Implicit large eddy simulation of shock-driven material mixing

F. F. Grinstein, A. A. Gowdhan† and J. R. Ristorcelli

Los Alamos National Laboratory, Los Alamos NM 87545, USA

Under-resolved computer simulations are typically unavoidable in practical turbulent flow applications exhibiting extreme geometrical complexity and a broad range of length and time scales. An important unsettled issue is whether filtered-out and subgrid spatial scales can significantly alter the evolution of resolved larger scales of motion and practical flow integral measures. Predictability issues in implicit large eddy simulation of under-resolved mixing of material scalars driven by under-resolved velocity fields and initial conditions are discussed in the context of shock-driven turbulent mixing. The particular focus is on effects of resolved spectral content and interfacial morphology of initial conditions on transitional and late-time turbulent mixing in the fundamental planar shock-tube configuration.

1. Introduction

Mixing of initially separate materials by the small scales of turbulent motion is a critical element in extremely complex Reynolds number (Re) flows of typical interest featuring a broad range of length and time scales and unavoidably under-resolved computer simulations. Material mixing predictability is a major concern in this context. Relevant computational fluid dynamics issues to be addressed relate to the modelling of the unresolved flow conditions at the subgrid scale (SGS) level—within a computational cell, and at the supergrid (SPG) scale—at initialization and beyond computational boundaries. Likewise, observables in laboratory experiments are always characterized by the finite scales of the instrumental resolution of measuring/visualizing devices and also by SPG aspects. It is thus important to recognize the inherently intrusive nature of observations based on numerical or laboratory experiments [1].
Direct numerical simulation (DNS) resolving all physical space/time scales is prohibitively expensive in the foreseeable future for most practical flows of interest at moderate-to-high $Re$. In the broadly defined coarse grained simulation (CGS), large energy-containing structures are resolved, smaller structures are spatially filtered-out and unresolved SGS effects are modelled; this includes classical large eddy simulation (LES) strategies [2] with explicit use of closure SGS models and implicit LES (ILES) [3] relying on SGS modelling implicitly provided by physics capturing numerical algorithms—briefly surveyed in §2.

An important unsettled issue is whether filtered-out and SGS spatial scales can significantly alter the evolution of the larger scales of motion and practical flow integral measures. The validity of the resolved/unresolved (outer/inner) scale separation assumptions underlying CGS needs to be carefully tested when potentially important SGS flow physics is involved; for example, for turbulent wall-bounded flows, for mixing of material scalars, which we consider in this paper, or in simulations of turbulence involving inertial particles [4], beyond the present scope. It is now recognized that for sufficiently large $Re$ the small-scale near-wall flow dynamics is enslaved to that of the larger scales, and CGS strategies used in conjunction with wall boundary condition models can provide a framework to capture physical outer flow features [5]. This suggests that it may be possible to extrapolate small-scale enslavement ideas to similarly explore difficult issues of under-resolved simulation of high-$Re$ mixing of material scalars.

Turbulent mixing of material scalars can be usefully characterized by the length scales of the fluid physics involved: (i) large-scale entrainment in which advection brings relatively large regions of the pure materials together, (ii) an intermediate length scale associated with the convective stirring owing to velocity gradient fluctuations, and (iii) a much smaller scale interpenetration resulting from molecular diffusion. Large-scale vortices and their interactions play a crucial role in controlling transitional growth and entrainment at moderately high $Re$—when convective time scales are much smaller than those associated with molecular diffusion. In this limit, we are primarily concerned with the numerical simulation of the first two processes above, advection and stirring, and to the extent that they can be emulated with CGS, it should be possible to capture scalar mixing driven by under-resolved turbulent velocity without use of an explicit model. We illustrate this ILES capability in §3, with the challenging problem of under-resolved mixing of material scalars promoted by under-resolved velocity and under-resolved initial conditions (ICs) in shock-driven turbulent flows. We focus on the effects of IC-resolved spectral content and initial interfacial morphology on transitional and late-time turbulent mixing in the fundamental planar shock-tube configuration. Finally, conclusions are presented.

