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Multiscale modeling and simulation of dynamic wetting

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ABSTRACT

In this paper, we present a multiscale analysis on dynamic wetting and liquid droplet spreading on solid substrates. In the proposed multiscale dynamic wetting model, we couple molecular scale adhesive interaction (the van der Waals type force) and the macroscale flow – that is: we combine a coarse-grain adhesive contact model with a modified Gurtin–Murdoch surface elasto-dynamics theory to formulate a multiscale moving contact line theory to simulate dynamic wetting. The advantage of adopting the coarse grain adhesive contact model in the moving contact line theory is that it can levitate and separate the liquid droplet with the solid substrate, so that the proposed multiscale moving contact line theory avoids imposing the non-slip condition, and then it removes the subsequent singularity problem, which allows the surface energy difference and surface stress propelling droplet spreading naturally.

By employing the proposed method, we have successfully simulated droplet spreading over various elastic substrates. The obtained numerical simulation results compare well with the experimental and molecular dynamics results reported in the literature.

1. Introduction

Wetting or droplet spreading on a solid substrate is an interesting and fascinating phenomenon in colloidal science that has many important applications in the fields of soft matter physics, chemistry, biology, and engineering, for example, cell motility, self-cleaning biological systems, wet friction between tire and pavement, pharmaceutical drugs manufacturing and delivery system, consumer electronics, e.g. hard disk drive, various bio- and soft matter sensors, etc.

In chemical physics, wetting is a physical process of liquid and gas phases concurrently interacting with the surface of a solid phase, resulting from intermolecular interactions of a triple phase system when the three are brought together. The degree of wetting is referred to as wettability, which is determined by the intermolecular force balance between adhesive, cohesive, and other contact forces. Wetting and the related surface tension and surface energy effects that control wetting are also responsible for other related physical phenomena, such as droplet spreading, capillary effect, surfactant assembly, wet friction, etc.

Because of vast applications and potential transformative impact, there is a long history and large body literature of attempting to establish a numerical method to simulate wetting and droplet spreading process at macroscale, e.g. [25,33,22,9,10,12,14] to name a few. Among them, the most notable one is the so-called moving contact line hydrodynamics theory [11,48,37,28]. However, there has been an outstanding challenge in the conventional moving contact-line

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hydrodynamics theory: a key technical ingredient of the moving contact line hydrodynamics is the non-slip boundary condition along the liquid/solid interface, which will lead to singularity in shear stress distribution at the front of the moving contact line between the liquid and solid phase (see Fig. 1 (a) and [51] for detailed discussion). In turn, the singular shear stress on the droplet will force the liquid droplet moving along the interface, which then violates the a priori assumption of non-slip condition. This technical difficulty has posted great challenge for macroscale simulation of dynamic wetting and droplet spreading.

In this work, we propose a multiscale dynamic wetting model (MDWM) that combines the conventional hydrodynamic contact line theory [11,48,37,28] and a modified Gurtin–Murdoch surface elasticity theory [16,17] with the coarse grain adhesive contact model developed by Sauer and Li [38–41], so that the droplet is levitated above the solid substrate (see Fig. 1(b)). In doing so, it completely eliminates singularity problem of the conventional hydrodynamic contact line theory (see recent discussions in [51]), while retaining the surface energy description in dynamics wetting modeling. To understand how the proposed method works, we have done a comparison simulation by using the conventional moving contact line method and MDWM method proposed in the work (see Fig. 1). In the moving contact line hydrodynamics simulation, a singular shear stress arises due to the fact that the initial contact line front between the liquid phase and solid phase forms a crack shaped cleavage (see Fig. 1(a)), and the abrupt change of surface tangent direction will cause stress concentration. On the other hand, if one can levitate the liquid droplet over the solid substrate, and it will separate the liquid phase and solid phase, i.e. creating a gap between the solid surface and liquid surface, as what really happens in reality. By doing so, the mechanical or mathematical modeling induced pathology will naturally go away, which is one of the main motivations and contributions of this work.

