Molecular Modeling of Nanofluidic Systems with Slip

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Abstract

In confined nanofluidic systems with slip the position where the Navier-Stokes boundary condition should be applied can make significant differences in the measurement of the system's transport coefficients such as the friction coefficient (or equivalently the slip length). It is generally accepted that this hydrodynamic height differs one atomic distance of the physical wall position and the most extended approach to compute it is by comparing Poiseuille and Couette flow simulations. The aim of our work is to accurately determine the hydrodynamic wall position from one single set of simulations discussing the suitability of three different approaches as well as showing the appropriateness of the method to measure the transport coefficients. Once the main system hydrodynamic parameters have been determined, our objective is to quantify the finite size effects in the measurement of the Self-Diffusion coefficient in the presence of slip.

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