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Nearly Discontinuous Chaotic Mixing*

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A new scientific approach is presented for a broad class of chaotic problems involving a high degree of mixing over rapid time scales. Rayleigh-Taylor and Richtmyer-Meshkov unstable flows are typical of such problems. Microscopic mixing properties such as chemical reaction rates for turbulent mixtures can be obtained with feasible grid resolution. The essential dependence of (some) fluid mixing observables on transport phenomena is observed. This dependence includes numerical as well as physical transport and it includes laminar as well as turbulent transport. A new approach to the mathematical theory for the underlying equations is suggested.

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Turbulent mixing is an important but unfinished subject. Acceleration driven mixing has been the subject of intense investigation for 50 years [1, 2]. The rarity of simulation-experiment [3–5] or simulation-theory comparisons [6, 7] is a measure of the unsolved nature of the problem.

In a controlled grid scaling study, over the range of grid resolution practical for today's computers, we observed a fundamental obstacle to computation: For scale invariant physics, with no physical transport in the fluid equations, we observed an interface between two phases in a chaotic mixture which scales as Δx^{-1} over the range of grids practical for 3D simulations today. Since, for any numerical code, an elementary error estimate (L_1 norm) is $\Delta x \times$ [Interface length or area], we conclude that the overall error is $\mathcal{O}(1)$; in other words, the error is not convergent [8] over this range of grid refinement.

A nonconvergent error, or a solution that converges to a code dependent limit is a very major problem for the goal of predictive simulation. In fact, related studies did reveal such code dependencies in apparently converged solutions for an identical problem [8, 9]. A related discrepancy between atomistic and continuum methods has been noted [10, 11]. In [10, 11], the atomistic simulations are in agreement with experiment, while the comparison continuum ones are not. To complement and add to the discussion in [10, 11], we observe the that the continuum simulations [3, 4] and theory [6, 7], are in agreement with both experiment and the atomistic simulations. Thus we regard the atomistic simulations as confirmation of our earlier work [3, 4, 6, 7].

Here we report a resolution to this problem, and a new approach to the science and mathematics of turbulent mixing.

For interface dominated problems, with fluid state variables discontinuous across the interface, the physics is ill posed. Regularization of the problem by nonzero transport is required to achieve a well posed problem. In the absence of regularization in a simulation, or when the physical regularization is very weak, the numerical transport features of the simulation dominate, and dictate the selection of a solution from among the possible nonunique solutions of the equations (when considered in a scale invariant, or transport-free). This situation is routinely encountered, as many problems have low levels of physical transport, and for practical grids, have more numerical transport than physical.

Methods have been developed for the resolution of subgrid physics, which is fundamentally what is in play here, and dynamic procedures determine of all model parameters, so that the these methods are parameter free [12, 13]. While these methods solve, in principle, the problems mentioned above, they are normally applied to problems far less dynamic than those considered here, and which have smoother and more highly diffusive solutions.

From a numerical perspective, our approach is to apply the subgrid models well outside of their normal sphere of applicability, to problems with small levels of physical transport and solutions with steep gradients and near discontinuities.

Why does the steepness of the gradient matter? It is easiest to answer this question in a comparison of physical and computational length scales. In turbulent mixing, the length scale of the smallest vortex is called the Kolmogorov scale. Resolution of the Kolmogorov scale is required for a fully resolved simulation of turbulence, refereed to as direct numerical simulation. In the case of small levels of mass diffusivity (typical of liquids), the ratio of the viscosity to the mass diffusivity, known as the Schmidt number, is large, for example $Sc \sim \mathcal{O}(10^3)$. The length scale associated with the mass diffusivity is known as the Batchelor scale. To resolve this scale requires additional mesh refinement of a factor of $\sqrt{Sc}$ in each spatial

dimension and time, with an increase of computational cost by a factor of Sc^2.

The difference between one and five mesh blocks to describe a rapid transition (approximate interface) as a blended boundary between two fluids is a factor of $5^4 = 625$ in computational cost. The difference between resolving the Batchelor scale or not is a factor of $Sc^2 = calO10^6$ in computational cost. The first is basically the difference between a teraflop computer and a petaflop computer. It is the difference between a \$10,000 computer and a \$6,000,000 computer, between achieving an answer, and getting the answer five years later. The second is the difference between getting the answer or not (ever). The resolution required and the length scales to be resolved are not simply arbitrary constants. They are fundamental measures of feasibility for the science of mixing.

