Three-Dimensional Simulation of a Richtmyer-Meshkov Instability with a Two-Scale Initial Perturbation

Ronald H. Cohen, William P. Dannevik, Andris M. Dimits, Donald E. Eliason,

Arthur A. Mirin, Ye Zhou

Lawrence Livermore National Laboratory, P.O. Box 808, Livermore CA 94550

David H. Porter, Paul R. Woodward

Laboratory for Computer Science and Engineering, University of Minnesota, Minneapolis, MN

(February 5, 2002)

Abstract

Three-dimensional high-resolution simulations (up to 8 billion zones) have been performed for a Richtmyer-Meshkov instability produced by passing a shock through a contact discontinuity with a two-scale initial perturbation. The setup approximates shock tube experiments with a membrane pushed through a wire mesh. The simulation produces mixing-layer widths similar to those observed experimentally. Comparison of runs at various resolutions suggests a transition from unstable to turbulent flow as the numerical Reynolds number is increased. At the highest resolutions, the spectrum exhibits a region of power-law decay, in which the spectral flux is approximately constant, suggestive of an inertial range, but with a weaker wavenumber dependence than Kolmogorov scaling, about $k^{-5/4}$. Analysis of structure functions at the end of the simulation indicates the persistence of structures with velocities largest in the stream-wise direction. Comparison of three-dimensional and two-dimensional runs illustrates the tendency toward forward cascade in

1

three dimensions, vs. inverse cascade in two dimensions. Comparison of the full simulation with a simulation of a single-scale perturbation indicates that the coupling of the disparate scales leads to destruction of the small-scale bubbles and spikes except near the spike growing from the large-scale perturbation. Finally, an analysis of the sub-grid-scale stresses in filtered data indicates significant correlation of the resultant forward and back transfer of energy with the determinant of the rate-of-strain tensor of the resolved scale flow. A possible relation between this trend and alignment of vorticity on small scales with the principle directions of strain on large scales is discussed. The observed correlation lends support to the use of sub-grid-scale models proportional to the determinant of the rate-of-strain tensor for large-eddy simulation.

Typeset using REVTEX

I. INTRODUCTION

Richtmyer-Meshkov instability [1,2] arises when a shock passes through an interface between two fluids. It is sometimes considered to be the impulsive limit of a Rayleigh-Taylor instability, but with the important distinctions that (a) instability occurs whether the acceleration is toward either side of the interface, whereas for Rayleigh-Taylor one has instability only for gravity in the direction of the lighter fluid; and (b) since the drive is impulsive, the evolution occurs largely during a time where the driving force is zero.

Richtmyer-Meshkov instability can occur in a number of natural and man-made settings, such as supernova explosions, the interiors and the wakes of jet engines, and combustion chambers. In addition there have been many laboratory shock-tube experiments to explore the basic physics of the interaction of shock waves with contact discontinuities.

A generic feature of these systems, as is the case for fluid turbulence in general, is the existence of fluctuations on multiple length scales. Multiple scales are generated through the hydrodynamic nonlinearities, but can often be present even in the initial conditions. Experiments set up to favor a single-wavelength initial perturbation often have a second, disparate, wavelength. So, for example, shock tube experiments with wire grids, such as those of Sturtevant and co-workers [3,4] will be characterized by the size scale of the grid as well as transverse dimensions of the shock tube. Since pairwise interaction of disparate-scale fluctuations is a fundamental building block in the physics of turbulence evolution, such experiments and their analysis provides a laboratory for investigation of turbulent dynamics.

In this paper we focus on simulations of Richtmyer-Meshkov instability for such a two-scale perturbation. We are motivated in particular by the shock-tube experiments of Vetter and Sturtevant [4], in which two fluids are intially separated by a membrane placed over a (two-dimensional) wire screen. In the particular experiments we have chosen to represent in our simulations, the shock pushes the membrane through the screen and ruptures it, creating a seed perturbation on the mesh scale, while deformation of the entire mesh creates a perturbation on the scale of the transverse dimensions of the shock tube. The experimental

setup is as shown schematically in Fig. 1.

Thanks to the advent of terascale parallel computers, simulation of disparate-scale initial conditions can be undertaken, in three dimensions, with sufficient resolution to meaningfully follow the disparate scales, and to allow energy to forward cascade from the largest energy-containing scales through a discernable inertial range, to be dissipated at short wavelengths.

Although many 2-D simulations have been performed of the RM instability, relatively few 3-D simulations have been reported. Previously reported 3-D RM simulations [5–15] have used either single-mode or "random" many-mode intial perturbations. The present study appears to be the first report of a 3-D RM simulation with a two-scale initial perturbation.

The simulations presented here lead to following conclusions: (1) Due to code limitations, the set-up of the Vetter-Sturtevant experiments could only by roughly approximated. Nevertheless, the macroscopic mixing behavior of the experiments is reproduced. In particular the mixing layer widths from the simulation are in perhaps surprisingly good agreement with the experiments; (2) The presence of the long wavelength perturbation has a notable impact on the evolution of the short wavelength perturbations, in particular destroying most of them, breaking them up into still-smaller perturbations. (3) Comparision of 2-D and 3-D runs illustrates the difference in 2-D vs. 3-D dynamics: The 2-D simulations are characterized by coalescence into structures comparable to or larger than the initial short-wavelength (mesh) scale, while the 3-D simulations evolve toward fine scales; this is as one would expect from the predominance of inverse and forward cascades, respectively. (4) Comparison of vizualizations at various resolutions suggests a transition from unstable to turbulent flow as the resolution is increased, consistent with arguments by Dimotakis [16] that such a transition should occur with increasing Reynolds number. In this case the Reynolds number is that attached to numerical dissipation. (5) As the resolution is increased, a kind of inertial range is evident; this is not a classic Kolmogorov inertial range as the spectrum is not continuously driven. The spectrum has a power-law region, but with a weaker wavenumber dependence than Kolmogorov scaling, about $k^{-5/4}$. The spectral flux is approximately constant in this region. (6) Analysis of structure functions at the end of the simulation indicates

the persistence of structures with velocities largest in the stream-wise direction. (7) There is a significant correlation between the forward- and bacward-trasfer of energy due to the sub-grid-scale stress and the determinant of the rate-of-strain tensor of the resolved-scale flow. This correlation suggests that a Smagorinsky-like model is a good candidate for a large-eddy-simulation (LES) model.

The remainder of this paper is organized as follows. In Sec. 2, we describe the codes, the simulation setups, and the relationship of these setups to the experiments of Vetter and Sturtevant [4]. Section 3 discusses macroscale properties of the temporal evolution, including comparison of the mixing-layer growth rate with experimental results. Section 4 is devoted to a resolution study, with regard to spectral convergence, the turbulence transition, and the nature of the "inertial" range. Section 5 presents a comparison of 2-D vs. 3-D dynamics. Section 6 presents results on the interaction of the short and long scales of the initial perturbation. Section 7 describes the comparison of the nonlinear stresses with possible model forms, including the gradient of the rate-of-strain tensor. Section 8 is a discussion and summary of the results.

II. SIMULATION SETUP

Vetter and Sturtevant performed a series of shock-tube experiments with various combinations of orientation of the high- and low-density gasses (respectively, SF_6 and air), the shock direction, and the positions of the membrane and the wire mesh. The particular simulation we have chosen is one where the shock passes from the low- to high-density fluids, and the membrane is initially on the same side of the mesh as the shock. Of the various combinations studied by the authors, this is the one that led to rupturing of the membrane and thus leads to subsequent mixing-layer growth unencumbered by properties of the membrane. Also because the membrane is pushed into the mesh, there is a distinct imprint of the mesh spacing on the initial contact discontinuity shape.

The simulations presented here, which were done in November 1998, were the result of

a unique opportunity: a large block of dedicated computer time was made available on a (then) uniquely large computing facility, the IBM Blue Pacific system at Lawrence Livermore National Laboratory, as part of the commissioning process for the facility. Exploiting this opportunity required the choice of code and numerical and physics compromises described below.

Our simulations were performed with the sPPM (simplified Piecewise Parabolic Method) code [17]. The Piecewise Parabolic Method [18] (PPM) is a Godunov method that uses parabolas to represent the dynamic fields within a grid cell. sPPM is a simple version of PPM that does not include a number of refinements, such as contact-discontinuity detection and steepening and the computation of a coefficient of numerical viscosity which adjust to the local needs of the flow in both space and time. sPPM has a number of restrictions, including periodic boundary conditions in two of its three dimensions, and a single ideal gas. However, sPPM is highly optimized for performance on hybrid distributed-plus-shared memory parallel computers such as the IBM Blue Pacific system at Lawrence Livermore National Laboratory; it is this feature which made the highest-resolution simulations reported here (ones with over eight billion computational zones) feasible.

