Transforming **ENERGY** Through Computational Excellence

NREL's Computational Science Center

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.

NREL's Computational Science Center (CSC) proudly focuses on providing the service of computing, advancing the science of computing, and enabling NREL's clean energy mission.

Provide the Service of Computing

The CSC is the steward of NREL's advanced computing capabilities. CSC researchers are deeply embedded in a wide range of scientific investigations, working across theory and experiment to develop groundbreaking, cross-disciplinary data acquisition and analysis, and tying these together with model development.

High Performance Computing (HPC)

Housed in the Energy Systems Integration Facility (ESIF) is the Kestrel supercomputing system—within the most energy-efficient data center in the world—and associated Insight Center. Onsite and offsite access are available for Kestrel and its applications, numerical and input/output libraries, development tools, toolchains (compiler and parallelization libraries), and environment modules. The data center also hosts computing capability architected to meet the needs of specific programs, such as Swift, an HPC resource dedicated to the needs of the vehicle technology program. The Insight Center's two- and three-dimensional, large-scale and immersive visualization installations support knowledge discovery through dynamic interaction exploration of extremely large, complex, experimental or simulation-based data.

Cloud and Hybrid Computing

The Vermillion HPC system is the cornerstone of NREL's institutional computing investment to support varied and data-centric workloads. Built on the OpenStack platform, Vermillion and related systems embrace virtualized and containerized computing with an eye to enabling hybridized HPC-on-premise/commercial cloud workflows as well as tight integration between experiment and computing. These capabilities are coupled with, and complemented by, self-service cloud computing services (Stratus) to enable researcher access, data sharing, and experimentation at multiple scales and locations.

The Power of Your Computing Resources

Through consulting and long-term collaborations, CSC researchers bring the capabilities and insights developed in the course of their own research to provide leveraged and durable impact. Together, we conceptualize new ways to use computing to achieve goals. Researchers who want to independently leverage advanced computing can benefit from seminars, user groups, and the community of computational science across the lab.

Advance the Science of Computing

Many challenges remain between implementing existing state-of-the-art computing practices in commercial and academic settings and enabling applied energy research. CSC researchers tackle challenges in abstracted forms that also benefit the broader community with three major objectives:

1. **Address fundamental computational science, visualization, and applied mathematics problems** in the applied energy space.
2. **Provide critical support of NREL's mission,** from fundamental research in artificial intelligence (AI) and visualization to computing and applied mathematics.
3. **Perform interdisciplinary research and development in an environment of "use,"** including analysis and control of integrated complex systems in collaboration with colleagues from across disciplines.

Insight Center Visualization Lab at the ESIF. Using NREL's supercomputer, data and analysis can be translated into a three-dimensional model to assist the resiliency study. *Visualization courtesy of Kenny Gruchalla and Nicholas Brunhardt-Lupo. Photo by Dennis Schroeder, NREL 58573*

NREL's advanced computing influence spans materials discovery, process modeling, fluid dynamics, resource mapping, and analysis of large-scale systems with real-time optimization.

Core Capabilities

Interdisciplinary skills make CSC staff key contributors across research domains.

Applied mathematics research focuses on techniques that enable simulations of practical challenges at the scale necessary for actionable insight. Techniques such as quantifying uncertainty and propagating it through multi-component models are essential for planning, while multi-scale and scale-bridging methods are needed to connect fundamental physics to practical designs. Faster and more robust linear systems solutions—and algorithms that enable codes to scale to the largest computers available—help generate the ground truth data that underpins AI and machine learning (ML).

Computational science research focuses on developing and solving models of the behavior and control of energy carriers, including chemical, biological, solar, wind, water, and electricity carriers. Targeted approaches include materials and chemistry theory, inverse design, development of digital twins for mobility, and network systems understanding and control.

Visualization and data science research into human-computer interaction, cognition, and immersive visualization enables researchers to make sense of their data and communicate their results, while exploring the workflows that leverage the unique capabilities of HPC, cloud, and data-centric computing. Specialized hardware builds the knowledge base to architect fit-for-purpose systems.

Energy-efficient systems operation research uses on-premise systems as a living lab. Operational research done in concert with operating the capability enables a reduction in energy usage within the data center and across the industry. Examples include parameter estimation for complex systems, physics-informed ML, understanding how to use multiple model fidelities together to enable optimization under uncertainty, visualization of complex data, co-simulation, and distributed control.

Enable a Clean Energy Mission

Grappling with the climate/energy nexus is a grand challenge of our time, and NREL's computing capabilities will play a critical role in defining paradigm shifts in cyber, climate resilience, environmental justice, and economy-wide modeling.

Sustaining Delivery of Computing Services

Successful innovation in computing requires both the hardware and the expertise to leverage the rapid advancements that continue at a lightning pace in the public and private sectors. NREL's computational facilities provide the right resources to test and develop new tools, libraries, and languages.

CSC data scientists, engineers, and mathematicians are performing basic and applied research and developing cross-cutting capabilities that provide the critical foundation upon which rapid breakthrough science is made possible across NREL and in support of DOE. CSC's high-impact expertise includes programming languages, petascale to exascale scientific data management and scientific visualization, distributed computing infrastructure, programming models for novel computer architectures, and code performance improvements.

Computational capabilities and expertise can empower the major changes and advances needed to achieve a decarbonized U.S. energy economy.

To access NREL stewarded computational resources please contact Center Director Ray Grout or visit nrel.gov/hpc for details.

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NREL Transforming ENERGY

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