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Molecular origins of continuum fluid mechanics: Atomic migrations of single-phase fluid and slip boundary conditions ALAN GRAHAM, SHIHAI FENG, TONY REDONDO, Los Alamos National Lab — We report the results of molecular dynamics simulations of pressure-driven flows of liquid argon in circular and planar conduits. We find that in inhomogeneous shear flows the molecules migrate to the center of the conduits and establish large radial density gradients under conditions that were previously assumed to be incompressible. These are the first predictions of shear-induced migration in pure fluids subjected to inhomogeneous shear flows. These density gradients increase monotonically with Péclet number. They result in a blunted velocity profile that deviates from the parabolic profile predicted by the Navier-Stokes equations for an incompressible fluid. Comparisons with simulations where the flow exhibits zero or linear shear indicate that this phenomenon is the result of the nonlinear shear flows and the finite size of the molecules.

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