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A fully 3-D molecular dynamics study of the initiation of the Kelvin-Helmholtz instability[1] ROBERT E. RUDD, K.J. CASPERSEN, D.F. RICHARDS, J.N. GLOSLI, Lawrence Livermore National Laboratory, J.A. GUNNELS, IBM, F.H. STREITZ, Lawrence Livermore National Laboratory — The modeling of hydrodynamic phenomena has almost exclusively been the purview of continuum mechanics, specifically, through the use of the Navier-Stokes equation and closely related variants. Nevertheless, at the smallest 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 62.5-billion-atom, fully 3-D molecular dynamics simulation of a cubic micron of molten copper and aluminum. The shear flow at 2 km/s exhibits complex phenomena associated with a Kelvin-Helmholtz (KH) instability. In this presentation we will discuss the initiation and early evolution of the KH instability, focusing specifically on the effects of full atomistic resolution.

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