Diffuse interface modeling of three-phase contact line dynamics on curved boundaries: A lattice Boltzmann model for large density and viscosity ratios

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Abstract

We introduce a simple and efficient lattice Boltzmann method for immiscible multiphase flows, capable of handling large density and viscosity contrasts. The model is based on a diffuse-interface phase-field approach. Within this context we propose a new algorithm for specifying the three-phase contact angle on curved boundaries within the framework of structured Cartesian grids. The proposed method has superior computational accuracy compared with the common approach of approximating curved boundaries with stair cases. We test the model by applying it to four benchmark problems: (i) wetting and dewetting of a droplet on a flat surface and (ii) on a cylindrical surface, (iii) multiphase flow past a circular cylinder at an intermediate Reynolds number, and (iv) a droplet falling on hydrophilic and superhydrophobic circular cylinders under differing conditions. Where available, our results show good agreement with analytical solutions and/or existing experimental data, highlighting strengths of this new approach.

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1. Introduction

Fluid-solid interactions are ubiquitous in nature. Common examples of practical interest include flow through porous media, aerodynamics, flow around structures, and colloidal suspensions, to name a few [1]. Within this context, three-phase (solid-liquid-gas) contact line dynamics is a challenging topic of significant global research interest with scientific and engineering applications spanning self-cleaning materials, oil and gas recovery, geological carbon sequestration, groundwater contamination by non aqueous phase liquids, inkjet printers, microfluidics, etc. [2]. While of critical importance, simulating such systems still poses challenges in terms of accuracy, efficiency, and numerical stability.

Various numerical approaches to tackle this problem exist [3]. Within these, diffuse interface models [4–9] present a promising framework for studying three-phase moving contact line dynamics. In part, this is due to their intrinsic capacity to handle the singularity at the three-phase contact point while not requiring a velocity-slip model on the solid surface. Among diffusive interface models, phase-field models are a popular choice, wherein the interface between different phases is usually obtained by solving a Cahn-Hilliard like equation [10] or a conservative phase-field equation [11, 12].

The interface tracking equation in phase-field models can be solved by any number of numerical methods, including finite differences or finite volumes [13], as well as Lattice Boltzmann Methods (LBM) [14–18], the focus of

23 this work here. Ease of implementation, straightforward handling of complex
 24 boundaries, highly scalable parallelization, and not having to solve an elliptical Poisson (pressure) equation are among the main reasons behind LBM’s
 25 success [19]. The fact that interphase boundaries are essentially mesoscopic
 26 in nature [8] makes LBM, a mesoscopic approach based on kinetic theory of
 27 dense fluids [14–16], a powerful candidate for dealing with interfacial phe-
 28 nomena in general and for three-phase contact line dynamics in particular.

30 Over the past three decades, several LB models for multiphase flows
 31 have been proposed in the literature, including the color model [20, 21],
 32 the pseudo-potential model [22–25], the free-energy model [26–28], and the
 33 mean-field model [29, 30]. All these models, in their primitive forms, share an
 34 undesired feature: the inability to model multiphase systems with large den-
 35 sity ratios. From first principles, He and Doolen [16] rigorously connected
 36 kinetic theory and LBM for multiphase flows. They then evaluated and
 37 identified weaknesses of the aforementioned models. This improved thermo-
 38 dynamic understanding enabled more advanced models to emerge [31–34].

39 Inamuro *et al.* [31] proposed an LB model for multiphase flows with
 40 large density ratios; the price for this achievement was the need to solve a
 41 time-consuming pressure-Poisson equation and inability to guarantee mass
 42 conservation due to using a cut-off value in updating of density. Lee and
 43 Lin [32] proposed a three-step (pre-streaming collision, streaming, and post-
 44 streaming collision) LBM by invoking the potential form of the surface-
 45 tension force in the interface tracking formula and the stress form in the
 46 momentum equation, as had been proposed by Jamet *et al.* [7]. Using a
 47 combination of central and biased finite-difference schemes, which is shown

48 to compromise mass conservation [35], they achieved numerical stability at
 49 high density ratios. The main criticism of this model is its complicated
 50 and inefficient algorithm. Later it was shown that the three-step algorithm
 51 could be reduced to the conventional, two-step collision-streaming without
 52 losing accuracy or stability [36]. Zheng *et al.* [37] proposed a modified free-
 53 energy-based LBM for multiphase flows intended for high density ratios, but
 54 it has been shown that it is limited to density-matched fluids [38]. Fakhari
 55 and Rahimian [38] presented a phase-field LBM for binary fluids at high
 56 Reynolds numbers which is limited to moderate density ratios. Based on
 57 the Cahn-Hilliard diffuse interface model [13], Lee and Liu [36] presented
 58 an improved version of the free-energy model, which was later extended to
 59 multiphase flows at high Reynolds numbers [39]. However, the inconsistent
 60 use of central and biased finite differences means that these models [36, 39]
 61 can violate mass and momentum conservation [40]. Mass conservation was
 62 remedied in Ref. [41] but momentum conservation issues remain.

63 Of important note to our problem of interest is that most of the aforemen-
 64 tioned studies only consider multiphase flow in the absence of solid bound-
 65 aries or with neutral wall boundary conditions at best [31–33, 38]. Unlike
 66 immersed boundary methods, which are readily used to tackle curved bound-
 67 aries on Cartesian grids [42], simulation of three-phase contact line motion
 68 on curved solid boundaries is still a challenging subject in LBM. The color
 69 model is widely used to this end [34], most likely due to its efficient imple-
 70 mentation. Despite this, even with improvements over time, the color model
 71 has had limited capabilities in dealing with realistic multiphase flows with
 72 large density differences [43], with a recent exception [44]. Additionally, the

73 resulting flow field can have very large so-called spurious currents or par-
 74 asitic velocities, which are unphysical and potentially undesirable artifacts.
 75 In order to control the spurious velocities in the color model, Leclaire *et al.*
 76 [45] proposed a relationship for scaling the interfacial thickness with grid
 77 resolution. Also, some correction terms can be added to improve the nu-
 78 merical stability and accuracy of the color model for simulation of two-layer
 79 Poiseuille flow at high density and viscosity ratios [44, 46]. The pseudo-
 80 potential model shares similar drawbacks with even larger spurious velocities
 81 reported [47]. The mean-field model [30] is in our view more appealing as
 82 it has a strong physical foundation based on kinetic theory for dense fluids
 83 and is versatile in handling complex flow phenomena with rapid topologi-
 84 cal changes such as interface disintegration and coalescence [48]. Improved
 85 versions of the mean-field model are even more practical particularly for sim-
 86 ulation of multiphase flows at high density ratios [36, 41], at high Reynolds
 87 numbers [38, 39], for thermocapillary fluids [49], and most importantly for
 88 this work with fluid-solid interactions [50].

89 Although wettability effects on a flat surface have been considered in
 90 some previous LB studies [36], for those cases the solid boundaries had to
 91 be co-located with lattice nodes, restricting their application to perfectly
 92 horizontal or vertical flat walls. In some other LB models, curved surfaces
 93 are approximated by stair-cased line segments in 2D (plain segments in 3D),
 94 potentially reducing the physical accuracy of the simulations. For example,
 95 in a recent color model [34], the actual wall location is only considered for
 96 constructing the color variable at the solid boundaries, and no treatment is
 97 performed for the distribution functions. Also, the model in Ref. [50] re-

quires significant care in dealing with boundary nodes and spatial derivatives at solid boundaries. It can also suffer violation of conservation laws.

