

An extended height function method for 3D VOF simulations of wetting phenomena on super-hydrophilic and hydrophobic surfaces

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Abstract

An extended height function method that can be consistently utilized for 3D VOF simulations of wetting phenomena on super-hydrophilic and super-hydrophobic surfaces, is proposed. First, the standard height function method is briefly explained. Then, 2D and 3D height function methods that reflect the contact angles reported so far are described, with their limitations discussed. Finally, specific treatments of contact line identification and height function construction reflecting the contact angle boundary condition, required to overcome such limitations, are presented in detail. Numerical tests for a sessile droplet reveal that the contact line identification and height function construction are conducted appropriately with respect to the imposed contact angles ranging from 15° to 165° in the proposed numerical scheme. Additionally, the present method shows approximately first- or second-order convergence of the curvature at the contact line for a wide range of contact angles. Moreover, simulations of droplet spreading driven by surface tension reveal that the proposed method can reasonably reproduce the behavior of a droplet reaching an equilibrium state defined by an imposed contact angle.

Keywords: Height function, Volume of fluid, Contact angle, Contact line, Interface curvature

1. Introduction

Many industrial applications such as inkjet printing and gas turbine engines involve gas-liquid two-phase flows. To numerically simulate such phenomena, capturing the topological changes of the gas-liquid interface while considering the effect of the surface tension force is necessary, which

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5 is achievable by applying interface capturing methods such as the volume of fluid (VOF) method [1], the level-set method [2], and the phase-field method [3]. Among these approaches, the VOF method is widely used owing to its good mass-conservation performance in numerous numerical simulations [4, 5, 6].

Within frameworks that use the VOF method, the surface tension force is commonly consid-
10 ered using the continuum surface force (CSF) model [7]. However, this model can potentially introduce an unphysical flow around the gas-liquid interface, which affects numerical results and decrease the prediction accuracy. It is known that such an unphysical flow can be reduced by discretizing the surface tension term appropriately and utilizing the optimal calculation method for interface curvatures [8, 9]. The discretization of the surface tension term should be consistent
15 with that of the pressure gradient [9]. For curvature estimation, the curvature is calculated by deriving the VOF function, a spatially filtered VOF function, or the level-set function within a framework using a coupled level-set and volume of fluid (CLSVOF) method [10]. However, these three methods do not exhibit grid convergence in the estimated curvature [11]. In contrast to these methods, the height-function (HF) method initially proposed by Torrey et al. [12] can
20 provide a converged estimation of the curvature with a fine mesh and is simpler than other mesh-convergent and high-order methods such as parabolic fitting (PROST) [8] or spline interpolation [13].

In the HF method on 2D Cartesian grids [11], the curvature is calculated using finite-difference approximations of the derivatives of the discretized height functions constructed by summing the
25 volume fractions in stencils in the x - and y -directions. In the case of the 3D Cartesian grids, height functions are also constructed in the z -direction. Although the HF method can provide an accurate estimate of the curvature with a fine mesh, the calculation of the height functions becomes inconsistent with the decreased grid resolution, more common in 3D cases and can result in curvature estimation with poor accuracy. To improve the estimation accuracy of the
30 curvature for such an under-resolved interface, alternative methods such as the parabolic interface interpolation method [14] and the mesh-decoupled height function method have been proposed [15]. So far, the HF method has been developed to provide practical estimates of curvature comparable in accuracy to the other calculation methods mentioned above.

However, considering the phenomena of interacting with a solid wall, its modeling becomes
35 more complicated because it requires the appropriate construction of height functions for a formed

contact line where the gas-liquid interface intersects with the solid wall, reflecting surface wettability. Surface wettability can be characterized by the contact angle which is defined as the angle between the gas-liquid interface and the solid wall at the contact line. To numerically consider surface wettability, Akfhami et al. [16] imposed a contact angle boundary condition for 2D cases
40 by constructing height functions near the contact line in the horizontal and vertical directions to the solid wall, reflecting the wettability. This construction in two orientations ensures that the method can be applied to wetting phenomena on super-hydrophilic and super-hydrophobic surfaces. By contrast, for 3D cases, Afkhami et al. [17] constructed height functions only in the horizontal direction because the construction of height functions in the vertical direction is much
45 more complex than that in the horizontal direction. Although few studies [18, 19] have proposed height function methods that consider the wettability for 3D cases, the construction of height functions has been limited to the horizontal direction in all methods owing to the complexity of the construction in the vertical direction, thus making all of the above-mentioned methods not suitable for wetting phenomena on super-hydrophilic and super-hydrophobic surfaces, corresponding to contact angles of $\theta < 45^\circ$ and $\theta > 135^\circ$, respectively, although these conditions are
50 necessary to simulate with high accuracy in terms of developing industrial applications.

