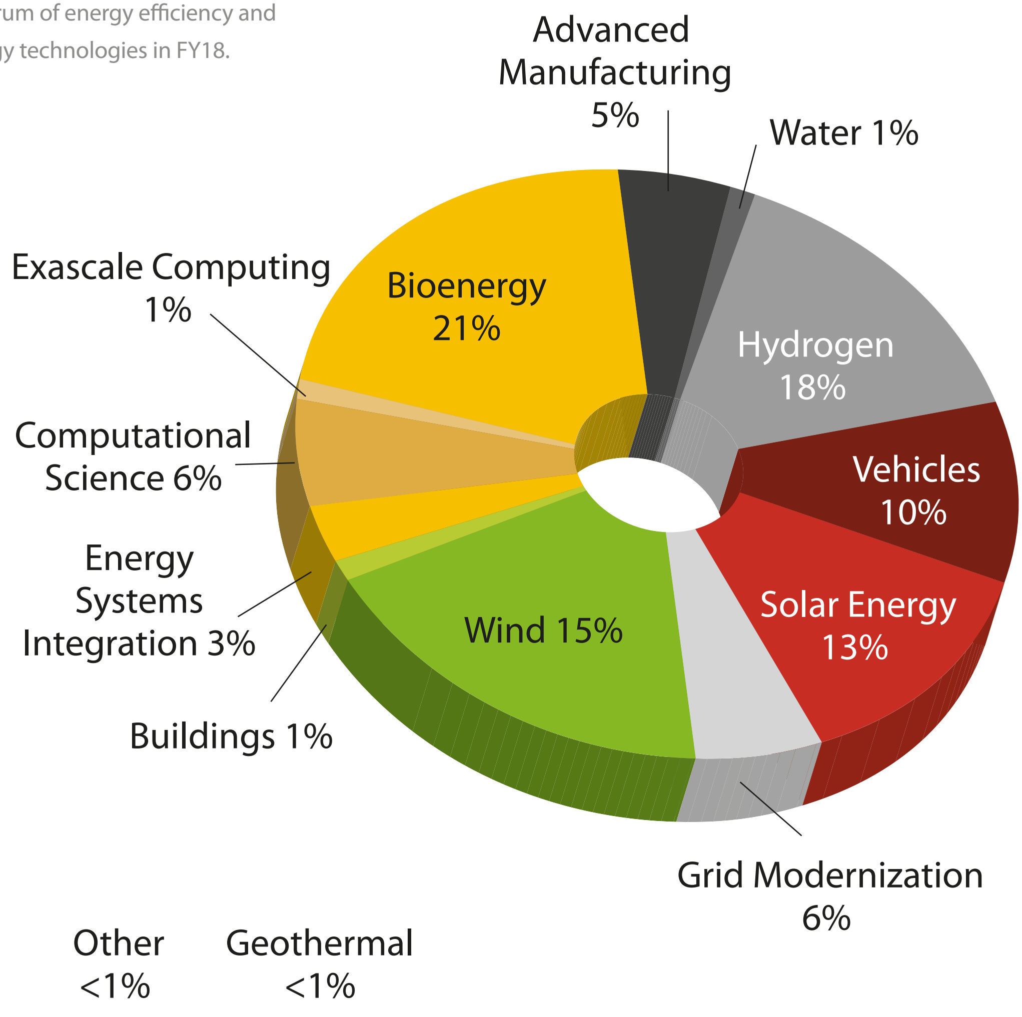


Eagle, NREL's new high-performance computer, will have a peak performance of 8.0 petaflops, meaning it can carry out 8 million-billion calculations per second—an approximately three-fold increase in the amount of scientific computing capability relative to Peregrine, its predecessor.

