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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 — A series of large-scale atomistic simulations of the Rayleigh-Taylor instability was performed using up to 5.7 billion particles. The results of these simulations, which included a wide range of time and length scales, suggest that atomistic fluid dynamics simulations exhibit a scaling similar to that predicted for Navier-Stokes solvers. Furthermore, quantitative comparison to a macroscopic Rayleigh-Taylor experiment further suggests that the results of atomistic simulations - even for complex non-stationary flows - can be scaled up to describe larger systems.

John Barber
Los Alamos National Laboratory

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