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Statistical Convergence of Multi-Phase Flow

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Abstract

We discuss the statistical convergence of interfacial two-phase averages in the Rayleigh-Taylor instability associated with steady acceleration. The statistical evolution of a planar, randomly perturbed interface subject to Rayleigh-Taylor instability is explored through direct numerical simulation in two space dimensions. We interpret interfacial averages theoretically, and explore that interfacial averages are convergent only in the outer portions of the mixing zone, where there is a coherent array of bubble and spike tips.

Keywords: multiphase flow, turbulence, interface average

AMS subject classifications: 76T99, 76F25

1 Introduction

In this paper, we discuss the statistical convergence of interfacial two-phase averages in the Rayleigh-Taylor (RT) instability associated with steady acceleration. This mixing process is nonlinear and chaotic, in the sense of sensitive dependence on initial data. As RT instability develops, small perturbations of a smooth contact surface rapidly grow into interpenetrating fingers of the distinct materials. Furthermore, only the statistical properties of the initial interface perturbations are known. These features point to a stochastic approach as the appropriate method to develop a predictive model for the deterministic properties of an evolving mixing layer.

We derive a formula of interfacial averages for $q = v,\ p,\ pv$ and interpret interfacial quantities. The computations of interfacial averages show convergence only in the outer portions of the mixing zone, where there is a coherent array of bubble and spike tips. There are three clearly distinguished physical regions comprising the mixing layer. In contrast, mixing models present a uniform description of the entire mixing layer, up to the setting of phenomenological coefficients. There is a physical basis for treating the bubble and spike regions in this manner, in the same way that gas bubbles in liquid bear a physical resemblance to liquid droplets in gas, but the middle region of the mixing zone is highly disordered. At present, when there is no comprehensive statistical description of this portion of the mixing layer, it makes sense to concentrate effort on the more important spike and bubble regions and use an interpolation scheme to bridge the gap. This approach has been followed to varying degrees in a number of two-phase flow treatments [8, 7, 15].

We report on results of numerical simulations of constant acceleration RT instability in two space dimensions. The data set that we have generated is highly resolved and covers a large ensemble of initial conditions, allowing a more refined analysis of closure issues pertinent to the stochastic modelling of chaotic fluid mixing. In particular, we closely approach statistical convergence of the mean two-phase flow under increasing ensemble size. The most stringent test of statistical convergence is performed at the latest possible time. Other quantities that appear in the two-phase averaged Euler equations are computed directly and analyzed for numerical and statistical convergence.

An interface between two fluids is subject to the RT instability when an external force is directed against the density gradient. This phenomenon is of importance in natural and technological problems encompassing a vast array of length scales, for example in supernova explosions, formation of salt diapirs, and laser implosion of inertial confinement fusion targets. See [12] for an overview of this problem, and [11] for further discussion.

2 Two-Phase Flow Equations

We study RT mixing of two immiscible, inviscid, non-heat conductiong gases. The Euler equations comprise the microphysical description, and a two-phase flow analysis begins with the ensemble average of these equations, with the averaging applied strictly within each material. The two-phase flow has a slab symmetry, with mean quantities varying only in the vertical (z) direction. There is also no shearing motion a time $t = 0$, which combined with the symmetry assumption implies no shearing motion for all t, hence zero transverse components of mean velocity. The averaged are then

$$\frac{\partial(\beta_k\rho_k)}{\partial t}+\frac{\partial(\beta_k\rho_k v_k)}{\partial z}=0\ , \tag{2.1}$$

$$\frac{\partial(\beta_k\rho_k v_k)}{\partial t}+\frac{\partial(\beta_k\rho_k v_k v_k)}{\partial z}+\frac{\partial(\beta_k p_k)}{\partial z}=\beta_k\rho_k g+\left\langle p\frac{\partial X_k}{\partial z}\right\rangle-\frac{\partial(\beta_k \mathbf{R}_k)}{\partial z}\ , \tag{2.2}$$

$$\frac{\partial(\beta_k\rho_k E_k)}{\partial t}+\frac{\partial(\beta_k\rho_k v_k E_k)}{\partial z}+\frac{\partial(\beta_k p_k v_k)}{\partial z}=\beta_k\rho_k v_k g+\langle p\mathbf{v}\cdot\nabla X_k\rangle-\frac{\partial(\beta_k \mathbf{S}_k)}{\partial z}\ . \tag{2.3}$$

