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Numerical methods, subgrid-scale modeling, and applications of large-eddy simulation (LES) — overview

The exponential rise in computational capability over the last few decades has enabled high-fidelity, unsteady calculations of multi-physics turbulent flows. The continued push to exascale computing in the next decade will not mitigate the necessity for efficient numerical methods and accurate modeling of unresolved subgrid physics. An exascale machine would provide approximately a factor of 100 in floating point operations; this corresponds to less than a factor of five in spatial resolution for an unsteady direct numerical simulation of a single-phase, non-reacting box of turbulence (Re^3 scaling in spatio-temporal degrees of freedom). As a result, modeling and numerical method development will be crucial to the success of high-fidelity calculations for the foreseeable future.

In addition to classical subjects in turbulence research (e.g., energy-conserving schemes, improved eddy viscosity closures for LES), several projects targeted the application of LES to complex flows (shock-wave/boundary layer interaction, boundary layer separation, near-wall roughness) and geometries. Specifically, the investigations performed by the twelve projects in this group pertained to: (a) efficiency of numerical methods for multi-scale simulations, (b) novel frameworks for subgrid-scale modeling, (c) near-wall roughness effects in turbulent flows, and (d) wall-modeled large-eddy simulations of high-speed flows, including turbomachinery. The results of these investigations are briefly discussed below.

(a) Efficiency of numerical methods: As the scale separation grows for many physical and engineering problems currently encountered, the reduction of the total time to solution for a given accuracy becomes increasingly important. Capuano *et al.* developed an energy-conserving Runge-Kutta time stepping scheme that reduces the total number of operations necessary for each step by a careful splitting of the advection term. Domino compared the efficiency for a given accuracy for low-order and high-order CVFEM schemes for the canonical Taylor vortex problem; a novel high-order scheme on unstructured grids was additionally developed.

(b) Frameworks for subgrid-scale modeling: Five projects developed novel subgrid-scale models and approaches, underscoring SGS modeling's continued importance in simulations of turbulent flows. Murman *et al.* derived a dynamic procedure for estimating coefficients in SGS models for the variational multi-scale method (VMM) offering a path to more predictive calculations. Balakumar *et al.* assessed the accuracy of different wall-modeling strategies on a separated flow behind a periodic hill at varying Reynolds numbers. The three wall models accurately predicted both the onset of separation and the boundary layer reattachment relative to DNS data. Verstappen *et al.* further developed an eddy-viscosity model that provides a minimal amount of dissipation in order to prevent the generation of eddies below the LES filter size by providing consistent discretizations of the SGS modeling terms. This resultant model was shown to discretely enforce the scale separation and accurately predict isotropic turbulence and turbulent channel flows. Lastly, high-fidelity simulations and high-resolution experiments continue to produce large databases of space-time evolutions of complex flows. The final two

projects leveraged machine learning and artificial neural networks to enhance existing phenomenological models and suggest new model forms. Duraisamy & Durbin utilized experimental skin friction measurements and an inverse modeling approach to infer an optimal intermittency field (for a particular RANS model) to accurately predict bypass transition. Vollant *et al.* used artificial neural networks to develop a new SGS model for the subgrid flux of a passive scalar; this model was shown to be more accurate than existing eddy and tensorial diffusivity models for transport of a passive scalar in LES calculations.

(c) Roughness effects in turbulent boundary layers: Two projects investigated the effect of wall roughness of near-wall turbulence for external (MacDonald *et al.*) and internal flows (Zhu *et al.*). MacDonald *et al.* generated a DNS database for rough-wall channel flows for different roughness elements, and developed drag laws to model the effect of unresolved roughness elements in LES calculations. These drag laws could be later used to help model geophysical flows where the ground topology is not resolved (for instance, in predicting wildfire spread). Zhu *et al.* performed wall-resolved LES calculations of a helically ribbed pipe used in thermal cracking applications. The losses were determined to be driven by pressure drag induced by the ribbing, which can be contrasted against a smooth wall case where the losses can be attributed to friction drag.

(d) Wall-modeled LES of high-speed flows: Prohibitive resolution requirements of near-wall turbulence have previously precluded large-eddy simulation of high Reynolds number external aerodynamics in high-speed flows. Three projects performed wall-modeled LES of supersonic flows ($0 < \mathrm{Ma} < 2$) with $\mathrm{Re} = 10^6 - 10^7$. Joo *et al.* simulated the NASA 37 compressor rotor; the study demonstrated that LES was capable of predicting boundary layer transition on the blade as well as the overall thermodynamic efficiency. Kim *et al.* calculated the loading of a steam turbine blade subject to highly unsteady inflow conditions (a companion experiment is forthcoming at Doosan Heavy Industries). Both simulations highlighted the sensitivity of turbomachinery simulations to thermal and inflow boundary conditions. Szubert *et al.* performed DES and LES of a shock wave-boundary layer interaction (SWBLI), relevant for next generation supersonic propulsion. Simulations are shown to accurately predict the non-equilbrium boundary layer in the vicinity of the SWBLI.

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