To test and develop these ideas, we examined a previously considered [14] 2D circular Richtmyer-Meshkov instability problem. We added terms describing physical transport and subgrid modeling terms describing turbulent transport to the equations. Not only does the solution depend on the values of the physical transport selected, but for a fixed selection of turbulent transport values (typical of fluid-fluid transport), we found convergence of both macroscopic and microscopic fluid observables. We include a chemical reaction rate with strongly nonlinear dependence on temperature as an example of a microscopic variable that shows convergence. For some of the cases considered (variation of Reynolds number and of transport parameters), we observed convergence of the reaction rate. In other cases, when the turbulent fluctuations in the chemical reaction rate were not removed by the spatial average employed, we observed small variation in mesh dependence about the finest grid value, but lack of convergence. A further ensemble average confirmed this picture.

We employ a range of meshes, for a variety of Reynolds numbers. The most refined of these resolve the Kolmogorov scale (DNS simulations). The others do not, and are thus known as Large Eddy Simulations (LES). No attempt was made to resolve the Batchelor scale for liquid mixing. We classify observables as macroscopic or microscopic. The former pertain to the large scale features of the flow. For the problem under study, it turns out that the macroscopic observables are essentially all convergent, and their limits are essentially independent of the specifics of transport, numerical or physical, laminar or turbulent. The microscopic observables, such as the temperature and the species concentrations are sensitive, however. Thus we study these variables. Even after a spatial average (over the mixing zone), we found some statistical fluctuations in the joint probability distributions for these variables. To regularize the observables under study, while retaining a vital scientific focus, we examined the chemical reaction rate for a temperature dependent reaction, with an activation temperature in the middle of the range of observed temperatures. Thus we had a meaningful, but difficult and nonlinear observable. We still found statistical fluctuations, but low enough to conclude that the chemical rate was mesh convergent, and for Reynolds numbers low enough to allow DNS on the fine grids, we found that the LES (coarse grid simulation) was verified, in the sense that it agreed with the DNS result. In this sense the strategy has been vindicated.

We examine the probability distribution functions for temperature. We form an ensemble of fixed-temperature cells, and compute the second moment of the concentrations in this ensemble. This second moment of the concentration f (or the expectation $\langle f(1-f)\rangle_T$ taken at fixed temperature T) enters in the chemical reaction rate w and its expected value at fixed T,

$$\langle w\rangle_T = \langle f(1-f)\exp(T/T_{\rm ACT})\rangle_T \ , \qquad (1)$$

where $T_{\rm ACT}$ is the activation temperature and $w = 0$ for $T \leq T_{\rm ACT}$. Finally,

$$\langle w\rangle = \int \langle w\rangle_T dT \qquad (2)$$

where no closure models are used in the evaluation of $\langle w\rangle$.

The dynamic subgrid models are parameter free. We further note some degree of skepticism regarding turbulent gradient diffusion models. For this reason, and in keeping with conventional scientific standards, we note that theories need validation (agreement with physical experiment) as well as verification (the mesh convergence study summarized here). For the low Reynolds number flows, the subgrid terms do not contribute, and the choice of turbulent coefficients has no role. For the moderate Reynolds number flows, the influence of these coefficients is not strong. But for the high Reynolds number flows, these coefficients have a large role. We have used 2D simulations throughout, as the plan of this study calls for examining a range of mesh and physical parameter values, and fine grid simulations in 3D were not practical in this context.

In Fig. 1, we show a density plot at late time of the circular Richtmyer-Meshkov instability studied here. The high degree of interface complexity is evident in this plot. In Figs 2 - 4, we show for three values of the Reynolds number (300; 6000; 600,000) a plot of the second moment of the concentration

$$\theta(T) = \langle f(1-f)\rangle_T / \langle f\rangle_T \langle (1-f)\rangle_T \ , \qquad (3)$$

evaluated at a constant temperature, and the pdf for the temperature. From these two plots, we compute the mean chemical reaction rate $\langle w\rangle$, assuming an activation temperature in the middle of the observed temperatures. Convergence properties of $\langle w\rangle$ are given in Table I. In

this table, we note that the entries for $Re = 300$ and $Re = 600,000$ are convergent in the conventional sense. In the case of $Re = 6000$, we see that the error for both coarse and medium grids is smaller than the ensemble variation. We interpret this as saying that both coarse and medium grids have converged, and remaining differences are due to statistical fluctuations, not completely removed by the spatial average used to compute $\langle w \rangle$. Visual inspection of Fig. 3 supports this conclusion.

FIG. 1: Late time density plot for circular Richtmyer-Meshkov instability. A circular shock, initially at the out region of the domain, has moved inward through a perturbed circular interface. Upon reaching the interface, it reflects as an outgoing circular shock wave. Upon recrossing the now strongly perturbed interface, the interface becomes extremely chaotic in its appearance.

