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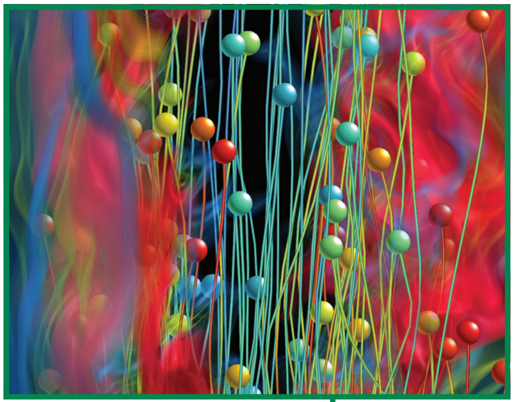
Simulations Explore Next-Generation Fuels for Cleaner Combustion



S3D combustion simulations focus on the underlying science that will help fuels burn cleanly in next-generation engines.

Simulations of turbulent combustion may help speed the achievement of fuel efficiencies at least 25 percent higher in next-generation engines. Employing compression ignition to burn dilute, lean fuels at lower temperatures than do today's engines will mean reduced emissions of unburnt hydrocarbons and pollutants.

Air and fuel violently mix during turbulent combustion. Such mixing is necessary to ignite fuel and sustain its burning in internal combustion engines, rockets, turbines for airplanes and power plants, and industrial boilers and furnaces. Fluid dynamics equations govern turbulent combustion, and solving them taxes even the Jaguar supercomputer at Oak Ridge National Laboratory, which is America's fastest with a peak speed of 3.3 petaflops, or quadrillion calculations per second. By the end of the year, this Department of Energy Office of Science machine will have even more computational power to bring to the problem with an upgrade to up to 20 petaflops with the addition of energy-efficient, high-performance scientific-application-code accelerators called graphics processing units (GPUs). The resulting hybrid supercomputer, Titan, will be able to run codes even faster, allowing increased complexity and realism in simulations. That accomplishment will accelerate research with S3D, a code to simulate combustion of diverse fuels that is advancing the development of predictive models for design of clean-energy technologies for power and propulsion. Resulting innovations that increase the efficiency of combustion could also increase energy security, create green jobs, strengthen the economy, and improve the environment.

"If low-temperature compression ignition concepts employing dilute fuel mixtures at high pressure are widely adopted in next-generation autos, fuel efficiency could increase by as much as 25 to 50 percent," said mechanical engineer Jacqueline Chen of Sandia National Laboratories, who with partners was allocated 113 million hours on Jaguar in 2008, 2009, and 2010 for S3D simulations.

S3D is one of six applications with which experts at the Oak Ridge Leadership Computing Facility (OLCF) work to demonstrate the promise of hybrid supercomputing. At the Center for Accelerated Application Readiness, they convene experts from the OLCF, computer maker Cray, GPU manufacturer NVIDIA, and the application teams to develop approaches for generating results from the hybrid system, which employs both GPUs and central processing units.

A direct numerical simulation (DNS) code, S3D simulates the finest microscales of turbulent combustion by solving the compressible reactive Navier-Stokes equations on a well-resolved 3D computational mesh. A burning flame can manifest chemical properties on small scales from billionths to thousandths of a meter. S3D provides underlying scientific insight and the benchmark simulation data needed to develop and validate a key subprocess model describing gas-phase combustion that would ultimately be part of an engineering computational fluid dynamics solver used to design engines. The solver would include models describing several key subprocesses such as sprays, heat transfer, and combustion.

S3D simulates fine-scale mixing and reaction processes in turbulent combustion required to understand finite chemical kinetic rate effects and their coupling with turbulence such as autoignition, extinction/reignition, stabilization of lifted flames in reactive environments, and compression ignition. Under low-temperature, high-pressure thermochemical conditions, mixed regimes of combustion may occur. For example, flames may propagate into a partially oxidized, autoigniting mixture. These more complex regimes are not well understood, nor are they encapsulated in current coarse-grained engineering models.

With GPUs Chen's team has dramatically increased the chemical complexity of combustion simulations, which can help engine developers better understand and tailor the combustion of gasoline and new, more complex fuels in next-generation engines. Ultimately, armed with this and other information in predictive design tools, automobile companies will be able to produce higher-performance, more-efficient combustion engines while significantly reducing emissions such as carbon and oxides of sulfur and nitrogen.

For today's state of the art, using Jaguar for a high-fidelity DNS with cells just 5 millionths of a meter wide, Chen's team directly simulated combustion in a canonical high-pressure, low-temperature domain to investigate homogeneous charge compression ignition combustion processes. The researchers identified different regimes of combustion in a compression ignition environment that are sensitive to details of ignition kinetics. Current coarse-grained models have difficulty accounting for multiregime combustion driven by nuances of chemistry and interaction with molecular and turbulent transport. Data like these will help guide the development of more predictive models.

Another state-of-the-art simulation on Jaguar used 7 billion grid points to explore hydrogen and syngas, a mix of carbon monoxide and hydrogen that burns more cleanly than coal and other carbonaceous fuels.

A 20-petaflop Titan system will give the team the ability to simulate more complex fuels, moving beyond simple fuels such as hydrogen and syngas to oxygenated fuels like ethanol and butanol (commercially important alcohols), to large-molecule hydrocarbon fuels such as isooctane (a surrogate for gasoline) and blends of methyl butanoate, methyl decanoate, and n-heptane (a biofuel surrogate).—*by Dawn Levy*

Contributors

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Publications

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