Here the ensemble average is denoted $\langle\cdot\rangle$. The function X_k is the phase indicator for material $k(k=1,2)$; *i.e.*, $X_k(t,\mathbf{x})$ equals 1 if $\mathbf{x}$ is in fluid k at time t, zero otherwise. The ensemble average of X_k is the expected fluid k concentration or volume of the density ρ and pressure p: $\rho_k=\langle X_k\rho\rangle\,/\,\langle X_k\rangle$, $p_k=\langle X_k p\rangle\,/\,\langle X_k\rangle$. The quantities v_k and e_k are, respectively, phase mass-weighted averages of the fluid z-velocity v_z and specific total energy E: $v_k=\langle X_k\rho v_z\rangle\,/\,\langle X_k\rho\rangle$, $E_k=\langle X_k\rho E\rangle\,/\,\langle X_k\rho\rangle$. The averaging of the nonlinear terms in the Euler equations contributes non-zero covariances which are redefined and put on the right hand side (RHS) of the equations of motion. These terms are defined through the relations

$$\mathbf{R}_k=\frac{\langle X_k\rho v_z v_z\rangle}{\beta_k}-\frac{\langle X_k\rho v_z\rangle^2}{\beta_k\langle X_k\rho\rangle}\ ,\quad \mathbf{S}_k=\frac{\langle X_k\rho v_z E\rangle}{\beta_k}-\frac{\langle X_k\rho E\rangle\langle X_k\rho v_z\rangle}{\beta_k\langle X_k\rho\rangle}\ .$$

We also average a material advection equation to obtain

$$\frac{\partial\beta_k}{\partial t}+\langle\mathbf{v}\cdot\nabla X_k\rangle=0\ , \tag{2.4}$$

which expresses the condition of no mass flux across material interfaces, promoted *via* averaging to an evolution equation.

Equations (2.1)-(2.4) contain no modelling assumptions beyond the underlying microphysics but the averaging of nonlinear terms introduces new unknowns: bulk averages of nonlinear terms such as $\mathbf{R}_k$, and interfacial averages such as $\langle p\partial X_k/\partial z\rangle$. The closures has been proposed systematically in [9, 10, 1].

The modelling of interfacial averages has been a major challenge of two-phase flow theory, whereas the volumetric or bulk averages of nonlinear terms capture fluctuation effects that are the focus of turbulence theory. Chaotic fluid mixing exhibits both fluctuation and interfacial phenomena, yet we are aware of few treatments [13, 4, 5, 14] that combine these effects in this context.

The simulated flows are weakly compressible, with negligible density fluctuations. Therefore the phase- and phase-mass averages of any variable are nearly identical. The quantities $\mathbf{R}_k$ and $\mathbf{S}_k$ are then the velocity-velocity and energy-velocity covariances strictly within material k, up to a factor of ρ_k.

It is important to distinguish between material-specific and global fluctuations. Interfacial effects contribute to global correlations, but they are mathematically separate from material specific correlations. For example, a mathematical identity derived in [3] gives the global Reynolds stress in terms of the material-specific $\mathbf{R}_k$ and a two-phase cross term,

$$\mathbf{R}_{zz} = \beta_1 \mathbf{R}_1 + \beta_2 \mathbf{R}_2 + \beta_1 \beta_2 \frac{\rho_1 \rho_2}{\bar{\rho}} (v_1 - v_2)^2 \qquad (2.5)$$

Note that the two-phase contribution does not introduce any new unknowns. Chen *et al.* demonstrated that the cross term in (2.5) is usually a major contribution to $\mathbf{R}_{zz}$ in weakly compressible RT mixing. Our work shows that their observation breaks down on finer computational grids, probably due to the enhanced velocity randomization arising from the resolution of smaller scale structures.

The mean pressures are dominated by hydrostatics, yet the motion induced by the instability is reflected in their non-hydrostatic components. Therefore, it is convenient to study the profiles of pressure after subtracting the hydrostatic contribution. Specifically, we define $p'_k = p_k - p_{h,k}$, where $p_{h,k}(z)$ is the pressure of fluid k at rest at height z at $t = 0$ (whether or not it is actually present). For an isothermal stratification,

$$p_{h,k} = p_{\text{int}} \exp \left[\frac{\gamma g (z - z_{\text{int}})}{c^2_{\text{int},k}} \right] , \qquad (2.6)$$

where p_{int} is the pressure at the initial mean interface height $z = z_{\text{int}}$ and $c^2_{\text{int},k}$ is the initial sound speed in fluid k.

