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On Implicit Large Eddy Simulations of Turbulent Mixing

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Mixing of materials by the small scales of turbulent motion is a critical element of many flow systems of interest in engineering, geophysics and astrophysics. Numerical simulation plays a crucial role and turbulent mixing predictability is a major concern. Small-scale resolution requirements focus typically on those of continuum fluid mechanics described by the Navier Stokes equations; different requirements are involved depending on the regime considered and on the relative importance of coupled physics such as multi-species diffusion and combustion as determined by Knudsen, Reynolds number (Re), Schmidt (Sc), Damköhler (Da), and other characteristic non-dimensional numbers. Direct numerical simulation (DNS) resolving all relevant physical space/time scales, is prohibitively expensive in the foreseeable future for most practical flows and regimes of interest at moderate-to-high Re. On the other end of the simulation spectrum are the Reynolds-Averaged Navier-Stokes (RANS) approaches – which focus on statistical moments for an ensemble of realizations and model the turbulent effects.

The small-scale turbulent flow dynamics is traditionally viewed as universal and enslaved to that of larger scales. In coarse grained simulation (CGS) large energy containing structures are resolved, smaller structures are spatially filtered out, and unresolved subgrid scale (SGS) effects are modeled; this includes classical LES strategies [1] with explicit closure SGS models, and implicit LES (ILES) [2], relying on SGS modeling implicitly provided by physics capturing numerical algorithms. Transition to turbulence involves unsteady large scale dynamics which can be captured by CGS but not by the single-point closures typical in RANS [3]. Our fundamental views of the so-called 'spectral gap' between large and small scales have significantly evolved over the past decade to provide a solid basis for the ideas of enslavement in turbulence as they relate to CGS [4]. The CGS strategy of separating resolved / unresolved physics constitutes the viable intermediate approach between DNS and RANS to address practical geometries and multiphysics.

Complex turbulent flow applications unavoidably involve under-resolved simulations, and robustness of CGS predictions is a frequently unsettled issue. If the information contained in the filtered-out smaller and SGS spatial scales can significantly alter the evolution of the larger scales of motion and practical integral measures, then the utility of CGS is questionable. The validity of the scale separation assumptions in CGS needs to be carefully tested when potentially important SGS flow physics is involved, specifically, for turbulent wall bounded flows, and for turbulent material mixing – the main focus of this talk. The talk reviews our understanding of coarse-grained turbulent mixing [5], its theoretical basis, verification, validation, and predictability aspects, and progress addressing difficult open issues in complex non-equilibrium applications involving turbulent flow.

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