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Transforming **ENERGY** Through Computational Excellence

High-Performance Computing for Energy Innovation

The challenges associated with energy efficiency of manufacturing and advanced materials often cannot be addressed through experimentation alone, whether because of scale, complexity, or practicality. High-performance computing (HPC) enables fast tackling of these challenges in the manufacturing sector—vital to achieving net-zero carbon emissions by 2050.

The National Renewable Energy Laboratory (NREL) and industry partners leverage HPC to apply advanced modeling, simulation, and data analysis to improve manufacturing efficiency, explore new materials for energy applications, and develop technologies to manage carbon across the life cycle. From improving additive manufacturing processes to increasing the energy efficiency of jet-engine components, advanced computing can help manage emissions produced by manufacturing in a wide variety of ways.

Scale-Up

Cost-effective, scalable solutions—and discovery and development of new energy materials, devices, and processes—are critical to industry's realization of clean, efficient energy and decarbonization. NREL modeling and simulation capabilities provide insights for planning and implementation, from fine-scale solutions through to solutions at the national level.

NREL's signature Energy Materials and Processing at Scale (EMAPS) Facility will incorporate multidisciplinary capabilities and create a direct path from materials and process innovations to at-scale integration and market readiness. Close connections between theory and experimentation are enabled by smart characterization, automation, and learning—aspects of EMAPS that will tightly couple NREL's modeling and simulation capabilities to key scaling challenges.

Industrial Decarbonization

Adopting new manufacturing processes can help companies reduce operational costs and greenhouse gas emissions while boosting production. Although changes are necessary to reach a carbon-free energy sector by 2035, tracking—which can have the greatest positive results—is a complex task. That's why NREL partners with industries to develop high-fidelity models to map these impacts.

Using world-class computational resources, like HPC for Energy Innovation (HPC4EI), NREL models how adding more renewable energy or battery storage might impact the reliability, flexibility, and cost of energy at a manufacturing plant. HPC can also monitor how new manufacturing processes—like using recyclable or reusable materials, using renewable biomass instead of less sustainable materials, or implementing more energy-efficient processes—could affect a company's carbon emissions, productivity, and costs.

Talon," the supercomputer purchased by the U.S. Department of Energy's Advanced Manufacturing Office, is located in NREL's `HPC Data Center. *Photo by Werner Slocum, NREL #67310*

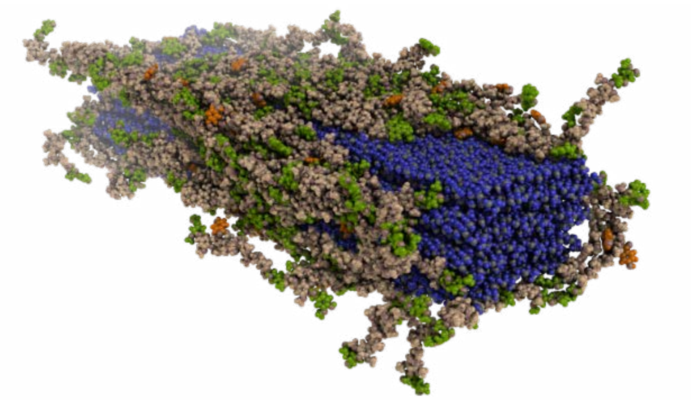
Project Examples

Rapid Design Optimization of Sulfur Thermal Energy Storage

With the computing expertise of NREL, Element 16 Technologies, Inc., will improve molten sulfur thermal energy storage product design with a high-fidelity HPC model validated by experimental data. The model outcomes can facilitate Element 16 thermal energy storage system deployment in various industry applications. Principal investigator: Zhiwen Ma.

Cellulose-Derived Packaging Materials

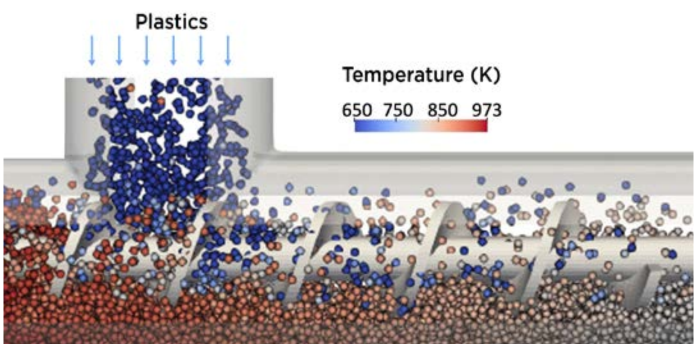
In collaboration, NREL and the Futamura Group will accelerate the development of next-generation recyclable cellulose-based packaging materials. Models of biopolymer assemblies are used to predict how molecular modifications of components impact performance metrics, such as mechanical strength, barrier properties, and wettability. Principal investigator: Peter Ciesielski.



An example of a molecular model of cellulose (shown in blue) with lignin polymer variations (beige, green, and orange) to assess properties of the composite material. *Illustration by Lintao Bu and Peter Ciesielski, NREL.*

Converting Waste to Fuels and Hydrogen

NREL and CHZ Technologies are advancing optimized methodologies for converting waste plastics to fuels and carbon-neutral hydrogen via NREL's multiphase chemically reacting flow models. These high-fidelity simulations have led to the discovery of optimal plastic feedstock mixtures, thermal conditions, and screw-fed pyrolysis reactor designs for optimal production of synthesis gas and hydrocarbon intermediates. Principal investigator: Hariswaran Sitaraman.



Simulations of granular flow and heat transfer in a screw-kiln plastic pyrolysis reactor. *Illustration by Hariswaran Sitaraman, NREL.*

Codes for Supercritical CO_2 Combustion

8 Rivers Capital, LLC, and NREL will develop a surrogate model to inform liner and turbine design along with material selection for supercritical CO2 combustion in a project titled "Development of Novel Combustion Codes for Supercritical CO2 Combustion." Principal investigator: Shashank Yellapantula.

Saving Energy Through Process Optimization

Dow Chemical Company will partner with NREL to model how flow in plastic impacts polymers at a molecular level in a project titled "Non-Equilibrium Molecular Simulations of Polymers Under Flow: Saving Energy Through Process Optimization." Principal investigator: Michael Crowley.

Learn More

NREL welcomes industry partners who seek to improve energy efficiency and understand how their manufacturing processes and systems can help drive decarbonization.

To learn more, visit: **https://www.nrel.gov/computational-science** or contact:

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