Details with additional parameter values will be published separately.

The scale invariant equations of fluid flow fall into the domain mathematically known as nonlinear conservation laws. Existence theories for equations are known in one spatial dimension, and even then require further restrictions. These theories come in two major branches, the first of which is based on a kind of perturbative theory of interaction strengths, and is applicable only to solutions

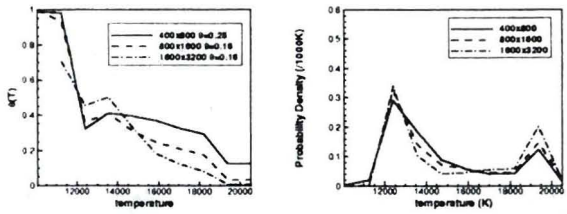

FIG. 2: Reynolds number 300. Left: $\theta(T)$ vs. T. Right: Plot of pdf for T.

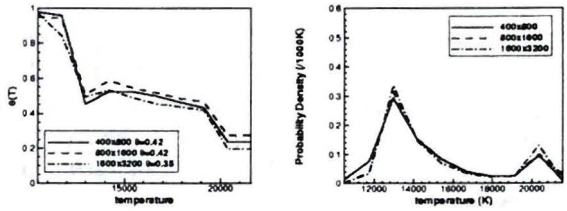

FIG. 3: Reynolds number 6000. Left: $\theta(T)$ vs. T. Right: Plot of pdf for T.

near a constant state [15]. Here we refer to the other main branch, which proceeds in two main steps [16, 17]. The first is to establish solutions in a very weak sense as measure valued distributions, and the second is to show that such solutions are in fact classical weak solutions. The scaling properties we have observed numerically suggest the following possible picture: The Euler equations (without transport) have solutions only as measure value distributions. These solutions in general do not reduce to classical weak solutions. Moreover, they are nonunique, and depend on details of some limiting process used in their derivation. Unique solutions and classical solutions require regularized equations, i.e. inclusion of transport terms.

To indicate the importance of this proposed change in point of view and of perspectives on the strategy for mathematical solutions of the higher dimensional Euler equations of compressible fluid dynamics, we can observe that an existence theory for measure valued solutions, while presently unknown, and possibly difficult, is surely orders of magnitude easier that a proof of existence of

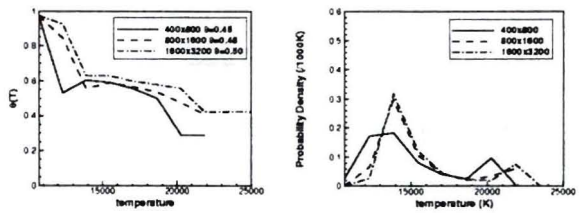

FIG. 4: Reynolds number 600,000. Left: $\theta(T)$ vs. T. Right: Plot of pdf for T.

Re	$2\sigma/\langle w\rangle$	c to f	m to f
≈ 300	0.62	3.33	1.25
≈ 6000	0.42	0.11	0.30
$\approx 600K$	0.17	0.29	0.12

TABLE I: Relative coarse grid ensemble fluctuations ($\pm 2\sigma$) divided by ensemble mean, and relative mesh errors for the mean chemical production term $\langle w\rangle$ for an activation temperature $T_{AC} = 15,000^o K$. Comparison is coarse mesh (c) to fine (f) and medium (m) to fine.

classical weak solutions. This later goal appears to be very unpromising. Not only does it appear to be technically extremely difficult, but conceivably it is false.

We summarize the principal points established in this paper. The problem of simulation of turbulent mixing is of wide importance; the specific example considered is suggestive of inertial confinement studies. Difficulties have been reported with convergence of simulations in the chaotic regime, especially when variables sensitive to microscopic or molecular level mixing are in question. The chemical reaction rate is a typical such variable. This variable, even when averaged over the mixing zone, displays a certain level of stochastic variability, shown in column 2 of Table I. When the course to fine grid error is larger than the variability ($Re \approx 300,\ \ 600K$), we observe convergence. When the coarse to fine grid error is smaller than the variabiity ($Re \approx 6000$), we regard coarse (and also the medium) grid to be converged, and without an extensive foray into stochastic modeling, with a convergence study of ensemble means and variances, there is no further convergence (at the level of a single realization) possible. In this sense, we achieve the main goal of this paper, which is to verify through a mesh convergence study a strategy for LES simulations of meaningful microscopic observables in a mixing or stirring dominated (as opposed to a diffusion dominated) flow, i.e. for a turbulent mixing flow having rapid dynamics.

The point of view developed here has implications for the mathematical theory of conservation laws, a secondary goal of this paper.

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