NREL HPC Usage Demographics

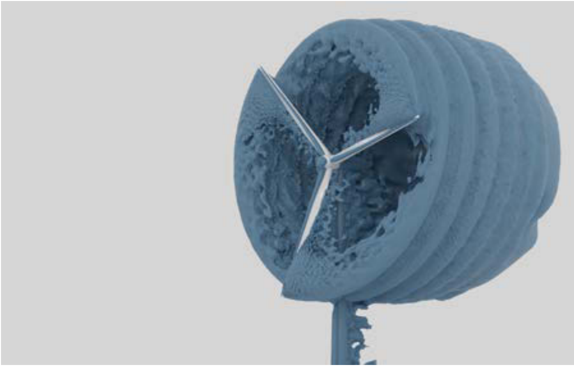
The NREL HPC user facility supported 106 modeling and simulation projects advancing the DOE mission across the spectrum of energy efficiency and renewable energy technologies in FY18.



Exascale Computing at NREL

Exascale computing refers to computing systems capable of at least one exaFLOPS, or a billion billion calculations per second—1,000 times the performance capability of today's supercomputers. Exascale computing will provide breakthrough modeling and simulation solutions that analyze more data in less time to address critical challenges in scientific discovery, energy reliability, economic competitiveness, and national security.

In FY18, NREL continued work on exascale computing projects for wind and combustion technology applications in support of DOE's Exascale Computing Project, which is funded through the Office of Science and National Nuclear Security Administration.



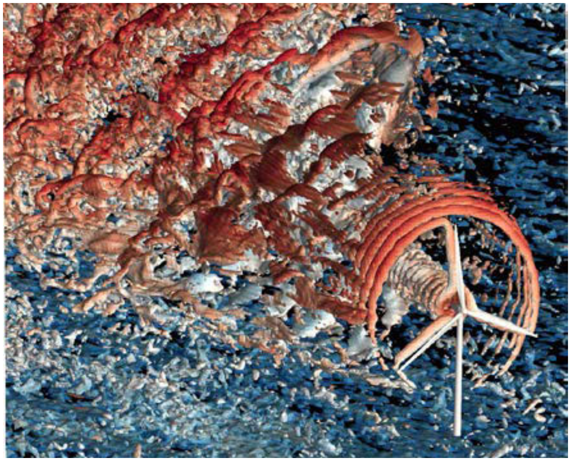
Geometry-resolved large-eddy simulation of the NREL 5-megawatt wind turbine created through the ExaWind project.

Exascale Predictive Wind Plant Flow Physics Modeling

NREL Principal Investigator: Michael A. Sprague

Partnering Institutions: Sandia National Laboratories, Oak Ridge National Laboratory, University of Texas at Austin

A key challenge to wide-scale deployment of wind energy in the utility grid without subsidies is predicting and minimizing plant-level energy losses—which are currently estimated to be 20% in relatively flat areas, and much higher in regions of complex terrain. Current HPC simulation tools and methods for modeling wind plant performance fall far short due to insufficient model fidelity and inadequate treatment of key phenomena, combined with a lack of computational power necessary to address the wide range of relevant length scales associated with wind plants.



Isosurfaces of vorticity colored by the instantaneous streamwise velocity in the wake of a wind turbine.

In the Exascale Predictive Wind Plant Flow Physics Modeling project, also referred to as ExaWind, NREL is leading the development of an exascale modeling and simulation capability (coupled fluid and structural mechanics) to understand the fundamental multiphysics, multiscale flow phenomena in large wind plants, including complex terrain. This involves blade-resolved simulations of O(100) multi-MW wind turbines in O(100) square kilometers and approximately 100 billion grid points.

The ExaWind project will result in advancements both in the development of a next-generation wind farm simulation capability, and in the understanding of how this capability can be applied to answer important science questions that are challenging the wind energy community. The project will also ensure that the new wind farm simulation code scales well on today's petascale systems and is well positioned to utilize first-generation U.S. exascale systems. Learn more at **exawind.org**.

