

Transforming **ENERGY** through Computational Excellence

Computational methods underpin advancing the science and engineering of energy efficiency, sustainable transportation, renewable power technologies, and developing a knowledge base to optimize energy systems. Researchers with access to enough computing, and the right type, can focus their ingenuity and creativity on addressing the energy challenges.

NREL's advanced computing influence spans several common themes across the Office of Energy Efficiency and Renewable Energy (EERE), including materials discovery, process modeling, fluid dynamics, resource mapping, and analysis of large-scale systems with real-time optimization.

Hardware & Facilities

Housed in the most energy-efficient datacenter in the world, the **Eagle supercomputing system** and associated **Insight Center** provide capability for highly complex, large-scale simulations, ensembles of simulations, and highly detailed visual analytics. This enables EERE to tackle energy challenges that cannot be addressed through traditional experimentation alone.

World-Class Researchers & Support

NREL computational science researchers are deeply embedded in a wide range of EERE-related scientific investigations, working across theory and experiment to develop ground-breaking cross-discipline data acquisition and analysis, and tie these together with model development. This engagement enables conceptualization of new ways to use computing to achieve NREL and EERE goals, and supports researchers across the complex in pursuing a new business as usual. Through consulting, leading by example, and long-term collaborations, computational science researchers provide leveraged and durable impact.

Core Capabilities

Applied Mathematics: Development of scalable algorithms to address uncertainty and solve multi-scale and inverse problems in continuous, discrete, and network domains. Techniques include stochastic optimization and control; adaptive methods in space, time, and fidelity; artificial intelligence; and linear solvers.

Computational Science: Development and solution of models for the behavior and control of energy carriers including chemical, biological, solar, wind, water, and electricity. Materials and chemistry theory. Inverse design, development of digital twins for mobility, and network systems understanding and control.

Planning for the Future

Successful innovation in computing requires both the hardware and the expertise to leverage rapid advances that continue at a lightning pace from the public and private sectors.

Kestrel, NREL's next high-performance computer (HPC), will provide an increase in computing power (over Eagle), with a mix of more capable nodes from new architectures to large memory. Kestrel includes upgraded network and data storage and will be installed in 2022. Designed to be **extensible to meet growing needs** of the energy efficiency and renewable energy community, Kestrel will enable more robust research with rigorous treatment of cyber, climate resilience, environmental justice, and economy-wide modeling.

Planned **Insight Center upgrades** include advances in both two- and three-dimensional large-scale and immersive visualization installations, supporting knowledge discovery through dynamic interaction and exploration of extremely large, complex experimental- or simulation-produced data. These NREL capabilities empower communities, utilities, and businesses to visualize and address the challenges of melding the plethora of clean energy technologies now available with aspirations to reduce their carbon footprints. Notable examples of NREL success here include the City of Los Angeles and Dallas Fort Worth (DFW) Regional Airport.

Computational capability and expertise can empower the major changes and advances in power generation, autonomous energy systems, transportation, buildings, and communities needed to achieve a carbon-free power sector by 2035 as a step toward a decarbonized U.S. energy economy in 2050.

Energy-Efficient System Operation: Scalable systems architecture, procurement, deployment, and operation; software stacks and toolchains; allocations processes; and scalable workflow support and user engagement.

Advanced Computer Science, Visualization, and Data: Human-computer interaction; immersive visualization; experimental design; hardware-in-the-loop/cloud integration; co-simulation; data centric workflows; code optimization; software quality; and data compression and anomaly detection.

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