In this work, we introduce a simple, yet robust, LB model for multiphase flows at high density ratios. The proposed model does not need biased or mixed finite differences, as are required in previous models for stability reasons [32, 36, 39], and therefore conserves both mass and momentum. Aside from two nonlocal distribution functions, the proposed model requires only one nonlocal variable (the phase field), compared with three to four nonlocal variables in some previous works [36, 39, 50]. This greatly enhances the simplicity and efficiency of the algorithm. We also propose a new algorithm for prescribing the three-phase contact angle on curved boundaries without using a stair-case approximation for the solid boundary. We start by presenting the macroscopic governing equations in Sec. 2, followed by introducing the conservative phase-field LB model in Sec. 3. The new algorithm for handling wetting boundary conditions on curved surfaces is described in Sec. 4. We test the proposed model by running various benchmark problems in Sec. 5 and conclude the paper with a summary in Sec. 6.

2. Governing equations

2.1. Interface tracking equation

While most phase-field models rely on Cahn-Hilliard theory [10, 9] for interface tracking, a fourth-order derivative that arises in taking the Laplacian of the chemical potential can cause difficulties and reduce the accuracy and efficiency of numerical approximations. In this study, we use a different form of phase-field equation that contains at most second-order derivatives, which

122 is called the conservative phase-field equation [11, 12].

123 For an incompressible binary-fluid system, we define a phase-field variable
 124 ϕ in such a way that it is zero in the light fluid and one in the heavy fluid. The
 125 following interface tracking equation is used to track the interface between
 126 different fluids [12]:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = \nabla \cdot \left[M \left(\nabla \phi - \frac{4}{\xi} \phi (1 - \phi) \hat{\mathbf{n}} \right) \right] \quad (1)$$

127 where t is time, $\mathbf{u}$ is the macroscopic velocity vector, M is the mobility, ξ
 128 is the interfacial thickness, and $\hat{\mathbf{n}}$ is the unit vector normal to the interface,
 129 with its direction pointing away from the heavy fluid, such that

$$\hat{\mathbf{n}} = \frac{\nabla \phi}{|\nabla \phi|} \quad (2)$$

130 In diffuse-interface models, the equilibrium phase-field profile for an interface
 131 located at $\mathbf{x}_0$ is usually assumed to vary according to

$$\phi(\mathbf{x}) = \frac{1}{2} \left[1 - \tanh \left(\frac{|\mathbf{x} - \mathbf{x}_0|}{\xi/2} \right) \right] \quad (3)$$

132 which is typically used to set the initial condition on ϕ .

133 In the absence of fluid interaction with solid walls, or in dealing with
 134 neutral wetting conditions (*i.e.* a 90° contact angle), Neumann boundary
 135 conditions are applied $\hat{\mathbf{n}}_{\text{w}} \cdot \nabla \phi|_{\mathbf{x}_{\text{w}}} = 0$, where $\hat{\mathbf{n}}_{\text{w}}$ is the unit vector normal
 136 to, and outwards from, the solid wall. To impose a specified contact angle at
 137 a solid boundary, the following boundary condition has been proposed [6]:

$$\hat{\mathbf{n}}_{\text{w}} \cdot \nabla \phi|_{\mathbf{x}_{\text{w}}} = \Theta \phi_{\text{w}} (1 - \phi_{\text{w}}) \quad (4)$$

138 where ϕ_{w} is the phase-field value at wall and Θ is related to the equilibrium
 139 contact angle θ by

$$\Theta = -\sqrt{\frac{2\beta}{\kappa}} \cos \theta \quad (5)$$

140 where coefficients β and κ are related to the surface tension σ and interfacial
 141 thickness ξ by $\beta = 12\sigma/\xi$ and $\kappa = 3\sigma\xi/2$.

142 Note that there are underlying differences between the present approach
 143 and other models for specifying the contact angle. The majority of previ-
 144 ous studies use a geometric formula [51] to impose the wetting boundary
 145 conditions. In addition to producing larger parasitic currents, the geometric
 146 approach works only on flat walls where the normal to the surface aligns with
 147 lattice nodes. On the other hand, specifying a potential, similar to the one
 148 in Eq. (4), to model the interaction of different fluids with a solid surface is
 149 more consistent with the nature of phase-field models [5, 6].

150 2.2. Navier-Stokes equations

The continuity and momentum equations that govern isothermal, incom-
 pressible, multiphase flows are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \quad (6a)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot (\mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]) + \mathbf{F}_s + \mathbf{F}_b \quad (6b)$$

151 where ρ and μ are the local fluid density and viscosity, respectively, p is the
 152 macroscopic pressure, $\mathbf{F}_b$ is the body force, and $\mathbf{F}_s$ is the surface tension
 153 force, which can take the following form [5]:

$$\mathbf{F}_s = \mu_\phi \nabla \phi \quad (7)$$

154 where

$$\mu_\phi = 4\beta\phi(\phi - 1)(\phi - 1/2) - \kappa\nabla^2\phi \quad (8)$$

155 is the chemical potential for binary fluids.

156 3. Multiphase flow solver: lattice Boltzmann method

157 3.1. LBE for interface tracking

158 The following LBE has previously been shown to recover Eq. (1) for the
159 conservative phase field [52]:

$$h_\alpha(\mathbf{x} + \mathbf{e}_\alpha \delta t, t + \delta t) = h_\alpha(\mathbf{x}, t) - \frac{h_\alpha(\mathbf{x}, t) - h_\alpha^{\text{eq}}(\mathbf{x}, t)}{\tau_\phi + 1/2} \quad (9)$$

160 where h_α is the phase-field distribution function, τ_ϕ is the phase-field relax-
161 ation time, and $\mathbf{e}_\alpha$ is the microscopic velocity set. For the D2Q9 lattice,
162 which is used in this study [15]

$$\mathbf{e}_\alpha = c \begin{cases} (0, 0), & \alpha = 0 \\ (\cos \theta_\alpha, \sin \theta_\alpha), & \theta_\alpha = (\alpha - 1)\pi/2, \quad \alpha = 1-4 \\ (\cos \theta_\alpha, \sin \theta_\alpha)\sqrt{2}, & \theta_\alpha = (2\alpha - 9)\pi/4, \quad \alpha = 5-8 \end{cases} \quad (10)$$

163 where $c = \delta x / \delta t = 1$ and δx and δt are the lattice length scale and time
164 scale, respectively (on uniform grids $\delta x = \delta t = 1$). The equilibrium phase-field
165 distribution function is given by

$$h_\alpha^{\text{eq}} = \phi \Gamma_\alpha + w_\alpha \frac{M}{c_s^2} \left[\frac{4}{\xi} \phi (1 - \phi) \right] (\mathbf{e}_\alpha \cdot \hat{\mathbf{n}}) \quad (11)$$

166 where

$$\Gamma_\alpha = w_\alpha \left[1 + \frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right] \quad (12)$$

167 $c_s = c/\sqrt{3}$ is the speed of sound in the system and w_α is the weight coefficient
168 set, where $w_0 = 4/9$, $w_{1-4} = 1/9$, and $w_{5-8} = 1/36$. Mobility M is related
169 to the phase-field relaxation time by

$$M = \tau_\phi c_s^2 \delta t \quad (13)$$

Equation (9) is usually solved with a two-step collision-streaming approach as

$$h_{\alpha}^*(\mathbf{x}, t) = h_{\alpha} - \frac{h_{\alpha} - h_{\alpha}^{\text{eq}}}{\tau_{\phi} + 1/2} \Big|_{(\mathbf{x}, t)} \quad (14a)$$

$$h_{\alpha}(\mathbf{x} + \mathbf{e}_{\alpha}\delta t, t + \delta t) = h_{\alpha}^*(\mathbf{x}, t) \quad (14b)$$

where the asterisk denotes the pre-streaming, or post-collision, state. After the streaming step, the phase field is updated by taking the zeroth moment of the phase-field distribution function

$$\phi = \sum_{\alpha} h_{\alpha} \quad (15)$$

and the density ρ is found by a simple linear interpolation

$$\rho = \rho_L + \phi(\rho_H - \rho_L) \quad (16)$$

where ρ_L and ρ_H are the densities of the light and heavy fluids, respectively.