2. Implicit large eddy simulation

Formal analysis of LES can be based on modified equation analysis (MEA) [3], a technique for generating the equations whose solution closely approximates the actual solution of the numerical algorithm underlying the simulation model. Detailed recent MEA of LES has been reported [6]. MEA provides a framework to reverse-engineer desirable physics into the numerics design. A crucial practical computational aspect is the need to distinctly separate the effects of spatial filtering and SGS reconstruction models from their unavoidable implicit counterparts owing to discretization. Indeed, it has been noted that in typical LES strategies truncation terms owing to discretization and filtering have contributions directly comparable with those of the explicit models [7]. Seeking to address the seemingly insurmountable issues posed to LES by under resolution, the possibility of using the SGS modelling and filtering provided implicitly by the numerics has been considered as an option: this is generally denoted as numerical LES by Pope [8]. Arbitrary numerics will not work for LES; good or bad SGS physics can be built into the simulation model depending on choice and particular implementation of the numerics.

The monotone integrated LES (MILES) approach first proposed by Boris [9] incorporates the effects of the SGS physics on the resolved scales through functional reconstruction of
the convective fluxes using locally monotonic finite volume (FV) schemes. The more broadly defined ILES [3] involves high-resolution non-oscillatory FV (NFV) algorithms [10] to solve the unfiltered Euler or NS equations. Popular physics capturing methods have been used in ILES, such as flux-corrected transport (FCT), the piecewise parabolic method, Godunov, hybrid and total variation diminishing algorithms. By focusing on inertially dominated flow dynamics and regularization of under-resolved flow, ILES follows on the precedent of using NFV methods for shock-capturing—requiring weak solutions and satisfaction of an entropy condition.

MEA was used in the early formal comparisons [11] between MILES and traditional LES, to show that a class of NFV algorithms with dissipative leading order terms provide appropriate built-in (implicit) SGS models of a mixed tensorial (generalized) eddy–viscosity type. Key features in references [6,11] were the MEA framework and the use of the FV formulation. Volume integrals in the FV representation naturally link with the discrete spatial filtering operation in LES—the so-called top-hat filtering. FVs and MEA have been also crucial ingredients in the analysis connecting ILES with the solution of finite scale NS equations for laboratory observables [12–14].

3. Under-resolved mixing in shock-driven turbulence

Recent ILES of turbulent mixing of a passive scalar by forced (equilibrium) compressible, isotropic turbulence with a prescribed mean scalar gradient [15], showed ILES is capable of accurately capturing the dominant aspects of the mixing transition as the function of the effective Reynolds number determined by grid resolution. Specifically, the SGS scalar model implicitly provided by a properly constructed ILES dissipative numerics was sufficient (by itself) to capture the mixing asymptotics and turbulent measure characteristics, e.g. Gaussian behaviour of fluctuating scalar PDF, increasing bias in the (non-Gaussian) PDFs of scalar derivatives with increasing effective \( Re \) and asymptotically constant scalar variance with increasing effective \( Re \). The substantially more challenging problem of non-equilibrium, under-resolved material mixing promoted by under-resolved velocity and under-resolved ICs in shock-driven turbulent flows is the subject of what follows.

In many areas of interest, such as inertial confinement fusion, understanding the collapse of the outer cores of supernovas and supersonic combustion engines, vorticity is introduced at material interfaces by the impulsive loading of shock waves, and turbulence is generated via Richtmyer–Meshkov instabilities (RMIs) [16]. RMIs 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 differences and material mixing fluctuation effects are not negligible. Because RMIs are shock-driven, resolution requirements make DNS approaches prohibitively expensive even on the largest supercomputers.

Classical LES approaches are particularly inadequate for flows driven by RMI because of the dissipative numerics required for shock-capturing; hybrid methods switching between shock-capturing schemes and conventional LES depending on the local flow conditions [17] have been proposed; high-order shock-capturing (e.g. fifth-order WENO) methods are typically chosen to ensure a smooth transition and matching of the inherently different simulation models. However, all shock-capturing methods degrade to first order in the vicinity of shocks because of the monotonicity requirements—and, in particular, at the very important initial stage at which shocks first interact with the material interface and generate the velocity field. Thus, severe resolution demands to address the competition between the (numerics provided) implicit and explicit subgrid models can be expected in the hybrid context. Alternatively, by combining shock and turbulence emulation capabilities based on a single (physics capturing numerics) model, ILES has the potential of providing a natural effective simulation strategy for RMI.