Therefore, this study aims to propose an extended height function method that can be consistently utilized for 3D VOF simulations of wetting phenomena on super-hydrophilic and super-hydrophobic surfaces. Specifically, the height functions are constructed in the horizontal and
55 vertical directions of the wall. For an under-resolved interface, the interface curvature is estimated using the parabolic interface interpolation method [14].

2. Numerical scheme

The numerical scheme adopted in this study is based on an in-house thermal flow analysis code called FK³ [20], applicable to multiphase flows, as described in our previous studies [5, 6].

60 In the following sections, an overview of the numerical scheme including the interface capturing method and governing equations, is provided. Then, a brief explanation of the height function method developed so far is described, followed by the details of the proposed height function method.

2.1. Interface capturing method

The gas-liquid interface is captured using the volume of fluid (VOF) method [1]. The VOF function C is governed by the following equation.

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = 0. \quad (1)$$

65 Here, $\mathbf{u}$ is the velocity vector. The advection equation is discretized in time using the directional-splitting method [21]. The interface is reconstructed using the piecewise linear interface calculation (PLIC) scheme [22, 23]. Details can be found in [6].

2.2. Governing equations

The governing equations for an incompressible two-phase flow are the following continuity equation and Navier-Stokes equations.

$$\nabla \cdot \mathbf{u} = 0, \quad (2)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla P + \nabla \cdot (2\mu \mathbf{S}) + \mathbf{F}_{st}. \quad (3)$$

Here, ρ is the density, P the pressure, μ the viscosity, and $\mathbf{S}$ the rate-of-strain tensor $S_{ij} = (\partial_i u_j + \partial_j u_i)/2$. The surface tension term $\mathbf{F}_{st}$ is considered by the continuum surface force (CSF) model [7] and calculated as

$$\mathbf{F}_{st} = \sigma \kappa \nabla C, \quad (4)$$

70 where σ is the surface tension coefficient, and κ is the local interface curvature which is estimated by the proposed height function method.

Physical properties are defined using the VOF function C as follows.

$$\zeta = \zeta_l C + \zeta_g (1 - C). \quad (5)$$

Here, ζ can be the density ρ and the viscosity μ . The subscripts l and g represent the liquid and gas phases, respectively.

The spatial derivatives for the advection term and diffusion term in the momentum equation are approximated using the Kawamura-Kuwahara scheme [24] and a second-order accurate central difference scheme, respectively. The third-order explicit TVD Runge-Kutta scheme is used for time integration of the advection term. The physical properties of the gas and liquid phases such as the density ρ and μ are calculated according to CHEMKIN [25, 26] and obtained from the database of NIST [27], respectively. The details of the numerical scheme can also be found in [6].

2.3. Height function method

The standard curvature estimation using the height function method [11] is performed as follows. The overview below is limited to the case wherein the local interface-normal vector has its largest component in the y -direction. In other directions, the height-function construction and curvature estimation can be performed similarly.

1. Evaluate the height function h in the coordinate direction by summing the volume fractions of the cells in the column lying in that direction. The height function in the y -direction h^y is calculated as follows.

$$h_{i,j,k}^y = \sum_j C_{i,j,k} \Delta. \quad (6)$$

Here, Δ is the grid spacing. In practice, the height functions are converted to the absolute interface coordinates so that they can be referred to for interpolating a parabolic interface, whose details are described later in this section.

2. Estimate the curvature κ using finite differences of the derivatives of the height functions.

$$\kappa = \begin{cases} \frac{h_{xx}^y}{(1 + h_x^{y2})^{3/2}} & \text{in 2D,} \\ \frac{h_{xx}^y + h_{zz}^y + h_{xx}^y h_z^{y2} + h_{zz}^y h_x^{y2} - 2h_{xz}^y h_x^y h_z^y}{(1 + h_x^{y2} + h_z^{y2})^{3/2}} & \text{in 3D.} \end{cases} \quad (7)$$

Here, h_x^y and h_{xx}^y are the first and second derivatives of the height function using a central difference scheme, respectively, i.e., $h_x^y = (h_{i+1,j,k}^y - h_{i-1,j,k}^y)/2\Delta$ and $h_{xx}^y = (h_{i+1,j,k}^y - 2h_{i,j,k}^y + h_{i-1,j,k}^y)/\Delta^2$ for the cell (i, j, k) .