It is worth noting that, aside from advantages in computational cost and efficiency, the conservative phase-field equation is much less dispersive when compared with the Cahn-Hilliard equation, particularly when implemented within the LBM framework. This lower-dispersion error hinders the phase-field variable from noticeably undershooting its lowest equilibrium value (here $\phi_{\min} = 0$). Therefore the density, which is linearly interpolated from the phase-field via Eq. (1), is less prone to unphysically becoming negative and leading to numerical instabilities at high density ratios. This is a key factor in achieving numerically stable solutions with a high density ratio.

3.2. LBE for hydrodynamics

Based on the explicit approach proposed by He *et al.* [29], we use an improved hydrodynamic evolution equation [38] to update the pressure and

187 velocity fields. The lattice Boltzmann equation for nearly incompressible
188 multiphase flows can be written as

$$\bar{g}_\alpha(\mathbf{x} + \mathbf{e}_\alpha \delta t, t + \delta t) = \bar{g}_\alpha(\mathbf{x}, t) + \Omega_\alpha(\mathbf{x}, t) + F_\alpha(\mathbf{x}, t) \quad (17)$$

189 where $\bar{g}_\alpha$ is the modified hydrodynamic distribution function for the nearly
190 incompressible fluids [30, 39], Ω_α is the collision operator, and the forcing
191 term is [41]

$$F_\alpha = \delta t [(\Gamma_\alpha - w_\alpha)(\rho_H - \rho_L)c_s^2 + \Gamma_\alpha \mu_\phi] (\mathbf{e}_\alpha - \mathbf{u}) \cdot \nabla \phi + \delta t \Gamma_\alpha (\mathbf{e}_\alpha - \mathbf{u}) \cdot \mathbf{F}_b \quad (18)$$

192 In this study we use a multiple-relaxation-time (MRT) model in the col-
193 lision operator [53], which has superior stability and accuracy over single-
194 relaxation-time (SRT) or Bhatnagar-Gross-Krook (BGK) models. The MRT
195 collision operator is

$$\Omega_\alpha = \Omega_\alpha^{\text{MRT}} = -\mathbf{M}^{-1} \hat{\mathbf{S}} \mathbf{M} (\bar{g}_\alpha - \bar{g}_\alpha^{\text{eq}}) \quad (19)$$

196 where the modified equilibrium distribution function is defined by

$$\bar{g}_\alpha^{\text{eq}} = g_\alpha^{\text{eq}} - \frac{1}{2} F_\alpha \quad (20)$$

197 and

$$g_\alpha^{\text{eq}} = p w_\alpha + \rho c_s^2 (\Gamma_\alpha - w_\alpha) \quad (21)$$

198 is the equilibrium distribution function for nearly incompressible fluids. $\mathbf{M}$
199 is an orthogonal transformation, which transforms the distribution functions
200 from physical space into moment space [53], and $\hat{\mathbf{S}}$ is the diagonal relaxation
201 matrix, which is chosen to be

$$\hat{\mathbf{S}} = \text{diag}(1, 1, 1, 1, 1, 1, 1, s_\nu, s_\nu) \quad (22)$$

202 where

$$s_\nu = \frac{1}{\tau + 1/2} \quad (23)$$

203 with τ being the hydrodynamic relaxation time (or simply the relaxation
204 time), which is related to the kinematic viscosity of the system by $\nu = \tau c_s^2 \delta t$,
205 and is calculated by using a harmonic interpolation from the phase field

$$\frac{1}{\tau} = \frac{1}{\tau_L} + \phi \left(\frac{1}{\tau_H} - \frac{1}{\tau_L} \right) \quad (24)$$

206 where τ_L and τ_H are the relaxation rates for the light and heavy fluids, respec-
207 tively. If all the relaxation rates in Eq. (22) are set to s_ν , the BGK model is
208 recovered.

After solving LBE (17) using a routine collision-streaming sequence, hydrodynamic properties are calculated as

$$\mathbf{u} = \frac{1}{\rho c_s^2} \sum_{\alpha} \bar{g}_{\alpha} \mathbf{e}_{\alpha} + \frac{\delta t}{2\rho} (\mathbf{F}_s + \mathbf{F}_b) \quad (25a)$$

$$p = \sum_{\alpha} \bar{g}_{\alpha} + \frac{\delta t}{2} (\rho_H - \rho_L) c_s^2 \mathbf{u} \cdot \nabla \phi \quad (25b)$$

209 Note that velocity is updated before pressure.

210 It is worth mentioning that the only non-local macroscopic quantity in
211 the proposed LB equations is the phase-field variable. Gradients of the phase
212 field in Eq. (2) and Eq. (7), and its Laplacian in Eq. (8) are calculated using
213 second-order, isotropic centered differences [54]. Moreover, we do not treat
214 the $\mathbf{e}_{\alpha} \cdot \nabla \phi$ term as a directional derivative along the lattice links [36], but
215 instead compute the gradient of the phase field $\nabla \phi$ using isotropic differences
216 and then execute the dot product, which improves the isotropy in the solu-
217 tion. We avoid using a combination of central and biased differences as was
218 done in previous studies [36, 39], because it leads to violations of mass and

219 momentum conservation [40]. Note that the main reason for using biased
 220 differences in Ref. [36] is to reduce the dispersion error in the numerical dis-
 221 cretization of the advection term. Compared with the Cahn-Hilliard-based
 222 model in Ref. [36], the conservative phase-field LBE in Sec. (3.1) produces
 223 much less numerical dispersion, even when central differences are employed.
 224 This allows us to attain a stable numerical scheme at large density and vis-
 225 cosity ratios using a minimal number (three) of supporting nodes.

226 4. Curved boundary treatment

227 4.1. Wetting boundary condition for the phase field

228 In order to apply the wetting condition given in Eq. (4) on a curved
 229 boundary, we need the unit vector normal to the solid wall ($\hat{\mathbf{n}}_{\mathbf{w}}$) along with
 230 the gradient of the phase field $\nabla\phi|_{\mathbf{x}_{\mathbf{w}}}$ and its value $\phi_{\mathbf{w}}$ at the wall. To this
 231 end we propose two different schemes.

