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The Scaling of Atomistic Fluid Dynamics Simulations JOHN BARBER, KAI KADAU, TIMOTHY GERMANN, Los Alamos National Laboratory, BERNI ALDER, Lawrence Livermore National Laboratory — In order to investigate the scaling properties of atomistic fluid dynamics simulations, we have performed a series of large-scale direct simulation Monte-Carlo simulations (containing up to 5.7 billion particles) of the Rayleigh-Taylor instability. The results, which include a wide range of length and time scales, suggest that such particle-based simulations exhibit the same scaling as predicted by the Navier-Stokes equation. In addition, a quantitative comparison with macroscopic Rayleigh-Taylor experimental results suggests that the results of micro-scale atomistic simulations can be scaled up to describe much larger systems, even in complex non-stationary flows.

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