

Using Supercomputers To Help Companies Advance Clean Energy Technologies

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Through DOE's High Performance Computing for Energy Innovation initiative, Argonne will partner with Ford Motor Company, Capstone Green Energy, Lakril Technologies and Power Manufacturing to help accelerate the development of clean energy technologies.

Research and development is an expensive undertaking for any company — which is why so many startups begin with a new patent, a brand new idea foundationally tested and ready to be scaled up.

For established companies, balancing R&D expenses with profit margins can be a delicate task. Advanced computer modeling is an essential component of product development today, saving companies millions of dollars on repeated fabrication and testing. Such modeling, whether it's in search of new chemicals or materials, or simulating mechanical engineering challenges, is time consuming and expensive, and new products take years to go from conception to production. And while many of the world's fastest computers are privately held, building that kind of computing infrastructure is both expensive and risky. This is why public funding for supercomputing is critical to the advancement of U.S. commerce.

The U.S. Department of Energy (DOE) recently announced funding for a new round of industry partnerships through its High Performance Computing for Energy Innovation (HPC4EI) program. These projects are aimed at linking DOE's high performance computing (HPC) resources with private industry to help them improve manufacturing efficiency and explore new materials for clean energy applications.

DOE's Argonne National Laboratory is supporting four of the projects, providing expertise and access to its supercomputing resources. This includes the powerful systems at the Argonne Leadership Computing Facility (ALCF), a DOE Office of Science user facility, and Argonne's Laboratory Computing Resource Center.

Companies will not only get the benefit of using advanced computing resources, but they will also receive the benefit of working with some of the world's foremost HPC experts. Argonne is home to researchers who are adept at using supercomputers and working with collaborators to optimize HPC and artificial intelligence workloads for the systems.

This year, Argonne's HPC4EI projects include partnerships with Ford Motor Company, Capstone Green Energy, Lakril Technologies Corporation and Power Systems Manufacturing.



"The breadth of these awards shows how DOE's investment in Argonne's massive HPC resources and deep expertise can help companies large and small improve their products while reducing carbon emissions," said David Martin, manager of industry partnerships and outreach at the ALCF.

Helping Ford with Battery Technology

Subramanian Sankaranarayanan, group leader at Argonne's Center for Nanoscale Materials, a DOE Office of Science user facility, leads the lab's efforts with Ford Motor Company's research to improve battery manufacturing efficiency. Sankaranarayanan in collaboration with Ford researchers will use HPC to model and improve solid-electrolyte interphase (SEI) formation, a critical process for developing stable long-cycling lithium batteries for electric vehicles. Currently, the formation of the SEI takes a week or more, one of the most time-consuming aspects of the battery manufacturing process. By speeding up SEI formation, researchers can help battery plants significantly reduce energy consumption and carbon dioxide (CO₂) emissions.

Power and Heat Generation with Microturbines

Capstone Green Energy's C200 microturbine system for power and heat generation is already a green technology, but the company plans to work with Argonne research scientist Debolina Dasgupta to redesign, optimize and refit the C200 to run completely on hydrogen fuel. Capstone's need for supercomputers comes in part from the computational fluid dynamics simulations required to assess and compare designs to produce a configuration that can ensure the optimization of the engine's design for combustion and fuel injection systems. This new modeling effort will help Capstone make the switch to hydrogen fuel, leading to reduced nitrogen oxide emissions.

Argonne Sketching Out a "Green" Paint

Working with Lakril Technologies, Argonne computational scientist John Low is engaged in removing some of the carbon from the \$10 billion dollar paint, coatings, adhesive and super

absorbent polymer (diapers) markets. By converting corn and other bio-derived sugar sources into paints and coatings, they aim to reduce the 16 million kilograms of CO₂ generated annually to produce the acrylic acid that is traditionally used to create these products. Using Argonne's HPC resources, the team aims to improve the performance of a new catalyst that will enable the transition to sustainable biomass feedstocks.

Reducing Hydrogen Flashback

Power Systems Manufacturing (PSM) provides advanced technology that enables gas turbines to co-fire with renewable gases such as hydrogen, leading to a net reduction of carbon in the power grid. Flashback is a common problem in hydrogen-fueled combustion systems wherein the flame from the combustion chamber passes into the nozzle, causing damage to the equipment. PSM, working with Argonne computational scientist Shashi Aithal, will use the lab's HPC resources, coupled with artificial intelligence, to run simulations of engine redesigns and optimizations to understand and reduce the risk of flashbacks. These advances will assist PSM in converting carbon-emitting equipment for power generation into greener, hydrogen-burning products, thereby lowering emissions and reducing production time and cost.

The HPC4EI program is sponsored by DOE's offices of Advanced Materials and Manufacturing Technologies and Industrial Efficiency and Decarbonization within the Energy Efficiency and Renewable Energy Office and the Office of Fossil Energy and Carbon Management.