232 A schematic implementation of the first approach for a typical boundary
 233 node is illustrated in Fig. 1. We use the fluid nodes, shown by blue dots,
 234 to obtain the unknown phase-field value at the boundary node ($\phi_{i,j}$), shown
 235 by a black dot, using the following procedure: first, we invoke a centered
 236 difference for the left-hand-side of Eq. (4) to obtain

$$\hat{\mathbf{n}}_{\mathbf{w}} \cdot \nabla\phi|_{\mathbf{x}_{\mathbf{w}}} = \left. \frac{\partial\phi}{\partial n_{\mathbf{w}}} \right|_{\mathbf{x}_{\mathbf{w}}} = \frac{\phi_{\mathbf{p}} - \phi_{i,j}}{2h} = \Theta\phi_{\mathbf{w}}(1 - \phi_{\mathbf{w}}) \quad (26)$$

237 where $h = |\mathbf{x}_{\mathbf{p}} - \mathbf{x}_{\mathbf{w}}|$ is the distance between the solid wall and the interpo-
 238 lated point, which is known *a priori* given the location of the wall boundary.
 239 We eliminate $\phi_{\mathbf{w}}$ in Eq. (26) by using $\phi_{\mathbf{w}} = (\phi_{\mathbf{p}} + \phi_{i,j})/2$. This yields a

Figure 1: Schematic depicting the bidirectional interpolation to obtain the unknown phase-field value, $\phi_{i,j}$, at a typical boundary node (black dots). Blue dots are fluid nodes and $\mathbf{n}_w$ is the normal vector pointing away from the solid wall.

240 quadratic equation, the solution of which gives

$$\phi_{i,j} = \frac{1}{a} \left(1 + a - \sqrt{(1+a)^2 - 4a\phi_p} \right) - \phi_p, \quad a = h\Theta \neq 0 \quad (\theta \neq 90^\circ) \quad (27)$$

241 For neutral wetting conditions ($\theta = 90^\circ$), the trivial solution would be $\phi_{i,j} =$
 242 ϕ_p . The only unknown quantity in Eq. (27) is ϕ_p , which can be determined
 243 by a biquadratic interpolation from the adjacent fluid nodes, as depicted in
 244 Fig. 1. The only caveat is that $\phi_{i,j}$ will appear in the resulting bidirectional
 245 interpolation scheme. As a remedy, we can either solve Eq. (27) iteratively
 246 or use the value of $\phi_{i,j}$ from the previous time step. For slowly evolving
 247 flows, especially close to a stationary solid wall, $\phi_{i,j}$ is not expected to vary
 248 rapidly. As such, and also to avoid a costly iterative scheme, we choose the
 249 latter approach and use the value of $\phi_{i,j}$ from the previous time step in the
 250 bidirectional interpolation that is needed to find ϕ_p .

251 Alternatively, for our second approach, we can use unidirectional inter-
 252 polations, either in the x -direction or in the y -direction, to find ϕ_p . A sketch
 253 demonstrating this approach is shown in Fig. 2. If the magnitude of the slope
 254 of the vector normal to the boundary is bigger than one, which is the case
 255 in Fig. 2(a), then the (linear or quadratic) interpolation is carried out in the
 256 x -direction; otherwise, the interpolation is carried out in the y -direction, as
 257 depicted in Fig. 2(b), to find the value of ϕ_p . Because the location of the
 258 solid wall $\mathbf{x}_w$ is no longer half-way between the boundary node $\mathbf{x}_{i,j}$ and the
 259 interpolated point $\mathbf{x}_p$, Eq. (26) must be modified. The final result is

$$\phi_{i,j} = \frac{s+h}{2ah} \left(1 + a - \sqrt{(1+a)^2 - 4a\phi_p} \right) - \frac{s}{h}\phi_p, \quad a = h\Theta \neq 0 \quad (\theta \neq 90^\circ) \quad (28)$$

260 where $s = |\mathbf{x}_w - \mathbf{x}_{i,j}|$ is the distance between the boundary node and the

Figure 2: Unidirectional interpolation schemes. Schematic of boundary nodes and fluid nodes around a curve boundary.

261 solid wall.

262 4.2. Boundary conditions for the distribution functions

263 In addition to the wetting boundary condition for the phase field at the
 264 wall, the incoming distribution functions from the boundary nodes towards
 265 the fluid nodes must be determined. Referring to Fig. 3 for a typical boundary
 266 node $\mathbf{x}_b$, and defining α^- such that $\mathbf{e}_{\alpha^-} = -\mathbf{e}_{\alpha}$, the value of $\bar{g}_{\alpha^-}^*(\mathbf{x}_b)$ before
 267 the streaming step is unknown (recall the asterisk denotes the pre-streaming,
 268 or post-collision, state). There are three common curved boundary models
 269 for specifying $\bar{g}_{\alpha^-}^*$ at the boundary:

270 1. Filippova–Hänel model [55]:

271 The boundary treatment of Filippova and Hänel [55], with the modifi-
 272 cations proposed by Mei *et al.* [56], is a widely used curved boundary

Figure 3: Schematic of boundary nodes and fluid nodes around a curved boundary.

273 condition in single-phase flows. Here, we use a variant of this model
 274 for a stationary solid boundary and a modified equilibrium distribution
 275 function to reduce the incompressibility error of the LBM. In essence,
 276 the following formula will be used to determine the unknown distribu-
 277 tion functions at the solid boundaries

$$\bar{g}_{\alpha-}^*(\mathbf{x}_b) = (1 - \chi)\bar{g}_{\alpha-}^*(\mathbf{x}_f) + \chi\tilde{g}_{\alpha-}(\mathbf{x}_{bf}) \quad (29)$$

278 where

$$\tilde{g}_{\alpha-}(\mathbf{x}_{bf}) = g_{\alpha-}^{eq}(\mathbf{x}_f) + \rho(\mathbf{x}_f)w_{\alpha}e_{\alpha} \cdot (\mathbf{u}_b - \mathbf{u}_f) \quad (30)$$

and

$$\mathbf{u}_b = \begin{cases} \mathbf{u}_{ff}, & \chi = \frac{2\Delta - 1}{\tau - 2}, \quad \text{for } 0 \leq \Delta < \frac{1}{2} \\ \frac{\Delta - 1}{\Delta}\mathbf{u}_f, & \chi = \frac{2\Delta - 1}{\tau}, \quad \text{for } \frac{1}{2} \leq \Delta < 1 \end{cases} \quad (31a)$$

$$\chi = \frac{2\Delta - 1}{\tau}, \quad \text{for } \frac{1}{2} \leq \Delta < 1 \quad (31b)$$

279 where

$$\Delta = \frac{|\mathbf{x}_f - \mathbf{x}_w|}{|\mathbf{x}_f - \mathbf{x}_b|} \quad (32)$$

280 2. Bouzidi–Firdaouss–Lallemand model [57]:

The following two-part formula was proposed by Bouzidi *et al.* [57]

$$\bar{g}_{\alpha-}^*(\mathbf{x}_b) = \begin{cases} 2\Delta \bar{g}_{\alpha}^*(\mathbf{x}_f) + (1 - 2\Delta) \bar{g}_{\alpha}^*(\mathbf{x}_{ff}), & 0 \leq \Delta < \frac{1}{2} \quad (33a) \\ \frac{1}{2\Delta} \bar{g}_{\alpha}^*(\mathbf{x}_f) + \left(1 - \frac{1}{2\Delta}\right) \bar{g}_{\alpha-}^*(\mathbf{x}_{ff}), & \frac{1}{2} \leq \Delta < 1 \quad (33b) \end{cases}$$

281

282 3. Yu–Mei–Shyy model [58]:

283 Yu *et al.* [58] proposed a one-step relation to establish the incoming
284 distribution functions according to

$$\bar{g}_{\alpha-}^*(\mathbf{x}_b) = \frac{\Delta}{1 + \Delta} [\bar{g}_{\alpha-}^*(\mathbf{x}_f) + \bar{g}_{\alpha}^*(\mathbf{x}_f)] + \frac{1 - \Delta}{1 + \Delta} \bar{g}_{\alpha}^*(\mathbf{x}_{ff}) \quad (34)$$

285 It is worth noting that both Eq. (33) and (29) recover the commonly
286 used mid-way bounce-back on the link [59] when $\Delta = 1/2$, while the one-
287 step formula (34) does not. Despite this, all the aforementioned methods
288 produce virtually identical results in all of our simulations. We will only
289 present the numerical results obtained using the first model [56].