In our recent simulations of RMI in shock-tube experiments surveyed below, the focus has been on IC effects on transition and late-time mixing and turbulence characteristics. The particular ILES strategy is based on using the Los Alamos National Laboratory (LANL) Radiation Adaptive Grid Eulerian (RAGE) code [18]. RAGE solves the multi-material compressible conservation
equations for mass–density, momenta, total energy and partial mass–densities, using a second-order Godunov scheme, adaptive mesh refinement (AMR), a variety of numerical options for gradient terms—limiters and material interface treatments (not used here). The van Leer limiter option was chosen for the present simulations. The simulation model is nominally inviscid, effectively models high-Re, Sc ~ 1, convection-driven flow and a miscible material interface is assumed. Simulations of planar [19,20] and gas-curtain [21] shock-tube experiments were examined, involving high-(SF6) and low-density (air) gases, with sharp and diffusive initial material interfaces, respectively, and Atwood number \( A = (\rho_{inner} - \rho_{outer})/(\rho_{inner} + \rho_{outer}) = 0.67 \), where outer values denote those the shock wave traverses before it impacts the material interface. We must deal here with inherently unsteady transitional and decaying turbulent flow. Suitable metrics for analysis of turbulence for this kind of flow are not established, and the state-of-the-art analysis largely relies on using suitable (unsteady) versions of diagnostics designed for the developed homogeneous isotropic regimes.

Richtmyer's [22] impulse analysis shows that the initial growth rate of RMI is given by \( \dot{a} = a_0 \Delta U A^+ \kappa_0 \), where \( a_0 \) is the initial amplitude of the interface perturbation between the two fluids, \( \Delta U \) is the change in the velocity of the mixing layer owing to the shock, \( A^+ \) is the post-shock \( A \), \( \kappa_0 \) is the initial wavenumber of the interface and \( \dot{a} \) is growth rate of the instability. The analysis is based on single-mode perturbation and is valid in the linear regime for very low initial wavenumber and amplitude (\( \kappa_0 a_0 \)) or low values of the material interface RMS slope at early time. Beyond the work surveyed in [16], investigation of IC effects on RMI have been the subject of many experimental [23–26], numerical [19–21,26–30] as well as theoretical studies [31].

We focus here on the planar shock-tube experiments of Vetter & Surtevant [23], involving presumed geometries of the membranes and the wire mesh initially separating the gases, and reshock off an end-wall (figure 1). The mixing-layer growth is affected by the initial interaction of the shock and material interface— with a direct distinct imprint of the initial contact discontinuity deformation specifics and significant further effects occurring after reshock. The contact discontinuity between air and SF6 is modelled as a jump in density using ideal gases with \( \gamma = 1.4 \) and \( \gamma = 1.076 \), respectively, with constant pressure across the initial interface at rest. Typical three-dimensional grids between 2.8–4.5 \( \times 10^7 \) and 1.7–3.2 \( \times 10^8 \) computational cells with smallest spacing \( \Delta_{min} = 0.1 \) cm and \( \Delta_{min} = 0.05 \) cm, respectively, were used in these simulations (table 1). A shocked air region is created upstream satisfying the Rankine–Hugoniot relations for a \( Ma = 1.5 \) shock. The shock propagates in the \( (x) \) direction through the contact discontinuity and reflects at the end of the simulation box on the right, where purely reflecting boundary conditions are enforced. Periodic boundary conditions are imposed in the transverse \( (y, z) \) directions. By design, the location of the left boundary of the computational domain is chosen far away enough so as to ensure that eventual reflections there are unable to affect the mixing region during the reported times of interest. Up to three levels of AMR are used.
modes, parametrized with perturbation was defined in terms of (top-hat or weighted) ranges of randomly superimposed power spectra by themselves [29,30].

Other studies (i) S + L deformation, combining a short (S) egg crate mode—chosen to represent the result of pushing the membrane through the wire mesh on a longer characteristic shock-tube scale L—chosen to be the transverse periodicity dimension of the computational domain. In later papers, the reshocked mixing layer was also simulated, and the IC modelling strategies have included a Weighted-short perturbation modes are weighted with $k^4 \exp[−(k/k_0)^2]$. 

