Non-Equilibrium Molecular Dynamics Simulations in the Hamiltonian Adaptive Resolution Method

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We discuss a recently-introduced open-boundary method to perform non-equilibrium molecular dynamics simulations [1]. The system of interest, described in atomistic resolution, is embedded in an infinite reservoir of non-interacting particles at a constant temperature, volume, and chemical potential [2]. To enforce this condition, we use the Hamiltonian adaptive resolution method, where an interface is defined between atomistic and ideal gas representations and a switching field smoothly connects both subdomains. An external potential, applied only in the interfacial region, balances the excess chemical potential of the system. To ensure that the size of the reservoir is infinite, we introduce a particle insertion/deletion algorithm to control the density in the ideal gas region. We show that it is possible to study non-equilibrium phenomena with this open-boundary molecular dynamics method. To this aim, we consider a prototypical confined liquid under the influence of an external constant density gradient. The resulting pressure-driven flow across the atomistic system exhibits a velocity profile consistent with the corresponding solution of the Navier–Stokes equation. This method conserves, on average, linear momentum and closely resembles experimental conditions. Moreover, this approach allows one to study various direct and indirect out-of-equilibrium conditions in complex molecular systems.

References

[1] M Heidari, K Kremer, R Golestanian, R Potestio, R Cortes-Huerto, Open-boundary Hamiltonian adaptive resolution. From grand canonical to non-equilibrium molecular dynamics simulations, Journal of Chemical Physics 152, 194104 (2020)

[2] M Heidari, K Kremer, R Cortes-Huerto, R Potestio, Spatially resolved thermodynamic integration: An efficient method to compute chemical potentials of dense fluids, Journal of Chemical Theory and Computation 14 (7), 3409-3417 (2018)