290 In order to eliminate mass leakage from the wall boundaries, and also for
291 stability reasons, we use mid-way bounce back to determine the unknown
292 phase-field distribution function at the boundary nodes such that

$$h_{\alpha-}^*(\mathbf{x}_b) = h_{\alpha}^*(\mathbf{x}_f) \quad (35)$$

293 Since we are dealing with stationary solid walls in this paper, the pro-
294 posed curved boundary conditions can be applied very efficiently by storing

the necessary data at the beginning of the simulation. Given a prespecified curved boundary we can identify the boundary nodes (shown by black dots in Figs. 1–3) and store their coordinate indices (i, j) together with the necessary parameters s, h, d_x, d_y , and Δ . For some problems (*e.g.* flow through complex porous media) the computations would be more efficient if the curved boundary treatment is turned off. We can easily achieve this while still using the proposed model by replacing curved boundaries with appropriate stair cases and implementing mid-way bounce-back. We can also deal with moving boundary problems by adding additional terms related to the motion of the boundary to the curved boundary models above. Here we only deal with stationary solid walls and leave the moving boundary problems to future studies.

5. Numerical results

In this section we test and validate the proposed LBM by considering various interesting problems involving three-phase contact line dynamics. We start simple with a drop on a flat wall, for which an analytical relation between the equilibrium contact angle and the height of the drop can be derived, and progressively add to the complexity of the problems. All input parameters will be presented in lattice units, or in dimensionless form, unless otherwise stated.

5.1. Test 1: wetting/dewetting of a droplet on a flat surface

As our initial condition we place a semi-circular droplet on top of a flat wall with an initial contact angle of 90° , which would be the equilibrium solution for neutral wetting conditions. We then specify different contact

Figure 4: Droplet wetting and dewetting on a (a) hydrophilic surface, and (b) hydrophobic surface.

angles by imposing boundary condition (4) and allow the droplet to evolve to
 its true equilibrium state. In the absence of gravity, the only mobilizing factor
 is interfacial tension. If $\theta < 90^\circ$ the solid wall is said to be *hydrophilic* and
 the droplet starts wetting the surface spreading to increase its contact area
 with the surface until the equilibrium contact angle is attained. On the other
 hand, if $\theta > 90^\circ$ then the solid wall is said to be *hydrophobic* and the droplet
 retracts in such a way as to reduce its contact area with the surface until the
 equilibrium contact angle is attained. Numerical results of these two states
 are shown in Fig. 4 for select contact angles. The simulation parameters are
 $\sigma = 0.01$, $M = 0.02$, $\rho_H/\rho_L = 1000$, and $\mu_H/\mu_L = 100$, where μ_L and μ_H
 are the bulk viscosities of the light and heavy fluids, respectively. The initial
 droplet is centered at $(L_0/2, 0)$, where L_0 is the length of the domain. The
 computational domain of size $L_0 \times L_0/2$ is resolved with 128×64 grid points.
 The initial radius of the semi-droplet is $R = L_0/8 = 16$. Periodic boundary
 conditions are applied in the x -direction and mid-way bounce-back is used
 on the top boundary.

To test the accuracy of the results, we compare an analytical relationship
 between the specified contact angle θ and the maximum height of the droplet

Figure 5: Contact angle (θ) between a droplet and a flat surface.

337 h_{max} above the flat surface, as demonstrated in Fig. 5, at equilibrium for two
 338 different values of interfacial thickness, $\xi = 3$ and $\xi = 4$. The mass per
 339 unit density (area) of the droplet is $A^{eq} = r^2 (\pi - \alpha + \sin \alpha \cos \alpha)$, where
 340 $\alpha = \pi - \theta$. Given an initial mass per unit density $A^0 = \pi R^2/2$, conservation
 341 of mass means

$$\frac{h_{max}}{R} = (1 - \cos \theta) \sqrt{\frac{\pi}{2\theta - \sin 2\theta}} \quad (36)$$

342 Figure 6 shows a good agreement between numerical results and analytical
 343 solution over a wide range of contact angles. The results for $\xi = 4$ are slightly
 344 more accurate than those with $\xi = 3$, particularly when the equilibrium
 345 contact angle is further away from 90° . The maximum error, which occurs
 346 for a hydrophilic surface with $\theta = 30^\circ$, is measured at 16% for $\xi = 3$ and 9%
 347 for $\xi = 4$. In the rest of the simulations we use $\xi = 4$ with $M = 0.02$.

Figure 6: Contact angle versus dimensionless height of the drop on a flat surface.

Figure 7: Schematic of the contact angle between a droplet with radius r and a solid cylinder with radius R_s .

348 5.2. Test 2: wetting/dewetting of a droplet on a cylindrical surface

349 Next we will evaluate the accuracy of the proposed wetting boundary
 350 conditions on curved surfaces by placing a droplet on top of a circular cylinder
 351 in the absence of gravity. We specify contact angles ranging from $45^\circ \leq \theta \leq$
 352 135° . The droplet evolves until the prescribed contact angle at the three-
 353 phase contact point is reached. A schematic of the shape of the droplet resting
 354 on the circular cylinder is shown in Fig. 7. At equilibrium, the interfacial
 355 tension forces tend to minimize the free energy in the system by minimizing
 356 the peripheral area. Therefore, an arc with radius r is formed on top of
 357 the cylinder with radius R_s . Referring to Fig. 7, we can calculate the mass
 358 per unit density (area) of the circular droplet with radius r , whose center is
 359 distance k from the center of the circular cylinder, in terms of r and $k(r, \theta)$.
 360 The resulting relation is

$$\begin{aligned}
 A(r, k) = & \pi r^2 - r^2 \cos^{-1} \left(\frac{k^2 + r^2 - R_s^2}{2kr} \right) \\
 & - R_s^2 \cos^{-1} \left(\frac{k^2 - r^2 + R_s^2}{2kR_s} \right) \\
 & + k \sqrt{R_s^2 - \left(\frac{k^2 - r^2 + R_s^2}{2k} \right)^2}
 \end{aligned} \tag{37}$$

361 where k is related to r and θ by the cosine law

$$k(r, \theta) = \sqrt{r^2 + R_s^2 - 2rR_s \cos \theta}. \tag{38}$$

362 We start the simulations by placing a circular cylinder centered at $(L_0/2, L_0/4)$
 363 and a droplet with radius $R = R_s = L_0/6$ centered at $(L_0/2, L_0/4 + R_s)$.
 364 The properties of the fluids are $\rho_H/\rho_L = 1000$ and $\mu_H/\mu_L = 100$. First we
 365 examine the grid independency of the results on three different grids with

Figure 8: Grid independency of the results for a droplet sitting on a cylindrical surface at $t\sigma/\mu_{\text{H}}R = 1800$. Comparison between three resolutions: 64×64 (dotted green line), 128×128 (solid blue line), and 256×256 (dashed red line).