### Table 1. Planar shock-tube simulations.

<table>
<thead>
<tr>
<th>case</th>
<th>dimension</th>
<th>$\Delta_{\text{min}}$ (cm)</th>
<th>AMR</th>
<th>$N_{\text{max}}$</th>
<th>$N_{\text{Ymax}}$</th>
<th>$N_{\text{Zmax}}$</th>
<th>$\phi$ (cm)</th>
<th>$(\lambda_{\text{min}}, \lambda_{\text{max}})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>w. short</td>
<td>three-dimensional</td>
<td>0.1</td>
<td>yes</td>
<td>1640</td>
<td>480</td>
<td>480</td>
<td>$A_2 = 0.025$</td>
<td>(0.2, 12)&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>w. short</td>
<td>three-dimensional</td>
<td>0.05</td>
<td>yes</td>
<td>1640</td>
<td>480</td>
<td>480</td>
<td>$A_2 = 0.025$</td>
<td>(0.2, 12)&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>short</td>
<td>three-dimensional</td>
<td>0.1</td>
<td>yes</td>
<td>820</td>
<td>240</td>
<td>240</td>
<td>$A_2 = 0.025$</td>
<td>(0.4, 4)</td>
</tr>
<tr>
<td>short</td>
<td>three-dimensional</td>
<td>0.05</td>
<td>yes</td>
<td>1640</td>
<td>480</td>
<td>480</td>
<td>$A_2 = 0.025$</td>
<td>(0.4, 4)</td>
</tr>
<tr>
<td>long</td>
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<td>yes</td>
<td>820</td>
<td>240</td>
<td>240</td>
<td>$A_2 = 0.025$</td>
<td>(4, 12)</td>
</tr>
<tr>
<td>no perturb.</td>
<td>three-dimensional</td>
<td>0.1</td>
<td>yes</td>
<td>820</td>
<td>240</td>
<td>240</td>
<td>$A_2 = 0$</td>
<td>—</td>
</tr>
</tbody>
</table>

<sup>a</sup>Weighted-short perturbation modes are weighted with $k^4 \exp[-(k/k_0)^2]$.

### (a) Initial material interface characterization and modelling

The accurate and reliable simulation of material interfaces is an essential aspect in simulating the material mixing fluid dynamics. Interfaces between fluids can be miscible or immiscible, with the character changing during the evolution of a system. This causes numerical approximations to the physics to be extremely challenging, because the basic features of the approximations need to be inherently dynamic, i.e. adapt to the evolution of the materials. For example, in many applications of interest (e.g. inertial confinement fusion capsules), an interface may begin as sharp and immiscible, but evolves into a state where it mixes at an atomic level with neighbouring material owing to the effects of temperature and diffusion or as it becomes a plasma. There exist a number of outstanding challenges in the material interface modelling area arising from the relative weakness of mathematical foundations associated with the techniques available for solutions [32]. Moreover, among the most crucial issue associated with interfaces is the sensitivity of most problems to the ICs: relatively small variations in the initial state of the interface can result in quite significant changes to even the integral character of a mixing layer at late times [29]. As we consider simulating RMI in the laboratory experiments, we must thus consider the effects of modelling insufficiently characterized initial contact-discontinuity deformations. The inherent difficulties with the open problem of predictability of material stirring and mixing by under-resolved multi-scale turbulent velocity fields are now compounded with the inherent sensitivity of turbulent flows to ICs [33].

The surface displacement of the material interface in RMI experiments [23] has been modelled using well-defined modes often combined with random perturbation components. In [28], the shocked planar RMI phase was examined in detail using $S + L$ deformation, combining a short (S) egg crate mode—chosen to represent the result of pushing the membrane through the wire mesh and superimposed distortion of the wire mesh on a longer characteristic shock-tube scale $L$—chosen to be the transverse periodicity dimension of the computational domain. In later papers, the reshocked mixing layer was also simulated, and the IC modelling strategies have included (i) $S + L + \phi$ deformation [27] and (ii) $S + \phi$ deformation [17], where $\phi$ is a spatially random distribution intended to break the presumed characteristic interface symmetries. Other studies have also used broadband $\phi$ multi-scale perturbations with prescribed standard deviation and power spectra by themselves [29,30].

An $S + \phi$ strategy was used here to model the initial interface conditions [19], where the perturbation was defined in terms of (top-hat or weighted) ranges of randomly superimposed modes, parametrized with $\lambda_o = \pi/\kappa_o$ (length scale of the egg crate mode) and characteristic amplitudes. Simulations were performed for a variety of grid resolutions and perturbations superimposed to the S mode (table 1).
Figure 2. (a–d) Instantaneous isosurfaces of the local mixedness function $\theta$ for the short perturbation case at the 0.1 cm resolution. (Online version in colour.)

