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Multiscale flow simulation of water past a fullerene

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INTRODUCTION: We present a three-dimensional multiscale flow simulation of water past a buckyball. We employ the Schwarz alternating method to couple molecular dynamics of liquid water and the C_{540} fullerene with the Lattice-Boltzmann (LB) description of the Navier- Stokes (NS) equations. Our approach allows for studying nanoscale flow phenomena that are out of scope of the pure atomistic simulation.

METHODS: The simulation model is shown schematically in Fig.1. We extend the Schwartz domain decomposition scheme [1] by a fully 3D atomistic-continuum coupling.

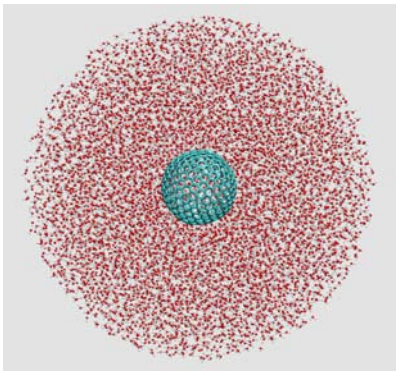

Fig. 1: Cross section of the water molecules that surround the C_{540} fullerene molecule.

The computational domain is cubical. Lattice nodes are centered in corresponding cubical MD sampling cells of size α. The spherical MD domain provides the LB method with velocity boundary conditions (BCs). The MD domain has non-periodic force BCs in all three directions in order to maintain the correct mean virial pressure [2]. Furthermore, we use a specular boundary to impose the ideal kinetic part of the system pressure. Liquid water is modeled with the rigid SPC/E water model. The simulations are performed at T = 300K and ρ = 997kg/m^3. Force field parameters for the rigid C_{540} fullerene molecule are taken from Refs.[3,4]. Long range electrostatic interactions are treated by the reaction field method with a cutoff of α. In order to correctly describe the hydrodynamics we employ in this study the linear momentum preserving Dissipative Particle Dynamics (DPD) thermostat.

RESULTS: The results from the multiscale simulations are compared with full MD reference simulations. In the inset of Fig.2 we monitor the evolution of the convergence rate. In the same figure we plot the x-component of the fluid velocity. In Fig.3 we present the tangential velocity radial profile, which shows that the slip velocity at the surface is not zero.

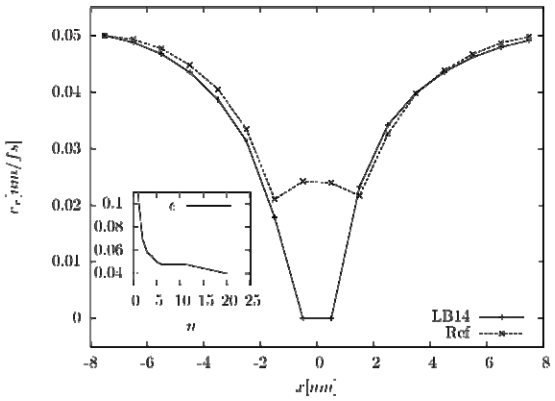

Fig. 2: The x-component velocity. The inset shows the convergence of the hybrid toward the reference solution.

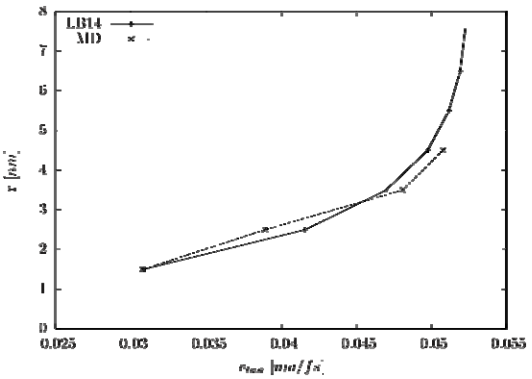

Fig. 3: The tangential velocity profile in the radial direction from the fullerene.

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