HPC Opens a New Frontier in Fuel-Engine Research

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Last year, the transportation sector consumed more than 15 billion barrels of oil worldwide. The output of combustion engines—an incredible engineering feat that has propelled not only people geographically but also entire trade markets and economies—is a mixture of chemical gases, particulates, and petroleum hydrocarbons. The chemical residues of burned petroleum can be found everywhere, from the cellular level of the human body to the ozone of the upper atmosphere, and in all the ecosystems and biomes in-between.

It is of significant economic and environmental impact to keep improving vehicle fuel consumption. Whereas the demand for gasoline products is projected to decline as more hybrid vehicles enter the passenger car fleet, the demand for diesel products is expected to rise as the global economy expands. Even a 1 percent improvement in engine efficiency can save billions of gallons of fuel annually.

Gasoline compression ignition is one efficiency-improving technology garnering attention, with considerable research efforts focused on understanding the relationship between fuel properties and combustion under autoignition conditions. Certain gasoline-like fuels have a lower cetane number than diesel, which leads to longer ignition delay and better fuel-air mixing before the onset of combustion. Together with the lower aromatic content, lower soot can be obtained with these fuels. But the longer ignition delays might produce elevated pressures on the engine components, which might affect the lifespan of the engine. Most research to date has focused on production engines with minor modifications to the engine hardware.

A team of researchers from Argonne National Laboratory's Virtual Engine Research Institute and Fuels Initiative (VERIFI) and from the Aramco Research Center–Detroit are using Argonne's Mira supercomputer to conduct a comprehensive design of experiments study—an optimization technique used in the engine industry—of a production engine to accelerate the development of an optimized fuel-efficiency focused design. This work matches engine combustion modes with improved fuel properties to create cleaner and more efficient transportation technologies. Aramco Research Center–Detroit is one of three US-based research centers operated by Saudi Aramco's North American subsidiary, Aramco Services Company.

The team recently conducted a computationally guided combustion system optimization of a heavy-duty diesel engine using a gasoline-like fuel. The goal was to utilize the fuel's high volatility and low sooting tendency to optimize the combustion system for better fuel consumption

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while maintaining nitrogen oxide emissions within production levels. The design exercise showed an improvement in fuel efficiency of up to 4.1 percent while maintaining the production-level emissions.

EXPERIMENT, SIMULATE, VALIDATE

Supercomputers have excelled at simulating physical phenomena that are difficult to reproduce in a laboratory setting, such as ignition or controlled explosions, or that are extremely complex, such as the movement of turbulent flow. They can also function as design tools, eliminating the need to build multiple costly physical prototypes of objects, or for testing under various operating conditions.

Traditional engine designs in industry are performed on smaller clusters with reduced design space that can take months to complete. Mira, Argonne's IBM Blue Gene/Q system, is a massively parallel computing resource with more than 780,000 cores and offers industry researchers the ability to explore a larger design and parameter space by being able to run many variations concurrently.

Even with such machine capability, however, the high-fidelity codes that enable the breakthroughs must first be optimized to take advantage of the speed and architecture of the system—in this case, to predictably and efficiently simulate complex fluid flow.

The team used a commercial computational fluid dynamics (CFD) software package, CONVERGE, to develop the model used in this study. Model predictions were validated against experimental results generated using the production engine hardware. Convergent Science, the maker of CONVERGE, previously worked with VERIFI staff to optimize CONVERGE's source code to perform large numbers of smaller, engineering-type simulations simultaneously. To do that, the VERIFI team used an Argonne-developed parallel-scripting language called Swift to automatically manage the workflows involved, opening up an entirely new computing capability for industrial partners seeking new advanced engine designs.

The team simulated about 2,000 high-fidelity engine design combinations on Mira in a matter of days, covering four different operating conditions, six bowl geometries, multiple fuel injector-related configurations, and various start of injection scenarios (see Figure 1).

SHARED MISSION, COMPETITIVE ADVANTAGE

Industry partnerships are a vital part of the Argonne Leadership Computing Facility's (ALCF's) user community, the US Department of Energy Office of Science User Facility where this work was performed. This work was done using an ALCF director's discretionary award on Mira, and involved researchers from Aramco Research Center–Detroit, mechanical engineers from Argonne's Energy Systems division, and engineering staff from Convergent Science. ALCF staff further optimized the CONVERGE code on Mira resulting in a 100x speedup in input/output (I/O), an 8x improvement in load balance, and a 3.4x improvement in time-to-solution, among other improvements, and assisted with visualizations.

Industry users of Argonne's supercomputing resources have always been a relatively small group compared to researchers from universities and other national laboratories. That is expected to change with the introduction of Argonne's Aurora 21 exascale machine, which will be installed at the ALCF in the 2021 timeframe and is expected to be the first exascale system in the nation. The ALCF will provide the broadest range of capabilities to the research community yet, including new services and workflows, and adding data science and machine learning projects to its portfolio of simulation projects.

Research teams using leadership-class computers can expect to drastically accelerate solutions to large-scale problems facing the nation in the realms of energy, security, and health. Some problems are borne out of sheer need—because many natural resources used today for energy and transportation, while possibly plentiful now, are ultimately finite. Finding better, cleaner, and renewable energy sources is a core pursuit of many research teams that use the open science computers at Argonne National Laboratory.

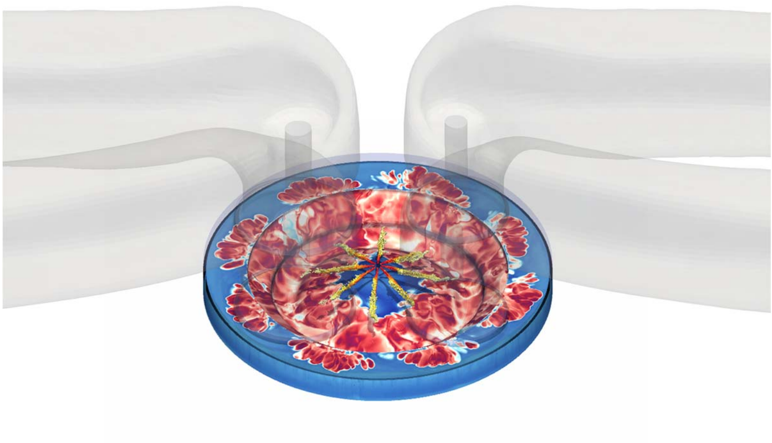

Figure 1. Visualization snapshot of a high-fidelity simulation of a heavy-duty engine fueled with a straight-run gasoline performed on the Mira supercomputer by researchers from Argonne National Laboratory, Aramco Research Center–Detroit, and Convergent Science Inc. The simulation has more than 100 million cells and is the largest engine simulation ever performed. This research provided unique insights about fuel-air mixing that enabled further engine optimization. Image: Yuanjiang Pei, Aramco Services Company: Aramco Research Center–Detroit.

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