(b) Evolution of mixing and turbulence characteristics

Analysis of the simulated mixing data is based on transverse-plane averaged quantities, $\langle f \rangle(x) = \int f(x,y,z) dy dz / \int dy dz$, $Y_{SF_6} = \rho_{SF_6}/\rho$, $\psi(x) = \langle Y_{SF_6} \rangle$, $M(x) = 4\psi(x)[1-\psi(x)]$, where $\rho$ is the mass–density, $\rho_{SF_6}$ is the $SF_6$ partial mass–density, $Y_{SF_6}$ is the $SF_6$ mass fraction, $M(x)$ are cross-stream averaged and integrated mixedness. The instantaneous mixing region is defined by a slab of volume $V$ about the centre of the mixing layer constrained in the $x$-direction by requiring $M(x) > 0.75$. Analysis of turbulence characteristics is based on data deviations around transverse planes within this mixing slab region. Following [17], the instantaneous material mixing zone thickness $\delta_{MZ}$ is defined in terms of the mixedness $M(x)$, by $\delta_{MZ} = \delta = \int M(x) dx$ designed to yield $\delta_{MZ} = h$ for $\psi(x) = [1 + \tanh(2(x-x_c)/h)]/2$, where $x_c$ defines the centre of the mixing layer.

The air–SF$_6$ interface is shocked at $t = 0$ ms, reshocked by the primary reflected shock at $t \sim 3.5$ ms, and then by the reflected rarefaction at $t \sim 5$ ms. The material mixing layer is further affected at later times by reflected compression and weaker secondary reflected shock waves (figure 2). Figure 3 compares the variation of the three-dimensional mixing-layer thickness $\delta_{MZ}$ as function of time for the different ICs considered at the baseline 0.1 cm resolution. Overall, the predicted mixing widths for all cases are very similar before reshock, when mixing width for the short (and weighted-short) perturbation case is slightly greater and a thicker mixing layer is associated with breaking of the egg crate mode by the perturbations. Late-time mixing measures are higher for the long IC perturbation case; short and weighted-short perturbation cases are fairly comparable, with the short case mixing measures being somewhat larger for late times—reflecting on higher longer wavelength IC content. Results for the non-perturbation case consistently appear as a limiting case of the long perturbation cases.

Effects of IC resolution were discussed in detail in [19], where it was found that a key IC posing issue that needs to be addressed is that of adequately resolving the $|\sin(\kappa_x y) \sin(\kappa_z z)|$ function used to prescribe the egg crate mode $S$ (introduced in [28] and historically used since...
in this context). Actual predicted mixing-layer thickness growth was shown to depend on the effective IC associated with the resolved egg crate function. The detailed late-time analysis for the weighted-short perturbation case showed that the presence of worms is accompanied by spectra consistent with Kolmogorov’s $\sim k^{-5/3}$ power law [19] for both the 0.05 and the 0.1 cm resolutions and by the noted good agreement of characteristic PDFs with those of (incompressible) isotropic-turbulence DNS data. As finer grids are used with ILES, increasingly smaller structures can be resolved and characteristic cross sections of the smallest resolved vortical worm structures scale with the ILES cut-off [34,35]. The observed resolution effects can be consistently characterized by a higher effective $Re$ associated with the higher resolution—as also noted previously [36]. As self-similar regimes are achieved for the late-times, spatial-velocity-derivative PDFs exhibit expected trends when scaling values with the RMS vorticity (as in the analysis of the DNS data): (i) the non-Gaussian tails, and (ii) the effects of increasing grid resolution (i.e. increasing effective $Re$ and resolved RMS vorticity) emulating effects of increasing physical $Re$. We regard this and the results in [36] as clear demonstration that predictive under-resolved simulations of the velocity in turbulent fluid flows are possible with ILES such as the one used here.

(c) Bipolar behaviour of Richtmyer–Meshkov instabilities

Our planar RMI studies [19] involving initially thin material interface showed mixing-layer growth rates fairly insensitive to IC specifics before reshock, very sensitive after reshock (figure 3) and very different growth trends as function of IC spectral content at shock and reshock time—pointing at the potentially significant role of morphological details in the thicker more complex mixing layers at reshock. These results motivated our systematic numerical study of evolution of RMI [20] by varying characteristic multi-scale spectral content and thickness of the initial interface between the two fluids, for fixed $Ma$ and $A$. The focus was again on the planar shock-tube configuration investigated above (figure 1), but now with IC prescribed only in terms of $\phi$ (no egg crate mode S) and no reshocks for the times considered.

