

Abstract Submitted
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Micron scale simulations of a Kelvin-Helmholtz instability: a direct comparison between molecular dynamics and Navier-Stokes hydrodynamics.¹ KYLE CASPERSEN, ROBERT RUDD, DAVID RICHARDS, JIM GLOSLI, WILLIAM CABOT, PAUL MILLER, FRED STREITZ, Lawrence Livermore National Lab — The modeling of hydrodynamic phenomena has largely been the purview of continuum mechanics, such as through the solution of the Navier-Stokes equations. Nevertheless, at small length scales, where atomistic effects become important, it is not clear that this continuum approach provides a complete description of fluid behavior. To understand the effects of atomistics, we have performed a 9 billion atom quasi-2D molecular dynamics simulation, and the corresponding Navier-Stokes hydrodynamic simulation, of an interface of copper and aluminum in a strong shear layer. The applied shear flow of 2 km/s produces complex phenomena associated with a Kelvin-Helmholtz (KH) instability. In this presentation we compare and contrast the initiation and early evolution of the KH instability modeled both by molecular dynamics and continuum hydrodynamics.

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