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Boundary conditions for coupling molecular dynamics simulations to continuum simulations[1] LIV HERDMAN, YVES DUBIEF, University of Vermont — Coupling continuum simulations to molecular dynamics simulations require implementing boundary conditions that constrain the atomic motions to match the physical properties of the large-scale simulations. The traditional wall and periodic boundary conditions used in molecular dynamics present difficulties for simulating non-equilibrium and spatially evolving flows. We are working toward creating an evolving boundary condition to match temperature and momentum conditions in atomistic simulations that are driven by coupled continuum simulations. We have developed an inlet boundary condition that utilizes a periodic buffer cell to drive the variable thermodynamic and flow conditions. In this work we demonstrate the new inlet boundary condition with simulations of a Lenard-Jones fluid in a channel and compare the effects of different outlet boundary conditions

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