Automated adaptive chemistry for LES of turbulent flames

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Abstract

Large Eddy Simulations (LES) of turbulent flames carried out with detailed kinetic mechanisms have a key role for the discovery of the physical and chemical processes occurring in combustion systems, and are essential for the development of efficient, stable, and non-pollutant technologies. Nevertheless, these simulations require huge computational resources, making their utilization for large-scale systems, such as industrial burners and gas turbines, impractical.

In this work, we combine state-of-the-art machine learning algorithms and model reduction methods to deliver a fully automated strategy for performing LES with adaptive chemistry. This strategy is based on the Sample-Partitioning Adaptive Chemistry (SPARC) algorithmic procedure, which consists of four steps: the generation of a training dataset, its partitioning in clusters, the generation of a set of reduced chemical mechanisms specifically tailored to each cluster and, lastly, the numerical simulation of the case of interest with adaptive chemistry enabled by an *on-the-fly* classification of every grid point. The SPARC approach has already been demonstrated to substantially reduce the computational effort of reactive flows simulations. However, a non-negligible level of user interventions is needed, upon which the method's success critically depend. Therefore, with the goal of boosting the performance of this workflow and minimise the user-specified degrees of freedom, we plug in and exploit the Local Principal Component Analysis augmented with an automated Bayesian-optimised search for optimal clustering solutions, and the Computational Singular Perturbation method with an additional layer of automation based on the Tangential Stretching Rate for minimally-sized reduced mechanisms. We employ a cheap and easy-to-generate 1-dimensional-flames training database and we demonstrate the efficiency, accuracy and robustness of this strategy with an application to LES of the Adelaide Jet in Hot Coflow (AJHC) burner, a turbulent reacting flow exhibiting intense turbulence-chemistry interactions.