The sPPM code solves the compressible Euler equations on a Cartesian computational grid. There is no explicit (Navier-Stokes) dissipation; the only dissipation present is numerical and takes the form of a strong damping of wavelengths comparable to the grid spacing. The solution procedure is directionally split and entails taking a Lagrangian step followed by a remap onto the original computational grid. Because of directional splitting, sPPM is formally 2nd order accurate in smooth flow. sPPM is 1st order accurate at discontinuities. Convergence tests of sPPM on decaying turbulence flows indicate that all effects of the numerical dissipation go up to wavelengths of about $32\delta x$, which corresponds to displacements of $16\delta x$. (Here δx is the computational grid size). The numerical viscosity of sPPM is very similar to previous versions of PPM. Convergence tests [19–22] and comparisons with resolved Navier-Stokes solutions [19,22] have been performed. Measures of rate of decay of sin waves in the velocity [21] indicate that the numerical dissipation of PPM leads to an effective

kinematic viscosity which scales as the $(\delta x / \lambda)^3$. Convergence tests of Navier-Stokes flows in 2-D [22] indicate that roughly eight mesh cells are required to resolve discontinuities, such as shock waves. By contrast, the PPM family of codes are designed to handle these kinds of discontinuities in about two mesh cells. The trade off is that Euler codes like PPM do not claim to describe the interior of discontinuities, but only their placement and interaction with larger scale flow.

We model the experimental setup approximately with sPPM, as follows. The air-SF$_6$ contact discontinuity is modeled as a discontinuity in density of a single ideal gas with a ratio of specific heats $\gamma = 1.3$. The temperature changes appropriately so as to maintain a constant pressure across the interface. The code uses dimensionless units such that the density and sound speed are 1.0 on the low-density (corresponding to air) side of the contact discontinuity (and the simulation box width is also 1.0, with x and y running from -0.5 to +0.5). The choice of length-scale normalization is discussed below. The density is set to 4.88 on the other (SF$_6$) side. A shock is created by moving this fluid into a higher-density, higher-pressure region where the density and pressure discontinuities are chosen so as to satisfy the Rankine-Hugoniot relations for a Mach 1.5 shock. A shock is then formed and propagates through the contact discontinuity and on out the end of the simulation box. Simple zero-derivative boundary conditions at the ends of the box suffice to produce negligible shock reflection for these parameters. The entire simulation is done in a reference frame in which the final contact discontinuity is approximately at rest. Empirically, the required initial velocity of the low-density fluid (and the contact discontinuity) is close to but not quite equal to that from a solution to the Riemann problem; the difference is due primarily to the effects of small but finite ($\sim 1\%$) shock reflections off of the ends of the simulation box.

To model the initial contact discontinuity deformation, we choose a surface displacement of the interface, of the form:

$$\Delta z = 0.01 \left(|\sin kx| \, |\sin ky| - \cos 2\pi x \cos 2\pi y \right) \tag{1}$$

with $k = 10\pi$. The terms $|\sin kx| |\sin ky|$ represent the result of pushing the membrane

7

through the wire mesh, while $\cos 2\pi x \cos 2\pi y$ represents the distortion of the wire mesh on the scale of the shock tube transverse dimensions. The simulation has different boundary conditions at the side walls and about a factor of two lower k as compared to the experiment. The different boundary conditions are due to code limitations. The lower value of k is in order for the simulation to be tractable.

The choice of $k = 10\pi$ was a compromise between having a ratio of scale lengths comparable to the experiment and having adequate numerical resolution to do interesting numerical and physics studies. We determined that about 8 billion computational zones was the maximum we could sustain and simulate an interesting physical time (one with significant nonlinear evolution) with the computer time made available to us. The simulation domain has to have an extent and resolution in the stream-wise direction at least comparable to that in the transverse directions in order that there be enough room for the mixing layer to grow and not be affected by the end boundaries. So this dictates having at most about 2000 cells in each of the transverse directions. Our exprience with the code in general and single-wavelength initial perturbations in particular indicates that a minimum of about 64 cells in the transverse (to the shock) directions is required to adequately follow the evolution of such perturbations through the nonlinear stage where secondary eddies form (stated another way, we need to be able to follow several harmonics of the fine scale perturbations to capture their nonlinear evolution). The above initial perturbation has $2k/(2\pi)$ fine-scale oscillations across the domain. Hence, the maximum allowed choice for k would be 30, which would be barely adequate to reproduce the experiment. However, this would allow no leeway for numerical convergence studies, or for observing such effects as increased forward cascade due to coupling of the short- and long-wavelength scales, transition to turbulence with increased resolution, etc. We chose to sacrifice quantitatively matching the experimental setup in order to be able to do such studies.

This brings us to the specification of the length-scale normalization in our dimensionless variables. Because the ratio of the short and long wavelength perturbations (corresponding to the mesh wire spacing and shock tube transverse dimensions, respectively) are different

8

in the simulation and experiment, two equally logical choices for length normalizaton are (1) normalizing all lengths to the transverse $(x, y$; see Fig. 1) dimension of the shock tube; or (2) normalizing all lengths to 10 times the distance between wires in the mesh (that is, requiring that the wire spacing in the experiment and simulation correspond.) In either case, we normalize time so that the sound speed is 1.0 in the lower density gas. We will compare our simulations with experiment using both normalizations. As a result of the various differences between the code and experiment, the comparisons can be expected to yield only semi-quantitative agreement.

III. MACROSCOPIC EVOLUTION

The growth of the Richtmyer-Meshkov instability and the consequent mixing is illustrated by the visualizations in Fig. 2. The variable plotted is the entropy

$$S = \ln P - \gamma \ln \rho \quad . \tag{2}$$

S is chosen because it vividly displays the contact discontinuity while, for the parameters of the simulation, it has a relatively small change across the shock. The color mapping is chosen to be red on the high-density (low-entropy, low-temperature) side and blue on the low-density side of the contact discontinuity. These figures indicate the early-time growth of Ricthmyer-Meshkov instability on the two initial perturbation scales (that of the simulation box and that of the wire array), an appearance of secondary instabilities before the $t = 1$ time slice (visualizations at intermediate times first show secondary instabilities at $t \approx 0.7$), and an onset of turbulent behavior at $t \sim 4$. In this and all subsequent work, time and length are given in the dimensionless code units obtained by normalizing to the transverse box dimension and to the time for a sound wave to cross the transverse dimension.

The growth of the combined perturbation is shown for the various resolutions studied in Fig. 3. The plotted data is obtained as follows. From horizontal slices of the data are extracted the minimum, maximum, and average values of S. Far away from the instability

layer, these values are approximately the same (but different on the two sides of the contact discontinuity). Denoting the values on either side as S_1 and S_2, and the average as $\overline{S}$, we define the layer width as extending from the value of z where the maximum value of S first becomes as large as $\overline{S}$ to the value of z where the minimum value of S is for the last time as small as $\overline{S}$.

Also shown in Fig. 3. is the experimental data [4], normalized in two different ways to the code's dimensionless units, as discussed in the preceding section. We see that the two sets of normalized data, while significantly displaced in time, both agree well with the simulation data. It is noteworthy that the two different normalizations correspond to two different normalized time intervals and hence are at different stages of the nonlinear evolution (particularly of the fine scales), as indicated by the simulation. There is, however, no indication in the experimental results presented in Ref. [4] of the nonlinear regime in which the data lives.

