Simulation of the Rayleigh-Taylor Instability Using Atomistic Methods

John L. Barber, Kai Kadau, Peter S. Lomdahl, T-14; Timothy C. Germann, Brad L. Holian, X-1-SMMP; Berni Alder, Lawrence Livermore National Laboratory

The Rayleigh-Taylor instability (RTI) occurs when a dense fluid lies on top of a light fluid in the presence of a vertical gravitational field. This arrangement is an unstable equilibrium, and the subsequent behavior of the two fluids is an archetypical example of turbulent fluid mixing. The RTI has applications in many diverse fields, such as astronomy, oceanography, and inertial confinement fusion, and it has been studied extensively via both simulation and experiment.

Most previous simulated studies of the RTI have involved the use of continuum techniques based on the Navier-Stokes (NS) or Euler equations. In this work [1,2], we instead make use of two atomistic methods: molecular dynamics (MD) and direct simulation Monte Carlo (DSMC) [3]. In MD, Newton's equations of motion for the positions and momenta of a large number of interacting particles are solved numerically. DSMC is similar in many respects to MD, except for the fact that the interparticle interactions are modeled stochastically, which results in a speed up factor of approximately 30–50 compared with MD.

There are several advantages to the use of atomistic methods to fluid turbulence. Continuum models, such as the NS equations, are known to fail in several regimes, such as in extremely rarified (high Knudsen number) flows, and flows at very small length scales. More fundamental atomistic methods are applicable in a much wider set of regimes. Furthermore, for applications involving interface dynamics, such as the RTI, MD, and DSMC have the advantage of allowing an initially flat interface, as opposed to the somewhat artificial initial perturbation spectrum that must be applied in a continuum simulation. In addition, it is much easier to control the degree of miscibility in atomistic methods (particularly MD). The main disadvantages of atomistic methods are the small length and time scales to which they are confined by the limits of current computational capacity. These limits are continually being pushed back, however, as evidenced by the simulations performed in this work.

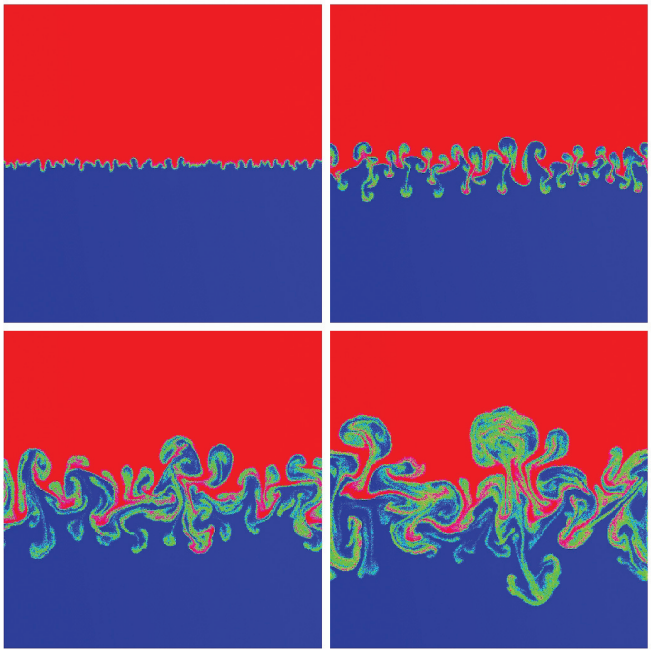
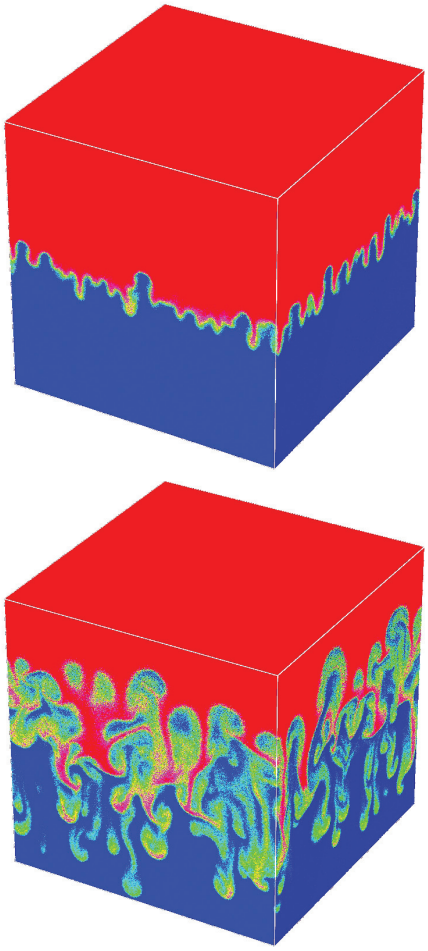


