Simulation of Shock-Driven Turbulent Mixing in High-Re Flows

Fernando Grinstein, Akshay Gowardhan, and Adam Wachtor
Computational Physics Division, XC-4 Methods and Algorithms, Los Alamos National Laboratory
MS F644, Los Alamos, NM 87545, USA

Background

The mixing of initially separate materials in a turbulent flow by the small scales of turbulent motion is a critical element of many programs, e.g., inertial confinement fusion, urban contaminant dispersal for consequences management, climate prediction, combustion, and material processing. Such extremely-complex high Reynolds number (Re) applications feature a broad range of length and time scales and will always require under-resolved computer simulations: it is simply not possible to simulate fully resolved practical high-Re turbulent flows. Instead, the effects of the small scales of motion that occur at length scales smaller than a computational cell size must be modeled. In large eddy simulation (LES) [1] 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. By necessity – rather than choice, LES becomes the half-way between engineering models and direct numerical simulation. The construction of SGS models is pragmatic and based primarily on empirical information. Implicit LES [2] (ILES, MILES) effectively addresses the seemingly insurmountable issues posed to LES by under-resolution – truncation terms due to discretization are comparable to SGS models in typical LES strategies [3], by relying on the use of SGS modeling and filtering provided implicitly by *physics capturing numerics.* Popular finite volume methods such as flux-corrected transport, the piecewise parabolic method, total variation diminishing, Godunov, and hybrid algorithms are being used for ILES. Extensive ILES verification and validation in areas of engineering, geophysics, and astrophysics has been reported [3]. *The substantially more difficult problem of under-resolved (Schmidt number ~ 1) material mixing driven by under-resolved velocity field and initial conditions (ICs) is the subject of the present paper.*

In many applications of interest, turbulence is generated by shock waves via Richtmyer-Meshkov instabilities (RMI) (e.g., [4,5]). The instability results in vorticity being introduced at material interfaces by the impulsive loading of the shock wave. RMI add the complexity of shock waves and other compressible effects to the basic physics associated with mixing; compressibility further affects the basic nature of material mixing when mass density and material mixing fluctuation effects are not negligible. Because RMI are shock-driven, resolution requirements make DNS impossible even on the largest supercomputers. State-of-the-art RMI simulations use ILES [5], or hybrid methods [6] which switch between shock capturing schemes and conventional LES depending on the local flow conditions. Given that ILES is based on locally adaptive NFV methods it is naturally suited to emulate shock physics. The unique combination of shock and turbulence emulation capabilities supports direct use of ILES as an effective simulation *anzatz* in RMI research.

In the present work, we test ILES in prototypical three-dimensional case studies [4,7] for which available laboratory and/or previous LES [6] data can be used for validation purposes. The particular ILES strategy discussed here is based on a nominally-inviscid simulation model using LANL's RAGE code [8] with adaptive mesh refinement (AMR). RAGE solves multi-material compressible-Euler equations using a 2nd-order Godunov scheme, with a variety of numerical options for gradient terms – limiters, as well as interface treatments. Progress in addressing relevant issues of grid resolution and convergence will be reported; the results show robustness of ILES in capturing established findings.

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