IV. RESOLUTION STUDY

The simulation was performed at various resolutions ranging from 192^3 to $2048^2 \times 1920$. The mixing layer width for the various resolutions is plotted in Fig. 3; it can be seen that the mixing layer width history is very nearly the same for all resolutions from 384^3 through the maximum resolution of $2048^2 \times 1920$. It might be argued that this is to be expected, since from Fig. 2 it can be seen that the large scale evolution is still not yet highly nonlinear. On the other hand the same figure indicates that the fine scales are strongly nonlinear, and their amplitude is non-negligible. A more sensitive test is provided by calculating the mixing-layer width with the long-wavelength (transverse-box-size) perturbation subtracted; the results of such a calculation is presented in Fig. 4, for three resolutions. This is accomplished by defining an average surface for the long-wavelength mode as follows. First a z-averaged entropy surface, $\overline{S(x,y)}$ is computed. The assumption is made that the change in entropy at the z-position of $\overline{S(x,y)}$, z_{avg}, is a simple jump, so that $S = S_1$, $z < z_{avg}$, while $S = S_2$,

10

$z > z_{avg}$. If the range of the z integration is z_{min} to z_{max} then

$$\overline{S(x,y)} = [(z_{max} - z_{avg}) * S_2 + (z_{avg} - z_{min}) * S_1]/(z_{max} - z_{min}) \tag{3}$$

so

$$z_{avg} = \left[z_{min} * \left(S_1 - \overline{S(x,y)} \right) + z_{max} * \left(\overline{S(x,y)} - S_2 \right) \right] /(S_1 - S_2). \tag{4}$$

This evaluation of z_{avg} is performed at each (x, y). This surface is then subjected to a low-pass Fourier filter, in which only the constant, fundamental (with wavelength equal to the transverse box dimension), second, and third harmonic modes are kept. Next, the data is sampled along this reference surface, and along a family of surfaces displaced from the reference surface by a constant displacement; from the data so sampled we extract layer widths as with the standard sampling along horizontal slices. It can be seen that the layer width growth is converging with resolution, but is somewhat more sensitive to resolution than the overall layer width plotted in Fig. 3; this is not surprising since inspection of the volume renderings indicates that, even at the end of the simulaton, the long-wavelength perturbation constitutes the majority of the overall "layer width" and is still in a near-to-linear regime, whereas the shorter wavelengths are in a highly nonlinear regime. It is perhaps surprising that the three curves agree as well as they do, particularly since the fine-scale structure is quite different at 512^3 than at the higher resolutions.

A sensitive indication of numerical convergence is provided by examining the power spectrum. In Fig. 5, $E^p(k_\perp)$, the 2-dimensional $(x - y)$ power spectrum of the normalized momentum $\hat{p} = \rho v/\langle \rho \rangle$ field [the square of the Fourier transform of p per unit interval in the magnitude of the perpendicular (to the shock direction z) wavenumber], in a horizontal slice which passes through the mixing layer, is plotted for each of the resolutions at the final time of the highest resolution run, $t = 9$. Here $\langle \rangle$ denotes a horizontal average, and v is the total speed $(v_x^2 + v_y^2 + v_z^2)^{1/2}$. We choose to plot spectra of $\hat{p}$ components rather than v as it is the equation for evolution of the momentum density that can be cast in conservative form and hence is more amenable to conservation arguments, etc. On the other hand, the momentum

11

density spectra have sizeable contributions from advection of the density contrast across the contact discontinuity. Remarkably, we find that the "inertial" ranges for either variable have about the same slope, but plots of the v spectra show a less extended inertial range and a steeper dissipation range.

Noteworthy in these plots are the remnants of the low- and high-wavenumber initial perturbations, a range dominated by numerical dissipation near the upper end of the range of wavenumber $k_\perp$, and, for the higher resolutions, a region possibly identified as an inertial range in between. These results are consistent with the notion of convergence for an Euler code with only numerical dissipation: a spectrum that tends to be consistent in the low- and intermediate-wavenumber range and then break away into a dissipation range at a wavenumber that depends on the resolution. The most notable exception to this trend is the variation in spectra at the odd harmonics at low wavenumber. The initial perturbation has an even symmetry with respect to the midplanes in the x and y directions; odd modes form only as a result of symmetry breaking due to finite numerical accuracy (*e.g.* roundoff errors). Hence the amplitude of the odd modes is a reflection of such error sources at any particular resolution, which cannot be expected to have any particular trend with resolution.

We consider the nature of the "inertial range" which appears in the highest-resolution simulations. Traditionally one looks for a $k^{-5/3}$ spectrum (or $k^{-8/3}$ for Kolmogorov turbulence integrated over a homogeneous direction), and a power spectral transfer rate (the rate of flow of kinetic energy in wavenumber space across a surface of specified k) that is independent of wavenumber k. But these results formally apply only to isotropic turbulence which is continuously driven, or decaying infintesimally slowly compared to dynamical timescales. Richtmyer-Meshkov instability is driven only impulsively, and the secondary instabilities which give rise to turbulence are driven by a decaying velocity shear.

To analyze this, it is most convenient to consider the equation for the z-integrated momentum density, as that can be written in conservative form with boundary source terms. Specifically, starting from the local momentum equation in conservative form, integrating over z, and dividing by the z domain length L_z, we obtain

12

$$\frac{\partial \overline{\rho \mathbf{u}}}{\partial t} + \nabla_\perp \cdot \overline{\rho \mathbf{u} \mathbf{u}} + (1/L_z)\Delta(\rho u_z^2)\mathbf{e}_z = -\nabla_\perp \overline{P} - (1/L_z)\Delta P \mathbf{e}_z \tag{5}$$

where $\Delta P = P(z_{\max}) - P(z_{\min})$, and similarly for (ρu_z^2). Here the line over a symbol denotes its z average, and $\nabla_\perp$ is the gradient in the x, y (perpendicular to the shock propagation) direction. It is assumed that the turbulent region is confined away from the ends so that $u_x = u_y = 0$ at the ends. Subtracting the horizontal average of the above equation from the equation itself removes the Δ terms, leaving

$$\frac{\partial \delta \left(\overline{\rho \mathbf{u}} \right)}{\partial t} + \nabla_\perp \cdot \overline{\rho \mathbf{u} \mathbf{u}} = -\nabla_\perp \overline{P} \tag{6}$$

where δ denotes the difference of a quantity from its horizontal average.

We define the spectral energy to be $\mathcal{E}_\mathbf{k} = |\mathbf{p}_\mathbf{k}|^2$, where $\mathbf{p}_\mathbf{k} = (\overline{\rho \mathbf{u}})_\mathbf{k}$ and $\mathbf{k}$ denotes the transverse (x, y) wavenumber. Fourier transforming Eq. (6) in x, y then yields an equation for spectral energy balance,

$$\frac{\partial \mathcal{E}_\mathbf{k}}{\partial t} + \mathcal{T} = -2\mathrm{Im}\left(\mathbf{k} \cdot \mathbf{p}_\mathbf{k}^* \overline{\mathrm{P}}_\mathbf{k} \right) \tag{7}$$

where the spectral transfer function $\mathcal{T}$ is given by

$$\mathcal{T}(\mathbf{k}) = 2\mathrm{Im}\, \mathbf{k} \cdot (\overline{\rho \mathbf{u} \mathbf{u}})_\mathbf{k} \cdot \mathbf{p}_\mathbf{k}^* \tag{8}$$

$$= 2\mathrm{Im}\, \mathbf{k} \cdot \sum_{\mathbf{k}'} \left(\overline{(\rho \mathbf{u})_{\mathbf{k}'} \mathbf{u}_{\mathbf{k} - \mathbf{k}'}} \right) \cdot \mathbf{p}_\mathbf{k}^* \tag{9}$$

The spectral transfer function, spectral energy, and other scalar statistical quantities are symmetric with respect to an interchange of the x and y directions, but, because of the square box cross-section wire mesh pattern, is not rotationally symmetric (though they may become so at short wavelengths).

The spectral energy flux is the integral of the transfer function,

$$\Pi = \int_{|\mathbf{k}'| < |\mathbf{k}|} d\mathbf{k}' \mathcal{T}(\mathbf{k}') \quad . \tag{10}$$

In particular, this should be equal to the rate of decay of the integral of the power spectrum over lower wavenumbers, plus the correction from PdV work, i.e.,

$$\Pi = -\int_0^{k_\perp} dk_\perp' dE(k_\perp')/dt - 2\mathrm{Im}\int_{|\mathbf{k}'|<|\mathbf{k}|} d\mathbf{k}'\mathbf{k}' \cdot \mathbf{p}_{\mathrm{kk}'}\overline{\mathrm{P}}_{\mathbf{k}'} \quad . \tag{11}$$

where $E_{k_\perp} = \int d\hat{\mathbf{k}}_\perp k_\perp \mathcal{E}_{\mathbf{k}}$ is the energy per unit thickness shell in $k_x - k_y$ space and $\int d\hat{\mathbf{k}}_\perp$ denotes integration over the direction of $\mathbf{k}_\perp$. Since the integrated spectral decay term is, at any fixed time, an increasing function of $k_\perp$, then, if the PdV term were negligible and the spectrum decaying at all wavenumbers, the spectral flux would increase with $k_\perp$, approaching a constant only at wavenumbers large compared to that at the transition between the energy-containing and inertial ranges.