366 $L_0 = 64, 128$, and 256 . Periodic boundary conditions are used in the x -
 367 direction and mid-way bounce-back is applied at the bottom and top of the
 368 domain. The results are shown in Fig. 8 for two different contact angles, cor-
 369 responding to a hydrophilic ($\theta = 45^\circ$) and a hydrophobic ($\theta = 120^\circ$) surface,
 370 at $t\sigma/\mu_{\text{H}}R = 1800$. As can be observed, the drop interface is indistinguish-
 371 able when increasing the number of grid points from 128×128 to 256×256 .
 372 Therefore, we will use the 128×128 grid, with $\sigma = 0.01$, to carry on the rest
 373 of the simulations in this section.

374 Figure 9 shows qualitative results for three different contact angles. Using
 375 $r = k = R_{\text{s}}$ in Eq. (37) gives us the initial mass per unit density of the drop

$$A(R_{\text{s}}, R_{\text{s}}) = \left(\frac{\pi}{3} + \frac{\sqrt{3}}{2} \right) R_{\text{s}}^2 \quad (39)$$

376 By equating the initial mass of the drop in Eq. (39) with its equilibrium

Figure 9: Equilibrium profile of a droplet on a cylindrical surface for three different contact angles.

377 mass in Eq. (37) we obtain an implicit relation between r and θ . We solve
 378 the resulting relation iteratively using the secant method. We can then mea-
 379 sure H_{max} (the distance between the top of the droplet and the center of
 380 the cylinder) in the simulations, and compare it with the analytical results
 381 ($H_{max} = k + r$). Variation of the dimensionless height of the drop (H_{max}/R)
 382 versus contact angle is plotted in Fig. 10. In addition to the numerical results
 383 obtained by the proposed curved boundary treatment, results obtained by
 384 approximating the curved wall as a stair-case (with bounce-back on the link),
 385 as is commonly done, are compared with the analytical solution. As can be
 386 seen in Fig. 10, approximating the curved wall with a stair-cased boundary
 387 leads to erroneous results, becoming progressively worse as the contact an-
 388 gle deviates more and more from neutral conditions. On the other hand,
 389 the numerical findings obtained by the present curved boundary model are
 390 in excellent agreement with the analytical solution. The maximum error,
 391 which occurs for a droplet in contact with a hydrophilic surface at $\theta = 45^\circ$,
 392 is less than 1% for the curved boundary model while it is about 5% for the

393 stair-cased approximation.

Figure 10: Comparison between the analytical solution and numerical results for a droplet in contact with a cylindrical surface.

394 5.3. Test 3: unsteady flow past a circular cylinder

395 Single-phase, incompressible, uniform flow past a circular cylinder is a
 396 standard and widely studied problem with very well documented results [60–
 397 68]. Once the Reynolds number supersedes a threshold value, $Re_{cr} \sim 49$ [63],
 398 the flow becomes unstable and the so-called von Kármán vortex street forms
 399 downstream of the cylinder. Here we extend this problem to a *multiphase*
 400 flow past a circular cylinder and compare the findings, particularly the drag
 401 and lift coefficients, with the available data for single-phase flow.

Figure 11: Schematic of the computational domain and boundary conditions for uniform flow past a circular cylinder.

402 The computational domain is shown in Fig. 11. A circular cylinder of
 403 diameter D is centered at $x = 8D$ from the inlet. The length and height
 404 of the computational domain are $L = 32D$ and $H = 16D$, respectively. In
 405 order to expedite initiation of vortex shedding, the cylinder is displaced from
 406 the centerline by one lattice node in the y -direction. The no-slip boundary
 407 condition on the surface of the cylinder is realized by applying the boundary
 408 conditions in Eq. (29). A uniform flow $(u, v) = (U_0, 0)$ is imposed at the inlet
 409 and along the top and bottom of the domain by invoking the nonequilibrium
 410 bounce-back rule after the streaming step [69]

$$f_{\alpha^-} = f_{\alpha} + f_{\alpha^-}^{eq} - f_{\alpha}^{eq} \quad (40)$$

411 where $f_{\alpha} \in (h_{\alpha}, \bar{g}_{\alpha})$ denotes the unknown incoming distribution function
 412 after the streaming step. For example, for the nearly incompressible LBM
 413 proposed by He and Luo [70], which is used in our single-phase flow simula-

414 tions, the non-equilibrium bounce back at the inlet gives

$$\bar{g}_{\alpha^-} = \bar{g}_{\alpha} + 2w_{\alpha}\rho_0 U_0 \quad (41)$$

415 where $\alpha^- \in \{1, 5, 8\}$, $\alpha \in \{3, 7, 6\}$, and ρ_0 is a constant representing the den-
 416 sity of the single-phase fluid. Convective boundary conditions for the macro-
 417 scopic properties (such as p , u , v , etc.) are applied at the outlet by solving
 418 the following equation using an implicit, upwind finite-difference scheme:

$$\frac{\partial q}{\partial t} + U_0 \frac{\partial q}{\partial x} = 0 \quad (42)$$

419 where q is a placeholder for the macroscopic properties. Then the non-
 420 equilibrium bounce-back is invoked at the outlet to find the incoming distri-
 421 bution functions. The initial condition is the potential flow solution around
 422 a circular cylinder in an infinite domain. The Reynolds number of the flow
 423 $\text{Re} = U_0 D / \nu$ is fixed at $\text{Re} = 100$. The momentum-exchange method [71] is
 424 used to calculate the force exerted on the cylinder such that

$$\mathbf{F}(t) = -\frac{1}{c_s^2} \sum_{\mathbf{x}_b} \sum_{\alpha^-} \mathbf{e}_{\alpha^-} [\bar{g}_{\alpha^-}^*(\mathbf{x}_b, t) + \bar{g}_{\alpha}^*(\mathbf{x}_f, t)] \quad (43)$$

425 where the summation at $\mathbf{x} = \mathbf{x}_b$ is taken over the α^- -directions that are
 426 pointing away from the circular cylinder. After calculating the force on the
 427 cylinder, the drag and lift coefficients are computed as

$$\begin{aligned} C_D &= \frac{F_x}{1/2 \rho_0 U_0^2 D} \\ C_L &= \frac{F_y}{1/2 \rho_0 U_0^2 D} \end{aligned} \quad (44)$$

428 Additionally we calculate the Strouhal number, defined as $\text{St} = f_s D / U_0$,
 429 where f_s is the shedding frequency determined from the alternation of the
 430 lift force on the surface of the cylinder.

Table 1: Average drag coefficient, peak-to-peak lift coefficient, and Strouhal number for unsteady flow past a circular cylinder at $Re = 100$.

