A Hybrid LES/FDF Framework for Low-Mach Turbulent Combustion with Adaptive Particle-Based Chemistry in AMR Grids

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This work presents the development and implementation of a high-fidelity computational framework for simulating low-Mach-number, turbulent, reactive flows. The solver is built around a semi-implicit predictor–corrector integration scheme applied to the governing transport equations. A hybrid modelling strategy combining Large Eddy Simulation (LES) with a transported Filtered Density Function (FDF) approach is employed to capture both large-scale turbulence and sub-grid-scale (SGS) scalar mixing effects.
Advective terms are discretized using the Total Variation Diminishing (TVD) CUBISTA scheme to ensure numerical stability and accuracy. Turbulence is modelled using the dynamic Smagorinsky closure, while the effects of unresolved scalar fluctuations on the filtered reaction rates are incorporated via a Lagrangian FDF formulation. In this framework, chemical composition is statistically represented by an ensemble of notional particles, with the Monte Carlo method used to solve the corresponding system of stochastic differential equations (SDEs).
To ensure the accuracy of the SDE solver in an Adaptive Mesh Refinement (AMR) context, a novel methodology is proposed that preserves at least the second-order statistical moments of the particle ensemble, even in cases involving extensive particle cloning or annihilation within a single time step. Validation against benchmark cases, including simulations using finite-difference solutions of the filtered species and energy transport equations, demonstrates excellent agreement. Furthermore, comparisons with conventional combustion models highlight the improved fidelity of the approach in both laminar and turbulent regimes when detailed chemical kinetics are accounted for.
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