Non-local hydrodynamic model for flow in slit nanopores

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There is a large interest in the understanding of the behaviour of fluids at nanoscales. At these short length scales, the fluid starts displaying features which are absent at the large scales where ordinary Navier-Stokes equations with the no slip boundary condition apply. The density field, for example, displays characteristic layering of the molecules near the walls. In many situations, the fluid slips against the walls. In order to address these problems we have recently formulated in Ref. [1] the equations of hydrodynamics near solid walls starting from first principles. The theory generalizes to non-equilibrium situations the successful Density Functional Theory of classical *simple* fluids [2]. In this hydrodynamic theory the effect of the walls is not through boundary conditions but rather through irreversible forces acting on the fluid and confined near a layer of molecular dimensions near the wall. These forces contain friction transport coefficients given in terms of Green-Kubo formulae [3].

In the present work we study by means of molecular dynamics (MD) simulations the predictions of the theory in planar shear flows. Space is binned and momentum of the fluid, forces due to the walls, and stress of the fluid are defined in terms of finite element basis functions [4, 5] and measured. From these, the Green-Kubo formulae are computed from equilibrium MD simulations. These transport coefficients which are non-local in space, are input of the discrete hydrodynamic equations and allow to predict the flow field in a decay situation from a given initial flow condition. We consider both plug flow and Couette flow that suddenly is left unforced and decay towards equilibrium. The predictions of the theory and the simulations are in a reasonable but not perfect agreement. We attribute the discrepancies to the fact that the Green-Kubo expressions suffer strongly from the plateau problem. This suggest that non-Markovian effects may play a role in this problem.

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