Reference	$\overline{C}_D$	C_L^{peaks}	St
Liu et al. [66]	1.350	± 0.339	0.165
Calhoun [67]	1.330	± 0.298	0.175
present ($L_0 = 256$)	1.377	± 0.324	0.170
present ($L_0 = 512$)	1.400	± 0.348	0.172
present ($L_0 = 1024$)	1.408	± 0.355	0.172

431 5.3.1. single-phase flow simulations

432 First, the time-averaged drag coefficient is calculated on three different
433 grids of differing resolution, which are 256×128 , 512×256 , and 1024×512 , to
434 examine grid independence of the results. The numerical findings, together
435 with available experimental and numerical data, are provided in Table 1.
436 As can be seen, the calculated drag coefficient and the Strouhal number
437 are in reasonable agreement with the available data in the literature. Also,
438 increasing the resolution from 512×256 to 1024×512 has minimal effect
439 on the predicted values for the drag and Strouhal number. Therefore, the
440 512×256 grid will be used for further simulations. Variation of drag and lift
441 coefficients versus dimensionless time $t^* = tU_0/D$ is also plotted in Fig. 12.

442 5.3.2. multiphase flow simulations

443 Now we consider the dynamics of binary fluid flow past a circular cylinder.
444 In order to study the effect of surface tension, the density ratio and the
445 viscosity ratio are set to one and the wettability of the cylinder is examined

Figure 12: Variation of the drag and lift coefficients for the unsteady single-phase flow past a circular cylinder at $Re = 100$.

Figure 13: Unsteady flow past a circular cylinder at $Re = 100$. Left: vorticity (flooded contour) in the single-phase flow; Right: vorticity (flooded contour) and interface location (black line) in the multiphase flow.

by changing the equilibrium contact angle. We consider two different contact angles: $\theta = 30^\circ$ and $\theta = 150^\circ$ with $\sigma = 0.002$. Qualitative comparison between the single-phase flow and multiphase flow simulations is shown in Fig. 13. Although the vorticity contours for both cases are similar, the interfacial tension forces in the binary fluid case compete with viscous forces and cause more dissipation in the flow field as is evident from the faded vorticity contours in the multiphase flow simulations.

Figure 14: Variation of the drag and lift coefficients for the unsteady multiphase flow past a circular cylinder at $Re = 100$.

Similar to the single-phase flow simulations, we can monitor the variation of drag and lift coefficients versus time and measure the resulting Strouhal number. The drag and lift coefficients are plotted in Fig. 14 for two different contact angles. As can be seen, the averaged drag coefficient for both cylinders are almost identical and the values are lower than those in the single-phase flow case. Similar reductions in drag coefficient have been ob-

Table 2: Average drag coefficient, peak-to-peak lift coefficient, and Strouhal number for multiphase flow past a circular cylinder at $\text{Re} = 100$.

	$\overline{C}_D$	$C_L^{\min}$	$C_L^{\max}$	St
$\theta = 30^\circ$	1.284	-0.131	0.078	0.159
$\theta = 150^\circ$	1.281	-0.077	0.167	0.159

served in simulations of viscoelastic polymeric flows around cylinder [72].
 With regard to the lift, it is interesting to note that the average lift coefficient for both cases is non-zero. The circular cylinder with $\theta = 150^\circ$ produces a slightly positive lift coefficient while the other cylinder with $\theta = 30^\circ$ results in a slightly negative value for the average lift coefficient. The magnitude of the peak-to-peak lift coefficient for both cylinders are almost identical (due to antisymmetry in the equilibrium contact angles) but with opposite direction. The reason for this phenomenon becomes clear by referring to Fig. 15, which shows the equilibrium profile of a quiescent two-layer fluid in the vicinity of the cylinder for both cases. As can be inferred from Fig. 15(a), the fluids exert a negative (downward) lift force on the cylinder with $\theta = 30^\circ$ while the net lift force experienced by the other cylinder with $\theta = 150^\circ$ in Fig. 15(b) is positive (upwards). This is the reason we observe a nontrivial average lift coefficient in Fig. 14.

5.4. Test 4: droplet falling on a circular cylinder

In order to show the versatility of the proposed model in dealing with three-phase contact line dynamics on curved surfaces, we consider droplet impact dynamics on a circular cylinder with different wettability properties.

Figure 15: Equilibrium profile of a two-layer binary fluid around a solid cylinder for (a) $\theta = 30^\circ$, and (b) $\theta = 150^\circ$.

477 Droplet impact onto spherical and cylindrical objects has been investigated
 478 experimentally [73–76] and numerically [77, 42]. Most of these are for drop
 479 impact at large velocities (high Weber numbers). Our computational setup
 480 is depicted in Fig. 16. A circular droplet with radius $R = L_0/10$ is cen-
 481 tered at $(L_0/2, 3L_0/2)$ in a domain of size $L_0 \times 2L_0$, where $L_0 = 128$. A
 482 circular cylinder with radius $R_s = R$ is also centered at $(L_0/2, L_0)$. The
 483 droplet accelerates from rest towards the solid cylinder due to gravity, which
 484 is incorporated in the LBE via a body force $\mathbf{F}_b = -\rho g_y \hat{\mathbf{j}}$, where g_y is the
 485 magnitude of gravitational acceleration. The pressure field is initialized with
 486 a hydrostatic distribution. Periodic boundary conditions are applied in the
 487 x -direction and link bounce-back are applied at the bottom and top of the
 488 domain.

489 This problem is characterized by contact angle and four other dimension-
 490 less groups: density ratio ρ_H/ρ_L , viscosity ratio μ_H/μ_L , gravity Reynolds num-
 491 ber $\text{Re}_{\text{Gr}} = \rho_H \sqrt{g_y D^3} / \mu_H$ and Eötvös or Bond number $\text{Bo} = g_y (\rho_H - \rho_L) D^2 / \sigma$.
 492 Gravity-based dimensionless time is defined by $t_g^* = t \sqrt{g_y / D}$. In the liter-
 493 ature, results are often also presented in terms of alternative dimension-

Figure 16: Computational domain for a droplet falling on a cylindrical surface.

less groups, the Reynolds and Weber numbers, where $\text{Re} = \rho_{\text{H}} U_i D / \mu_{\text{H}}$ and $\text{We} = \rho_{\text{H}} U_i^2 D / \sigma$, respectively. These are based on the velocity of the droplet at the instant of impact, U_i . They can be combined to form the Ohnesorge number $\text{Oh} = \sqrt{\text{We}} / \text{Re}$, which quantifies the ratio of viscous forces to surface tension forces. In all examples here we set the properties of the fluids such that $\rho_{\text{H}} / \rho_{\text{L}} = 1000$, $\mu_{\text{H}} / \mu_{\text{L}} = 100$, and $\text{Re}_{\text{Gr}} = 25$. We then examine the effects of surface tension and contact angle at relatively small Bond numbers, $\text{Bo} \sim \mathcal{O}(1)$.

