Designing Simulations to Overcome the Surface Layer Overshoot of Mean Shear in Large-Eddy Simulation of the Neutral Atmospheric Boundary Layer

Tie Wei and James G. Brasseur

Department of Mechanical Engineering, The Pennsylvania State University
University Park, PA 16802, USA

A long-standing problem in large eddy simulation (LES) of the shear-dominated atmospheric boundary layer (ABL) with eddy viscosity models is the over-prediction of mean shear near the surface, leading to other errors and infecting the entire boundary layer structure. Although a number of researchers have found it possible to alter the overshoot by adjusting the subfilter-scale (SFS) model, none have succeeded in fully eliminating the error, primarily because the underlying mechanisms are not understood. Recently we have uncovered the underlying mechanisms, to be presented in a companion talk by J.G. Brasseur. We found that two inter-related parameters are critical to eliminating the overshoot: the ratio between mean resolved shear stress to mean SFS shear stress at the first grid level, $\Re$, and a "LES Reynolds number", Re_{LES} that is defined with a "numerical LES viscosity." $\Re$ and Re_{LES} are adjustable through the SFS model constant, grid resolution, and grid aspect ratio. In particular, for the Smagorinsky closure, $\Re \sim \left[C_s^2 (AR)^{4/3} \right]^{-1}$ and $Re_{LES} \sim N_\delta \left[C_s^2 (AR)^{4/3} \right]^{-1}$, where C_s is the Smagorinsky constant, AR is the grid aspect ratio, and N_δ is the grid resolution in the vertical.

A series of simulations have been carried out using eddy viscosity closures in which the model constant, grid resolution and grid aspect ratio were systematically varied to cover the parameter space $0 < \Re < 2$ and $0 < Re_{LES} < 700$. Consistent with our theoretical analysis, these simulations show that the overshoot of mean shear can not be eliminated unless $\Re$ and Re_{LES} for the simulation reside within a particular region of $\Re$ - Re_{LES} parameter space which we shall call the "High Accuracy Zone (HAZ)." From our simulations, we estimate the critical vales of $\Re$ and Re_{LES} to be $\Re^* \sim 0.85$ and $Re_{LES}^* \sim 350$. Most previous studies have focused on the SFS model, for example, by modifying dynamic schemes, adding stochastic forcing, and/or applying different levels of reconstruction. All modifications affect $\Re$ and $Re_{LES,}$ but our estimates suggest that in none of these reported studies is the simulation within the HAZ for LES of the ABL.

We find that as the simulations are adjusted to reach the HAZ in the parameter space and the overshoot of mean shear is largely eliminated, new "secondary" issues arise that must be addressed. The most obvious issue is the development of numerical instability, appearing as an oscillation in the mean velocity gradient at the first couple grid levels and spreading into the computational domain as $\Re$ and Re_{LES} increase within the HAZ. We find that the instability is sensitive to several issues when the simulations enter the HAZ, including lower wall boundary conditions, dealiasing, numerical dissipation, and details of the SFS model structure.

In this presentation we shall focus on the High Accuracy Zone, the way in which LES of the neutral ABL changes as the simulation moves into the HAZ, and the "secondary" issues that must be addressed as the simulations enter the HAZ. We find that the balance between the location of the simulation within the HAZ and numerical instability depends on the level of fluctuation in the model for total surface shear stress. We further find, in agreement with previous studies, that the overshoot of mean shear is relatively insensitive to the details of the lower boundary conditions when the simulation is well outside the High Accuracy Zone. However, when the simulation is in the HAZ, the model for surface stress fluctuations has a major influence on numerical instability.