In Fig. 6, we plot the spectral flux versus wavenumber for the $2048^2 \times 1920$ simulation at the final time ($t = 9$). A striking feature is the large flux out to the 9th harmonic (just below the shorter initial perturbation), followed by a rapid falloff. It is evident that spectral transfer is contributing to a filling in of the scales between the two initial wavelengths, at the expense of the longer one. Another significant feature is that the flux is everywhere positive, indicative of forward transfer; we will see later that this is not the case for early times, low resolution, or two-dimensional simulations. Is there anything in this diagnostic suggestive of an inertial range? The spectral flux is fairly constant beyond about the 30th harmonic (wavenumber 200), perhaps suggestive of an inertial range; but note that the integral definition we have used will produce a near-constant flux even in the dissipation range, so long as the fluctuating fields are significanlty weak there.

We note that the "correction" from PdV work, the last term in Eq. (11), is not small; it is in fact an order of magnitude larger than Π even at the final time of the simulation. However Π is the only term that can account for the transfer of energy between wavenumbers. We will return to a discussion of the spectral flux in conjunction with the "transition to turbulence", below.

Another issue governing the spectral shape is isotropy. In addition to the previously noted absence of rotation symmetry in the $x - y$ plane, the direction of shock propagation (z) is different than the other two coordinate directions, and the initial growth of structures on the scale of the initial perturbations is preferentially in this direction. A convenient way

to quantify this effect, and its dependence on the perturbation scale length, is to plot the second-order structure function

$$\mathcal{S}_i(\delta x_j) = \langle(u_i(\mathbf{x} + \mathbf{e}_j \delta x_j/2) - u_i(\mathbf{x} - \mathbf{e}_j \delta x_j/2))^2\rangle \quad , \tag{12}$$

where the average is over the position $\mathbf{x}$ and $\mathbf{e}_j$ is a unit vector in the j direction ($j = x, y, z$). For isotropic turbulence, and more generally for any "cubically symmetric" turbulence (independent of arbitrary interchange of the x, y, z directions), there would be two independent components; all of the diagonal (longitudinal) components would equal one another, as would all of the off-diagonal (transverse) components. As can be seen in Fig. 7, this is the case for relatively short wavelengths: about a factor of 30 up from the short-wavelength cutoff for the diagonal components, and about a factor of ten for the off-diagonal components. In particular, as the scale length is increased, the stream-wise on-diagonal component becomes progressively larger than the other two, corresponding to the preference for structures extended in, and/or velocities largest in, the streamwise direction. The asymmetry in the off-diagonal components may help sort out these two possibilities, since at the longest scales there is a strong asymmetry in favor of components containing u_z, and a weak asymmetry between the remaining components which favors components that involve streamwise separation.

Returning now to the local-in-z spectra plotted in Fig. 5, inspection indicates that the mid-range wavenumber spectrum is falling off more slowly than $k^{-5/3}$ [the rate we would expect for the inertial range of homogeneous, isotropic (Kolmogorov) turbulence]. We find that a semi-compensated spectrum $k_\perp^{5/3} E(k_\perp)$ shows a distinct power-law rise with $k_\perp$ over this range; a good fit is provided instead by $k_\perp^{-5/4}$, as indicated by the compensated spectrum $k_\perp^{5/4} E(k_\perp)$ plotted in Fig. 8.

A recent analysis [23] suggests that for Richtmyer-Meshkov turbulence the spectrum should decay as $k_\perp^{-3/2}$, which is closer, but still not as shallow a fall-off, as our data. In this analysis, Kolmogorov phenomenology is extended to form a general framework to incorporate the case with an external time scale (Zhou, 2001). Here "external time scale" is

used to represent any time scale other than the nonlinear eddy turnover time. The key of the analysis is to estimate the time scale for decay of transfer function correlations, τ_T, which is responsible for inducing turbulent spectral transfer. The external time scale associated with Richtmyer-Meshkov intability is $\tau_{RM} = (kAV)^{-1}$, where k is the wave number of the initial perturbation, A is the Atwood number, and V is the change in the velocity produced by the impulsive acceleration. When τ_{RM} is dominant, one identifies $\tau_T = \tau_{RM}$. Dimensional reasoning gives

$$E(k, z) = C_{RM}[AV\epsilon(z)]^{1/2}k^{-3/2},$$

where C_{RM} is a constant. This theoretical prediction is for the mildly nonlinear regime; for later times, a transition to the steeper Kolmogorov spectrum is expected.

Our results are less steep than either a Kolmogorov spectrum or that of Ref. [23]. A referee has kindly pointed out that the difference between the computations and the Kolmogorov or Zhou decays is possibly due to the fact that, within the period that was computed, the present results comprise two dominant length scales. In contrast, both the Kolmogorov and Zhou results assume a smooth spectrum from the large to the small scales. We note two additional effects that can contribute to a flatter spectrum: (1) the presence of an additional timescale, namely that of the decay of the energy-containing scales, not well separated from the timescale for spectral transfer (used to derive the Kolmogorov spectrum) and that associated with shock passage (used for the Richtmyer-Meshkov analysis of Ref. [23]); (2) advection of near-step-wise discontinuities in velocity and density by the instability; and (3) growth of the spectral flux with $k_\perp$ resulting from the contribution of a larger number of decaying modes, as discussed following Eq. (11).

We consider first effect (1). Turbulent energy in the inertial range gets there by a finitely fast cascade rate from the inertial range. Turbulence deep in the inertial range will have originated from the energy-containing range longer ago than turbulence in the near (close to energy-containing) inertial range, at a time when the energy-containing turbulence was stronger. This should lead to a spectrum that falls more slowly than that which would

cascade from a steady energy-containing range. Mathematically, Ref. [23] notes that the spectrum is of the form

$$E(k) = C\varepsilon^p k^{-q} \tag{13}$$

where for Richtmyer-Meshkov instability, $p = 1/2$ and $q = 3/2$, whereas for Kolmogorov (homogeneous, isotropic) turbulence, $p = 2/3, q = 5/3$. Usually it is argued that the dissipation rate ε is constant. However, under the present circumstance, we may expect ε to be a decaying function of time, decaying with the available energy to transfer and dissipate. More specifically, we expect that ε would be constant for a packet of turbulent energy as it makes its way through the spectrum, but that at fixed time, ε at any k will depend on the value of ε in the energy containing range ($k \sim k_0$) at some time $t - \Delta t$ in the past, *i.e.*, $\varepsilon(k, t) = \varepsilon(k_0, t - \Delta t)$. For example, if the time τ for a perturbation to propagate a distance Δk scales as $\tau(k) \sim K(\Delta k)^m$, (where for example m would be $1/2$ for a diffusive model in k space), and if the spectral energy is decaying as $(1 + \alpha t)^n$, then we would expect that

$$\varepsilon(k_\perp, t) \sim \varepsilon(k_0, t - Kk_\perp{}^m) = \varepsilon_0(t = 0)\left[1 + \alpha(t_0 - Kk_\perp{}^m)\right]^{-n} \tag{14}$$

and hence $E(k_\perp)$ decays more slowly.

Effect (2) arises from for example advection of the density contrast across the contact discontinuity, by the Richtmyer-Meshkov instability dynamics. For a slice through the bubbles and spikes of an initial monochromatic disturbance, the density changes as a two-dimensional square wave, smoothed only be the resolution of the contact discontinuity. Since the Fourier transform of a two-dimensional square wave is $1/k$, we would expect to see such a component in the spectra. A similar phenomenon occurs even in the velocity field, as the passage of the shock sets up tangential velocity discontinuities across the perturbed interface. (At later times, as the bubbles and spikes develop secondary instabilities, the square-wave pattern becomes blurred, and this spectral feature would be less distinct.)

A comparison of the volume renderings at $t = 9$, and even more dramatically, a comparison of renderings of vertical slices of the volume at various resolutions, shown in Fig. 9,

indicates a qualitatively different behavior at the higher resolutions (1024^3 and $2048^2 \times 1920$) than at the lower ones (192^3, 384^3 and 512^3). The lower resolution runs are characterized by well-defined structures which become sharper with resolution; the higher-resolution simulations show abundant fine-scale features and "look turbulent". This is suggestive of a transition to turbulence with increasing Reynolds number, as suggested by Dimotakis [16], though in the present case the finiteness of the Reynolds number is due to numerical dissipation. The transition is thought to arise from the development of sufficient separation between energy-containing and dissipation-scale wavenumbers that a true forward energy cascade can develop.

