

COARSE GRAINED SIMULATION OF SHOCK DRIVEN TURBULENT MIXING

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We focus on simulating the consequences of material interpenetration, hydrodynamical instabilities, and mixing arising from perturbations at shocked material interfaces, as vorticity is introduced by the impulsive loading of shock waves -- e.g., as in ICF capsule implosions. Because of the shock-driven instabilities, resolution requirements to resolve all relevant space and time scales are computationally prohibitive in the foreseeable future. In the coarse grained simulation [1] (CGS) paradigm small scales are presumed enslaved to the dynamics of the largest, or put in other words, the spectral cascade rate of energy (the rate limiting step) is determined by the initial and boundary condition constrained large-scale dynamics. CGS includes classical large-eddy simulation (LES) using explicit subgrid scale (SGS) models, implicit LES (ILES) [2] relying on SGS modeling implicitly provided by physics capturing numerics, and mixed strategies combining explicit / implicit SGS modeling. By combining shock and turbulence emulation capabilities based on a single (physics capturing) numerics, ILES provides an effective simulation framework for shock driven turbulent mixing. Beyond the complex multi-scale resolution issues of shocks and variable density turbulence, we must address the equally difficult problem of predicting flow transition promoted by energy deposited at the material interfacial layer during the shock interface interactions. A typical laboratory shock-tube experiment involves transitional non-equilibrium flow at first-shock and subsequent reshocks, relaxing to quasi-equilibrium decaying turbulence between shock events. Transition involves unsteady large-scale coherent-structure dynamics capturable by a CGS strategy but not by an unsteady Reynolds-Averaged Navier-Stokes (URANS) approach based on single-point-closure modeling [3].

Robust CGS for dissipative turbulent phenomena exhibiting enslavement of small-scale dynamics is achievable with suitable SGS modeling, enough scale separation, and well-resolved initial conditions (IC). However, because of chaotic variability associated with unavoidable uncertainties of presumed IC, it may be impossible even within a mathematically well-posed dissipative flow simulation framework to provide realistic late-time deterministic predictions of shock driven turbulent material mixing [4]. Ensemble averaged CGS over a suitably complete set of realizations covering the relevant IC variability is then a strategy of choice. Hybrid URANS/CGS is current industrial standard to drastically cut computational costs for 3D simulations of complex full-scale flows of interest [5] while offering computationally feasible ways of implementing the CGS ensemble averaging goals.

We consider the simulation of canonical shock-tube (AWE [6] and CEA [7]) (Fig.3) experiments, using ILES and URANS. We report recent validation studies [8] benchmarking ILES with the available turbulence velocity and mixing data from the CEA laboratory studies. In turn, the ILES generated flow data is used to initialize and as reference to assess the URANS. We compare state-of-the-art ILES and 3D URANS using the LANL RAGE code in the ILES and URANS modes [6] -- RAGE-clean and RAGE-BHR, respectively (e.g., Fig. 2 from [8]). We find that by prescribing (ILES generated) physics-based 3D IC and allowing for 3D convection with just enough resolution, the computed dissipation in 3D URANS (vs. 2D URANS) blends effectively with the modeled dissipation -- rather than multiple-counting turbulent effects -- to yield significantly improved statistical predictions (Fig.4). We will discuss our ongoing strategy to extend the hybrid URANS/CGS *flow simulation methodology* [9] for applications involving variable-density turbulent mixing applications, and report progress testing such hybrid methods for the shock-tube problems.

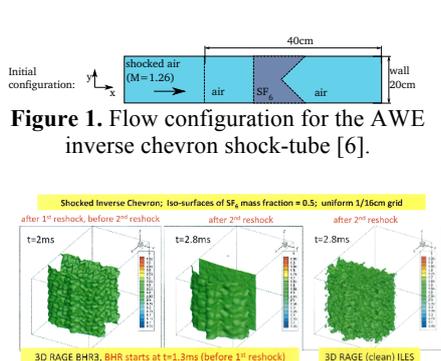


Figure 1. Flow configuration for the AWE inverse chevron shock-tube [6].

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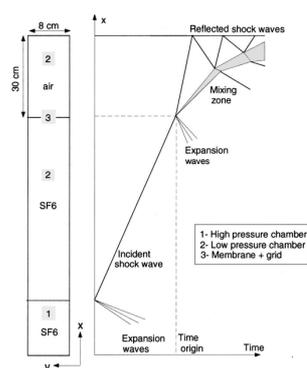


Figure 3. Schematic of the CEA shock-tube experiment [7].

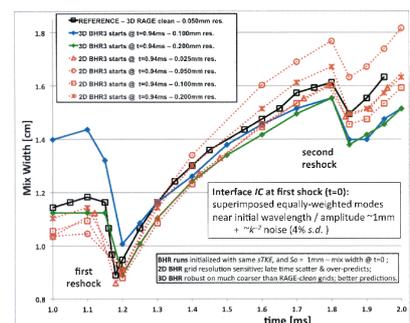


Figure 4. Mix width for RAGE BHR3 vs. 3D RAGE-clean (ILES) [8]. BHR starts at $t=0.94\text{ms}$ just before first reshock; 3D BHR3 is more robust and accurate between first and second reshock.