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A Multiscale Algorithm to Drastically Reduce Computational Times when Simulating Liquid/Solid Interaction at Atomic Resolution with Realistic Hydrodynamics Effects

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Abstract. A hybrid multiscale model that incorporates both continuum fluid dynamics effects including thermal fluctuations and molecular dynamics is presented for the challenging 3D liquid-solid interface problem of gap water flows between the moving tip of the Atomic Force Microscope (AFM) cantilever and a material substrate surface. Highlights of the method include the all-atom resolution in the vicinity of material surfaces, thereby avoiding the empiricism of interface boundary treatments of continuum mechanics approaches, with considerable computational savings in comparison with direct single-scale approaches such as Non-Equilibrium Molecular Dynamics (NEMD) methods. All components of the multiscale method are systematically described and verified. To optimise the coupling of the continuum fluid dynamics solution with the molecular dynamics solution a simple iterative method is used. Predictions of the multiscale method are compared with the reference equilibrium molecular dynamics solutions and discussed in the context of available AFM measurements in the literature. Computational performance of the suggested multiscale method is analysed in comparison with that of the NEMD method for a relevant range of the AFM problem parameters. In particular, in comparison with the single-resolution MD method, the implemented multiscale model leads to an eight order of magnitude acceleration of the solution for a slowly moving AFM tip typical of the existing experiments. Perspectives of further development and application of the suggested multiscale method are discussed. The current model is implemented in the open-source GROMACS software, and the source code of which is also provided.

AMS subject classifications: 76A99, 76-04, 76-10, 65M32, 65M22, 70G99, 68U99

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1 Introduction

Many applications in science and engineering involve interface-flow processes that span across a great range of spatial and temporal scales from continuum to atomic. For example, the microfluidic devices used in biomolecular separation involve water flows passing through custom-designed micro-channels, whose walls are functionalised to have hydrophobic or hydrophilic properties [1]. In such applications, water molecules away from the liquid-solid interface are mainly driven by hydrodynamics forces due to the collective motion of molecules, where short-range intermolecular forces are well-balanced on average. At the same time, the intermolecular forces close to the liquid-solid interface play a crucial role. The effect of such forces and the corresponding liquid-solid interactions at microscale cannot be described by continuum fluid mechanics models without introducing crude approximations, for example, using an empirical partial slip boundary condition.

To resolve the intermolecular effects at atomic level, Non-Equilibrium Molecular Dynamics (NEMD) methods have been traditionally used, for example, to explicitly simulate water atoms slipping along solid surfaces under external force [2]. In the past, the application of NEMD methods allowed revealing surprising properties of microscale flows, such as a several orders of magnitude faster flow rate through a carbon nanotube (CNT) in comparison with the continuum model predictions [3,4], a strong dependency of the slip length of ice-like water formed between graphene surfaces on the shear rate [5], the blockage of water flow in CNT by Ions [6], and the emerging water transport in a polyamide membrane under pressure gradient [7]. Despite many successful applications of NEMD methods for non-equilibrium molecular systems, there is a great number of applications where the usage of a single-resolution method remains inefficient because of the diversity of spatial and temporal scales, which leads to an excessively high computational cost. Hence, there is a pressing demand to develop application-tailored multiscale methods that seamlessly combine macroscale and microscale models to simulate the interfacial flow processes in an efficient way, whilst retaining the essential interactions between the atoms.

Two types of multiscale frameworks have been proposed in the literature: (i) Heterogeneous Multiscale Methods (HMM) [8–10] and (ii) Domain Decomposition Methods (DDM) [11–14]. A schematic of both these methods is shown in Fig. 1. HMM typically embeds a micro model described by an interaction potential between discrete particles in the nodes of a uniform Cartesian grid that covers the entire macroscopic simulation domain where Navier-Stokes (NS) equations are solved (Fig. 1(a)). Several techniques were proposed to transfer information between the micro to the macroscopic parts of the