

Dynamic Scale-Resolving Paradigm for Coarse Grained Simulations of Turbulent Mixing

Fernando F. Grinstein

fgrinstein@lanl.gov

Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Abstract: We report progress developing and testing a dynamic blended hybrid paradigm based on LANL's xRAGE eulerian hydrodynamics code with the BHR unsteady RANS option. Proof-of-concept test cases to be discussed include a shock tube experiment prototyping shock-driven turbulent mixing, and a canonical Rayleigh-Taylor driven flow and mixing case. We have also examined in this context the impact of newly available numerical hydrodynamics in xRAGE, including a Low-Mach Correction (LMC) option to address the well-known issue of excessive numerical diffusion of upwinding schemes for low Mach numbers.

Keywords: Turbulence Modeling, Large-Eddy Simulation.

Background

We are interested in detailed understanding of the late-time consequences of mixing driven by hydrodynamical instabilities promoted by initial conditions at accelerated material interfaces, as in Inertial Confinement Fusion (ICF) capsule implosions. The flow physics is driven by flow instabilities such as Richtmyer-Meshkov, Kelvin-Helmholtz, Rayleigh-Taylor, and vortex stretching. The initial conditions dependent flow involves, transition to turbulence, turbulence decay, and non-equilibrium turbulence –capturable with a Coarse-Grained Simulation (LES/ILES) strategy [1] – where small-scale flow dynamics is presumed enslaved to the dynamics of the largest scales.

Unsteady RANS involving ensemble-averaged flow on typically-coarser than LES grids are preferred for faster turnaround for engineering and design purposes. RANS typically presumes equilibrium turbulence and enstrophy production slaved to kinetic energy production, and reduced dimensional computations (1D / 2D) are often involved [2]. There are outstanding problems using such RANS for shock-driven turbulence, specifically: 1) transitional initial-conditions-dependent flow physics is 3D and non-equilibrium; 2) enstrophy generation is inherently very different from energy production. RANS can be effectively used to capture each shock-triggered transitional event with suitable initialization, but cannot capture well the consequences of subsequent (e.g., reshock) transitional events. Crucial to note here is the fact that transition to turbulence is driven by large-scale vortex dynamics, which can be captured with CGS, but not by RANS based on single-point-closure modeling [3]. It is thus timely to explore the possible impact of hybrid RANS/LES paradigms for shock-driven turbulent multi-material mixing.

A dynamic blended RANS/ILES bridging strategy for applications involving variable-density turbulent mixing applications was recently proposed [4]. The bridging approach exploits the structure similarity of RANS & LES equations. It is based on the *Flow Simulation Methodology* [5], locally blending a high-resolution computational strategy with RANS modeling – depending on how much of the turbulence is resolved at given resolution, and providing a sophisticated LES strategy in-between. How much dissipation is modeled and how much is computed is decided based on having the RANS models locally morph into LES SGS models with a contribution function $f=f(\Delta/L)$, $0 < f < 1$, where Δ is the smallest grid size and L is a resolution reference length scale. Our bridging paradigm involves ILES at the high-resolution limit $f \rightarrow 0$, and pure RANS at the low-resolution limit $f \rightarrow 1$.

We follow a proposal by Germano [6] to **solve for f** dynamically, based on decomposing the full stress into modeled and resolved components, and using a differential filter as secondary filtering operation [7] to define the resolved part. This is in contrast with classical FSM [5] where $f(\Delta / L)$ is defined explicitly in empirical ad hoc fashion. Although present focus is on LANL's xRAGE Eulerian hydrodynamics code with BHR unsteady RANS [4] – our *Dynamic BHR* paradigm formulation is expected to be applicable with other single-fluid RANS approaches.

To be Presented

We report progress testing the *Dynamic BHR* implementation for a shock tube experiment prototyping shock-driven turbulent mixing [8], and for a Rayleigh-Taylor driven flow and mixing case [9]. We have also examined in this context the impact of higher order algorithms in xRAGE, including a Low-Mach Correction (LMC) to address the well-known issue of excessive numerical diffusion of upwinding schemes for low Mach numbers. The LMC leads to transition to turbulence with higher late-time turbulence Reynolds number and small-scale population [12,13].

LANL is operated by TRIAD National Security, LLC for the US DOE NNSA.

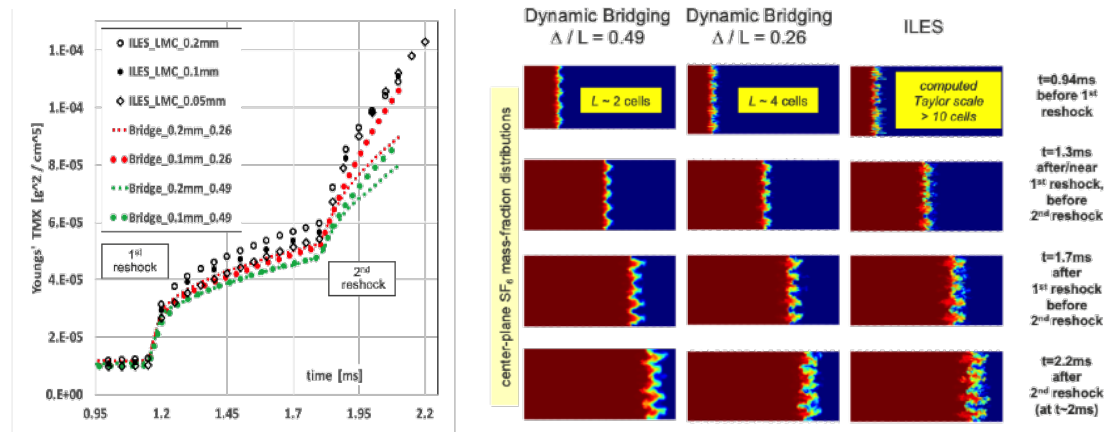


Figure 1: Representative CEA shock tube simulations results, comparing *Dynamic BHR* mixing predictions with 3rd-order LMC xRAGE ILES – from [4].

References

- [1] Grinstein, F.F., *Coarse Grained Simulation and Turbulent Mixing*, Cambridge, 2016.
- [2] Schwarzkopf, J.D., et al. *J. Turb.*, **12**, pp. 1-35, 2011; *Flow Turb. Comb.*, **96**:1-43, 2016.
- [3] George, W.K., Davidson, L., *AIAA Journal*, **42**, 438-446 (2004).
- [4] Grinstein, F.F., et al., *Comp. Fluids* **199**, 104430, (2020); *Phys. Fluids* **33**, 035131 (2021).
- [5] Speziale, C. G., *AIAA Journal*, **36**(2), 173-184, 1998;
Fasel, H.F., et al., *J. Appl. Mech.*, **73**, 405-412 (2006).
- [6] Germano, M., *AIAA Journal*, **36**(9), 1766-1767 (1998).
- [7] Germano, M., *Physics of Fluids*, **29**(6):1755-1757 (1986).
- [8] Grinstein, F.F., *Computers and Fluids*, **151**, 58-72, 2017.
- [9] Pereira, F.S., Grinstein, F.F., et al., *Physics of Fluids*, **33**:115118, (2021).
- [10] Grinstein, F.F., et al., *Comp. and Math. with Applns.*, **78**, Issue 2, pp. 437-458 (2019).
- [11] Grinstein, F.F., and Pereira, F.S., *Phys. Fluids* **33**, 035126 (2021)
- [12] Zhou, Y., Grinstein, F.F., et al., *Phys. Review E*, **89**, 013303 (2014).