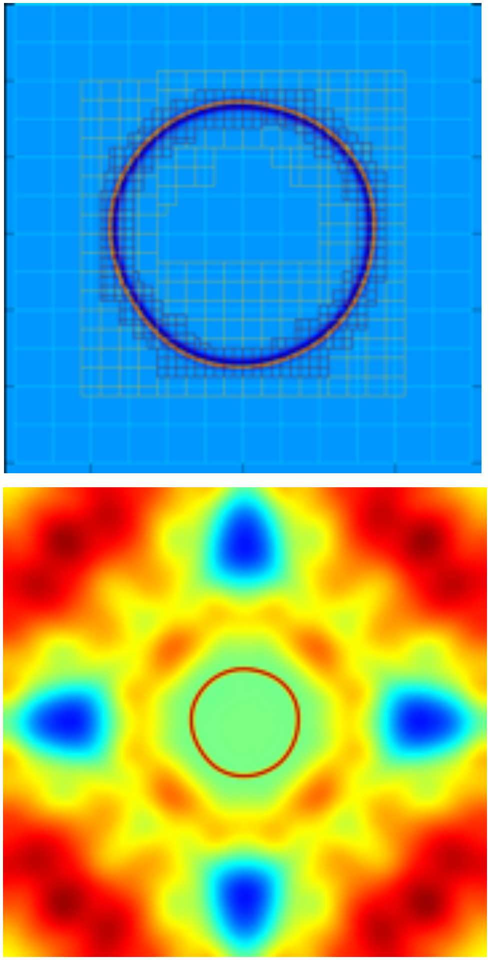
Transforming Combustion Science and Technology with Exascale Simulations

NREL Principal Investigator: Ray Grout

Partnering Institutions: Sandia National Laboratories, Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, Argonne National Laboratory

NREL is playing a key role in developing an exascale computing simulation framework for modeling multiphysics reacting flows for combustion applications. This simulation capability will enable unique first-principles and near-first principles simulations of mixing, spray vaporization, auto-ignition, flame propagation, and soot/radiation in conditions relevant to practical combustion devices.

Computer hardware is fundamentally changing, with performance now coming from parallelism, rather than increasing clock frequency. Current combustion codes will not perform well on evolving hardware without a major re-working of algorithms and implementation. The exascale combustion simulation framework offers a tremendous opportunity for advancing design technology for energy generation and propulsion.



H_2-Air Flame Kernel propagation demonstrating adaptive mesh refinement-based reacting flow simulation tool, Pele. Simulation performed in collaboration with John Bell and Marc Day of Lawrence Berkeley National Laboratory. Top: Reaction rate of HO_2 showing the length scales of heat release. Bottom: Pressure waves resulting from the combustion process associated with kernel propagation.

Science 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. The work performed on NREL's HPC systems leads to increased efficiency and reduced costs for these technologies, including wind and solar energy, energy storage, and the large-scale integration of renewables into the electric grid.

This section presents a selection of research highlights from FY18 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

Engineering Low-Cost Magnesium for Lightweight Vehicles

If we can reduce the weight of a vehicle, less energy is required to get from A to B, regardless of the energy source. Magnesium is light—but a bottleneck preventing its increased use in vehicles is difficulty processing it into a sheet that can be formed into parts. NREL is modeling how magnesium behaves at the atomic scale in order to ultimately determine how to make rollable sheets for the auto industry.

The work involves quantum-mechanics-based simulations to understand how magnesium deforms and how it changes in different chemistries. NREL researchers are leveraging the power of high-performance computing to examine plastic deformation and inform changes in composition.

The data is not only being used to inform the broader project but can also be used for future modeling. Industry can use NREL data in fine-element modeling to investigate how this sheet metal will perform.

POTENTIAL IMPACT

Engineer low-cost magnesium sheets for manufacturing lighter-weight and more energy-efficient cars

