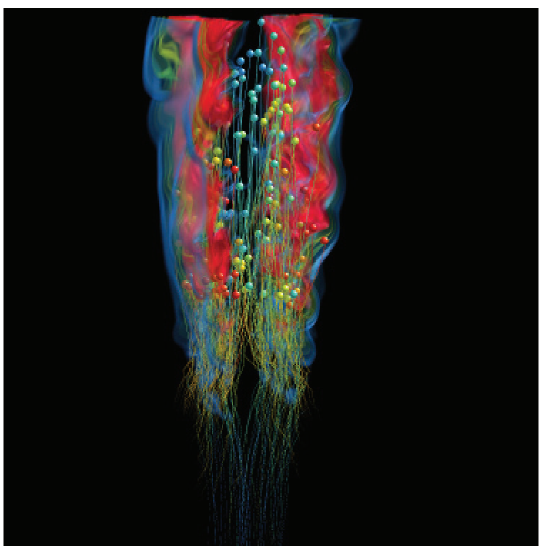
Burn, Baby, Burn

Jaguar lights the way to energy independence

America's dependence on foreign oil is becoming more than a thorn in the country's side—it's now widely viewed as an unsustainable, and potentially dangerous, liability.

One of the more promising remedies for our import addiction is the deployment of engines, furnaces, and power-generation devices that burn alternative fuels and use advanced technologies. These next-generation combustion systems will not only reduce our dependence on foreign oil but also likely help reduce the amount of pollution generated by traditional internal combustion engines in automobiles.



Simultaneous volume rendering of a lifted ethylene/air slot jet flame. The particles are colored by temperature: cold (blue), hot (red). Image courtesy Jackie Chen, SNL, and Kwan-Liu Ma, UC–Davis.

Considering that two-thirds of the petroleum Americans use goes for transportation, while the remaining one-third heats buildings and generates electricity in steam turbines, the necessity for advanced combustion devices is a no-brainer. Their deployment directly addresses two key DOE mission objectives: energy security and environmental responsibility.

To bring these technologies to market, a team led by Jacqueline Chen of Sandia National Laboratories (SNL) is simulating the combustion of various fuels on the NCCS's Jaguar supercomputer, research that is creating a library of data that captures complex aero-thermo-chemical interactions and provides insight into how flames stabilize, extinguish, and reignite. Chen's data libraries will assist engineers in the development of models that will be used to design the combustion devices of tomorrow.

"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," Chen said. With mechanical engineer Chun Sang Yoo of SNL and computational scientist Ramanan Sankaran of the NCCS, Chen used Jaguar to simulate combustion of ethylene, a hydrocarbon fuel. The simulation generated more than 120 terabytes (120 trillion bytes) of data.

In an effort to revolutionize combustion technology, the NCCS granted Chen and her team time on Jaguar following the system's upgrade to 263 teraflops. Running computationally demanding applications after a major machine upgrade is part of a transition-to-operations (T2O) activity that begins when a commissioned NCCS system passes a formal acceptance test and its performance is monitored and assessed. Essentially, researchers with compelling science problems and codes that could use a large fraction of the machine were selected to run on one of the most powerful supercomputers in the world. Chen's direct numerical simulation (DNS) code, known as S3D, was a perfect fit.

Exploring Lifted Flames

Advanced combustion technology depends on lifted flames, which result when cold fuel and hot air mix and ignite in a high-speed jet. If the speed increases too much, lifted flames can blow out. For flames to stabilize, or continue to burn downstream from the burner, turbulence, which mixes fuel with air to enable burning, must exist in balance with key ignition reactions that occur upstream of where the flames appear.

Proper positioning of lifted flames in advanced engines could burn fuel so cleanly that emissions of nitrogen oxide, a major contributor to smog, would be nearly undetectable. To explore processes underlying ethylene combustion, the group uses DNS, a high-fidelity numerical approach that fully resolves all of the temporal and spatial scales associated with both turbulence and flames. The technique employs a computational

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mesh of more than a billion points to capture both fast ignition events and the slower motion of turbulent eddies.

"Direct numerical simulation is our numerical probe to measure, understand, or see things in great detail at the finest scales where chemical reactions occur," Chen said. "That's particularly important for combustion because reactions occurring at the finest molecular scales impact global properties like burning rates and emissions."

S3D runs on multiple processing cores to model compressible, reacting flows with detailed chemistry. The 2008 T2O simulations used up to 30,000 of Jaguar's 31,000 processing cores and 4.5 million processor hours. Furthermore, Chen and her colleagues created the world's first fully resolved simulation of small lifted autoigniting hydrocarbon jet flames, designed to represent some of the fine-grained physics relevant to stabilizing in a direct-injection diesel engine.

Chen's simulations also showcased the relationship between the NCCS liaisons and principal investigators. For the T2O allocation, the NCCS's Ramanan Sankaran developed a new feature for the S3D code that allowed the team to track tracer particles throughout the simulated flames.

The tracer, which doesn't alter the data and can be programmed to track different phenomena in the flame, is analogous to dropping a bottle with a tracking device in the ocean, said Sankaran. As the ocean currents move the bottle across the sea, the tracking device records all sorts of information, not only telling the recipient where the bottle has been, but also what it has been through. "It gives us a better look at what's going on inside the flame," said Sankaran, adding that "it also enables a different view of the same data."

Because of the large number of particles transported, mechanical engineer Ray Grout and computer scientist Hongfeng Yu from SNL developed a graphics processing unit–enhanced framework for interactive Lagrangian particle query and analysis on the analytics machine at ORNL known as Lens.

The sheer scale of Chen's simulations has enabled an unprecedented level of quantitative detail in the description of both turbulence and chemistry and their interactions. And while ethylene is not a common transportation fuel, it is an important reference fuel in research. Ethylene's relatively simple chemistry makes it a good candidate for DNS. Moreover, it is easy to work with in the lab, and its chemical properties are well known, so it is feasible to test results from experiments against predictions from numerical simulations.

"DNS of turbulence-chemistry interactions requires the horsepower of machines like Jaguar and beyond to simulate the coupling between complex hydrocarbon ignition kinetics and turbulent mixing," said Chen. "It is particularly important to understand how differences in chemical properties of various fuels—biofuels and petroleum—impact combustion phenomena such as ignition and extinction in a turbulent environment."

Chen's simulations are helping engineers develop unprecedented models of combustion in a variety of environments. These models will eventually be used in engineering computational fluid dynamics simulations to optimize the design of engines and power-generation devices, a crucial ingredient in America's quest for both cleaner energy and energy independence.—by Scott Jones

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