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Oriented ordering parameters for free energy lattice Boltzmann methods using the bounce-back boundary condition

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ABSTRACT

We evaluate the Lattice-Boltzmann model that combines the free energy approach for multiphase flow with the bounce-back boundary condition. This method requires a virtual ordering parameter to be assigned to the wall nodes. Existing literature has assigned a single ordering parameter for the entire wall node, but this is too coarse to give accurate simulations since it allows for a spurious interaction of different phases through the wall nodes. The consequences are illustrated by examining rough and hydrophobic surfaces where contact angles can be predicted using the Cassie–Baxter equation. It is found that the single value approach gives a large systemic error in the measured contact angles. Considerable improvement can be obtained by assigning different values of the ordering parameter to each side of the wall node.

1. Introduction

The behavior of fluids on different forms of surfaces is a field of study with multiple scientific and industrial applications. The chemical and structural characteristics of a surface can determine whether water tends to stick to or roll off it. These attributes are significant, for example for applications that require surfaces to be as dry as possible.

If a surface attracts water, the droplet will spread out giving a contact angle θ less than 90°. Such a surface is called hydrophilic. In contrast, a water droplet on a surface that repels water will curl up and have a contact angle greater than 90°. Such a surface is called hydrophobic. Very hydrophobic surfaces with contact angles greater than 150° are called superhydrophobic and are of great industrial interest.

Several proposals for manufacturing superhydrophobic surfaces exist, many with the aim of achieving characteristics such as ice-phobicity and durability, see for example [1,2]. Many of these publications report on laboratory testing of the results, but fluid dynamics simulations by using mesoscopic methods such as the Lattice Boltzmann method have also been applied [3]. Laboratory tests require the production of a physical test surface, something that is not needed for computer simulations.

In this article we examine the feasibility of using the popular bounce-back boundary condition for the solid–fluid interface when using the free energy approach [4,5] for multiphase flow. We aim to improve on the method offered in the previous literature [6,7] and show that this gives simulated contact angles that are more consistent with classical fluid theory. This is applicable to any domain with a complex solid boundary.

The classical fluid theory for rough surfaces is covered in Section 2. The Lattice Boltzmann method and the associated boundary conditions that are the focus for this article is covered in Section 3. Simulation results are covered in Section 4, and the conclusions are drawn in Section 5.

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2. Fluid theory of rough surfaces

A roughness is required to make a surface superhydrophobic. The contact angle of droplets on heterogeneous and rough surfaces has been the subject of considerable study. The simplest equations for estimating the contact angle on rough surfaces are the Wenzel [8] and Cassie–Baxter [9] equations. The Wenzel equation applies when a droplet fills the cavities of a rough surface. The apparent contact angle θ_c is then given by

$$\cos\theta_c = r\cos\theta_0, \tag{1}$$

where θ_0 is the contact angle the material would give on a smooth surface and the roughness parameter r is the ratio between the actual surface area and the projected surface area.

In its original form, the Cassie–Baxter equation applies on a smooth surface with n components with surface fractions $\xi_1, \xi_2, \ldots, \xi_n$ with different contact angle parameters $\theta_1, \theta_2, \ldots, \theta_n$. For a smooth surface made of different components, the sum over surface fractions will be 1. The resultant contact angle θ_c on a composite surface is given by

$$\cos\theta_c = \sum_{i=1}^{n} \xi_i \cos\theta_i. \tag{2}$$

The Cassie–Baxter equation has also been applied to some rough surfaces where the droplet is suspended above the cavities. In this case air, which has a contact angle parameter of 180°, is treated as a separate component. If the surface fraction of the solid component is ξ, one obtains simplified version of Eq. (2) which has been used in a majority of articles that deal with contact angles on a rough surface [10]:

$$\cos\theta_c = \xi\cos\theta - (1-\xi). \tag{3}$$

Eq. (3) assumes that the solid part of the surface is made up of a single component with an initial contact angle θ that covers a fraction ξ of the surface, and that the droplet does not penetrate into the surface at all. While these assumptions are commonly made, real droplets often exhibit more complex behavior by penetrating somewhat into the surface in which case Eq. (2) should be used without the assumption that the sum over all ξ_i is equal to 1. As the droplet penetrates deeper into the surface ξ_{solid} approaches the roughness factor and ξ_{air} approaches 0. Consequently, Eq. (2) approaches the Wenzel equation (1) [10].

The Cassie–Baxter and Wenzel equations can be derived from thermodynamic analysis [11] and provide a means for analytical predictions of the contact angle for simple cases of stationary droplets that are entirely on top of the surface or entirely penetrated into the surface. However the validity of the equations has been the subject of skepticism [12] and the fluid dynamics for the transitional states or droplets in motion cannot be described fully by the equations. There is therefore an interest in a computational fluid dynamic approach to studying such surfaces and the scales involved invite the use of mesoscopic approaches.

3. Lattice Boltzmann method

The Lattice Boltzmann method is a computational fluid dynamics (CFD) model originally introduced by Mcnamara and Zanetti [13] and later interpreted as a discretization of the Boltzmann equation [14,15]. The method is commonly used on a mesoscopic scale and based on the discrete particle distribution function $f_i(x, t)$ which gives the number of particles moving at a given velocity at site x at time t. For two-component flow, two distribution functions are needed. One option is to have a separate distribution function for each component. The other option, used here, is to let the first distribution function $f_i(x, t)$ account for the sum of the components while the second distribution function $g_i(x, t)$ accounts for the difference between them. The distribution functions evolve according to the equations

$$f_i(x + e_i\delta t, t + \delta t) = f_i(x, t) + \Omega_{f,i} + F_i \tag{4}$$

$$g_i(x + e_i\delta t, t + \delta t) = g_i(x, t) + \Omega_{g,i} \tag{5}$$

F_i accounts for any external forces such as gravity. Ω_i is the collision operator where we have used the single relaxation time operator [16],

$$\Omega_{f,i} = \frac{f_i - f_i^{eq}}{\tau_f}, \qquad \Omega_{g,i} = \frac{g_i - g_i^{eq}}{\tau_g} \tag{6}$$

where the superscript eq represents an equilibrium distribution and $_f$ and $_g$ are the relaxation times. The relaxation time for f_i gives the kinematic viscosity ν by

$$\nu = \frac{2\tau_f - 1}{6}\delta t. \tag{7}$$