Accelerating direct numerical simulation of turbulent reacting flows with time-dependent bases

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Abstract

I will present a novel *on-the-fly* reduced-order modeling strategy based on time-dependent bases and CUR factorization (TDB-CUR), Jung et al. *Comput. Methods Appl. Mech. Engrg.* 437 (2025) 117758, to significantly reduce computational cost as well as memory and storage requirements of deterministic turbulent reacting flow direct numerical simulations. The methodology was previously applied to systems of stochastic partial differential equations, Donello et al. *Proc. R. Soc. A* 479 (2023) 20230320. The species transport equations are reformulated as a matrix differential equation (MDE) to leverage the instantaneous low-rank structure of the resulting species mass fraction matrix, constraining the solution of the species MDE to the manifold of low-rank matrices and integrating it explicitly in its low-rank form. In this formulation, the rows represent the grid points and the columns correspond to the species mass fractions. The species matrix contains significantly more rows than columns and is found to be amenable to accurate low-rank approximations. A CUR algorithm is employed to construct the low-rank approximation of the species matrix by sampling only a dominant subset of its columns and rows, extracted *on-the-fly*. We develop a time-explicit integration algorithm for the CUR low-rank approximation, constraining the selected columns (species) to only include slow species. The selected rows (grid points that include the fast species) have significantly fewer entries and are sub-cycled with smaller effective time steps, yielding implicit-like time-stepping while maintaining explicit-like computational costs. Further computational efficiency gains are obtained through reduction in the rank of the ROM through local manifolds. The proposed methodology is validated across a hierarchy of combustion problems on massively parallel supercomputers, demonstrating considerable reduction in computational cost without compromising accuracy or relying on training data.