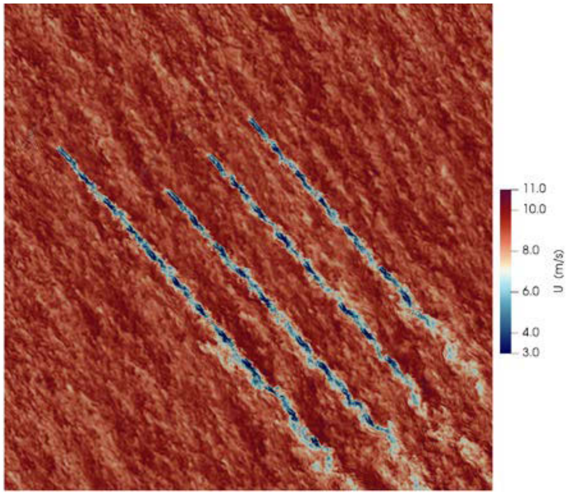
WIND

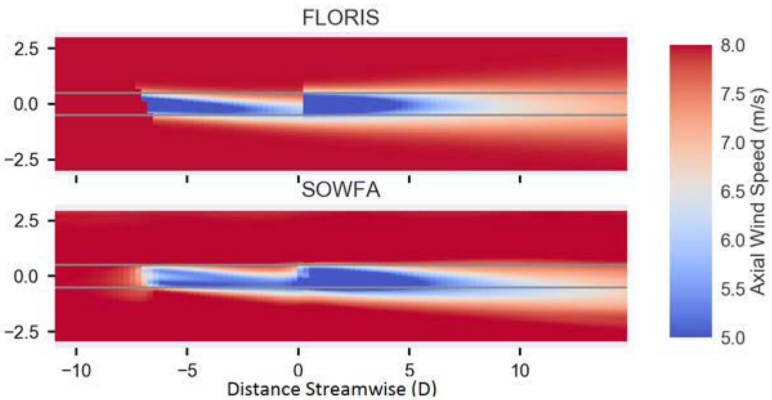
Improving Wind Farm Controls

NREL is using high-performance computing to model the wake interactions in wind farms—how air flows through turbines and affects performance.

The modeling focuses on wake steering, which is a form of wind control in which an upstream turbine intentionally offsets its yaw angle to generate a deflection in its wake away from downstream turbines and thereby improve windfarm overall performance. The models allow researchers to adjust turbine controls to find what an upstream turbine could do to minimize wake losses downstream and produce better overall power.

High-performance computing has been crucial to developing this research area, which could ultimately inform improvements to existing farms to produce more energy, as well as inspire new farms to be designed differently. This would ultimately reduce the cost of wind energy because wind farms would produce more energy from the same capital investment—only the turbine controls software would change.





POTENTIAL IMPACT

Generate more energy from wind farms by coordinating turbine controls to account for how multiple turbines interact in the flow

Accelerating Materials Development for Improved Thermal Control

Insulation is key to energy-efficient buildings, and for decades, fiberglass has been one of the best materials for it. NREL is exploring alternative low-thermal-conductivity materials with the goal of using modern materials-science approaches to develop an even better insulation material than fiberglass.

NREL's approach is based on what are called packed-bed systems. Packing keeps air from flowing, but the packed bed also has the advantage of forcing heat to route only through pinch points where spheres are touching, which leads to lower thermal conductivity because thermal energy must take winding paths through the spheres.

Through computational work performed in concert with experimental efforts in buildings and materials science research, NREL aims to calculate and accurately predict the thermal conductivity of arrays of nanoparticles with different surface coatings (ligands), and understand the mechanisms by which energy is transfered form one particle to another—all with the goal of creating a better insulation material for thermal control.

POTENTIAL IMPACT

Develop a cost-effective insulation material that performs better than fiberglass in preventing energy losses and gains from heat conductivity—a huge source of air conditioning and heating costs

GRID INTEGRATION

Informing Optimal Pathways for Renewable Integration

NREL's Resource Planning Model (RPM) is an optimization model that finds least-cost investment and dispatch solutions for power systems over a decadal-scale planning horizon. The model makes investment decisions for multiple conventional and renewable generation technologies, storage technologies, and transmission. RPM has high spatial resolution down to the individual unit, as well as multiple solar and wind spatial resource regions.

In FY18, NREL analysts used RPM to run a set of forward-looking scenarios with high solar photovoltaic (PV) penetrations. The scenarios were run in three different focus regions and included a reference case with midline assumptions, along with cases corresponding to fictitious renewable energy goals in either a focus region or across the entire Western Interconnection. Some of the scenarios with fictitious renewable energy goals also varied technology costs (for PV and battery energy storage) and fuel prices (for natural gas).

