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**Simulation of the Rayleigh-Taylor instability using atomistic methods** JOHN BARBER, KAI KADAU, TIM GERMANN, PETER LOMDAHL, BRAD HOLIAN, Los Alamos National Laboratory, BERNI ALDER, Lawrence Livermore National Laboratory — Recent increases in computational capacity and speed have allowed the application of particle-based algorithms, such as molecular dynamics (MD) and direct simulation Monte Carlo (DSMC), to the simulation of turbulent fluid behavior. The use of such techniques has a number of advantages. In particular, they capture several physical effects not resolved by more traditional continuum methods, for example the discontinuous breakup of flow features and the influence of micro-scale fluctuations. In addition, they can be used for length and time scales at which the continuum approximation does not hold. In this work, we present the results of various MD and DSMC simulations of the Rayleigh-Taylor instability, in which a heavy fluid lies on top of a light fluid in the presence of gravity. Our results for the initial growth spectrum of the interface and the development in time of the mixing zone width are compared with the analogous results from both continuum simulations and experiment.

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