The initial interfacial morphology is defined statistically by $\eta_o = \kappa_o \delta_o \sim (\nabla \chi \nabla \chi)^{1/2}$, the initial RMS slope, where $\chi(y,z)$ is the local deviation of the initial material interface around the mean interface location, $\kappa_o = 2\pi/\lambda_o$, $\lambda_o$ is a representative wavelength of the multi-scale perturbation in
Figure 4. Schematic of the initial interface.

Figure 5. Zero-crossings of $\rho'$; $L$ is the transverse dimension of the computational domain.

Table 2. Planar shock-tube simulations II.

<table>
<thead>
<tr>
<th>$(\lambda_{\text{min}}, \lambda_{\text{max}})$</th>
<th>$L(1/24, 1/6)$</th>
<th>$L(1/12, 1/4)$</th>
<th>$L(1/6, 1/3)$</th>
<th>$L(1/4, 1/2)$</th>
<th>$L(1/24, 1/6)$</th>
<th>$L(1/12, 1/4)$</th>
<th>$L(1/6, 1/3)$</th>
<th>$L(1/4, 1/2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta_o$ (cm)</td>
<td>0.5 (low $\eta_o$)</td>
<td>5 (high $\eta_o$)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$\kappa_o$ (cm$^{-1}$)</td>
<td>$\pi$</td>
<td>$\pi/2$</td>
<td>$\pi/4$</td>
<td>$\pi/6$</td>
<td>$\pi$</td>
<td>$\pi/2$</td>
<td>$\pi/4$</td>
<td>$\pi/6$</td>
</tr>
</tbody>
</table>


The initial interface and $\delta_o = \delta(t = 0)$ denotes the initial interface thickness (figure 4). Thus, a high value of $\eta_o$ denotes a highly corrugated interface with high RMS slope.

The quantity $\kappa_o$ is used in the study of homogeneous stochastic processes, where it is called the mean zero-crossing frequency [37]. In practice, the initial material interface value of $\kappa_o$ is computed by checking for sign changes of the mass–density fluctuation over lines within transverse planes and averaging their occurrences (figure 5); for $t > 0$, $\kappa = \kappa(t)$ is similarly evaluated within the mixing region. Mathematically, $\kappa(t)$ is related to the Taylor microscale [20].

Various simulation-based experiments were performed in terms of well-defined initial material interface perturbations. The material interface deformation is defined by $
abla(y, z) = \Gamma \sum_{n,m} a_{m,n} \sin(\kappa_{n}y + \phi_{n}) \sin(\kappa_{m}z + \phi_{m})$, $\kappa_{i} = \frac{2\pi i}{L}$, where we use random coefficients $-1/2 < a_{m,n} < 1/2$, $\Gamma$ is used to prescribe $\delta_o$, $\{\phi_{n}, \phi_{m}\}$ are random phases, and the participating modes are constrained by the requirement, $\lambda_{\text{min}} \leq L/[2\pi \sqrt{(n^2 + m^2)}] \leq \lambda_{\text{max}}$. For completeness, we note that for the single-mode analysis [22] cited above, $\delta_o = a_o$. A variety of IC perturbations and grid resolutions (using up to two levels of AMR refinement) were considered. The baseline resolution involved a $820 \times 240 \times 240$ grid ($\Delta_{\text{min}} = 0.1$ cm); a much finely resolved $1640 \times 480 \times 480$ grid ($\Delta_{\text{min}} = 0.05$ cm) was used for selected representative cases. The various cases are organized into two distinct categories having significantly different (low and high) initial RMS slope ($\eta_o$) with prescribed spectral content but different interfacial thickness (table 2).