Dimotakis indicates that the transition should occur for a macroscale Reynolds number of order 10^4. Hence we derive an approximate Reynolds number for our simulations, as follows: We take the integral scale length L_{int} to be the transverse $(x-y)$ correlation length,

$$L_{\text{int}} = \frac{\sum_i \int dx dx' dy \, (u_i(x,y)u_i(x-x',y))}{\sum_i \int dx dy \, (u_i(x,y))^2}$$
$$= \frac{3\pi}{4} \frac{\int dk_\perp k_\perp^{-1} E(k_\perp)}{\int dk_\perp E(k_\perp)} \tag{15}$$

where the second form is presented in Ref. [24]. Following Dimotakis, [16], we take the Kolmogorov scale $k_{\text{kol}} \equiv 2\pi/L_{\text{kol}}$ to be $50k_\nu$, where the dissipation scale k_ν is defined to be the value of $k_\perp$ at which the spectrum begins to drop below the extrapolation of the inertial range; then, we take the (numerical) Reynolds number Re to be

$$\text{Re} = \left(\frac{L_{\text{int}}}{L_{\text{kol}}}\right)^{4/3} \tag{16}$$

Using this defintion, we obtain Re = 1700, 4700, and 8200 for, respectively, the 512^3, 1024^3 and $2048^2 \times 1920$ simulations. Thus the change in character of the turbulence is roughly consistent with Dimotakis's criterion. Whether there is a fairly abrupt transition or a smooth change as the resolution is increased from 512^3 to 1024^3 is not settled; additional simulations at intermediate resolutions would be required.

Another possible indicator of the turbulence transition is the spectral flux Π defined by Eq. (10). We note from Fig. 6 that, at the final time of the $2048^2 \times 1920$ simulation,

its value at large wavenumber (above the energy-containing range) is positive, indicating forward transfer of wave energy. The corresponding plot for 1024^3 resolution (shown in the next section; see Fig. 13) shown, is qualitatively similar, again with positive Π at high k. The volume renderings of these simulations look qualitatively similar, namely turbulent. In contrast, as shown in Fig. 10, the large-wavenumber value is *negative* at lower resolution (512^3) and also for the $2048^2 \times 1920$ simulation at an early time ($t = 2$); in both of those at which the volume rendering looks non-turbulent. Thus it seems that the sign of Π is an indicator of forward cascade to a turbulent state. A corroborating piece of evidence, the negativity of Π at high k for a two-dimensional high-resolution simulation, will be discussed in the next section.

The turbulence transition criterion might be described in a somewhat different way, as follows. In three-dimensional turbulence simulations [25] and experiments [26], there has been observed a "bottleneck" in the spectra, over a factor of about 4 in wavenumber extending downward from the beginning of the dissipation range. This bottleneck is thought to be due to the inhibition of forward cascade as a result of suppression of modes in the dissipation range that would otherwise be involved in triad mode couplings [27]. The result is an excess of spectral energy in the upper end of the inertial range. There may be a suggestion of such a bump in Fig. 8. For a turbulent cascade to proceed, one needs a finite range, presumably at least a factor of 2–4, of uninhibited inertial range. This then translates to a minimum separation of 8–16 between the energy-containing and dissipation ranges, which is consistent with the transition we observe.

V. 2-D VS. 3-D DYNAMICS

As discussed in the review article by Kraichnan and Montgomery (Two-dimensional turbulence, Rep. Prog. Phys. vol. 43, p.547, (1980)), "Two dimensional turbulence has the special distinction that it is nowhere realised in nature or the laboratory but only in computer simulations. Its importance is two-fold: first, it is idealises geophysical phenomena in

the atmosphere, oceans, and magnetosphere and provides a starting point for modeling these phenomena; second, that it presents a bizarre and instructive statistic mechanics. Phenomena characteristic of two-dimensional turbulence also play essential roles in the confinement of thermonuclear plasmas and in superfluid and superconductive behaviour of thin films". As a very recent example, Schorghofer and Gille [28] found that simple forced two-dimensional turbulence simulations agree with upper ocean observations (data from TOPEX satellite altimeter measurements) with regard to probability density functions and conditional averages of velocity gradients.

It is well-known that two-dimensional and three-dimensional turbulence have a fundamental difference, in that two-dimensional turbulence can exhibit a dual cascade, with energy inversely cascading to longer wavelengths while enstrophy forward-cascades. In contrast, in three dimensions there can only be a forward cascade. Hence one would expect the structure of the mixing layer to be quite different in two and three dimensions. To observe this distinction in simulations, one must have sufficient resolution to allow a significant separation between energy-containing and dissipation scales, as noted in the preceding section. With the high resolution in three dimensions now available, such an examination is feasible.

In Fig. 11, we show a rendering of the entropy field for a 1024^2 two-dimensional simulation and for a vertical slice of the 1024^3 simulation. The contrast is evident: a predominance of sizeable structures with sharp edges in the two-dimensional results, versus predominantly fine-scale structure in the slice of the three-dimensional simulation.

As one might expect, the two-dimensional and three-dimensional cases differ substantially in their spectra, as shown in Fig. 12. The 3-D case shows a Kolmogorov-like (though less steep) inertial range as discussed earlier, while the 2-D case has a much steeper spectrum between the energy-containing and inertial ranges, k_x^{-p}, where p is found to be in the range 2.8–4.3 (depending on the wavelength range fitted; all are about equally good fits). This is as one would expect for a two-dimensional inverse cascade process. For the fit and fitting range shown in the figure, $p = 4.3$.

Another indication of the difference is provided in Fig. 13, where the spectral flux is

plotted for the 1024^2 two-dimensional and 1024^3 3-dimensional cases. We see that the high-k value is negative for the former case and positive for the latter, consistent with the dominance of inverse cascade dynamics in two dimensions and forward cascade in three dimensions, and consistent, as noted in the previous section, with a transition to turbulence in 3-D, but not in 2-D.

VI. TWO-SCALE INTERACTIONS

In order to assess the effect of having two disparate scales of perturbations present, we have compared the full three-dimensional simulation to a smaller one which follows only a single bubble and spike. The smaller one has enough grid points to represent the single bubble and spike with as much resolution as the comparable portion of the full simulation.

A rendering of the entropy from a vertical slice at the final time are plotted in Fig. 14. The single-bubble simulation, replicated 20 times in each of the transverse (to the shock propagation) directions, would represent the result of an experiment with only the short wavelength (wire mesh spacing) perturbation and no noise to break the perfect periodicity. If we imagine this construction and compare to the full two-scale simulation, we see that the presence of the long-wavelength perturbation leads to a break-up of most of the wire-spacing-scale bubbles and spikes; only the ones closest to the middle of the long-wavelength spike survive. Examining renderings of sub-volumes of the full simulation shows a circular ring around the center of the long-wavelength spike, with a diameter of about five wire-mesh spacings, within which the wire-spacing-scale bubbles and spikes survive. Most of the mixing region is thus filled with fine-scale turbulent features.

There are several possible interpretations of these results. One is that there is more vorticity deposition on the sides of the large-scale spike than at its peak. This is certainly true of the large-scale feature by itself. But for the combination of two scales, there is also an effect: while $\nabla P \times \nabla \rho$ passes through zero for each small-scale bubble, it does so asymmetrically on the sides of the long-wavelength structure; the extrema and the average of the

magnitude over the short wavelength is larger on the sides than at the extrema of the long-wavelength structure. An expression for the circulation deposition (integral of the vorticity deposition across the contact discontinuity) per unit length has been derived by Samtaney, Ray and Zabusky [29], Eq. (2.24) of their paper. We have evaluated this expression for our initial perturbation and display the results for a slice in the stream-wize direction that passes through the middle of the simulation volume in Fig. 15. We notice, as expected, that the circulation deposition is oscillatory on the scale of the short-wavelength perturbation, and that the magnitude is largest on the sides of the long-wavelength perturbation. There is, however, no obvious difference between the peak magnitude or average around the maximum and minimum of the long-wavelength perturbation.

Hence the variation in circulation deposition contributes to the more complete breakup of the bubbles and spike on the sides of the large-scale perturbation, but cannot account for the apparent asymmetry between the long-wavelength bubble and spike with regard to survival of the short-scale bubbles and spikes. One possible explanation for the asymmetry is that the fine-scale spikes grow in a direction close to the local normal to the long-wavelength perturbation rather than perpendicular to the unperturbed shock propagation direction (see sketch in Fig. 16, and simulation results in Figs. 9 and 14). Hence the fine-scale spikes grow apart from one another (i.e. are further apart at their tips than the midpoints of their bases) about the large-scale spike peak, whereas the reverse is true about the peak of the large-scale bubble. (Also, the midpoints of the bases might be expected to be further apart near the large-scale spike than near the large-scale bubble, as the former grows faster than the latter. But this effect, if present,is small.) The small-scale spikes may as a result have less interaction with one another and hence survive better.

