Boundary-controlled barostats for slab geometries in molecular dynamics simulations

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The simulation of confined fluids at well defined normal pressures requires the use of barostats which, on the one hand, impose the required target pressure to the system while, on the other hand, should interfere as little as possible with the dynamics of the confined liquid. There are a number of schemes in the literature used to maintain a confined fluid system at a target pressure. In our work we have derived and tested barostat schemes for achieving a given normal pressure for a thin liquid or solid layer confined between two parallel walls which are built on the boundary-controlled barostat scheme of Lupkowski and van Swol [J. Chem. Phys. 93, 737 (1990)]. Two classes of barostat are explored, one in which the external load is applied to a virtual regular lattice to which the wall atoms are bound using a tethering potential, the other type in which the external force is applied directly to the wall atoms, which are not tethered. The first class of barostats can suffer from anomalous dynamical signatures and resonances which are sensitive to the effective mass of the virtual lattice, whose value lacks any rigorous definition. The second type of barostat performs much better under equilibrium and wall-sliding nonequilibrium conditions and in not being so prone to resonance instabilities in the wall separation and does not require so many largely arbitrary parameters. Exploratory simulations which characterize the dynamical response of the model systems for both dry and wet or lubricated systems using the different barostats also show that the barostats which have an inherent damping mechanism, such as the ones analogous to a damped harmonic oscillator, reduce the occurrence of large fluctuations and resonances in the separation between the two walls, and they also achieve a new target pressure more quickly [1].