Transforming **ENERGY** Through Computational Excellence

NREL Computational Fluid Dynamics Modeling Complex, Dynamic Systems

Computational fluid dynamics (CFD) enables modeling, analysis, and visualization of phenomena that would usually be impossible or extremely expensive to measure experimentally.

These dynamics govern the physics of wind generation, chemical reactions and electricity flow in materials—problems fundamental to informing the evolution of clean energy technologies as well as their integration into the grid. Modeling fluid behavior in complex systems can be an enormous undertaking. Complexity can arise from the need to address a range of scales, both in space and time, and as the ranges of scales increase, so does the magnitude of the computer simulation required to capture them.

NREL's CFD and supporting tools provide:

- Solution-adaptive automatic mesh refinement
- High-order accurate computational approaches
- Solvers for linear and nonlinear systems
- Advanced time-evolution strategies for coupled systems
- Complex, moving domain geometries
- Strategies to couple CFD with machine learning diagnostics, model development, inference, and training of artificial intelligence control algorithms
- Cutting-edge, accelerator-based computing hardware.

At the National Renewable Energy Laboratory (NREL), we create and customize cutting-edge tools designed to tackle the barriers to decarbonization, leveraging the expertise of a diverse team of developers, applied mathematicians, and engineers. NREL also collaborates with partners in universities, industry, and other national laboratories to accelerate energy research and development.

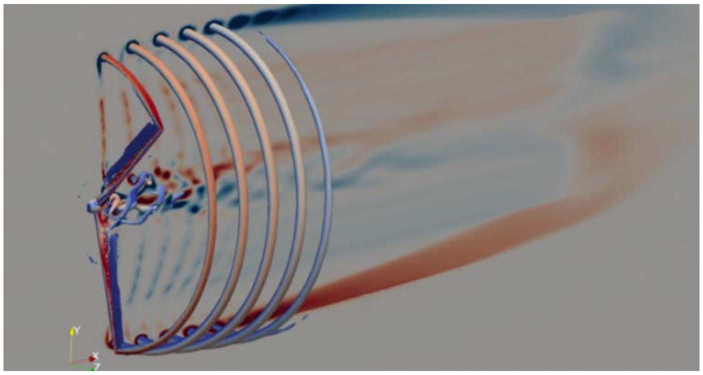
Our work is funded through both public and private sources, and involves a variety of multiphysics fluid-based systems and applications involving complex chemical and physical interaction such as particle/fluid interactions; multiphase transport; chemically reacting flows; turbulence; multiscale, coupled phenomena; fluid-structure interactions; electrically charged flows; and flows in porous media complex chemical and physical interaction.

We continuously expand our toolkit to support research to solve real-world problems. The following example projects illustrate how advancing the state of the art can address increasingly complex scenarios.

ExaWind

ExaWind is an open-source suite of physics codes and libraries that enables blade-resolved simulation of wind turbines and wind-based power plants. Simulations span a massive range of relevant scales, from millimeter-high boundary layers that form along the curved blades of wind turbines to kilometer-scale atmospheric wind patterns.

Powerful CFD solvers work together to explore these complex systems, from modeling the flow near the turbine blades and nacelle structures, to capturing the atmospheric boundary layers and interacting downstream wakes of multiple



Simulated flow around an NREL 5-megawatt wind turbine rotor generated by the ExaWind high-performance computational codes. *Image by Shreyas Ananthan, NREL*

turbines in a wind farm. This allows scientists to understand, for example, the impact of blade-design details on power plant performance. Active development includes expansion of the ExaWind framework to include multiphase processes necessary to simulate off-shore floating wind-turbine installations.

Modeling Each Step in Converting Biomass to Fuels To Improve Yields

A diverse set of coupled tools enable reactor and mesoscale modeling of biochemical and thermochemical biomass conversion processes. Across unit operations—from biomass feedstock processing to catalytic fuel upgrading—NREL applies predictive modeling to address important challenges, including reactor scale-up and whole-plant analysis. Recent developments aid in the design of high-performance biofuel plants at scale through system-level tools that couple high-fidelity CFD models with techno-economic analysis. Cutting-edge modeling capabilities allow NREL scientists to study alternative fuel production pathways such as gas fermentation of CO_2, conversion of renewable hydrogen to natural gas photobioreactors, and production of sustainable fuels using large-scale algae ponds.

Reacting Flows

Reacting flows are at the heart of several applications pertaining to renewable energy, such as clean combustion, electrochemistry, and material synthesis. NREL is actively developing a suite of libraries and tools for reacting flow modeling, called Pele. Pele performs extremely high-resolution simulations required to resolve turbulence chemistry interactions, such as those within chemical vapor deposition chambers and piston and gas turbine combustors.

In addition to the extraordinary computing resources provided by DOE's leadership-class supercomputers, these simulations require a broad array of innovative mathematical algorithms and software engineering, which NREL has developed. Current modeling efforts span several applications, including CO_2 capture, chemical vapor deposition, electrochemistry, and turbulent combustion.

Software Development and Applied Mathematics

A critical aspect of each CFD application is the effective development of novel algorithms for both physics modeling and linear and nonlinear solver techniques. NREL's CFD teams use modern software engineering practices to develop high-performance implementations of these algorithms that can effectively leverage a broad range of emerging high-performance computing platforms. Most importantly, our algorithms are publicly shared in packages such as Lawrence Berkeley National Laboratory and NREL's co-developed AMReX and Lawrence Livermore National Laboratory's Hypre software libraries. NREL scientists are committed to developing robust and supported software that is useable across the scientific community.

Why Partner With NREL?

NREL's expertise in CFD enables virtual experiments that are impractical in the real world and empowers researchers, businesses, and government agencies to make well-informed technical, economic, and policy decisions.

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Cover image: Using the Pele code for compressible reacting flows, NREL researchers use CFD to evaluate the stability and efficiency of supersonic hydrogen combustion when fuel is injected directly into the turbulent recirculating flow generated by a shaped cavity along the walls of a high-speed channel. *Visualization by Nicholas Brunhart-Lupo, NREL*

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