VII. TOWARD A SUB-GRID-SCALE MODEL

A major challenge facing the hydrodynamics community is to develop sub-grid scale models that capture the fine-scale effects for use in large-eddy simulations (LES). A successful

22

model must be able to relate the effect of sub-grid-scale terms to resolved-scale quantities. There has been very little work deriving such models for Ricthmyer-Meshkov turbulence.

We can make use of the high resolutions now available to test candidate models. In particular, here we construct the sub-grid scale stress, and its constituent components (Reynolds, Leonard, and cross), and determine their correlation with various macroscopic quantities.

We can think of a numerical simulation as an attempt to follow the equations of motion of the large scale component of a flow. This large scale component might be expressed as either the values of the fluid quantities on a given computational mesh or by a finite series of modes. Our approach is to take the results of a well resolved numerical simulation and decompose the flow in to two components (resolved and unresolved) in terms of a spatial filter which is much broader that the original computational mesh resolution. For the present discussion we choose a Gaussian filter. For field, Q, and filter wavenumber, k_f, we express the filtered, or resolved, field as

$$\bar{Q}(x) = \frac{1}{N} \int e^{-(k_f(x-x_1))^2} Q(x_1) d^3 x_1 \quad , \tag{17}$$

where

$$N = \int e^{-(k_f x)^2} d^3 x \quad . \tag{18}$$

The original field Q is written as the local sum of its filtered and fluctuating components

$$Q(x,t) = \bar{Q}(x,t) + Q'(x,t) \tag{19}$$

We wish to assess the influence of the unresolved fields on the equations of motion of the resolved fields. In order to have relatively simple equations, we follow the custom for large-eddy simulation and choose as variables to diagnose, the density ρ, presure P, and velocity $\mathbf{v}$, with averages defined by Eq. (17) for ρ and P, but density-weighted (Favre) for velocity, $\tilde{\mathbf{v}} = \overline{\rho \mathbf{v}}/\bar{\rho}$.

With these decompositions, as is well-known, the continuity equation for the filtered fields is identical to the continuity equation for the raw fields, while the equation for the filtered velocity

$$\partial_t\left(\overline{\rho}\tilde{u}_i\right) + \partial_j(\overline{\rho}\tilde{u}_i\tilde{u}_j) = \partial_i\bar{P} + \partial_j\tau_{ij} \tag{20}$$

includes an additional term, the subgrid-scale stress

$$\tau_{ij} = \overline{\rho u_i u_j} - \bar{\rho}\tilde{u}_i\tilde{u}_j \tag{21}$$

In the following, we concentrate on an analysis of τ_{ij} in terms of its influence on the evolution of the kinetic energy of the filtered fields

$$K_f = \frac{1}{2}\bar{\rho}\tilde{u}^2 \tag{22}$$

Evolution of this component of the kinetic energy, which may be derived from the continuity and momentum equations, is given by

$$\partial_t K_f = \frac{1}{2}\tilde{u}_i\partial_j\left(\rho\tilde{u}_i\tilde{u}_j\right) + \frac{1}{2}\tilde{u}_i\rho\tilde{u}_i\partial_j(\tilde{u}_j) + \tilde{u}_i\partial_i\bar{P} + \tilde{u}_i\partial_j\tau_{ij} \quad . \tag{23}$$

The first three terms on the right hand side of this equation involve only resolved fields. The last term is the influence of the fluctuating part of the velocity field on the resolved kinetic energy. We split this last term into two pieces

$$\tilde{u}_i\partial_j\tau_{ij} = \partial_j(\tilde{u}_i\tau_{ij}) - \tau_{ij}\partial_j\tilde{u}_i \tag{24}$$

While $\tilde{u}_i\partial_j\tau_{ij}$ is not Galilean invariant, the term $(\partial_j\tilde{u}_i)\tau_{ij}$ is invariant under a velocity boost. The term $\partial_j(\tilde{u}_i\tau_{ij})$ is the effect on K_f of the kinetic energy flux $(\tilde{u}_i\tau_{ij})$ due to the SGS stresses: it only spatially redistributes kinetic energy of the resolved scale flow in the same way that stresses due to the resolved pressure field does. Hence, the term $\partial_j(\tilde{u}_i\tau_{ij})$ does not correspond to any forward or back transfer of energy between the resolved and unresolved components of the flow. We identify

$$\epsilon_f = -(\partial_j\tilde{u}_i)\tau_{ij}$$

as the contribution of the subgrid-scale stress to the energy flux from the resolved to the unresolved components of the flow. ϵ_f is a scalar function, defined locally in both space and

time, and depends on the SGS stresses. Hence, the equation above can be considered as one constraint equation on the six independent components of the subgrid-scale stress tensor τ_{ij}.

We examine the $2048^2 \times 1920$ Richtmyer-Meshkov simulation at time $t = 9$. We filter the flow with a Gaussian filter with a filter wavenumber $k_f = 16$, corresponding to a wavelength of $L/16$. Figure 17a shows a visualization of the sgs forward transfer, ϵ_f, in the entire simulation volume. Figure 17b shows the probability distribution function (pdf) of ϵ_f taken over the entire volume at time 9. Probability distribution functions shown in Figure 17, and thereafter, were computed by counting the number of zones which had values falling in bins linearly distributed across the range of the respective quantity. The counts in each bin were then normalized by the total number of counts and the bin size so that the resulting curve integrates to unity. Most of the volume is filled with regions of weak energy transfer (i.e., small values of ϵ_f) which are rendered transparent. Regions of strong transfer, with forward transfer shown in blue-green and inverse transfer shown in red-yellow, are seen to be entirely in the mixing layer. It is of interest to relate these regions of forward and inverse transfer with the geometry of the large scale flow.

We correlate ϵ_f with components of the rate of strain tensor of the resolved velocity field. The velocity gradient tensor $A_{ij} = \partial_i \tilde{u}_j$ may be decomposed

$$A_{ij} = \frac{1}{2}(R_{ij} + S_{D,ij} + S_{I,ij}) \tag{25}$$

into a rotational component

$$R_{ij} = A_{ij} - A_{ji} \quad , \tag{26}$$

a deviatoric component

$$S_{D,ij} = A_{ij} + A_{ji} - \frac{2}{3}\delta_{ij}A_{kk} \quad , \tag{27}$$

and a compressional component

$$S_{I,ij} = \frac{2}{3}\delta_{ij}A_{kk} \tag{28}$$

of the flow. We start by examining the rotational invariants of A_{ij} and of its components.

The modulus squared of R is the enstrophy. The pdf of enstrophy is shown in Fig. 18. The enstrophy of the filtered velocity, $\omega_f^2 = |\nabla \times \tilde{\mathbf{u}}|^2$, is strong in the mixing layer and is seen to be organized in vortex rings, or tightly curved vortex tubes. These rings correspond to the heads of the plumes seen in entropy. A cross correlation of the ω_f^2 and ϵ_f (see Fig. 19) shows little or no spatially local correlation between these two fields. This is expected from the standard argument that enstrophy corresponds to solid body rotation, which produces no deformation of local flow structures.

The compressional component of the flow, $S_{I,ij}$, is parameterized by $d_f \equiv \mathrm{Trace}(A_{ij}) = \nabla \cdot \tilde{\mathbf{v}}$. Figure 20 shows the pdf of d_f. Like ω_f^2 and ϵ_f, d_f is only large in the mixing layer. The cross correlation between d_f and ϵ_f (Fig. 21) shows a positive correlation with a large spread. This positive correlation is due to converging or diverging flow carrying structures through the filter plus pressure dilatation work.

The pdf for the modulus squared of the deviatoric component of the flow, $|S_D|^2$ is shown in 22. Again, it is large only in the mixing region. Figure 23 shows a strong correlation of large $|S_D|^2$ with large forward transfer, corresponding to $\epsilon_f << 0$. Standard sub-grid scale models of turbulence (such as the Smagorinsky and k-ϵ models) typically use a factor which scales with $|S_D|^2$ in the sgs dissipation. $|S_D|^2$ seems to be able to identify regions of strong forward transfer in this flow. The modulus squared of the deviatoric strain, $|S_D|^2$, is positive definite and can not distinguish between forward and inverse energy transfer. Even expressing the sgs stress purely as a function of S_D, such as

$$\tau_{ij} = \nu_{turb} |S_D| \, S_{D,ij} \quad , \tag{29}$$

being of the same form as the Navier-Stokes diffusion term, can only produce forward transfer. However, large forward transfer is always associated with a large modulus of S_D in this flow. This motivates the question of whether there is some other invariant of S_D which tracks both forward and inverse transfer.

