TERASCALE 3D DIRECT NUMERICAL SIMULATIONS OF TURBULENT COMBUSTION WITH DETAILED CHEMISTRY

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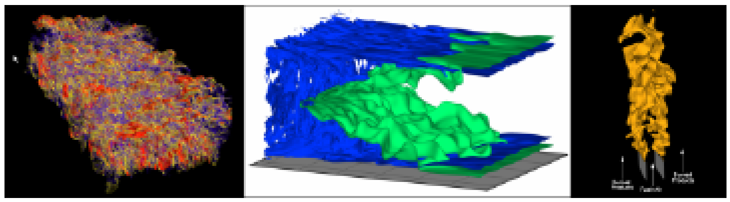

In recent years, the rapid growth of computational capabilities has presented both opportunities and challenges for high-fidelity simulations of turbulent combustion flows. Realistic simulations that address complex multi-physics interactions, such as the so-called "turbulence-chemistry" interactions in combustion flows, have become accessible through the growth of processor speed, computer memory and storage, and significant improvements in computational algorithms and chemical models. While the opportunity exists for gleaning fundamental physical insight into fine-grained chemistry-flow interactions in simplified two-dimensional physical configurations, it remains a formidable challenge to directly simulate three-dimensional turbulent flames with detailed chemistry. In the past several years, the advent of terascale computers in the U.S. and in Japan, has made it possible to begin to study fundamental issues such as flame stabilization, extinction and reignition, and flame structure in three-dimensional laboratory configurations at moderate Reynolds numbers with multi-step chemistry using the DNS approach. These simulations are costly, requiring several million cpu-hours on a terascale computer with up to 0.5 billion grid points and ~20 transported variables. While costly, three-dimensional turbulent direct numerical simulations with detailed chemistry enable both turbulence dynamics and chemical reaction to be accurately represented concurrently, thus opening new realms of possibility for the understanding of turbulence-chemistry interactions and the development and validation of models. Improved closure models for turbulent transport and reaction are required in coarse-grained approaches, RANS and LES, which are used ultimately to predict the efficiency, stability and emissions of pratical devices. In this presentation the results from two recent terascale 3D DNS simulations of premixed and nonpremixed turbulent combustion will be presented to illustrate some of the cyberinfrastructure requirements for combustion science. Significant challenges remain to extract salient information from terascale combustion data sets, to generate reduced mechanisms suitable for computationally-intensive DNS, and to manage data movement, storage, workflow and sharing over the wide-area-network.

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