To accomplish this goal, in this work we have proposed a multiscale dynamic wetting model, and have established its finite element formulation, and have carried out several numerical simulations. The paper is organized into eight sections. We begin in Section 2 by setting forth the multiscale dynamic wetting model (MDWM) in terms of its mathematical strong form, and subsequently in Section 3, we state and derive the Galerkin weak formulation of MDWM theory. With these preparations, we discuss finite element discretization and implementations of MDWM in Section 4. In Section 5, we discuss a special but important case of moving contact line theory, in which the surface stress is assumed to be constant in each surface element; and in Section 6, we discuss the general surface contact line theory, in which the surface stress is non-uniform. In Section 7, several numerical examples are presented, and finally in Section 8, we conclude the presentation by assessing the advantages and limitations of the proposed MDWM model.

2. Multiscale dynamic and wetting model (MDWM)

We consider a general triple phase system of gas, liquid, and solid phase as shown in Fig. 2, in which $\Omega_\alpha,\ \alpha = G, L,$ and S are the bulk volumes for gas (G), liquid (L), and solid (S) phases. One can see from Fig. 1. that along each interphase, there are two surfaces. For example, Γ_{GL} is the gas surface of the gas–liquid interphase, whereas Γ_{LG} is the liquid surface of the gas–liquid interphase (see the order of letter G and L). By the same convention, we denote that Γ_{LS} is the liquid surface of the liquid–solid interphase, whereas Γ_{SL} is the solid surface of the liquid–solid interphase; Γ_{GS} is the gas surface of the gas–solid interphase, whereas Γ_{SG} is the solid surface of the gas–solid interphase. For the triple system configuration shown in Fig. 2, we have $\partial\Omega_L = \Gamma_{LG} \cup \Gamma_{LS}$, $\partial\Omega_S = \Gamma_{SL} \cup \Gamma_{SG}$, and $\partial\Omega_G = \Gamma_{GL} \cup \Gamma_{GS}$.

As a hybrid multiscale model, we model the bulk medium by using continuum mechanics formulations, i.e.

$$\frac{\partial \boldsymbol{\sigma}_\alpha}{\partial \mathbf{x}} + \rho_\alpha \mathbf{b}_\alpha = \rho_\alpha \ddot{\mathbf{u}}_\alpha, \quad \alpha = G, L, \text{ and } S \tag{1}$$

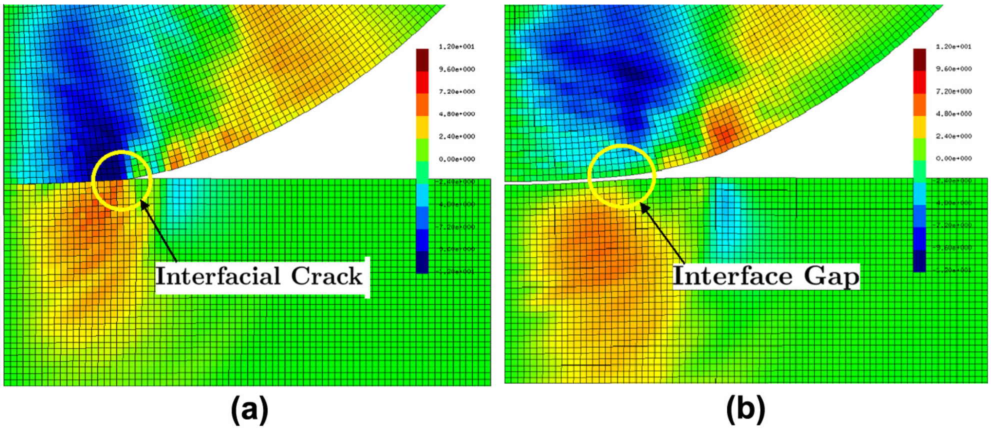

Fig. 1. Comparison simulation results of (a) Singularity in shear stress (σ_{12}) distribution obtained from the moving contact line hydrodynamics simulation, and (a) shear stress (σ_{12}) distribution from a MDWM simulation of adhesive contact and droplet spreading.