While point by point there seems to be no correlation between ω_f^2 and ϵ_f, volume visual-

izations indicate a tendency for pairs of regions of positive and negative ϵ_f to straddle vortex rings in the filtered flow; see for example Fig. 17b. This is most clearly evident in the head of the central plume shown in the upper left corner of this figure. The only invariant of the rate of strain tensor with opposite signs on either side of a vortex ring is the determinant of S_D : ahead of a vortex ring (in the direction of propagation) S_D has two positive eigenvalues and one negative leading to $\text{Det}(S_D) < 0$; behind a vortex ring two eigenvalues are negative and one is positive leading to $\text{Det}(S_D) > 0$. Intriguingly, both ϵ_f and $\text{Det}(S_D)$ scale as $(\partial_i u_j)^3$.

A rate of energy transfer, such as ϵ_f, has units of

$$\text{(Energy Density)}/\text{(Time)} \sim \text{(Mass Density)}\text{(Velocity)}^3/\text{(Length)} \sim \lambda_f^2 \rho (\partial_i u_j)^3 \qquad (30)$$

Here, λ_f is a characteristic wavelength of the filter. Two invariants of A which scale as $(\partial_i \tilde{u}_j)^3$ include $\nabla \cdot \mathbf{v}|A|^2$ and $\text{Det}(S_D)$. So we construct two terms with units of ϵ_f

$$R_1 = \lambda_f^2 \bar{\rho} \text{Det}(S_D) \quad . \qquad (31)$$

and

$$R_2 = \lambda_f^2 \bar{\rho} \nabla \cdot \tilde{\mathbf{u}} |A|^2 \quad , \qquad (32)$$

The first term is motivated by the correlation between div(u) and ϵ_f seen in Fig. 21. A factor like $\bar{\rho} \lambda_f^2 |A|^2$ can be thought of as an estimate of the local energy on the scale of the filter, while $\nabla \cdot \tilde{\mathbf{v}}$ is the rate at which structures are carried across the filter by the compressibility of the flow. Comparison of visualizations of R_1 with those of ϵ_f indicate a fairly strong agreement both in regions of forward and inverse transfer. Figure 24 shows the cross correlation. Note the linear relation between $\lambda_f^2 \bar{\rho} \text{Det}(S_D)$ and ϵ_f for strong forward transfer. There is a kink at (0,0) with inverse transfer (i.e., positive values of ϵ_f) being positively and linearly related to R_1 but with a different slope.

Finally, we consider a fit of the form

$$\epsilon_f = A \lambda_f^2 \bar{\rho} (\text{Det}(S_D) + B \nabla \cdot \tilde{\mathbf{u}} |A|^2) = A (R_1 + B R_2) \quad . \qquad (33)$$

For the $2048^2 \times 1920$ data at time 9, with a filter width of $k_f = 16$, best fit values of the two unitless coefficients are $A = 0.032$ and $B = 2.0$. This fit is shown in Fig. 25. Note, this fit, which minimizes the mean square error

$$(\epsilon_f - A\lambda_f^2 \bar{\rho}(\text{Det}(S_D) + B\nabla \cdot \tilde{\mathbf{u}}|A|^2))^2 \tag{34}$$

also produces a common linear slope (i.e., $A = 0.032$) for both positive and negative values of ϵ_f. This same analysis was also performed for filter widths $k_f = 8/L$ and $k_f = 32/L$ with similar results, despite the proximity of the dissipation and energy containing scales. On a mesh where $\delta x = L/2048$, the dissipative effects are expected to span wavenumbers down to about $k = 64/L$. The energy containing scale spans wavenumbers up to $k = 10/L$ in this problem.

One possible reason for the agreement between $\text{Det}(S_D)$ and ϵ_f is that when $\text{Det}(S_D)$ is positive, only one eigenvalue of S_D is positive, which tends to align the vorticity field along the corresponding eigenvector direction. In these regions the flow tends to behave like a 2D flow with the associated inverse transfer of energy. When $\text{Det}(S_D)$ is negative, two eigenvalues of S_D are positive, vortex stretching can occur along any direction in the plane spanned by the corresponding eigenvectors, and forward transfer is enhanced.

VIII. SUMMARY

The simulations described in this paper lead to a number of conclusions:

Simulations such as these can reproduce the macroscopic mixing behavior of experiments. In particular the mixing layer widths from our simulation are in remarkably good agreement with the Vetter et al [4] experiments.

The two scales present in the initial perturbation interact. The presence of the long wavelength perturbation has a notable impact on the evolution of the short wavelength perturbations, destroying most of them, breaking them up into still-smaller structures. This is particularly evident on the sides of the long wavelength structures. One effective mechanism

of interaction is that, on the sides of the long-wavelength perturbation, the maximum angle between the gradients pressure and density is increased,thereby increasing the vorticity deposition, as found in Fig. 15. There is also an asymmetry in the survival of the short-wavelength features between the bubbles and spikes of the long-wavelength perturbation, with survival greatest around the peak of the long-wavelength spike. Our results suggest that this asymmetry is associated with the tendency of short-wavelength spikes to "grow apart" around the long-wavelength spike, versus growing together around the long-wavelength bubble.

The well-known differences between 2-D and 3-D fluid dynamics is dramatically illustrated in our simulation visualizations. The 2-D simulations are characterized by coalescence into structures comparable to or larger than the initial short-wavelength (mesh) scale, while the 3-D simulations evolve toward fine scales. This is consistent with the predominance of inverse and forward cascades, respectively.

Comparison of visualizations at various resolutions suggests a transition from unstable to turbulent flow as the resolution is increased, consistent with arguments by Dimotakis [16] that such a transition should occur with increasing Reynolds number. In this case the Reynolds number is that attached to numerical dissipation. More generally, they provide a warning about resolution requirements in three-dimensional hydrodynamics simulations: with inadequate resolution, qualitatively wrong conclusions can be drawn about the structure of the fluid flows. The resolution required is surely problem-dependent (beyond a simple Reynolds number dependence). The example studied here indicates that billion-zone simulatons may be required even for relatively simple flows.

As the resolution is increased, a kind of inertial range is evident; this is not a classic Kolmogorov inertial range as the spectrum is not continuously driven. The spectrum has a power-law region, but with a weaker wavenumber dependence than Kolmogorov scaling, about $k^{-5/4}$. The spectral flux, defined as the integral over magnitude of wavenumber of the nonlinear transfer function, is approximately constant in this region, which is consistent with, but not necessarily indicative of, an inertial range.

Analysis of structure functions at the end of the simulation indicates the persistence of

structures with velocities largest in the stream-wise direction, and a weaker indication of predominance of structures spatially extended in the streamwise direction.

Finally, our analysis of quantities smaller and larger than a post-processing filter indicate that there is a significant correlation between the (sub-grid-scale) nonlinear stress and the (resolved) rate-of-strain tensor. This suggests that a Smagorinsky-like model is a good candidate for a large-eddy-simulation (LES) model.

IX. ACKNOWLEDGMENTS

REFERENCES

[1] R. D. Richtmyer, "Taylor instability in shock acceleration of compressible fluids," Pure Appl. Math **13** 297 (1960).

[2] E. E. Meshkov, "Instability of the interface of two gases accelerated by a shock wave," Sov. Fluid Dyn. **4**, 101 (1969).

[3] M. Brouillette, and B. Sturtevant, "Experiments on the Richtmyer-Meshkov instability: single-scale perturbations on a continuous interface", J. Fluid Mech., **263**, 271 (1994).

[4] M. Vetter and B. Sturtevant, "Experiments on the Richtmyer-Meshkov instabilities of an air/SF6 interface", Shock Waves **4**, 247 (1995).

[5] L.D. Cloutman and M.F. Wehner, "Numerical simulation of Richtmyer-Meshkov instabilities," Phys. Fluids A **4**, 1821 (1992).

[6] R.H. Cohen, W.P. Dannevik, A.M. Dimits, D.E. Eliason, A.A. Mirin, D.H. Porter, O. Schilling, and P.R. Woodward, "Three dimensional high-resolution simulations of the Richtmyer-Meshkov mixing and shock turbulence interaction," in Proceeding of the 6th International Workshop on the Physics of Compressible Turbulent Mixing, Marseille, France, 18-21 June 1997, pp. 128–133.

