This dissertation studies the behaviour of a fluid in contact with a solid in the nanoscale. Theoretical formulations of non-local continuum and discrete hydrodynamics are presented in which the interaction of the solid with the fluid appears explicitly in terms of extended forces on the fluid, confined to the vicinity of the solid object. The discrete theory is validated through MD simulations, where we encounter the plateau problem in the determination of the transport coefficients. We offer a method that solves the problem and allows us to evaluate the transport coefficients unambigously.

In the course of the MD investigation we find that the Markovian assumption implicit in the theoretical derivations is not satisfied near the wall when the hydrodynamics is resolved at molecular scales. However, for sufficiently large bins in which the discrete hydrodynamic variables are defined the behaviour is fully Markovian.

The final outcome of the present dissertation is the derivation of the slip boundary condition from the microscopically formulated discrete hydrodynamic theory. The slip length and the position of the wall are defined through Green-Kubo formulas. We test the validity of the slip boundary condition thus obtained in a particularly challenging flow, an initial plug flow that is discontinuous near the wall at initial stages of the flow.

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UNIVERSIDAD NACIONAL DE EDUCACIÓN A DISTANCIA

2019