COMPUTING FOR A RENEWABLE FUTURE

Computational Science at NREL Accelerates Energy Research

The National Renewable Energy Laboratory (NREL) is the nation's primary laboratory for renewable energy and energy efficiency research and development. NREL's mission and strategy are focused on advancing the U.S. Department of Energy's and our nation's energy goals. The laboratory's scientists and researchers, including those involved in high-performance computing and simulation, support critical market objectives to accelerate research from scientific innovations to market-viable alternative energy solutions.

Biofuels

Cellulosic Ethanol

Focus on dramatically reducing the cost of producing ethanol from cellulose, the woody part of plants:

•Pursue modeling and simulation aimed at understanding the structure-function relationships in cellulose-degrading enzymes and systems. The system sizes of interest range up to several million atoms.

•Used RedMesa and RedSky, in collaboration with Sandia Scientific Computing, and amassed *more* than 15 million processor hours for molecular dynamics simulations.

•Utilizing simulation in collaboration with **Genencor** to rationally design improved cellulases.

Wind

Turbine Modeling

Coupled atmospheric wind and turbine models to optimize design and operation of wind turbines:

•Simulate "inflow" characteristics affecting design of large wind turbines.

•Model and minimize impact of upwind turbines and wakes on "downwind" turbines.

•Predict and maximize wind energy capture potential.

The **National Wind Technology Center** has research and development collaborations and partnerships with industry partners such as **Seimens**, **Alstom,** and **Gamesa** for turbine aerodynamics, rotor testing, and performance.

Solar

Organic Photovoltaics

Design efficient and low-cost solar materials by combinatorial screening of organic photovoltaic candidates.

•Use electronic-structure calculations of energy levels to find suitable co-polymer pairs.

•Screened more than 50,000 pairs, and imported them into database/Web app for automated analysis.

•Identified more than 100 promising new materials; currently working with two industry partners to synthesize novel materials.

The **National Center for Photovoltaics** has partnerships and collaborations with industry partners such as **Konarka**, **Plextronics**, **ConocoPhillips**, **Luna nanoWorks**, **Solarmer**, **Nano-C** and others, and is also involved in collaborations with universities such as **Stanford University**, **Colorado School of Mines**, **University of Arizona**, and others.

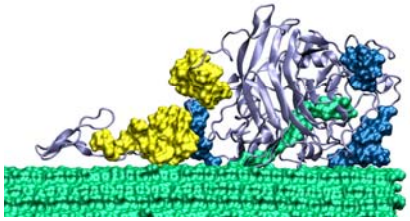
High-Performance Computing (HPC)

Red Mesa

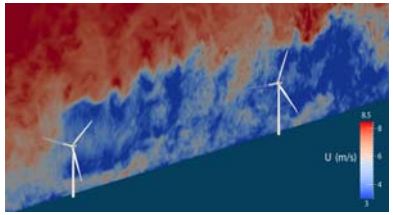
As part of an HPC collaboration, Sandia National Laboratories and NREL have deployed the tenth-fastest high-performance computing system in the world, RedSky-RedMesa. RedMesa is the fastest system dedicated to advancing research on energy efficiency and renewable energy technologies.

Red-Mesa alone has a peak performance of 180 teraFLOPS, with over 15,000 Intel Xeon 5570 Nehalem cores. It is the fastest system in the world dedicated to advancing research on energy efficiency and renewable energy technologies.

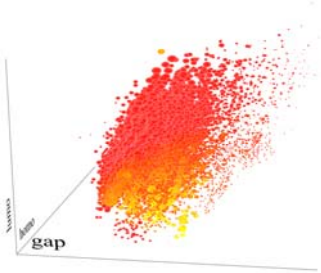
NREL researchers are using RedMesa to conduct modeling and simulation in the areas of bioenergy, energy-efficient building design, fuel cells, solar energy, vehicles, and wind turbines to accelerate progress toward meeting national energy goals.



Large-scale microsecond simulation of cellulase digesting cellulose, showing new insights into role of linker and its glycosylation. Ribbon/string cartoon is protein; yellow is space-filling representation of glycosylation (sugars) on linker peptide; blue is glycosylation of catalytic domain; green is cellulose.



High-resolution simulation of turbulence affecting a 5-megawatt wind turbine in the wake of another turbine ~900 meters upstream. Generated by OpenFOAM (computational fluid dynamics model) coupled with FAST (NREL-developed turbine simulator) on NREL's RedMesa supercomputing cluster.



Bubble plot showing five dimensions of predicted properties for ~10,000 organic photovoltaic materials. Bubble size is proportional to overlap of the material's absorption spectrum with sunlight. Color indicates predicted solar cell efficiency (yellow denotes higher efficiencies).

RedMesa is the cornerstone of a successful collaboration in high-perfomance computing between NREL and Sandia to deploy and use a world-class capability for studying complex issues related to renewable energy technologies.

U.S. DEPARTMENT OF ENERGY
Office of Science

NREL
NATIONAL RENEWABLE ENERGY LABORATORY