On LES Modeling for Predictive Mixing

Fernando F. Grinstein [1]
[1]Applied Physics Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Accurate prediction of material mixing with quantifiable uncertainty is essential to achieving a predictive science for many important applications in engineering, geophysics, and astrophysics. Typical applications in realistic regimes and configurations exhibit extreme flow complexity, due to broad range of length scales of physical processes and problem geometry, and will always require utilizing under-resolved computer simulations. In this context, it is crucially important to have theory and computational evidence as to what type of flows and quantities can (or can not) be usefully predicted with insufficient resolution. Developing predictive numerical tools based on rational scientific principles for unresolved simulation of macroscale and microscale material mixing is very important in this context.

It is not feasible to compute high Reynolds-number (Re) turbulent flows by directly resolving all scales of motion and material interfaces; instead, macroscale portions of the unsteady turbulent motion are computed while the rest of the flow physics including molecular diffusion and other microscale physics (e.g., combustion) remains unresolved. One major approach in the turbulence community is large eddy simulation (LES) in which the large energy containing structures are resolved whereas the smaller, presumably more isotropic, structures are filtered out and their unresolved subgrid scale (SGS) effects are modeled. The construction of SGS models is pragmatic, and often based primarily on empirical information. Adding to the physics-based difficulties in developing and validating SGS models, one is faced with simulations where contributions from numerical truncation terms can be as significant as those from SGS models in typical LES strategies.

Extensive recent work [1] has demonstrated that predictive unresolved simulations of turbulent velocity fields are possible using any of the class of nonoscillatory finite-volume (NFV) numerical algorithms. This strategy is called implicit LES (ILES). This is a new area of research undergoing rapid evolution; scientific understanding and theory explaining the success of these methods have been proposed; truncation terms associated with NFV methods implicitly provide SGS models capable of emulating the physical dynamics of the unresolved turbulent velocity fluctuations by themselves; the connection of these truncation terms to the physical theory of inviscid dissipation and ultimately to irreversible thermodynamics has been demonstrated. The extension of the ILES approach to the substantially more difficult problem of material mixing by an unresolved velocity field has not yet been investigated numerically, nor are there any theories as to when the methodology may be expected to be successful. Progress in addressing these issues with ILES in the cases of passive and shock-driven scalar mixing will be reported.

1. F.F. Grinstein, L.G. Margolin, and W.J. Rider 2007, Eds., *Implicit Large Eddy Simulation: Computing Turbulent Flow Dynamics*, Cambridge University Press.