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Large Eddy Simulation Applied to Advanced Engine Combustion Research

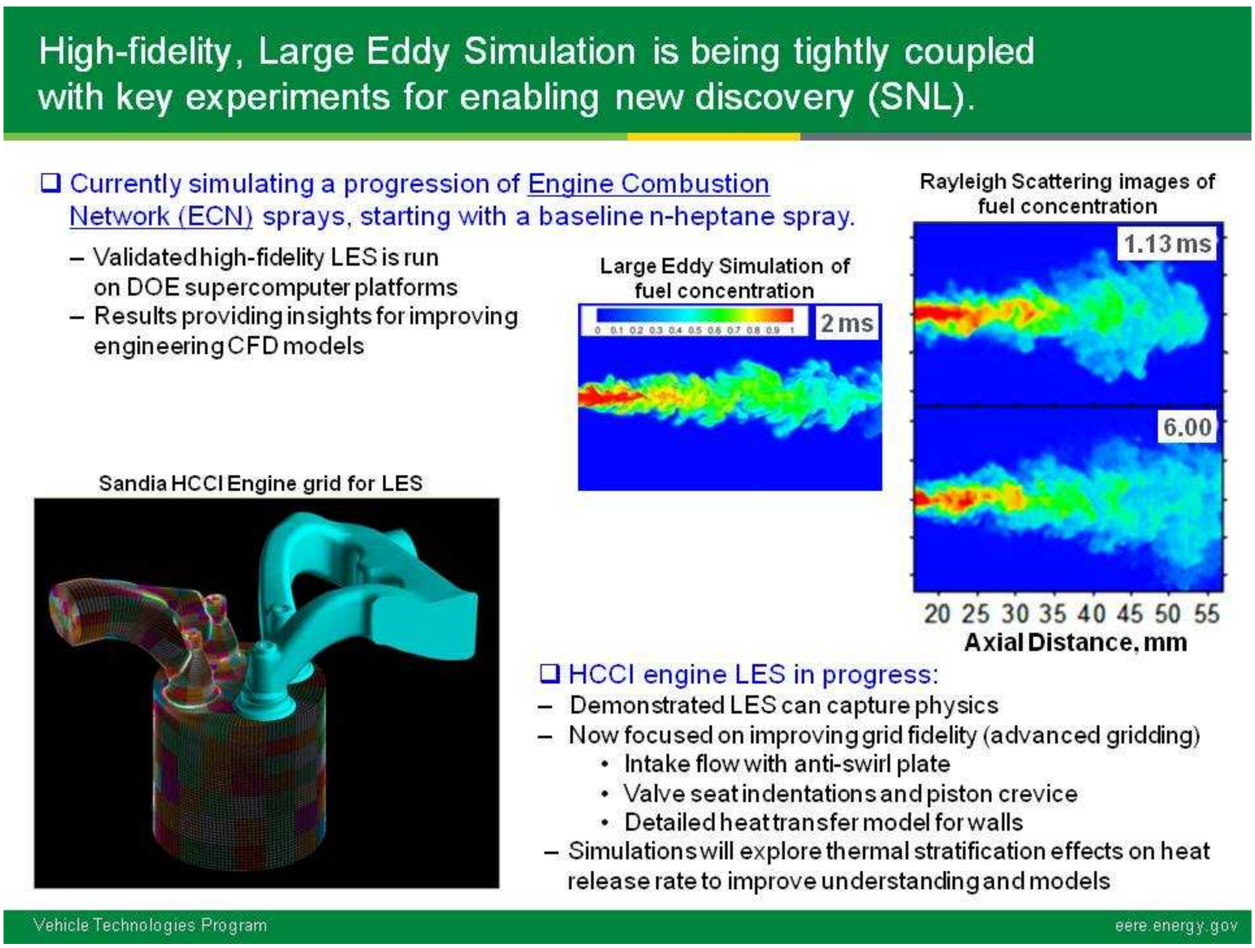
The combination of High Performance Computing (HPC) and the Large Eddy Simulation (LES) technique has significant potential to provide new insights into the dynamics of IC-engine flow processes. At the CRF, we integrate the combined merits of HPC and LES in a manner that provides some of the highest-fidelity, most detailed calculations ever performed to investigate turbulent reacting flow processes in IC-engines. Core activities in this area are funded by the DOE Office of Energy Efficiency and Renewable Energy (EERE), Vehicle Technologies Program. The primary objective is to establish high-fidelity computational benchmarks that match the geometry and operating conditions of key experiments using a single unified theoretical-numerical framework.