The results from the model have been used to probe for ways in which current planning methodologies fall short at very high PV penetrations—including whether a region might be overbuilt or underbuilt from a peak demand perspective, and whether ramping needs are sufficiently captured and subsequently met by the planned build-out.

NREL is currently working to publish these FY18 results, and generally publishes the methods developed and used in RPM so they can be incorporated into other planning tools. Currently, the City of Los Angeles is using this model with the assistance of NREL analysts to examine pathways toward its goal of a 100% renewable energy power system.

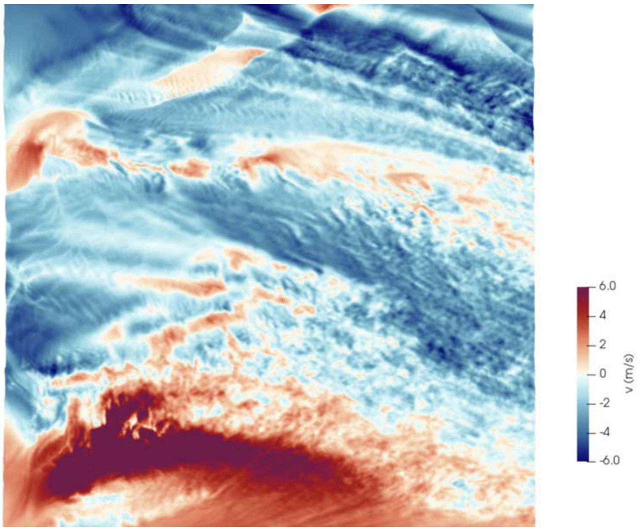
POTENTIAL IMPACT

Research and document new methodologies for high-resolution planning of the electricity sector to inform cities, states, and regions of different possible routes they can take to reach their renewable energy goals

WIND

Optimizing Wind Plant Design Through High-Fidelity Physics Simulations

The first step to better managing wind for energy production is to have a better physical understanding of it and its interaction with the wind turbines within a wind power plant. The wind field surrounding and flowing through a wind power plant is extremely complex. The winds within a wind power plant directly affect each wind turbine and their wakes. Locally, the winds are turbulent and are influenced by the terrain and the turbines themselves; at the same time, these turbulent winds are influenced by the surrounding regional-scale weather patterns that extend hundreds of kilometers away from the wind power plant.



In this project, NREL aims to improve physics-based high-fidelity computational models to calculate flow through a wind power plant. Examining the fluid dynamics of wind turbine wakes helps us gain a better understanding of how wind turbine wakes evolve and flow through a wind plant and interact with other turbines, surrounding winds, and complex terrain. Coupling wind-plant scale computational models with regional-scale weather models allows us to better understand how regional-scale weather affects wind power plant performance.

The winds within a wind power plant can be measured in the field, but the measurement resolution is much coarser than that achieved with supercomputer-based wind power plant flow simulations. Using high-performance computing, NREL can simulate the entire wind power plant flow field along with the wind turbine response and performance. With simulations, we can examine nearly any aspect of the wind flow, from animated slices through wakes to time series of point measurements. Virtual sensors can even be placed in simulated turbines to assess mechanical loads. Through these simulations, not only do we gain knowledge, but we can also use them to guide very specific field measurement campaigns, design wind plant controllers of the future, and innovate new turbine designs.

POTENTIAL IMPACT

Optimize the design of new wind turbines and wind power plants using high-fidelity modeling

News and Innovations

Read on for highlights of NREL's innovative HPC partnership, facility, and sustainability initiatives in FY18.

Eagle, Powerful New High-Performance Computer, Arrives at NREL

In January 2019, NREL put into production use its new, more powerful supercomputer, Eagle. The Hewlett Packard Enterprise-built supercomputer includes the latest Intel Xeon processors and boasts a peak performance of 8.0 petaflops, meaning it can carry out 8 million-billion calculations per second. This equates to an approximately three-fold increase in the amount of scientific computing capability relative to Peregrine, NREL's prior supercomputer.