Note that the stencils used to evaluate the height function can be asymmetric, depending on the interface geometry [14]. Referring to the local interface-normal vector, the stencils are extended in both directions until empty ($C = 0$) and full cells ($C = 1$) are found. In this study, the maximum length of the stencil in each direction is set to six. On the other hand, the blocklength of message communications between different processors by Message Passing Interface (MPI) required for parallel computing is set to four in our in-house code FK³. Because the maximum length of the stencil is larger than the blocklength, only the VOF function C has a blocklength of six for the stencil extension. The reference normal vector is estimated using the reconstructed distance function (RDF) [11, 28].

For an under-resolved interface, the curvature estimation becomes inaccurate because in such a case, empty and full cells cannot be found during the stencil extension, making the evaluation of the height function inconsistent. To address this problem, the curvature is estimated using the parabolic interface interpolation method [14] only when the number of consistent height functions required for the curvature calculation is less than three (resp. nine in 3D). The procedure for the parabolic interface interpolation method is as follows.

1. Check if the number of independent interface positions is more than three (resp. six in 3D).
2. Compute the coordinate of the barycenter of the independent interface positions.
3. Compute the transformed coordinates of each interface position.
4. Fit a parabola (resp. paraboloid in 3D) below as a minimization problem referring to independent interface positions.

$$f = \begin{cases} a_0x^2 + a_1x + a_2 & \text{in 2D,} \\ a_0x^2 + a_1z^2 + a_2xz + a_3x + a_4z + a_5 & \text{in 3D.} \end{cases} \quad (8)$$

5. Calculate the interface curvature as follows.

$$\kappa = \begin{cases} \frac{2a_0}{(1 + a_1^2)^{3/2}} & \text{in 2D,} \\ 2 \frac{a_0(1 + a_4^2) + a_1(1 + a_3^2) - a_2a_3a_4}{(1 + a_3^2 + a_4^2)^{3/2}} & \text{in 3D.} \end{cases} \quad (9)$$

First of all, it is checked if the number of independent interface positions is more three (resp. six in 3D) in Step 1. Two different interface positions are regarded as independent if the distance between them is greater than a grid spacing. Then, the coordinate of the barycenter of the independent interface positions are computed in Step 2. Then, based on the barycenter, the coordinates of each interface position are transformed using Rodrigues' rotation formula in Step 3. Then, a parabola (resp. paraboloid in 3D) is fitted to the transformed interface positions by solving a 3×3 (resp. 6×6 in 3D) linear system using PLU-decomposition for a robust computation in Step 4. Finally, referring to the parabola, the interface curvature is calculated in Step 5.

2.4. Height function method reflecting contact angles

When the gas-liquid two-phase flow interacts with a solid wall, a contact line is formed, where the gas-liquid interface intersects with the wall surface. In such phenomena, surface wettability is considered to have a great influence, which can be characterized by the contact angle θ defined as the angle formed between the gas-liquid interface and the wall surface at the contact line. To numerically simulate such phenomena, the height functions must be appropriately constructed near the contact line in a manner reflecting the contact angle. The proposed method which can be consistently applied to wetting phenomena on super-hydrophilic and super-hydrophobic surfaces is partially based on the method in the previous work [17] although their method is limited to the conditions of $45^\circ < \theta < 135^\circ$. After identifying the contact line, the height functions are constructed such that an appropriate contact angle boundary condition is imposed near the contact line. The constructed height functions are used to estimate the curvature. Details of this process are described in the following Sections 2.4.1-2.4.3. For sake of simplicity, the explanations below are limited to the case wherein the wall lies at the bottom and its surface is perpendicular to the y -direction.

2.4.1. Arrangement of contact-line cells and adjacent cells

The contact line is identified by arranging both contact-line and adjacent cells near the contact line just above the wall surface. Note that although the definition of the 'contact-line cells' is similar to that used in a prior study [17], the definition of the 'adjacent cells' is different, described in detail later in this section.