Fig. 1.
Four snapshots in time from a 2-D, 500-million particle simulation of the RTI using DSMC.

Several large-scale DSMC simulations of the RTI were performed using the Scalable Parallel Short-range MD code [4] on Livermore's BlueGene/L machine. Figure 1 shows the results of a 2-D run involving 500 million particles, corresponding to length and time scales of 5 μm and 140 ns, respectively. Figure 2 shows some results from a 3-D run of 7 billion particles (a new world record), corresponding to 1 μm and 20 ns. The bubble-formation and merger process characteristic of the RTI is evident in both.

During the initial stages of the RTI, linear stability analysis predicts



that the various modes present on the interface will grow independently and exponentially with a growth rate n(k), where k is the wavenumber [5]. As a test of how well atomistic simulations agree with continuum predictions, we have used MD to calculate the growth rate for two different gravities. The results are shown in Fig. 3. Note that the shaded envelopes are not error bars, but are instead an estimate of the intrinsic physical spread in the growth rate, which occurs due to the fact that all macroscopic fields (such as density or fluid velocity) become random variables subject to microscale fluctuations at these small length scales. There is good agreement with the continuum prediction at small wave numbers, but increasing discrepancies at larger k, due to the effects of capillary waves, compressibility, and fluctuations.

For more information contact John L. Barber at jlbarber@lanl.gov.

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[3] G.A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press, Oxford, England, 1994).
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Fig. 2.
Two snapshots in time from a 3-D, 7-billion particle simulation of the RTI using DSMC.

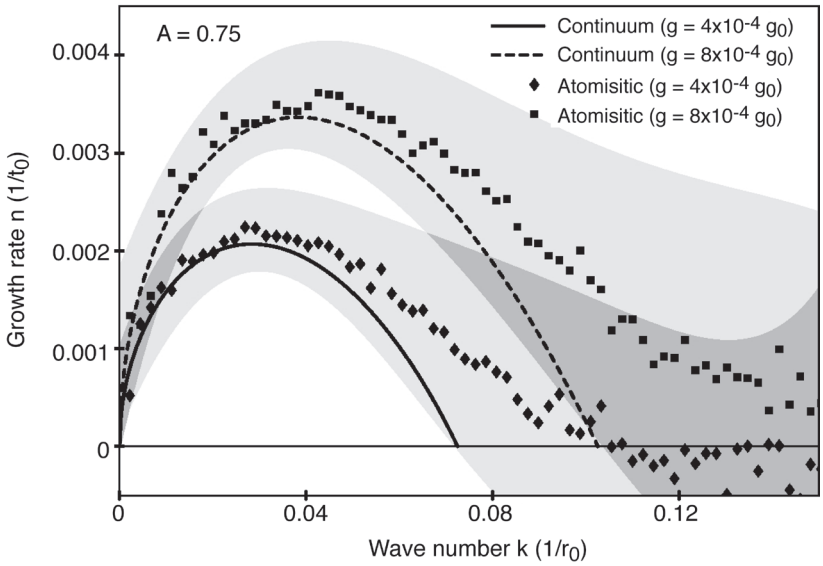

Fig. 3.
The initial growth rate spectrum as calculated via MD for two different gravities. The lines represent the theoretical continuum predictions, and the shaded envelopes reflect an estimate of the physical spread in growth rate at these length scales. (Results in simulation units.)