Eagle is installed in NREL's ESIF, and like Peregrine, it is a warm-water liquid cooled system in which all of the waste heat will be captured and available for re-use in office and lab space. In addition to the computational capability, the acquisition includes a high-speed parallel centralized file system and data storage components.

Like Peregrine, Eagle will give NREL researchers the unique capability to run increasingly detailed modeling work and simulate complex processes, systems, and phenomena, providing valuable new perspective to drive innovative energy research. Whether it's used to predict the fundamental properties of materials or advance our understanding of the complex turbulence in whole wind plants, the new HPC system will provide a much-needed boost in computational capability to the research community.

Award-Winning Team Revolutionizes Data Center Water Savings with Thermosyphon System

HPC systems like Eagle produce a lot of heat. NREL's HPC data center cooling system was designed to be super effective in managing that heat—using evaporative towers that are more efficient and less expensive than energy-demanding chillers. But the towers consumed approximately 2.5 million gallons of water annually to support cooling of the IT load—approaching an hourly average of 1 megawatt. Driven by a mission to push the leading edge for data center sustainability, NREL recognized the need to make the data center not just energy efficient, but water efficient, too.

So, thanks to NREL's David Sickinger, Roy Fraley, and Kevin Regimbal, along with partners from Johnson Controls and Sandia National Laboratories, the BlueStream Hybrid Cooling System was born on the roof of the ESIF in August 2016. It saved 1.16 million gallons of water in its first year of operation, cutting the data center's onsite water usage in half while continuing to operate at optimal energy efficiency. In combination with the existing evaporative towers, this advanced dry cooler that uses refrigerant in a passive cycle to dissipate heat—called a thermosyphon—forms an extremely water- and cost-efficient hybrid cooling system.

And the project's success did not go unnoticed: NREL engineers David Sickinger and Kevin Regimbal received 2018 DOE Federal

Energy and Water Management Awards for this outstanding achievement in energy and water efficiency and conservation. Annually, these Federal Energy Management Program awards recognize individuals and organizations who have made significant contributions to energy and water efficiency within the federal government. Tom Carter of Johnson Controls, David Martinez of Sandia, and DOE's Matt Graham were also honored for their contributions to the project.

Water is not relatively expensive, but it's not readily available in every environment either. As a result, improving water efficiency in data centers is important to their sustainability. NREL has taken the lead in this area, and its groundbreaking work is paving the way for others to follow suit.

World's Most Energy-Efficient Data Center Demonstrates Hydrogen Fuel Cell Concept

NREL's data center is the most energy efficient in the world. It effectively cools IT equipment, captures and re-uses waste heat, and minimizes water usage in those processes. The waste heat is used as the primary heating source throughout its parent facility, the entire ESIF.

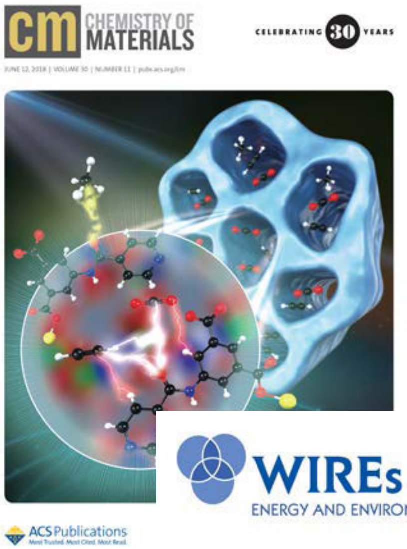
Envisioning a future in which data centers will be supplied entirely by renewable energy, NREL is working with industry partners to implement a prototype carbon-free data center concept based on automotive-scale hydrogen fuel cells within the HPC data center. When electricity generated from renewables (e.g., from solar and wind) exceeds the electrical power demands of the IT equipment, the excess energy is converted to hydrogen using electrolysis and stored. When the energy supply is less than the IT demand, a hydrogen fuel cell converts hydrogen into electricity to provide continuous power through intermittent sources.