Instantaneous visualizations of $Y_{\text{SF}_6}$ at the selected time, $t = 3000$ $\mu$s shown in figure 6 suggest material (interpenetration) mixing increasing with $\eta_o$. Following [22], the passage of a shock through the material interface has the effect of having baroclinic vorticity ($\sim \kappa_o \dot{\alpha} = \Delta U A^+ \kappa_o \eta_o$) deposited as function of $\eta_o$. For low $\eta_o$, less baroclinic vorticity is generated. When the initial
characteristic wavelength is greater than its characteristic amplitude, crests and troughs are well separated and the vortices are weaker, and consequently do not interact strongly. In the low $\eta_0$ regime, the modes mainly grow in the shock direction in a ballistic (non-interacting) fashion. For these (low $\eta_0$) flows, the zero-crossing frequency $\kappa$ is virtually unchanged with time as shown in figure 7a, indicating that no new modes are produced. For high $\eta_0$, more baroclinic vorticity is generated. The initial characteristic wavelength is less than its characteristic amplitude, thus crests and troughs of the perturbations are closer together and the vortices are stronger and create new modes through nonlinear processes. For these flows, there is an unmistakable jump in $\kappa$ indicating rapid production of smaller scales. Consistent with this notion, figure 7a shows that the higher the $\eta_0$, the sooner the jump occurs. The borderline case is $\lambda_0/2 \sim \delta$ or $\eta_0 \sim \pi$. Representative selected cases were also analysed based on the higher-resolution simulations. Integral measures such as the mixing width were found to be virtually insensitive to grid resolution; as the flow becomes nonlinear (high $\eta_0$), finer resolution results depict increased small-scale production as indicated by higher $\kappa$ (figure 7a) and longer self-similar ranges in the spectra of $R$ (figure 7b)—which can be associated with higher effective $Re$ [19,36].
Inversely proportional to time shocked mixing-layer growth rate $\eta$ same direction and increased the mixing-layer widths. However, for the shock is mostly in the shock direction and leads to growth of the initial modes in that same direction and increased the mixing-layer widths. However, for $\eta_0 = \pi/2$, the theory is valid only for a very short time after the material interface is shocked. Soon thereafter, the growth rate drops, and this is not consistent with linear theory. By contrast, for high $\eta_0$ ($\eta_0 \gg \pi$), the growth is inversely proportional to $\eta_0$. For higher $\eta_0$, there is a much larger deposition of baroclinic vorticity.

Inspection of the evolution of the mixing-layer width $\delta(t)$ (figure 8a) for relatively small $\eta_0$ (for $\eta_0 = \pi$) shows growth rates ordered in agreement with predictions of classical linear impulse theory (growth proportional to $\eta_0$) [22]. For the high $\eta_0$ cases, higher $\eta_0$ results in larger deposition of baroclinic vorticity and leads to thicker mixing layers initially. The energy produced by passage of the shock is mostly in the shock direction and leads to growth of the initial modes in that same direction and increased the mixing-layer widths. However, for $\eta_0 = \pi/2$, the theory is valid only for a very short time after the material interface is shocked. Soon thereafter, the growth rate drops, and this is not consistent with linear theory. By contrast, for high $\eta_0$ ($\eta_0 \gg \pi$), the growth is inversely proportional to $\eta_0$. For higher $\eta_0$, there is a much larger deposition of baroclinic vorticity.

Interestingly, the increase in $\eta_0$ does not result in increase in the mixing-layer width but leads to production of more small scales, and thus more dissipation.

As in the work of Jacobs & Sheeley [24], we found it useful to plot each layer thickness $\kappa_0 (\delta - \delta_0)$ versus time scaled with $\kappa_0 \delta_0$ (figure 8b), using the corresponding computed early-time shocked mixing-layer growth rate $\delta_0$. Such plotting tends to collapse the data into two distinctly different groups. Depending on the initial RMS slope of the interface, RMI evolves into linear or nonlinear regimes, with different flow features, growth rates, turbulence statistics and material mixing rates. We called this the bipolar RMI behaviour. For interfaces with low initial RMS slope $\eta_0$, the mixing-layer growth is ballistic with no mode coupling, the evolution of RMI is linear ($\sim t$) and follows the linear scaling [22]. Increasing $\eta_0$ in the low-$\eta_0$ group increases the deposition of baroclinic vorticity on the initial material interface and leads to higher layer growth. By contrast, increasing $\eta_0$ in the high-$\eta_0$ group also increases the deposition of baroclinic torque but this leads to a reduced mixing width growth rate ($\sim t^{0.5}$) associated with the production of small scales by nonlinear mode coupling that are additionally dissipative. Early-time data scatter apparent in figure 8b reflects a historical (rather than fundamental) issue: our original study did not focus on early time aspects and, in hindsight, dumps in time were not frequent enough to ensure uniformly accurate computed $\delta_0$ for all cases compared.

