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Molecular Dynamics to extract friction factor at the nanoscale

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Abstract: We perform Non-Equilibrium Molecular Dynamics simulations to describe the detailed atomistic behaviour of fluids moving in nanochannels. For some cases, flows at the nanoscale can still be investigated with Navier-Stokes equations, however, the modification scheme that has to be adjusted to the classical equation forms has a key-role and seems to depend on flow geometrical characteristics [1-2]. The question is how to incorporate phenomena existing at the nanoscale, such as shear stresses, slip lengths, non-constant viscosity and fluid density values, at the macroscale [3]. Molecular Dynamics (MD) is a common method for interpretation and investigation of nanoscale phenomena, describing particle interactions at the atomic scale. In this work we incorporate MD atomistic results in order to extract nanoscale properties to be used in the continuum N-S equations, such as the slip velocity at the wall and the shear viscosity profile. We find that classical continuum theory predictions of power dissipation do not apply in the case of nanochannels and have to be modified accordingly. However, the mathematical form of the friction factor expressions persists for quite small nanochannel widths and breaks down only when the channel walls are hydrophilic.

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