**Far-from-equilibrium Flow in Nanopores from Molecular Simulation**

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Fluids in small nanopores have properties that differ from bulk fluids at the same state point due to the restriction of motion, wall-fluid interactions and layering effects, especially close to the wall. Of particular interest is the change in rheological properties and nonequilibrium flow due to confinement. It has been found that the onset of nonlinear behaviour can occur at lower flow rates when a fluid is confined, and when this occurs linear response theory cannot be applied and the flux will no longer be proportional to the force. We show how nonlinear response theory [1] can be applied to these systems and how it can be used to improve the results obtained from simulations, if nonlinearity sets in at relatively low forcing. Simulations of Poiseuille will be used to demonstrate the behaviour. [2]

Study of lubrication is an area where changes in behavior due to flow is important. In many cases lubrication occurs at high strain rates and under high confinement. In this work we evaluate the response of a fluid under shear flow in a nanopore. The movement of the boundaries in opposite directions induces the shear. The viscous heat generated inside the pore is removed by a thermostat applied exclusively to the atomic walls, leaving the dynamics of the fluid as realistic as possible. [3] We will also discuss the characterization of slip in these small pores.

References

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