Nanoscale hydrodynamics near solids

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We propose a generalization of Equilibrium Density Functional Theory (DFT) for simple fluids in motion in the presence of solid walls. The theory gives the structure of the fluid at nanoscales, and allows one to study effects like how the structure of the fluid near a wall is modified by the flow field.

We use the Theory of Coarse-Graining for the derivation of this Dynamic DFT. The selected relevant variables are the mass density field (as in usual approaches to Dynamic DFT[1]) *and* the momentum density field of the fluid. The CG description provides the structure of the equations that govern the dynamics of the fluid and describes the irreversible forces that arise in the fluid because of the interaction with the walls that ultimately give rise to boundary conditions in a macroscopic description. These forces contain slip coefficients and viscosity kernels that are defined microscopically in terms of Green-Kubo expressions.

The theory is completely general, and requires a free energy functional and a dissipative matrix. The free energy functional is exactly the same as the equilibrium free energy functional. The dissipative matrix contains non-local transport kernels that need to be obtained beforehand in order to be predictive. Being tensorial quantities, we need in principle up to 50 different functions in order to make dynamic predictions.

To reduce the number of transport coefficients needed, in the present work we consider situations in which symmetries of the solid surface and fluid flow can be exploited. In particular, we work with planar geometries and planar flows (Fig. 1). In this configuration the number of non-local transport kernels is reduced to a wall friction, a slip friction, and a viscous friction. All of them can be computed from their Green-Kubo expressions from MD simulations. This is ongoing work[2, 3, 4] that should allow to describe flow situations in nanochanels as those depicted in Fig. 2.

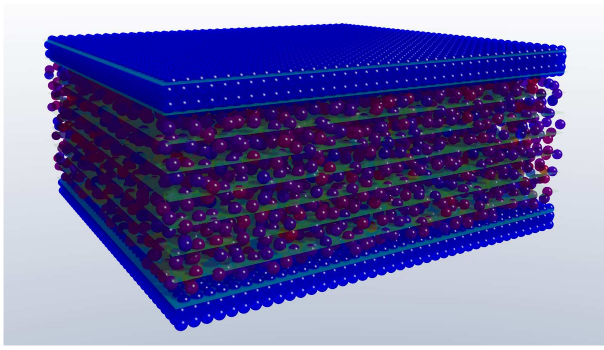

Figure 1: Representation of the MD simulation with a sketch of the binning used. Normalized velocity of the particles is indicated by color scale ($\mathrm{blue} = 0$, $\mathrm{red} = 1$). In green are depicted the nodal planes used to obtain the relevant variables.

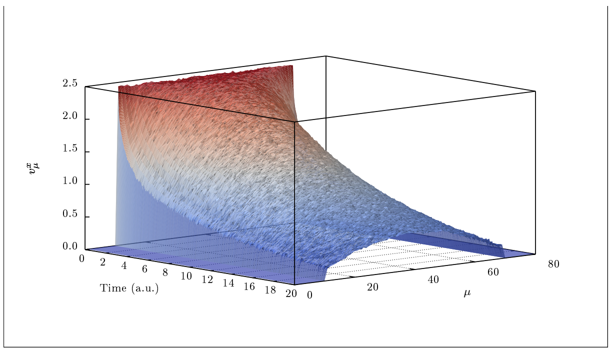

Figure 2: Velocity profile decay in a planar flow between two parallel walls, obtained from MD simulations. Initially the fluid has a constant velocity in the x direction.

[1] J. A. de la Torre, P. Español, and A. Donev, J. Chem. Phys. **142**, 094115 (2015).

[2] D. Camargo, J. A. de la Torre, P. Español, R. Delgado-Buscalioni, and F. Chejne, *Nanoscale hydrodynamics near solids. I Theory*, in prep., (2017).

[3] D. Camargo, J. A. de la Torre, P. Español, R. Delgado-Buscalioni, and F. Chejne, *Nanoscale hydrodynamics near solids. II Simulations*, in prep., (2017).

[4] D. Camargo, J. A. de la Torre, P. Español, R. Delgado-Buscalioni, and F. Chejne, *Nanoscale hydrodynamics near solids. III Boundary conditions*, in prep., (2017).