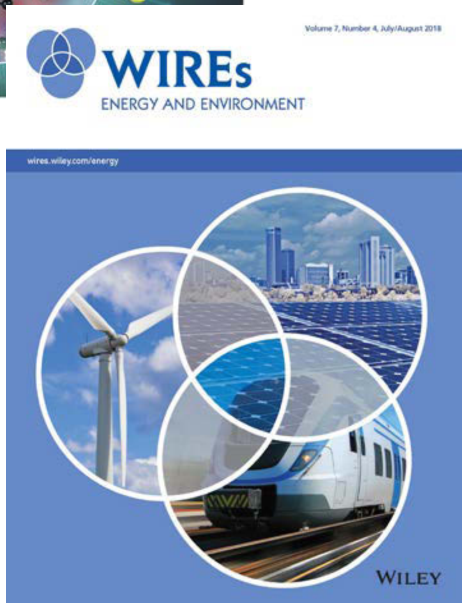
NREL has tested a Daimler-produced, Mercedes-Benz, 65-kW hydrogen fuel cell and in FY18 moved it into the data center to provide power directly to two racks of IT equipment. Daimler, in addition to NREL, collaborated with Hewlett Packard Enterprise and Power Innovations on this proof-of-concept project to make use of its automotive fuel cells in non-transportation sectors. Fuel cells provide resilience and can serve either as the primary or backup energy supply for the data center.

Publications

In FY18, 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 see a comprehensive list of publications and presentations, visit www.nrel.gov/computational-science/publications.html.



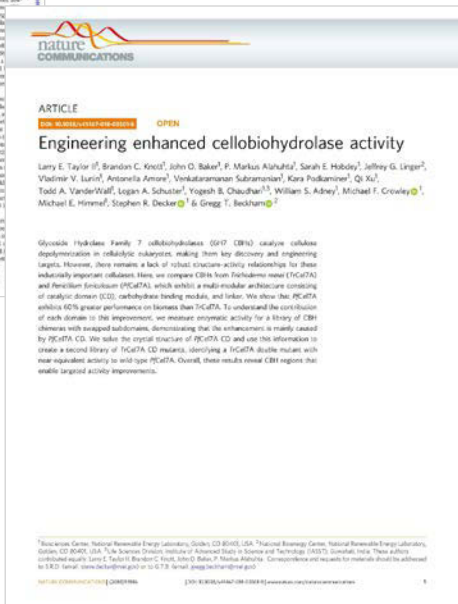


RESEARCH

SUSTAINABLE CHEMISTRY

Renewable acrylonitrile production

Acrylonitrile (ACN) is a petroleum-derived compound used in resins, polymers, acrylics, and carbon fiber. We present a process for renewable ACN production using 3-hydroxypropionic acid (3-HP), which can be produced microbially from sugars. The process achieves ACN molar yields exceeding 90% from ethyl 3-hydroxypropanoate (ethyl 3-HP) via dehydration and nitrilation with ammonia over an inexpensive titanium dioxide solid acid catalyst. We further describe an integrated process modeled at scale that is based on this chemistry and achieves near-quantitative ACN yields (98 ± 2%) from ethyl acrylate. This endothermic approach eliminates runaway reaction hazards and achieves higher yields than the standard propylene ammoxidation process. Avoidance of hydrogen cyanide as a by-product also improves process safety and mitigates product handling requirements.



nature COMMUNICATIONS

ARTICLE

OPEN

Engineering enhanced cellobiohydrolase activity

Larry E. Taylor II, Brandon C. Knott, John O. Baker, P. Markus Alahuhta, Sarah E. Hobdey, Jeffrey G. Linger, Vladimir V. Lunin, Antonella Amore, Venkataraman Subramanian, Kara Podkaminer, Qi Xu, Todd A. VanderWall, Logan A. Schuster, Yogesh B. Chaudhari, William S. Adney, Michael F. Crowley, Michael E. Himmel, Stephen R. Decker & Gregg T. Beckham

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