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Reducing Computational Load in Turbulent Reacting Flows with Adaptive Chemistry and Cell Agglomeration

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High-fidelity modeling of reactive systems requires detailed chemical kinetics to capture system behavior but is computationally expensive due to numerous species and diverse timescales. However, such simulations are essential for accurate combustion predictions, aiding in efficiency optimization, stability, and emission estimates. In this study, we employ the SPARC (Sample-Partitioning Adaptive Reduced Chemistry) [1] and Cell Agglomeration (CA) [2] techniques to enhance the efficiency of turbulent reacting flow simulations. SPARC creates a training dataset, partitions it into clusters, generates reduced mechanisms, and applies adaptive chemistry through real-time grid point classification. CA groups cells with similar thermochemical states, significantly accelerating simulations by lowering the cost of chemistry calculations while maintaining accuracy. Traditionally, CA relies on user-selected thermochemical variables to determine cell similarity. Here, we propose an unsupervised clustering approach using Principal Component Analysis (PCA) [3] within the CA framework to improve adaptability across cases and reduce user dependency, eliminating the need for prior simulation knowledge.
To demonstrate the effectiveness of the combination of SPARC with PC based CA, we applied them to two benchmark cases involving the Adelaide Jet in a Hot Coflow (AJHC) burner: (i) Reynolds-Averaged Navier–Stokes (RANS) simulations using a reduced kinetic mechanism for n-C_7H_{16} [4], and (ii) Large Eddy Simulation (LES) of the same burner fired with an equimolar mixture of CH_4 and H_2 [5].

References

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