The three interfacial averages that appear in Eqs (2.1)-(2.4) are directly computed and nomalized as follows

$$v^* \equiv \frac{\langle \mathbf{v} \cdot \nabla X_k \rangle}{\partial \beta_k / \partial z} , \quad p^* \equiv \frac{\langle p \partial X_k / \partial z \rangle}{\partial \beta_k / \partial z} , \quad (pv)^* \equiv \frac{\langle p\mathbf{v} \cdot \nabla X_k \rangle}{\partial \beta_k / \partial z} . \qquad (2.7)$$

These quantities are well defined despite the appearance of the index k in their definitions because we ignore surface tension and assume perfect fluid immiscibility. The interfacial average of the primitive variable q, $q = v$, p, pv, is $q_{\rm int} = \langle q\hat{n}_k \cdot \nabla X_k \rangle \,/\, \langle \hat{n}_k \cdot \nabla X_k \rangle$, where $\hat{n}_k$ is the unit normal vector into fluid k at interface points. It is shown in Sec. 3 that that q^* in (2.7) is actually a weighted average of q at interface points. However, both $q_{\rm int}$ and q^* have the same boundary values, namely

$$\lim_{\beta_k \to 0+} q^* = \lim_{\beta_k \to 0+} q_{\rm int} = q_k \; . \tag{2.8}$$

3 Statistical Convergence of Interfacial Two-Phase Averages

In this section, we discuss the statistical convergence of interfacial two-phase averages. Since the fluid flow is chaotic, the most stringent test of statistical convergence is performed at the latest possible time. Unless indicated otherwise, the times referred to in the following discussion are $gt/c_2 = 1.42$ for the Atwood number $A \equiv (\rho_2 - \rho_1)/(\rho_2 + \rho_1) = 0.5$ and $gt/c_2 = 1.07$ for $A = 0.8$. At these times, the material interface in any realization has evolved to a stage exemplified by the snapshot [2].

The sample size for fluid k bulk averages is proportional to $N\beta_k$. Despite the small fluid k sample size near mixing zone edge k (due to small β_k), the microphysical flow is highly ordered in this region and the fluid k averages are likewise stable. In the center portion of the mixing layer, the large fluid k sample size ($\beta_k \sim 1/2$) suppresses any statistical noise due to the highly disordered material interface.

The evalution of interfacial averages uses only material interface points. The material interface is stored and tracked as a set of piecewise linear curves. Each curve contains a linked list of the (x, z) coordinates of each linear segment-connecting point. For each point, there are also left and right fluid states that are computed explicitly using Riemann problem solvers. The left or right state at any location on a material interface is therefore available *via* interpolation between the surrounding connecting points. The normal vector at a location on the interface is the normal to the line segment connecting the surrounding points.

In two dimensions, an interface average at a given height z uses state and geometric information everywhere the material interface intersects a horizontal line of this height. Near the center of the mixing zone, where the number of such crossings is maximized, there are 50 to 100 crossings in any realization. The total maximum number of crossings for $N = 20$ was approximately 1100 for $A = 0.5$ and 1400 for $A = 0.8$. Despite these seemingly large numbers,the interfacial averages are plagued by severe noise in the disordered region of the mixing zone.

The extraction of an interfacial average $\langle q\nabla X_k \rangle$ or $\langle \mathrm{q} \cdot \nabla X_k \rangle$ from numerical data is not obvious. Here, we relate an interfacial average to a single flow realization assuming (2.1) two-dimensional flow; (2.2) scalar q; and (2.3) a horizontal average. After deriving Eq. (3.8) below, we relax these assumptions.

The material indicator X_k is a generalized function. To remove the delta function behavior at material interface points, we combine the horizontal average with a spatial average over an ϵ interval of z, evaluate the integral, and then take the limit $\epsilon \to 0$. Thus we integrate over a narrow horizontal strip. If the fluid domain extends from $x = x_l$ to $x = x_u$, then the ϵ-strip average of a field variable q is

$$\langle q \rangle_\epsilon (t, z) = \frac{1}{(x_u - x_l)\epsilon} \int_{z-\epsilon/2}^{z+\epsilon/2} dz' \int_{x_l}^{x_u} dx \; q(t, x, z') \; . \tag{3.1}$$

Consider the evaluation of $\langle q\nabla X_1 \rangle_\epsilon$, where q is any scalar field. The integral in Eq. (3.1) has contributions only where $\nabla X_1 \neq 0$, namely everywhere the contact surface (curve) crosses the strip. We need analyze only one arbitrarily chosen crossing, and then sum the contributions of all crossings to complete the evaluation. We close up a section of the ϵ-strip that is crossed once by the contact surface. We label the left and right handed fluids 1 and 2, respectively, and by convection the normal vector $\mathbf{n}$ points into fluid 1.

