Temperature Control and Flow Manipulation for Nano-Confined Fluids by Molecular Dynamics Simulations

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The control of temperature for molecularly structured fluids under flow conditions in molecular dynamics computer simulations is of critical importance for useful applications. As computational power continues to improve, the ability to perform simulations of very large and complex molecular systems is now feasible. The complexity of a system increases considerably when the system is both highly confined and under the application of an external field that drives fluid flow far from equilibrium. For such systems it has been demonstrated that thermostatting the fluid directly can induce simulation artefacts, and that the most reliable method is to thermostat only the confining walls, allowing heat to flow from the fluid into the walls as would typically happen in nature [1]. However, for complex wall structures, this can add an additional degree of difficulty, which can increase the required simulation time beyond feasible limits. In this presentation we propose a new method whereby instead of thermostatting the wall particles directly, we position vibrating "virtual" particles tethered to the walls that assume the role of a heat sink [2]. These particles do not interact with the walls and can pass straight through them. They do however interact with fluid atoms, thereby exchanging both energy and momentum. The new thermostat is compared to systems of thermostatted walls and shown to be reliable and efficient, without the introduction of unwanted artefacts. We use the new method to simulate the flow of water confined to physically realistic asymmetric planar walls composed of hydrophobic graphene and hydrophilic silica and thereby show that by spinning water molecules by the application of a rotating electric field we can induce unidirectional flow with only moderate temperature rise in the fluid [3].

References

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