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An efficient finite element method for simulation of droplet spreading on a topologically rough surface ☆

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ABSTRACT

We study numerically the dynamics of a three-dimensional droplet spreading on a rough solid surface using a phase-field model consisting of the coupled Cahn–Hilliard and Navier–Stokes equations with a generalized Navier boundary condition (GNBC). An efficient finite element method on unstructured meshes is introduced to cope with the complex geometry of the solid surfaces. We extend the GNBC to surfaces with complex geometry by including its weak form along different normal and tangential directions in the finite element formulation. The semi-implicit time discretization scheme results in a decoupled system for the phase function, the velocity, and the pressure. In addition, a mass compensation algorithm is introduced to preserve the mass of the droplet. To efficiently solve the decoupled systems, we present a highly parallel solution strategy based on domain decomposition techniques. We validate the newly developed solution method through extensive numerical experiments, particularly for those phenomena that can not be achieved by two-dimensional simulations. On a surface with circular posts, we study how wettability of the rough surface depends on the geometry of the posts. The contact line motion for a droplet spreading over some periodic rough surfaces are also efficiently computed. Moreover, we study the spreading process of an impacting droplet on a microstructured surface, a qualitative agreement is achieved between the numerical and experimental results. The parallel performance suggests that the proposed solution algorithm is scalable with over 4,000 processors cores with tens of millions of unknowns.

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1. Introduction

The study of the wetting phenomenon is of critical importance in many industrial applications such as coating, ink-jet printing, and microfluidics. Interesting wetting behavior occurs when micrometric spatial dimension comes into play, as a result roughness-enhanced wetting has become the subject of extensive investigation. When a droplet spreads on a topo-

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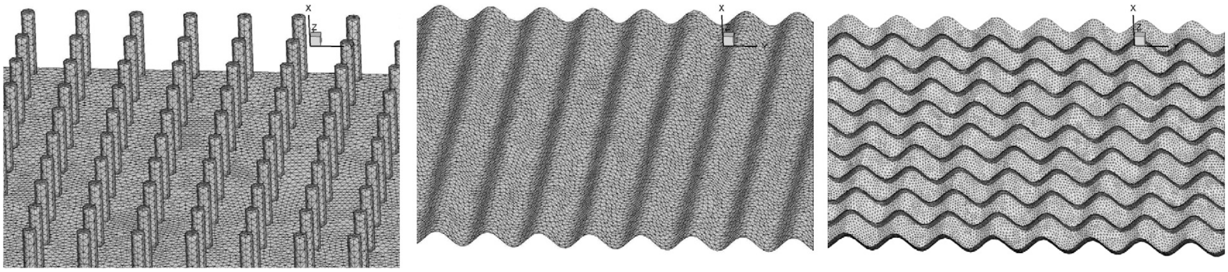

(a) circular posts (b) parallel strips (c) periodic waves

Fig. 1. Surfaces with various roughness.

logically rough surface with, for example, a pillar microstructure as illustrated in Fig. 1 (a), it may appear in two possible states: either the Wenzel state where the droplet infiltrates into the grooves and wets the bottom substrate between the posts, or the Cassie state where the droplet sits on top of the posts with pockets of air beneath it. The latter state results in a composite surface that exhibits superhydrophobic properties. The morphology of the liquid microstructures depends sensitively on the dimensions and spacing of the posts and may undergo a wetting transition between the Wenzel state and the Cassie state. Some authors have considered the conditions for the existence of different wetting regimes for sessile droplets, by means of analytic or numerical simulations based on the minimization of free energy [8,13,19,18,28,4,23]. In [18], the authors investigated the transition between the two states on a superhydrophobic surface by numerical simulations. They concluded that the equilibrium state of the droplet depends on the intrinsic contact angle and the position of the posts. Ren [23] used a string method to study the wetting transition on hydrophobic surfaces textured with a square lattice of pillars. The dependence of the energy barrier on the droplet size and the gap between the pillars was studied.

In systems involving three-dimensional droplets on rough surfaces, there are various contact angles along the contact line, and the droplets may assume a variety of shapes. Some applications require the knowledge of the contact angle as well as the contact angle hysteresis (CAH), i.e., the difference between maximum and minimum contact angles, which is generally attributed to surface heterogeneities and roughness. Lots of effort have been made to understand the effect of chemical heterogeneities on CAH for smooth surfaces, including striped patterns and regular chemical patches [2,14,18,29]. Studies for CAH on topologically rough surfaces were also attempted for some simplified model problems, such as the two-dimensional (or axisymmetric three-dimensional) problems of a droplet spreading on posts or sinusoidal surfaces [13,21,18,28]. These papers focused on the steady state prediction of the CAH, pinning of the contact line, and the existence of multiple local energy minima. Quasi-static results were obtained by increasing or decreasing the volume of the droplet.

In this paper, we study the CAH in dynamic cases by numerical simulation of a droplet spreading on a topologically rough surface. Different from the energy-based approaches in previous studies, the motion of the droplet and the surrounding air is described by a two-phase flow containing the liquid phase and the vapor phase. An issue in hydrodynamics with solid boundary is the incompatibility between the moving contact line and the no-slip boundary condition, as the latter leads to a non-integrable singularity, implying infinite viscous dissipation (see e.g. [20,7]). In [22], a phase field model consisting of the Cahn–Hilliard–Navier–Stokes equations with the GNBC is proposed to resolve the issue. This model has been used to simulate two-phase flows in two-dimensional channels with chemically patterns [27], as well as the dynamics of a three-dimensional droplet on smooth surface with chemical patches [10]. For the regular domains in these simulations, a finite difference scheme was used to discretize the governing equations on structured meshes. In the present work, we develop a new three-dimensional finite element solver on unstructured meshes and generalize the GNBC to arbitrarily complex surfaces. In order to construct a stable and efficient scheme for two-phase flows with large density and viscosity ratio, we combine a stabilized scheme [9] for the Cahn–Hilliard equation and a projection scheme [12,25] for the Navier–Stokes equations to fully decouple the phase function, the velocity, and the pressure. The GNBC is included in the weak form of the velocity system along different normal and tangential directions. Due to the truncation error, the total mass changes with small magnitude [5]. The accumulation of this effect usually causes the droplet to shrink and even to disappear [15,30]. To handle this issue, we apply a mass compensation algorithm to preserve both the total mass and the mass of the droplet by truncating and separately redistributing the phase field variable. For the three-dimensional simulations, the overall problem is computationally very demanding. To accelerate the convergence, we adopt a scalable domain decomposition method in which the computational mesh along with its associated data are distributed over many processors. We validate the newly developed solver through extensive numerical experiments on various rough surfaces (see Fig. 1). In particular, we study how wettability and droplet dynamics depend on the geometry and roughness of the surface.

The paper is organized as follows. In Section 2, the three-dimensional phase field model for two-phase flows is described. In Section 3, we recast the model into a variational form with a weak GNBC. The numerical scheme, the mass compensation algorithm, and the parallel solution strategy are demonstrated. In Section 4, numerical experiments of a droplet spreading on surfaces with various textures are presented. The paper is concluded in Section 5.

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