Figure 8. (a) Mixedness measures as a function of time; (a) low $\eta_0$, (b) high $\eta_0$. The air–SF$_6$ interface is shocked at $t = 0$ µs. (b) Mixedness measures suitably shifted and scaled with IC parameters (time scaling first proposed in [24]).
Transition to turbulence is traditionally viewed in terms of a rapid increase in the population of motions with smaller length scales, which can lead to an inertial subrange in the turbulent kinetic energy spectra [38,39]. The spectral bandwidth of fully developed turbulence can be scaled by the turbulent Re [38], usually taken as a ratio of integral-to-Kolmogorov length scales. In our context, we use the thickness of the layer $\delta(t)$ as a measure of the integral scale and the mass–density Taylor microscale $\lambda(t)$—related to the spatial zero-crossing frequency through $\lambda(t) \sim 1/\kappa(t)$—as proxy for the small scales. We can use $\eta(t) = \kappa(t)\delta(t)$ as measure suggestive of the spectral bandwidth (figure 9a). Our observations [20] suggest that sudden increase in $\eta(t)$ (and $\kappa(t)$) can be consistently used to indicate transition as it corresponds to increase in number of active modes of smaller length scales. Figure 9b exemplifies PDFs of $Y_{SF_6}$ over the mixing-region slab (at $t = 2500 \mu s$). Similar to the spectral bandwidths (figure 9a), the PDFs also increase monotonically with $\eta_0$, indicating that as we increase the initial RMS slope we get more material (interpenetration) mixing for both linear (low-$\eta_0$) and nonlinear (high-$\eta_0$) regimes.

Vorticity production at shock time and eventual mode coupling thereafter will depend on the initial interfacial characteristics, as well as on the particular $A$, $Ma$ and (light/heavy or heavy/light) configuration considered. However, the initial RMS slope of the material interface $\eta_0$ appears to be a relevant parameter in determining whether the flow is in the linear ballistic regime, or in nonlinear mode-coupling regime. In the linear regime, the impulsive theory [22] predicts the mixing-layer growth trends: as the initial RMS slope increases the growth rate increases. Less mode coupling is seen, as inferred by the smaller spectral bandwidth, and the primary production of enstrophy is baroclinic. In the nonlinear regime, the mixing-layer growth rate trends are the inverse of that predicted by Richtmyer [22]. There is significant mode coupling and our proxy for spectral bandwidth makes a sudden jump; this suggests that stretching becomes an important enstrophy production mechanism. Important practical consequences of our results are addressed separately [40,41]: (i) reshock effects on mixing and transition can be emulated at first shock if $\eta_0$ is high enough and (ii) simple turbulence models cannot handle both classes of ICs, i.e. current moment closure models are not general enough to predict RMI flow with sequential shocks.

4. Conclusion

Accurate predictions with quantifiable uncertainty are essential to many practical turbulent flow applications exhibiting extreme geometrical complexity and broad ranges of length and time scales. Under-resolved computer simulations are typically unavoidable in such applications, and
CGS (and more typically ILES) becomes the effective simulation strategy mostly by necessity rather than by choice. SGS modelling issues have motivated intense research in the last four decades. A particular focus here has been on addressing some of the challenging issues of under-resolved RMI-driven turbulent material mixing simulation. Because RMI is shock-driven, resolving all physical space/time scales in numerical simulations is prohibitively expensive even on the largest supercomputers. By combining shock and turbulence emulation capabilities on a single model, ILES has the potential for providing a natural effective simulation strategy for the study of RMI. The noted inherent sensitivity of laboratory and computational experiments to initial and other boundary conditions is also a crucial aspect to be addressed in this context. Our work addressed the importance of IC characterization and modelling and their effects on three-dimensional transition and mixing in RMI.

Shocked driven mixing is fairly insensitive to ICs before reshock, but very sensitive after reshock. Vorticity production at shock time and eventual mode coupling (and transition) thereafter will generally depend on the initial interfacial characteristics, as well as other ICs, such as $Ma$ [25,26], $Re$ [28], and magnitude and sign of $A$ [42]. The presence of small-scale material-concentration fluctuations in the ICs—and their consequences on the morphology of thicker (high RMS slope $\eta_o$) mixing layers at reshock time, promote disorganization, larger spectral bandwidth and late-time features typically associated with transition to turbulence [21]. A single IC parameter characterizing the initial RMS material interface slopes can be usefully identified as relevant in determining whether the RM-driven flow is in a linear ballistic regime or nonlinear mode-coupling regimes [41].

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