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Atomistic simulation of the Rayleigh-Taylor instability

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Abstract. Large-scale atomistic simulations are performed using both the molecular dynamics and direct simulation Monte Carlo algorithms. These simulations are used to investigate several aspects of turbulent behavior, focusing on the Rayleigh-Taylor instability, in which a heavy fluid lies on top of a light fluid in the presence of a gravitational field. The use of atomistic techniques allows us to capture various physical effects not resolved by more traditional continuum methods, such as the discontinuous breakup of flow features, and the effects of micro-scale fluctuations. In addition, we compare with both experiment and continuum simulations such properties as the initial growth spectrum of the interface, and the development in time of the mixing zone width.

1. Introduction
The Rayleigh-Taylor (RT) instability [1, 2], in which a heavy fluid lies on top of a lighter fluid in the presence of a gravitational field, has wide applicability to problems in fields such as astrophysics, oceanography, inertial confinement fusion, etc. Furthermore, it serves as an archetype for more general instances of turbulent mixing. The RT instability has been studied extensively by theory, experiment, and simulation. Until recently, most simulations have been carried out using continuum methods. In this work, we perform simulations of the RT instability using molecular dynamics (MD) [3] and Direct Simulation Monte Carlo (DSMC) [4], a faster, stochastic atomistic algorithm.

There are several advantages to the use of atomistic schemes. The traditional continuum models of fluids have had great success in describing fluid flow in the regimes with which we are most familiar. However, this success has tended to obscure the various approximations inherent in such models. In any extended parameter space for fluid behavior, which might include the Knudsen number (the ratio of particle mean free path to the length scale of the flow), distance from equilibrium, Mach number, etc, there are regions in which continuum models do not apply. The passage of a spacecraft through the rarified gas high in a planet’s atmosphere, or the discontinuous breakup of nanojets [10] are two of many real world examples. More fundamental atomistic methods, however, should have applicability across the entire parametric spectrum.

The major drawbacks of atomistic methods are the small length and time scales to which they are confined by their computationally-intensive nature. For example, the largest runs described in this work correspond to a few microns for about 140 nanoseconds. Nevertheless,
advances in technology have allowed multi-billion-particle simulations to be performed [9], and computational capacity is rapidly expanding to the point where atomistic simulations on the length scale of millimeters (the size of several real-world experiments) will soon be possible. For these reasons, it is important to explore the use of atomistic methods in applications beyond those to which it has been traditionally confined.

2. Computational Details
This work incorporates data from MD simulations previously described in [8], as well as several new large-scale DSMC simulations. Both types of simulation were performed using the Scalable Parallel Short-ranged MD code (SPaSM) [11]. Two different domain geometries were considered: quasi-2D (or “thin-slab”) geometry, and 3D. Thin slab geometry was used in order to emulate a truly two-dimensional system while at the same time maintaining finite transport coefficients. A vertical gravitational field was maintained in all runs, which had a magnitude of approximately $10^9$ to $10^{10}$ Earth gravities. Such a high gravity was necessary due to the small length and time scales to which we were limited.

The MD simulations were run on up to 1,600 central processing units (CPUs) of the ASCI Q computer system at Los Alamos National Laboratory. The largest of these runs consisted of 100 million particles simulated for 250,000 integration time steps. The DSMC simulations were done using the BlueGene/L machine at Lawrence Livermore National Laboratory. The largest 2D DSMC run consisted of 500 million particles run for 210,000 time steps on 65,536 processors. The length and time scales represented by this run were approximately 5 microns and 140 nanoseconds, respectively. The 3D DSMC simulation consisted of 7 billion particles run for 30,000 time steps on 32,768 processors. Its length and time scales were approximately 1 micron and 20 nanoseconds. It should be noted that this latter simulation sets a new world record for the number of particles in an atomistically-based production run. This was made possible by the fact that DSMC is at least 50 times as efficient as MD on a parallel architecture, due to the low level of communication between processors.

3. Homogeneous Turbulence Results
As a validation of the use of atomistic methods in a realm traditionally dominated by continuum algorithms, we performed an additional simulation of homogeneous turbulence in 2D. This simulation was done in 12 hours on a single processor, using DSMC with 38 million particles. Turbulence was generated using a linear forcing scheme as described in [12]. A thermostat was used to prevent the temperature from growing due to viscous effects.