Our unique linkage with both EERE and the DOE Office of Science has enabled the development of formal collaborations with the National Center for Computational Sciences at Oak Ridge National Laboratories (ORNL) under the DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. These collaborations have led to unprecedented amounts of CPU allocations on the ORNL CRAY XT systems (i.e., jaguar, see http://www.nccs.gov). Using a combination of local mid-scale computer clusters and leadership platforms, we combine LES with key target experiments related to high-pressure fuel-injection studies under Spray Combustion and HCCI/SCCI combustion under HCCI/SCCI Fundamentals.

In addition to providing a unique massively-parallel multiscale modeling framework based on LES, we have established direct collaborations with two of the "flagship" experimental efforts at the CRF. A scientific foundation for development of advanced subgrid-scale models for combustion has been established as a direct extension of the "International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames" (i.e., the "TNF Workshop," www.ca.sandia.gov/TNF). Similarly, under this program we have established collaborative research activities that focus on key IC-engine related experiments that are part of the Engine Combustion Network (ECN, see www.ca.sandia.gov/ECN), which analogous objectives to those of the TNF workshop but with emphasis on engine combustion processes.

Example studies include "LES of Direct Injection Processes for High-Pressure, Low-Temperature Engine Applications with emphasis on Hydrocarbon Fuels," and "LES of the CRF Homogeneous-Charge Compression-Ignition (HCCI) Engine." The importance of understanding and predicting fuel injection, atomization and dense spray dynamics in advanced engine systems is widely recognized. The difficulties in measuring spray phenomena, especially in the dense regime, are also well recognized. One aspect that is not as well understood is the effect of pressure on the fundamental physics of injection. Depending on the pressure, injected fuel jets exhibit two distinctly different sets of evolutionary processes. At subcritical cylinder pressures the classical situation exists where a well defined interface separates the injected liquid from ambient gases due to the presence of surface tension. Dynamic shear forces and surface tension promote primary atomization and secondary breakup processes that evolve from a very dense state, where the liquid exists as sheets filaments or lattices intermixed with sparse pockets of gas; to a very dilute state, where drop-drop interactions are negligible and the theory associated with isolated drops can be used. As chamber pressures exceed the critical pressure of the fuel, however, the situation becomes quite different. Under these conditions, a distinct gas-liquid interface does not exist. Instead, injected jets undergo a transcritical change of state as interfacial fluid temperatures rise above the critical temperature of the local mixture. Effects of surface tension become diminished, and the lack of these inter-molecular forces promotes diffusion dominated mixing processes prior to atomization. The injected jets evolve in the presence of exceedingly large (but continuous) thermophysical gradients in a manner that is markedly different from the classical picture typically assumed. To investigate issues related to pressure at conditions relevant to an engine, Dahms, Pickett and Oefelein (ILASS 2011), applied a real fluid approximation to account for the nonideal effects described above. Using this model, LES results were compared to the available mixture fraction measurements by Pickett et al. (i.e., Baseline n-heptane case, www.ca.sandia.gov/ECN). The simulations qualitatively reproduce key experimental features such as the flow structure and spatial evolution. At the same time, significant questions were raised regarding what was really being represented by widely used light-scatter measurement techniques at these conditions.

Likewise, thermal stratification is critical for practical HCCI operation. Increasing the thermal stratification has a large potential for extending HCCI to higher loads and higher efficiencies. From this perspective, LES modeling offers the capability of capturing the essential aspects of thermal stratification and the mechanisms responsible for producing it. Here, we combine LES with the experimental efforts of Dec et al. to contribute to a more complete understanding of methods for enhancing thermal stratification and the related combustion processes. Calculations will be performed using identical operating conditions and geometry as the experiment. Experimental pressure traces and measurements of thermal stratification will be used for validation. Recently, we have demonstrated that LES can capture the basic physics of the thermal stratification process. On-going efforts are aimed at improving the fidelity of the LES and extend the analysis to reacting cases by including improved grid resolution of the intake-flow including the anti-swirl plate, adding detailed features of the valve-pocket crevices, and providing improved treatment of wall heat transfer processes inside the cylinder. With these changes appropriately verified, our collaboration will focus on using LES to determine the dynamic processes responsible for producing the thermal stratification and how this impacts combustion.



Oefelein’s code (RAPTOR) and unique linkage with the Office of Science has enabled the development of formal collaborations with the National Center for Computational Sciences at Oak Ridge National Laboratories (ORNL) under the DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. These collaborations have led to significant amounts of CPU allocations on the ORNL CRAY XT systems (i.e., jaguar, see http://www.nccs.gov). The total allocation in 2011 was 30-million CPU hours, which were used to continue to validate high-pressure injection models; and subsequently to perform detailed simulations of the optically accessible HCCI engine being studied by Dec *et al*. (as shown above).