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Petascale direct numerical simulation of turbulent combustion—fundamental insights towards predictive models

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Abstract

The advent of petascale computing applied to direct numerical simulation (DNS) of turbulent combustion has transformed our ability to interrogate fine-grained 'turbulence-chemistry' interactions in canonical and laboratory configurations. In particular, three-dimensional DNS, at moderate Reynolds numbers and with complex chemistry, is providing unprecedented levels of detail to isolate and reveal fundamental causal relationships between turbulence, mixing and reaction. This information is leading to new physical insight, providing benchmark data for assessing model assumptions, suggesting new closure hypotheses, and providing interpretation of statistics obtained from lower-dimensional measurements. In this paper the various roles of petascale DNS are illustrated through selected examples related to lifted flame stabilization, premixed and stratified flame propagation in intense turbulence, and extinction and reignition in turbulent non-premixed jet flames. Extending the DNS envelope to higher Reynolds numbers, higher pressures, and greater chemical complexity will require exascale computing in the next decade. The future outlook of DNS in terms of challenges and opportunities in this regard are addressed.

Keywords: Direct Numerical Simulation (DNS); Turbulent; Combustion Models; High-Performance Computing; Complex Chemistry

1. Background and significance

1.1. Direct numerical simulation computational approach

The rapid growth in computational capabilities in the past two decades has presented both opportunities and challenges for high-fidelity simulations of turbulent reacting flows [1–8]. The advent of petascale computing power made it possible to glean fundamental physical insight into fine-grained 'chemistry-turbulence' interactions in canonical and laboratory-scale turbulent flames with detailed chemistry using three-dimensional direct numerical simulations [9–15]. In direct numerical simulation (DNS), the instantaneous governing equations are solved without averaging or filtering; all relevant continuum scales are resolved on the grid with no closure models for turbulence or combustion using accurate numerical methods. Constitutive models representing chemical kinetics, molecular transport, and other physics are still required. Such simulations are costly, requiring tens of million of cpu-hours on a petascale computer, containing up to several

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billion grid points, and generating 100's of terabytes of raw data. High performance computing at the petascale and beyond is enabling direct simulation of a large dynamic range of scales ($O(10^4)$ for incompressible turbulence) and the transport of dozens of species representative of hydrocarbon fuels of practical interest. The ability to combine turbulent transport with complex chemistry in DNS is providing greater realism and quantitative predictability, complementing experimental measurements in providing information critical to understanding new combustion regimes characteristic of future internal combustion engines and gas turbines for power and transport.

1.2. Direct numerical simulation of relevant archetypical configurations

Next-generation alternative-fuel internal combustion engines will operate in unconventional, mixed-mode, turbulent combustion under previously unexplored 'turbulence-chemistry' regimes. Compared to current engines, combustion in next-generation engines are likely to operate at higher pressures, lower temperatures, and higher levels of dilution. Similarly, in gas turbines for power generation hydrogen-enriched fuels are being considered for pre-combustion capture of CO_2 to minimize greenhouse gases from fossil fuel power plants. A hydrogen-rich fuel supply poses challenges downstream of fuel delivery in terms of thermal efficiency, emissions, and flashback safety. Combustion processes in these new environments, combined with diverse physical and chemical fuel properties associated with non-petroleum based fuels, may result in complex interactions that are poorly understood even at a fundamental level.

Therefore, there is an increasing role for high-fidelity simulation approaches that capture these fundamental fine-scale turbulence-chemistry interactions, and in particular, capture and discriminate the effects of variations in fuel composition. DNS can uniquely isolate and reveal fundamental causal relationships between turbulence, mixing, and reaction that are required for physical understanding and to develop predictive models. With petascale computing many turbulence-chemistry interactions have recently become accessible by DNS, for example, – stabilization of autoignitive lifted turbulent jet flames, stabilization of reactive turbulent fuel jets in crossflow, premixed flame propagation, structure, and NO formation in intense turbulence, extinction and reignition in turbulent jet flames, and stratified flame propagation and structure in turbulent flames. In addition to gleaning fundamental insight into specific 'turbulence-chemistry' interactions, the DNS benchmark data are increasingly being used to validate and develop models for turbulent combustion. In recent years, the emphasis in modeling formalisms has shifted towards capturing multi-regime or mixed-mode combustion, i.e. not purely premixed or non-premixed combustion, and often propagating flames or ignition fronts through dilute, autoigniting mixtures. Because of the increased prevalence of finite-rate kinetic effects, small-scale mixing and reactive chemical scales play a more significant role in determining macroscopic combustion quantities e.g. the overall burning rate and emissions. Hence, this imposes more stringent requirements of models to capture detailed chemical effects. In this regard, DNS with complex chemistry is complementing experiments in providing essential spatially and temporally resolved three-dimensional reactive scalar and velocity field data for model evaluation. Finally, DNS data have also been used to aid in the interpretation of measurements by relating scalar statistics obtained from lower-dimensional measurements to those of the true three-dimensional quantity.

In the following sections the governing Navier–Stokes, energy and species continuity equations and constitutive models for molecular transport are presented for both compressible and low-Mach number DNS formulations together with numerical algorithms, boundary conditions, parallel domain decomposition, chemical reduction strategies, and some potentially useful tricks-of-the-DNS-trade. Next, the various roles of large-scale DNS are illustrated by selected examples, loosely organized by phenomena: stabilization of autoignitive lifted turbulent jet flames, stabilization of reactive turbulent fuel jets in crossflow, premixed flame propagation, structure, and NO formation in intense turbulence, stratified flame propagation and structure in turbulent flames, and extinction and reignition in turbulent jet flames. In the examples, implications for model formalisms that warrant further development are discussed in light of the greater significance placed on finite-rate chemical kinetics interactions with turbulence and mixed regimes of combustion. Finally, the future outlook of DNS is discussed in light of the changing landscape of high performance computing in its expected evolution from petascale to exascale supercomputers in the next decade. In particular, lessons learned from recent refactorization of a compressible Navier–Stokes solver for an existing hybrid architecture utilizing cell broadband engines are discussed, and examples of in situ feature extraction/tracking and visualization methods for addressing the data deluge accompanying large-scale simulations are presented.

There are many review articles related to advances in DNS of turbulent combustion [1,6–8,15–17]. The present intent is to illustrate the roles of large-scale 3D DNS focusing on turbulence-chemistry interactions rather than to provide a comprehensive review of the DNS literature. As such, many important multi-physics phenomena – thermal radiation, soot and multiphase flows – are beyond the present scope.