There is an extensive literature of theoretical results for 2D turbulence, derived largely from continuum models such as the Navier-Stokes equation. However, there was no a priori reason for these results to apply to particle-based simulations. We therefore chose to compare our results

![Figure 1. Energy spectra for homogeneous 2d turbulence at several values of Re, along with power-law reference lines.](image)
for the turbulent energy spectrum with those predicted by the Batchelor-Kraichnan (BK) theory of 2D turbulence, which follows largely from dimensional considerations, and is therefore model independent [13, 14]. Energy spectra for a few values of the Reynolds number $Re = UL/\nu$ are shown in Figure 1. It can be seen that there is good agreement with the general BK theory. At low $Re$, the flow is dominated by the so-called “enstrophy cascade” $k^{-3}$ power law. At high $Re$, the Kolmogorov “inertial range” $k^{-5/3}$ scaling is apparent. At intermediate $Re$, both regimes coexist, with a smooth cusp between the two.

In addition to the $k^{-3}$ and $k^{-5/3}$ ranges predicted by the BK theory, there is also a $k^1$ range evident at large $k$. It should be noted that this is not a numerical artifact of the atomistic scheme used to model the fluid. Instead, it is a very real physical effect that results from the fact that, at small length scales, macroscopic fields such as velocity and density become random variables subject to thermal fluctuations. The $k^1$ scaling is indicative of two-dimensional spatial white noise.

4. Rayleigh-Taylor Instability Results
Several images from various stages in the development of the RT instability in 2D and 3D are shown in Figures 2 and 3, respectively. These examples were generated using DSMC, and represent the typical behavior of the RT instability. Driven by bouyancy, the light fluid (blue) penetrates the heavy fluid (red) in large, round features known as “bubbles”. At the same time,
Figure 4. The initial growth rate $n$ of the interface as a function of the wavenumber $k$.

Figure 5. $h_B$ and $h_S$ as a function of $t^2$ for a typical DSMC simulation.

the heavy fluid moves downward in somewhat longer, thinner shapes known as “spikes”. The fraction of the domain covered by the bubbles and spikes is known as the “mixing region”.

For small times, linear stability analysis predicts that each Fourier coefficient present in the interface will grow as $e^{nt}$, where the growth rate $n$ is a function of wavenumber $k$. Results for $n(k)$ computed from MD simulations are shown in Figure 4, along with Chandrasekhar’s continuum prediction [5]. It can be seen that there is good agreement except at large $k$, where the MD data lies above the theoretical prediction of no growth. This occurs because high-$k$ features lie closer to the length scale of particles. Thus, for these $k$ values, the continuum hypothesis breaks down. Note that the “error bars” in Figure 4 are actually estimates of the fluctuation-induced standard deviations of the growth rates, which become random variables at these small scales.

At larger $t$, the size of the mixing region grows to the point where linear stability no longer applies. In this regime, it has been observed that the depths $h_B$ and $h_S$ to which the bubbles and spikes penetrate the heavy and light fluids, respectively, grow as $h_B = \alpha_B A g t^2$ and $h_S = \alpha_S A g t^2$. (Here $A = (\rho_h - \rho_l)/(\rho_h + \rho_l)$ is the Atwood number, where $\rho_h$ and $\rho_l$ are the heavy and light mass densities at the interface.) The bubble and spike $\alpha$-values are of particular interest, and they have been extensively measured by both experiments and continuum simulations. Figure 5 shows the bubble and spike penetration depths as a function of $t^2$ for a typical DSMC simulation, along with the associated estimates for $\alpha_B$ and $\alpha_S$. The linear scaling of $h_B$ and $h_S$ with $t^2$ for small-to-moderate $t$ can clearly be seen, although (for the spikes especially) this behavior breaks
down at large $t$ due to the discontinuous breakup of spikes and bubbles. In order to compare experimental results with those of the various simulation methods, Figure 6 shows bubble and spike $\alpha$ values calculated via experiment [6], MD, and several continuum simulations in the literature [7]. It can be seen that the particle-based results compare at least as favorably with experiment as the continuum results.

5. Conclusion

Though the size of the systems that may be studied by atomistic methods is limited by computational capacity, the generality of these algorithms and the results of this work suggest that they can be applied to much broader sets of problems than have previously been contemplated. In particular, they are essential in the study of nanoscale fluid dynamics, high-Knudsen number flows, and other examples of non-continuum turbulence. Furthermore, particle-based simulations of truly macroscopic flows (i.e. $\geq 1$ mm in size) will soon be possible. These can serve as a powerful alternative, first-principles method for predicting the properties of fluid flows.

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