The crossing contact surface divided this section of strip into two pieces, labeled P_1 and P_2. We also label the lower and upper boundaries of P_i as L_i and U_i, respectively, and we define R_1 to be the right hand boundary of P_1. We re-arrange $\langle q\nabla X_1 \rangle_\epsilon$ as follows

$$\langle q\nabla X_1 \rangle_\epsilon = \langle \nabla(qX_1) \rangle_\epsilon - \langle X_1 \nabla q \rangle_\epsilon \tag{3.2}$$

and evaluate each term on the righthand side of this expression. Applying the divergence theorem to $\langle \nabla(qX_1) \rangle_\epsilon$,

$$\int_{P_1 \cup P_2} \nabla(qX_1)\, dA = \int_{L_1 \cup L_2 \cup U_1 \cup U_2} qX_1 \, dS = \int_{L_1 \cup U_1} q \, dS \; . \tag{3.3}$$

Since $X_1 = 0$ on the strip edges L_2 and U_2, this integral reduces to

$$\int_{P_1 \cup P_2} \nabla(qX_1) dA = \int_{L_1 \cup U_1} q\, dS \; . \tag{3.4}$$

For the same reason, the second term, $\langle X_1 \nabla q \rangle_\epsilon$, is evaluated only on the section of strip where $X_1 = 1$, *i.e.*, on P_1. Applying the divergence theorem to the area integral of ∇q on P_1, we have

$$\int_{P_1 \cup P_2} X_1 \nabla q\, dA = \int_{L_1 \cup U_1 \cup R_1} q\, dS \; . \tag{3.5}$$

Combining the last two expressions as in Eq. (3.2), the integrals on the upper and lower boundaries of P_1 cancel, leaving

$$\int_{P_1 \cup P_2} q \nabla X_1 dA = -\int_{R_1} q\, dS \; . \tag{3.6}$$

This integral is easily evaluated in the limit of small ϵ, so that R_1 is a straight line segment and q is nearly uniform on R_1. Then

$$\int_{P_1 \cup P_2} q \nabla X_1\, dA = \left. \frac{\epsilon \mathbf{n}}{|n_x|} q \right|_{R_1} \; . \tag{3.7}$$

If q is not continuous across R_1, then $q|_{R_1}$ is evaluated on the fluid 1 side of R_1.

To evaluate $\langle q \nabla X_1 \rangle_\epsilon$, we apply Eq. (3.7) to every intersection of the contact surface with the ϵ-strip at height z. Then the factor of ϵ in Eq. (3.7) cancels the normalization factor in Eq. (3.1), and the $\epsilon \to 0$ limit is trivial, leaving

$$\langle q \nabla X_1 \rangle = \frac{1}{x_l - x_u} \sum_{\text{xings}} \frac{q\mathbf{n}}{|n_x|} \; . \tag{3.8}$$

The sum is over all points of intersection of the contact surface with the horizontal line at height z, and the summed is evaluated at each such point. If q is continuous across material interfaces, then $\langle q \nabla X_2 \rangle = -\langle q \nabla X_1 \rangle$.

The extension of this result to vector q follows by replacing $q\mathbf{n}$ with $\mathbf{q} \cdot \mathbf{n}$ in Eq. (3.8). The extension to a combined horizontal/ensemble average is obvious, because we can imagine aligning all of the realizations side by side and then applying a horizontal average to the combined system. If there are

N realizations, then the normalization constant in Eq. (3.8) is $N(x_u - x_l)$ and the sum is over all crossings at height z in all realizations.

The result for 3D flow has a similar, but more complicated derivation, and we state it here without proof. The intersection of the contact surface with the horizontal plane at height z is a set of curves. The sum in (3.8) is replaced by the line integral of $q\mathbf{n}/(n_x^2+n_y^2)^{1/2}$ along all curves of intersection, and the normalization constant is replaced by the lateral area of the fluid domain.

