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Combined Temperature/Momentum Boundary Conditions for Molecular Dynamics Simulations of Flow in Nanofluidic Systems[1]
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— Molecular dynamics (MD) is a useful technique for scientific investigations of nanofluidic processes as it explicitly represents the dynamics of every atom in a system. In order to model systems of interest, e.g. nanochannels, it is necessary to constrain atomic motions to conform to conditions corresponding to large-scale information, e.g. thermodynamic variables. However, many engineered configurations involve complex interactions between the system and its environment, and take place in non-trivial geometries. To accurately simulate these phenomena, methods to apply boundary conditions to MD systems are required that simultaneously regulate the temperature (i.e., energy) and momentum of the atoms in a local manner. This work uses an atomistic-to-continuum formulation to generate boundary conditions by using finite elements (FE) and their associated shape functions to define "boundaries" for a particle system. By projecting onto the FE basis, coarse-scale observables are identified for regulation based on separating the mean and fluctuating velocity components defining the momentum and temperature. Regulating the MD system is achieved by applying constraints posed on the coarse-grained variables. The method is illustrated by application to several nanofluidic systems.

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