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Modeling Primary Atomization of Liquid Fuels using a Multiphase DNS/LES Approach

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As part of a Laboratory Directed Research and Development project, we are developing a modeling-and-simulation capability to study fuel direct injection in automotive engines. Predicting mixing and combustion at realistic conditions remains a challenging objective of energy science. And it is a research priority in Sandia's mission-critical area of energy security, being also relevant to many flows in defense and climate. High-performance computing applied to this non-linear multi-scale problem is key to engine calculations with increased scientific reliability.

Our team has developed a two-fold computational strategy to assess with unprecedented detail how fuel sprays are injected, atomize, and burn in engines. First, a state-of-the-art multiphase sharp-interface formalism with adaptive mesh refinement can track fuel injection on a time-scale of nanoseconds, capturing fragmenting liquid interfaces with micrometer resolution near the injector. This capability is unique since it does not require pre-existing knowledge of spray characteristics (computer code name: CLSVOF). Second, the sequence leading to combustion is explored within the large eddy simulation (LES) framework (computer code name: Raptor). Major advances underlie a state-of-the-art Euler-Euler solver describing the dynamics of sprays strongly coupled to multicomponent gases. Multiple sizes of droplets interact, as described by a Multi-Fluid (MF) model, a sectional/high-order moment method with advanced velocity closures. The accurate numerics we developed for MF-LES achieve unprecedented robustness and parallel efficiency on target injection cases.

The knowledge from direct simulation of atomization at engine conditions (Figure 1) is summarized and input in the high-fidelity MF-LES (Figure 2). The high computational resolution is key: finely discretized physical and phase spaces alleviate spray and turbulent sub-model uncertainty. Thanks to low-dissipation numerics, the novel approach crisply renders injection and auto-ignition despite large density and temperature fluctuations.

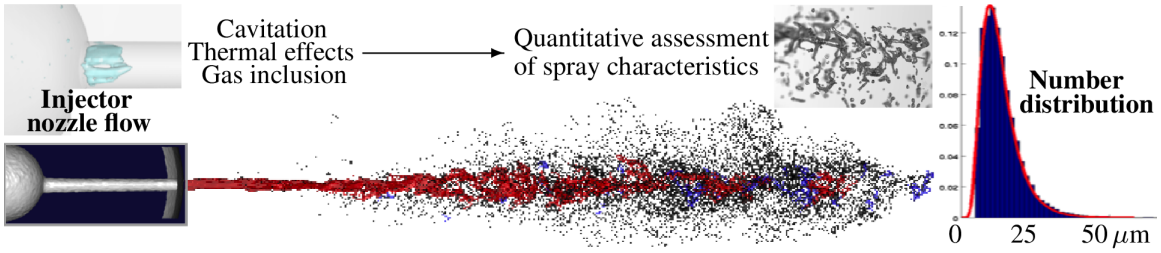

Figure 1. Direct numerical simulation of fuel injection (from CLSVOF) with commanded needle opening at t = 40 μs.

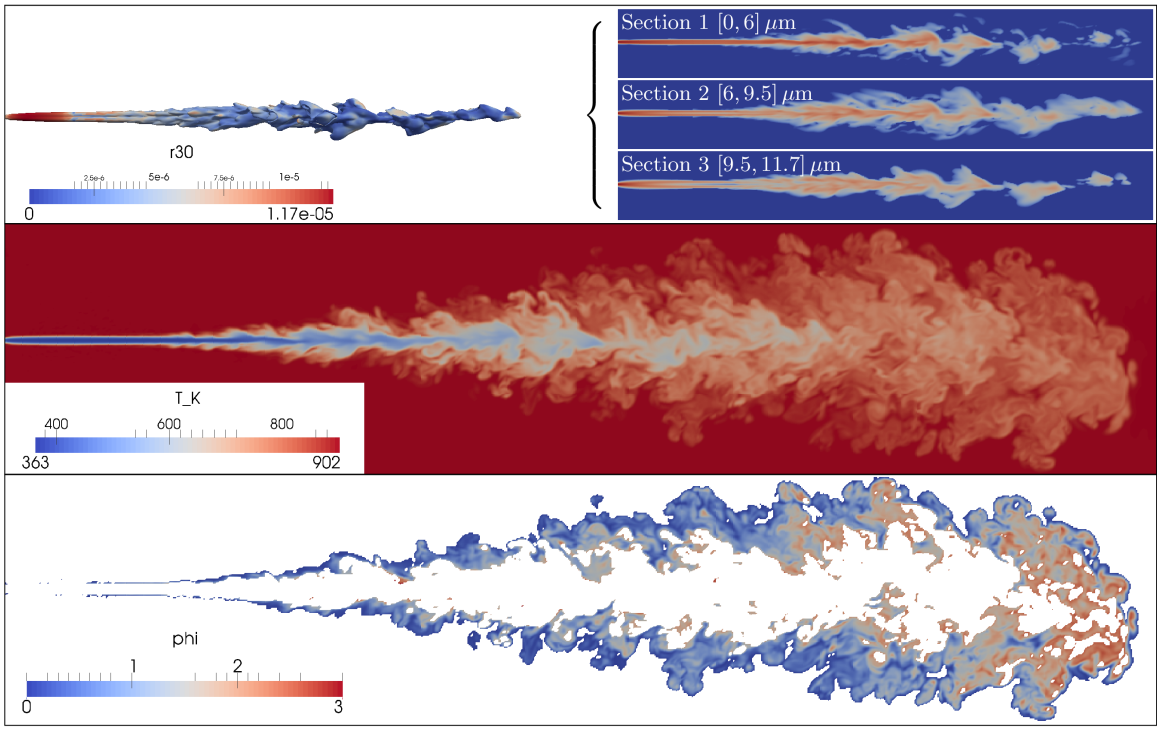

Figure 2. Large eddy simulation of polydisperse spray flame (from Raptor) at t = 400 μs. Liquid fuel contour (top), gas temperature (middle) and equivalence ratio Φ in warm regions (800 < T_g < 899 K) (bottom).