Setting $q = 1$ in Eq. (3.8) yields a method to calculate the volume fraction gradient directly from the interface information, as opposed to the usual method of numerically differentiating the volume fraction itself. Consequently, direct evaluation of $q^* = \langle q\partial X_k/\partial z\rangle / (\partial\beta_k/\partial z)$ is accomplished. Eq. (3.8) makes clear the fact that q^* is not the interfacial average of q, but rather a weighted sum of interfacial values of q, where the weights have positive and negative values. The interfacial average of q is

$$q_{\text{int}} = \frac{\langle q\mathbf{n}_k \cdot \nabla X_k\rangle}{\mathcal{A}} = \frac{1}{\mathcal{A}(x_u - x_l)} \sum_{\text{xings}} \frac{q}{|n_x|}\,, \tag{3.9}$$

where $\mathcal{A}$ is the average interfacial area per unit volume,

$$\mathcal{A} = \frac{1}{x_u - x_l} \sum_{\text{xings}} \frac{1}{|n_x|}\,. \tag{3.10}$$

It would be interesting and useful to develop a statistical characterization of the complex interface geometry, in the framework of a set of evolution equations for moments such as β_k and $\mathcal{A}$. These ideas are discussed by Drew and Passman [6].

We observe that there is a strong correlation between the region of non-monotonicity of β_k and the extreme noise in the profiles. In the regions near the edges both quantities exhibit roughly linear behavior with minor noise. In view of our data, a more pragmatic modelling approach may be to focus effort on the more important outer regions of the mixing zone, and bridge the central region by interpolation.

4 Conclusion

A formula for interfacial two-phase averages is derived theoretically. Our simulations of two-dimensional Rayleigh-Taylor instability achieve a good statistical convergence of mean two-phase properties under increasing ensemble size. The numerical data is suitable for an order-or-magnitude understanding of the mixing zone physics.

References

[1] W. Bo, H. Jin, D. Kim, X. Liu, H. Lee, N. Pestieau, Y. Yan, J. Glimm, and J. Grove. Compressible multi species multi phase flow models. 2006. In preparation. Stony Brook University Preprint Number SUNYSB-AMS-XX-XX, Los Alamos National Laboratory LAUR Number LAUR-XX-XXXX.

[2] Y. Chen. *Two Phase Flow Analysis of Turbulent Mixing in the Rayleigh-Taylor Instability.* PhD thesis, University at Stony Brook, 1995.

[3] Y. Chen, J. Glimm, D. H. Sharp, and Q. Zhang. A two-phase flow model of the Rayleigh-Taylor mixing zone. *Phys. Fluids*, 8(3):816–825, 1996.

[4] C. W. Cranfill. A multifluid turbulent-mixing model. Technical Report LA-UR-91-403, Los Alamos National Lab., 1991.

[5] C. W. Cranfill. A new multifluid turbulent-mixing model. Technical Report LA-UR-92-2484, Los Alamos National Lab., 1992.

[6] D. Drew and S. Passman. *Theory of Multicomponent Fluids.* Applied Mathematical Sciences. Springer-Verlag, New York, 1999.

[7] N. Freed, D. Ofer, D. Shvarts, and S. Orszag. Two-phase flow analysis of self-similar turbulent mixing by Rayleigh-Taylor instability. *Phys. Fluids A*, 3(5):912–918, 1991.

[8] F. Harlow and A. Amsden. Flow of interpenetrating material phases. *J. Comp. Phys.*, 18:440–464, 1975.

[9] H. Jin, J. Glimm, and D. H. Sharp. Compressible two-pressure two-phase flow models. *Phys. Lett. A*, 353:469–474, 2006.

[10] H. Jin, J. Glimm, and D. H. Sharp. Entropy of averaging for compressible two-pressure two-phase models. *Phys. Lett. A*, 360:114–121, 2006. Stony Brook University Preprint number SUNYSB-AMS-06-08 and Los Alamos National Laboratory.

[11] H. J. Kull. Theory of the Rayleigh-Taylor instability. *Phys. Reports*, 206:197, 1991.

[12] D. H. Sharp. An overview of Rayleigh-Taylor instability. *Physica D*, 12:3–18, 1984.

[13] D. L. Youngs. Modeling turbulent mixing by Rayleigh-Taylor instability. *Physica D*, 37:270–287, 1989.

[14] D. L. Youngs. Three-dimensional numerical simulation of turbulent mixing by Rayleigh-Taylor instability. *Phys. Fluids A*, 3:1312–1319, 1991.

[15] D. L. Youngs. Numerical simulation of mixing by Rayleigh-Taylor and Richtmyer-Meshkov instabilities. *Laser and Particle Beams*, 12:725–750, 1994.