Results for a droplet impacting a hydrophilic surface with $\theta = 40^\circ$ are shown in Fig. 17 for $\text{Bo} = 2.2$ ($\text{Oh} = 0.06$) and in Fig. 18 for $\text{Bo} = 6.6$ ($\text{Oh} = 0.11$). For the lower Bond number in Fig. 17 the drop tends to adhere to the surface of the hydrophilic cylinder and evolve slowly. It then engulfs

Figure 17: Droplet impact on a hydrophilic cylindrical surface with $\theta = 40^\circ$. $\rho_H/\rho_L = 1000$, $\mu_H/\mu_L = 100$, $\text{Re}_{\text{Gr}} = 25$, $\text{Bo} = 2.2$ ($\text{Oh} = 0.06$). See supplementary materials for simulation videos.

the perimeter of the hydrophilic cylinder at $t_g^* = 6$ and starts stretching at $t_g^* = 8$ due to the influence of gravity. External gravitational forces are not strong enough compared with the surface tension force between the droplet and the hydrophilic cylinder, causing the drop to momentarily hang from the circular surface while covering its whole area. On the other hand, the gravitational force in Fig. 18 is strong enough to prevail over the interfacial tension between the drop and the solid surface, causing the droplet to break up and detach from the surface of the hydrophilic cylinder.

In order to consider wettability effects of the cylindrical surface we increase the contact angle to $\theta = 170^\circ$, which corresponds to a *superhydrophobic* surface. Dealing with a superhydrophobic surface numerically is rather challenging and its simulation poses interesting interfacial dynamics. As such, we consider droplet impact on the superhydrophobic cylinder for three different Bond numbers. Results are shown in Fig. 19 for $\text{Bo} = 2.2$ ($\text{Oh} = 0.06$), in

Figure 18: Droplet impact on a hydrophilic cylindrical surface with $\theta = 40^\circ$. $\rho_H/\rho_L = 1000$, $\mu_H/\mu_L = 100$, $\text{Re}_{\text{Gr}} = 25$, $\text{Bo} = 6.6$ ($\text{Oh} = 0.11$). See supplementary materials for simulation videos.

520 Fig. 20 for $\text{Bo} = 3.3$ ($\text{Oh} = 0.07$), and in Fig. 21 for $\text{Bo} = 6.6$ ($\text{Oh} = 0.11$).

Figure 19: Droplet impact on a superhydrophobic cylinder with $\theta = 170^\circ$. $\rho_H/\rho_L = 1000$, $\mu_H/\mu_L = 100$, $\text{Re}_{\text{Gr}} = 25$, $\text{Bo} = 2.2$ ($\text{Oh} = 0.06$). See supplementary materials for simulation videos.

521 For the lowest Bond number in Fig. 19, the droplet retracts after hitting
522 the cylindrical surface. The superhydrophobicity of the cylinder clearly over-
523 comes the gravitational pulling force, causing the droplet to bounce on top of

the surface a couple of times until it settles. This phenomenon is similar to the bouncing of a droplet after impact on a flat hydrophobic surface [78], and is also in line with recent numerical simulations in axisymmetric coordinates [42].

Figure 20: Droplet impact on a superhydrophobic cylinder with $\theta = 170^\circ$. $\rho_H/\rho_L = 1000$, $\mu_H/\mu_L = 100$, $\text{Re}_{\text{Gr}} = 25$, $\text{Bo} = 3.3$ ($\text{Oh} = 0.07$). See supplementary materials for simulation videos.

Comparing Fig. 19 and Fig. 17 at $t_g^* = 8$, we can see the effect of wettability of the cylindrical surface on the outcome of droplet impact. The hydrophilic surface in Fig. 17 allows the drop to wet its entire perimeter while the superhydrophobic surface in Fig. 19 repels the drop. By increasing the Bond number to 3.3 in Fig. 20, the drop gains enough momentum to break up upon contact with the upper pole of the cylinder, while being repelled from the superhydrophobic surface. Eventually, the drop disintegrates into two daughter droplets which are completely detached from the surface of the cylinder at $t_g^* = 4.4$, experiencing a free fall. Further increasing the Bond number to 6.6 leads to an interesting disintegration of the impacting drop

538 into several droplets of various sizes in Fig. 21. Interested readers can refer
 539 to supplementary materials for simulation videos of these droplet impacts on
 540 the cylindrical surface.

Figure 21: Droplet impact on a superhydrophobic cylinder with $\theta = 170^\circ$. $\rho_H/\rho_L = 1000$, $\mu_H/\mu_L = 100$, $\text{Re}_{\text{Gr}} = 25$, $\text{Bo} = 6.6$ ($\text{Oh} = 0.11$). See supplementary materials for simulation videos.

541 The film thickness, h_f on top of the cylindrical surface can be measured
 542 and compared with experimental data [75]. The normalized film thickness is
 543 defined by $h^* = h_f/h_i$, where h_i is the height of the drop at the instant
 544 of impact. Another dimensionless time is defined as $t^* = (t - t_i)U_i/D$,
 545 where t_i is the instant of impact between the drop and solid surface. The
 546 temporal variation of the film thickness at the north pole of the cylinder is
 547 plotted in Fig. 22 alongside theoretical and experimental expectations [78,
 548 75]. According to [75] the film thickness is expected to vary as $h^* = 1 - t^*$ at
 549 early times, and as $h^* = 0.15t^{*-2}$ at intermediate times [75]. As can be seen
 550 in Fig. 22, our simulations approximately obey the power-law fitted curves
 551 of [75]. Any deviations are likely due to the unrealistic nature of our 2D

552 simulations as well as the lower impact velocities in the current simulations
 553 compared with the experiments [75], which are conducted for a drop impact
 554 on a spherical surface with a drop diameter to target diameter ratio of 2.6/3.2
 555 at $Re = 4806$ and $We = 131$. Despite these obvious limitations, our results
 556 are qualitatively promising.

Figure 22: Temporal variation of the film thickness on top of the solid cylinder. $\rho_H/\rho_L = 1000$, $\mu_H/\mu_L = 100$, and $Re_{Gr} = 25$. Solid black line and dashed red line are the power-law curves from experimental data [75]; red squares correspond to $\theta = 40^\circ$ and $Bo = 2.2$ ($Re = 30$ and $We = 3$); green circles correspond to $\theta = 40^\circ$ and $Bo = 6.6$ ($Re = 32$ and $We = 12$); blue triangles correspond to $\theta = 170^\circ$ and $Bo = 2.2$ ($Re = 21$ and $We = 2$); and gray deltas correspond to $\theta = 170^\circ$ and $Bo = 6.6$ ($Re = 26$ and $We = 7$).

557 6. Summary and conclusion

558 In this paper we proposed a numerical technique to implement wetting
559 boundary conditions on curved surfaces without approximating the curved
560 boundary as a stair-case. We introduced a rather simple lattice Boltzmann
561 method, implemented on uniform Cartesian grids, which is capable of simu-
562 lating multiphase flows with large density ratios. In contrast to other existing
563 LB models for multiphase flows, there is only one nonlocal macroscopic prop-
564 erty in our model – the phase field. This feature is advantageous for parallel
565 implementation of the algorithm. We conducted various benchmark studies,
566 looking at three-phase contact line dynamics, to assess the proposed model.
567 Where available, the numerical results were found to be in good agreement
568 with analytical solutions and experimental data. The successful simulation
569 of drop impingement on a superhydrophobic cylinder highlights the great po-
570 tential of the proposed model for multiscale study of contact line dynamics
571 within diffuse-interface models. Although some major studies have addressed
572 the sharp-interface limit of Cahn-Hilliard-based models [9, 79], there is little
573 to no work on this issue for conservative phase-field models [11], particularly
574 when contact line motion is considered. Moreover, parameterizing the in-
575 terplay between the mobility and interfacial thickness is another important
576 topic worthy of investigation for accurate modeling of multiphase flows using
577 the phase-field models. Both these issues present important future research
578 avenues.

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