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Direct Numerical Simulation of Combustion Using Principal Component Analysis¹ OPEOLUWA OWOYELE, TAREK ECHEKKI, North Carolina State University — We investigate the potential of accelerating chemistry integration during the direct numerical simulation (DNS) of complex fuels based on the transport equations of representative scalars that span the desired composition space using principal component analysis (PCA). The transported principal components (PCs) offer significant potential to reduce the computational cost of DNS through a reduction in the number of transported scalars, as well as the spatial and temporal resolution requirements. The strategy is demonstrated using DNS of a premixed methane-air flame in a 2D vortical flow and is extended to the 3D geometry to further demonstrate the computational efficiency of PC transport. The PCs are derived from a priori PCA of a subset of the full thermo-chemical scalars' vector. The PCs' chemical source terms and transport properties are constructed and tabulated in terms of the PCs using artificial neural networks (ANN). Comparison of DNS based on a full thermo-chemical state and DNS based on PC transport based on 6 PCs shows excellent agreement even for species that are not included in the PCA reduction. The transported PCs reproduce some of the salient features of strongly curved and strongly strained flames. The 2D DNS results also show a significant reduction of two orders of magnitude in the computational cost of the simulations, which enables an extension of the PCA approach to 3D DNS under similar computational requirements.

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