Combustion

Combustion-Pele: Transforming Combustion Science and Technology with Exascale Simulations

Aggressive national goals for significantly reducing petroleum use and greenhouse gas emissions require major improvements in all aspects of our nation's energy use. Combustion processes have historically dominated electrical power production and transportation systems. Despite major advances in improving the efficiency and reducing the costs of alternative energy sources, combustion-based systems are projected to dominate the marketplace for decades. Consequently, these systems need to be optimized for energy efficiency and reduced emissions.

The motivating problem underlying this project is a sufficiently realistic simulation of the in-cylinder processes in an internal combustion engine utilizing low-temperature combustion, for which reactivity-controlled compression ignition (RCCI) is the exemplar. The enabled exascale-era simulations will address key scientific questions regarding mixture formation effects, multistage ignition of a diesel surrogate fuel, lifted flame stabilization, jet reentrainment affected by cylinder–wall geometry, and emissions. The simulation will account for isentropic compression, subsequent injection of the high-reactivity fuel, and combustion processes in a compression ignition engine. Necessary physics include gas compression and models of fuel injection process; spray vaporization (i.e., injection of liquid fuel sprays into high-pressure conditions); and mixing. Combustion processes include autoignition, flame propagation, and soot/thermal radiation, all in a nontrivial engine geometry. The scenario involves kinetically controlled processes in turbulent combustion including ignition, extinction, and emissions. The application used for this project, Pele, implements a hybrid large-eddy simulation (LES)/direct numerical simulation (DNS) approach in both the compressible and low-Mach limits where, using the machinery of adaptive mesh refinement (AMR), the project team will refine the mesh to the DNS limit where necessary to capture turbulence/chemistry interactions, while restricting grid resolution to that required for a high-fidelity LES model far from the flame.

This project is structured around providing a combination of first-principles DNS and near-first-principles DNS/LES hybrid simulations to advance the scientific community's understanding of fundamental turbulence–chemistry interactions in device-relevant conditions. The exascale motivating problem is to perform high-fidelity simulations of the relevant processes in an RCCI internal combustion engine. The relevant processes include turbulence, mixing, spray vaporization, low-temperature ignition, flame propagation, and soot/radiation. RCCI is thermodynamically favorable relative to existing engines and hence holds the promise of groundbreaking efficiencies while operating in a regime that limits pollutant formation. The roadmap toward this exascale-era motivating problem includes simulations of a multi-injection low-temperature diesel jet into an open domain with a large alkane fuel undergoing two-stage ignition processes, dilute spray evaporation and mixing, and multi-injection with fuels of varying reactivity in a geometry that influences the mixing field. The multi-injection simulation forms the challenge problem to demonstrate new exascale capability.

The specific science-based challenge problem is derived from the roadmap toward the motivating exascale-era problem. Specifically, the challenge problem demonstrates the ability to simulate the interaction of two fuels with varying reactivity under a multipulse injection strategy into an engine-relevant geometry. It will serve as a baseline for a series of simulations that will enable isolating the impacts of effects such as spray evaporation on mixture fraction and temperature, alternative fuels, and design of strategies to control combustion phasing and subsequent combustion rate. The problem will be tractable under a realistic allocation using the full capabilities of an exascale machine.

PI: Jacqueline Chen, Sandia National Laboratories

Collaborators: Sandia National Laboratories, National Renewable Energy Laboratory, Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory, Argonne National Laboratory, Massachusetts Institute of Technology, University of Connecticut

Progress to date

- Extended Pele with tiling approach for data-parallel shared memory parallelism.
- Extended Pele with embedded boundary geometry capability.
- Extended Pele with non-ideal equation of state capability.
- Ported Pele compressible hydrodynamics to GPUs using OpenACC and CUDA.
- Completed demonstration calculations of multi-injection diesel ignition using tiled Pele.

Exascale computing is being used to investigate and validate new low-emission, high-efficient combustion engine designs.