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REQUIREMENTS TO PREDICT THE SURFACE LAYER WITH HIGH ACCURACY AT HIGH REYNOLDS NUMBERS USING LARGE-EDDY SIMULATION

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It was pointed out in a 1992 paper by Mason & Thomson (JFM 242) that large-eddy simulation (LES) of the high Reynolds number rough-surface boundary layer systematically over-predicts mean velocity gradients in the shear-dominated surface layer. (Subsequent authors have shown a similar phenomenon in mean temperature gradient.) The error is apparent in LES of all high Reynolds number boundary layers where the viscous layer either does not exist (rough surface) or is not resolved. The "overshoot" in mean shear produces a wide range of negative effects in the surface layer that originate from the over-prediction of streamwise turbulence production. These include the tilting of the Reynolds stress tensor towards the mean flow, a strongly enhanced stream-wise coherence in all turbulence variables, and an incorrect eddy structure near the surface. The spurious effects infect the outer boundary layer as well. This is particularly the case in the moderately unstable atmospheric boundary layer (ABL) because the buoyancy-driven vertical motions originate within the shear-driven structure at the surface and the near-surface errors infect the entire structure of the ABL. Consequently, the overshoot adversely alters LES predictions of vertical transport of temperature, humidity, greenhouse gases and other pollutants, and indirectly affects other numerical predictions such as cloud formation, albedo, and radiative heating.

It has been found that increasing the grid resolution moves the overshoot towards the surface, but does not reduce its strength or its negative consequences. Over the past 16 years, attempts to rectify the overshoot have focused entirely on adjustments to the closure for subfilter-scale (SFS) stress tensor. Whereas numerous studies have shown that the details of the SFS model influence the overshoot, attempts to fully eliminate the overshoot and predict a well-defined law-of-the-wall layer have not been successful, in large part because the mechanisms underlying the overshoot have not been understood. The connection between grid and overshoot suggests that the explanation extends beyond the SFS model to include an inherent lack of resolution of integral-scale motions at the first few grid levels (Khanna & Brasseur, JFM 345, 1997; Juneja & Brasseur Phys. Fluids 11, 1999).

In this study we discover and describe the source of the overshoot. From this new understanding, we develop the framework in which a LES should be formulated to resolve the overshoot and its consequences. Our study shows that, to first order, the accuracy of LES in the high Reynolds number surface layer is a consequence of three inter-related issues near the surface that must be understood in terms of the discretized dynamical system (rather then the continuous system it approximates): (1) the net level of dissipation in the discretized dynamical system that arises from a mix of the SFS stress model, the discretization method, and algorithmic additions such as dealiasing and added numerical viscosity, (2) the effective aspect ratio of the grid near the surface, taking into account explicit dealiasing and the anisotropic consequences of the implicit spectral filter from all dissipative effects, and (3) the vertical resolution of the surface layer by the grid.

We explain the existence of a two-parameter space within which LES experiments should be developed. The first parameter is the ratio of mean resolved shear stress to mean SFS shear stress ($\Re$); the second is a "numerical LES Reynolds number" (Re_{LES}) based an "LES viscosity" that parameterizes the mean viscous content of the SFS stress. These parameters are independent of the details of the SFS closure. However, by scaling these parameters using the Smagorinsky representation for eddy viscosity, we show that $\Re$ and Re_{LES} are determined by a specific mixture of SFS model constant, grid aspect ratio and vertical resolution of the surface layer by the grid, N_δ. Within the $\Re - \mathrm{Re}_{LES}$ parameter space we define three critical parameters, $\Re^*$, Re^*_{LES} and N^*_δ, that must be simultaneously exceeded to remove the overshoot. These critical parameters define a subregion of the $\Re - \mathrm{Re}_{LES}$ parameter space that we label the "*High-Accuracy Zone*," or HAZ. In theory, large-eddy simulations of the high Reynolds number boundary layer must reside within the HAZ to eliminate the overshoot and its negative consequences.

To validate the theory we have carried out over 70 simulations of the neutrally stable ABL broadly covering the $\Re - \mathrm{Re}_{LES}$ parameter space. We find that as the LES moves systematically into the HAZ, the overshoot is systematically suppressed, in close correspondence with the theoretical arguments. We have estimated the critical values of $\Re$, Re_{LES} and N_δ that define the HAZ for LES of the neutral ABL. We further find that a large-eddy simulation with surface layer resolution below critical not only incorrectly predicts the surface layer, but the mean velocity is erroneously predicted *throughout* the ABL. Thus, the first requirement for accurate prediction of the boundary layer is that the grid designed for the LES have sufficient vertical grid resolution to properly resolve the surface layer. Our simulations suggest that at least 9-10 grid points are required in the lower 20 % of the ABL, roughly the surface layer.

Whereas we have validated three necessary conditions for high-accuracy LES of the boundary layer and have established a "High-Accuracy Zone" within the $\Re - \mathrm{Re}_{LES}$ parameter space, we also find that as the LES moves into the HAZ, higher-order affects appear that require attention to further improve details of the surface-layer simulation. In particular, we find that a balance arises between the suppression of overshoot and the appearance of numerical instability that originates at the surface and extends into the computational domain as the simulation moves farther into the HAZ. The establishment of the HAZ provides a framework within which further advances in accuracy can be explored. This exploration involves an interaction between boundary layer physics, the SFS model, the grid, boundary conditions, and ad-hoc regularization techniques. We shall explore some of these issues in a companion discussion.