[7] N. Cowperthwaite, M. Philpott, A.V. Smith, A.D. Smith, and D. Youngs, "Shock-induced instability experiments on gas interfaces featuring a single discrete perturbation," in Proceedings of the 5th International Workshop on Compressible Turbulent Mixing, Stony Brook, NY, 18–21 July 1995, pp. 147–157.

[8] V.V. Demchenko, "Analytical and numerical study of sequential contact surface turbulization in Richtmyer-Meshkov instability," in Proceedings of the 5th International Workshop on Compressible Turbulent Mixing, Stony Brook, NY, 18–21 July 1995, pp. 331–337

[9] I.G. Lebo, V.B. Rozanov, V.F. Tishkin, V.V. Nikishin, I.V. Popov, and A.P. Favorsky,

"Numerical simulation of Richtmyer-Meshkov instability," in Proceedings of the 5th International Workshop on Compressible Turbulent Mixing, Stony Brook, NY, 18–21 July 1995, pp. 346–356

[10] X.L. Li and Q. Zhang, "A comparative numerical study of the Richtmyer-Meshkov instability with nonlinear analysis in two and three dimensions," Phys. Fluids **9** 3069 (1997).

[11] D.I. Meiron, R. Samtaney, D.I. Pullin, and B. Kosović, "Contributions to the computation of compresssible turbulence," AIAA Paper 99-3646 (1999).

[12] D.L. Youngs, "Numerical simulation of mixing by Rayleigh-Taylor and Richtmyer-Meshkov instabilities," Laser Part. Beams **14**, 725 (1994).

[13] O.M. Belotserkovskii, V.V. Demchenko and A.M. Oparin, "2D and 3D Comparative Study of the Richtmyer-Meshkov Instability Development", in Proceeding of the 6th International Workshop on the Physics of Compressible Turbulent Mixing, Marseille, France, 18-21 June 1997, pp. 86-89.

[14] I.G. Lebo, V.B. Rozanov, V.F. Tishkin, and V.V. Nikishin, "Computational Modeling of the Hydrodynamic Instability Development in Shock Tube and Laser Driven Experiments", in Proceeding of the 6th International Workshop on the Physics of Compressible Turbulent Mixing, Marseille, France, 18-21 June 1997, pp. 312-317,

[15] V.V. Nikishin, V.F. Tishkin, N.V. Zmitrenko, I.G. Lebo, and V.B. Rozanov, "Numerical Simulations of Nonlinear and Transitional Stages of Richtmyer-Meshkov and Rayleigh-Taylor Instabilities", in Proceeding of the 6th International Workshop on the Physics of Compressible Turbulent Mixing, Marseille, France, 18-21 June 1997, pp. 381-387.

[16] P.E. Dimotakis, "The mixing transition in turbulent flows", J. Fluid Mech **409**, 69 (2000).

[17] S.   E.   Anderson   and   P.   R.   Woodward,   "The   sPPM

benchmark code", http://www.lcse.umn.edu/research, Laboratory for Computational Science and Engineering, U. Minnesota (1995).

[18] P. Colella and P. R. Woodward, "The piecewise-parabolic method for gas dynamical simulations", J. Comp. Phys. **54** 174 (1984).

[19] I. V.Sytine, D. H. Porter, P. R. Woodward, S. H. Hodson, and Karl-Heinz Winkler, "Convergence Tests for Piecewise Parabolic Method and Navier-Stokes Solutions for Homogeneous Compressible Turbulence," J. Computational Physics, Vol. 158, pp. 225-238 (2000).

[20] D. H. Porter, and P. R., Woodward, 2000, "3-D Simulations of Turbulent Compressible Convection" Astrophys. J. Supplement, **127**, 159, March 2000. http://www.journals.uchicago.edu/ApJ/journal/contents/ApJS/v127n1.html

[21] D. H. Porter and P. R. Woodward, "High Resolution Simulations of Compressible Convection using the Piecewise- Parabolic Method", Astrophys. J. Supplement **93**, 309 (July 1994)

[22] D. H. Porter, A. Pouquet, and P. R. Woodward, "A Numerical Study of Supersonic Homogeneous Turbulence", J. Theor. Comp. Fluid Dyn. **4**, 13 (1992).

[23] Y. Zhou, "A scaling analysis of turbulent flows driven by Rayleigh-Taylor and Richtmyer-Meshkov instabilities," Phys. Fluids **13**, 538 (2001).

[24] J. Jimenez, A. A. Wray, P. G. Saffman, and R. S. Rogallo, "Structure of intense vorticity in isotropic turbulence", J. Fluid Mech. **255**, 65 (1993).

[25] D. Lohse and A. Muller-Groeling, "Bottleneck effects in turbulence: Scaling phenomena in r verse p space", Phys.R̃ev.L̃ett.~**74**, 1747 (1995).

[26] S. G. Saddoughi and S. V. Veeravalli, "Local isotropy in turbulent boundary layers at high Reynolds number", J. Fluid Mech.~**268**, 333 (1994).

[27] G. Falkovich, "Bottleneck phenomenon in developed turbulence", Phys. Fluids **6** 1411 (1994).

[28] Schorghofer and Gille, "Statistics of velocity gradients in two-dimensional Navier-Stokes and ocean turbulence", Phys. Rev. E, **65**, 026307 (2002)

[29] R. Samtaney, J. Ray and N. J. Zabusky, "Baroclinic circulation generation on shock accelerated slow/fast gas interfaces", Phys. Fluids **10**, 1217 (1998).

FIGURES

FIG. 1. Schematic representation of Vetter-Sturtevant shock-tube experiment

FIG. 2. Volume renderings of the simulation at successive times

FIG. 3. Computed and experimental mixing-layer widths. The squares denote the experimental data normalized to the transverse dimension of the shock tube; the "x"'s denote the data normalized to the wire spacing

FIG. 4. Computed mixing-layer width with box-size perturbation subtracted out.

FIG. 5. Kinetic energy power spectrum for various resolutions, averaged over four transverse (fixed-z) slices through the mixing layer

FIG. 6. Spectral kinetic energy flux versus wavenumber for $2048^2 \times 1920$ simulation at the final time

FIG. 7. Structure functions for components of velocity (a) longitudinal to and (b) transverse to the spatial separation. u_x and u_y refer to the components of velocity in the plane of the mixing layer, while u_z refers to the component of velocity normal to the mixing layer. Similarly, dx, dy and dz refer to structure functions in each of these three directions, respectively.

FIG. 8. Compensated power spectrum vs. transverse wavenumber

FIG. 9. Vertical slices of entropy at various resolutions

FIG. 10. Spectral kinetic energy flux versus wavenumber for (a) the $2048^2 \times 1920$ simulation at $t = 2$, and (b) the 512^3 simulation at $t = 9$

FIG. 11. Entropy from two-dimensional simulation vs. slice of 3-D simulation

FIG. 12. Kinetic energy spectrum from two-dimensional simulation vs. slice of 3-D simulation

FIG. 13. Spectral flux in two-dimensional simulation (a) vs. 3-D simulation (b), both for 1024^3 resolution at $t = 9$

FIG. 14. Comparison of (a) a slice through the midplane of the full two-scale simulation with (b) a slice of a single-wavelength (fine-scale) perturbation, plotted at the same scale. The The solid black line shows the z-location of the spike and the dashed black line shows the z-location of the bubble.

FIG. 15. Normalized circulation deposition vs. position along interface in slice, from Samtaney *et al.* formula

FIG. 16. Sketch of small-scale spikes on large-scale bubble and spike. Arrows depict direction of growth of small-scale bubbles

FIG. 17. Energy flux across a spatial filter due to SGS stresses, ϵ_f, shown volume rendered (a), and the corresponding PDF (b). Negative values of ϵ_f correspond to forward transfer of energy and are colored yellow and green in the volume rendering.

FIG. 18. Probability distribution function of enstrophy

FIG. 19. Cross-correlation of enstrophy and ϵ_f

FIG. 20. Probability distribution function of $\nabla \cdot \mathbf{v}$

FIG. 21. Cross-correlation of $\nabla \cdot \mathbf{v}$, ϵ_f

FIG. 22. Probability distribution function of $|S_D|^2$

FIG. 23. Cross-correlation of $|S_D|^2, \epsilon_f$

FIG. 24. Cross-correlation of R_1, ϵ_f

FIG. 25. Cross-correlation of $R_1 + BR_2, \epsilon_f$