First, contact-line cells are arranged, referring to the the y -component of the RDF-based interface-normal vector n_y^{RDF} . Fig.1 shows contact-line cells arranged just above the wall surface in 2D, which are indicated by the red-colored solid squares. A contact-line cell is defined as the cell which satisfies the conditions that its volume fraction C is between ϵ and $1 - \epsilon$ with ϵ of 0.01 and it neighbors at least one cell along a wall surface that is empty ($C < \epsilon$) in the case of $n_y^{\text{RDF}} < 0$ or full ($C > 1 - \epsilon$) in the case of $n_y^{\text{RDF}} > 0$. Note that the arrangement of the contact-line cell is classified on the basis of not the contact angle θ as in [17] but n_y^{RDF} . In an equilibrium state, n_y^{RDF} is negative and positive under the conditions of $\theta < 90^\circ$ and $\theta > 90^\circ$, respectively. In contrast, in an unsteady state, n_y^{RDF} can be inconsistent with θ , i.e., n_y^{RDF} can be positive and negative under the conditions of $\theta < 90^\circ$ and $\theta > 90^\circ$, respectively. In this sense, n_y^{RDF} is a more suitable criterion to reflect the actual state of the gas-liquid interface.

Then, adjacent cells are arranged along the wall surface so that they neighbor at least one contact-line cell, referring to n_y^{RDF} and the contact angle θ . Fig.2 shows the adjacent cells arranged just above the wall surface in 2D, which are indicated by the blue-colored squares. In the case of $\theta < 90^\circ$, an adjacent cell is placed on the opposite side of the droplet and has to satisfy the condition of $C < \epsilon$ and $C < 1 - \epsilon$ for $n_y^{\text{RDF}} < 0$ and $n_y^{\text{RDF}} > 0$, respectively (corresponding to the cases (a) and (b) in Fig.2). On the other hand, in the case of $\theta > 90^\circ$, an adjacent cell is placed on the same side of the droplet and has to satisfy the condition of $C > \epsilon$ and $C > 1 - \epsilon$ for $n_y^{\text{RDF}} < 0$ and $n_y^{\text{RDF}} > 0$, respectively (corresponding to the cases (c) and (d) in Fig.2).

Both the contact-line and adjacent cells can be arranged similarly in 3D, as shown in Figs.3 and 4, respectively. The only difference between 2D and 3D is that determining whether the cell neighbors at least one cell which satisfies a given condition is performed by checking the cells in a 3×3 stencil.

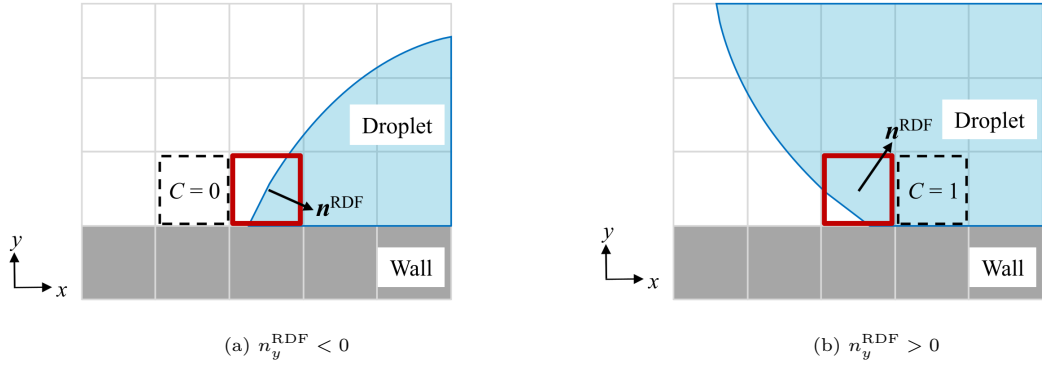


Figure 1: Arrangement of a contact-line cell indicated by the red-colored solid square just above the wall surface in 2D, referring to the y -component of the RDF-based interface-normal vector n_y^{RDF} . The contact-line cell is defined as the cell which satisfies the conditions that its VOF function C is between zero and one, and it neighbors at least one cell with $C = 0$ when n_y^{RDF} is negative (corresponding to the case (a)) or neighbors at least one cell with $C = 1$ when n_y^{RDF} is positive (corresponding to the case (b)). The cell neighboring the contact-line cell is indicated by the black dashed square.

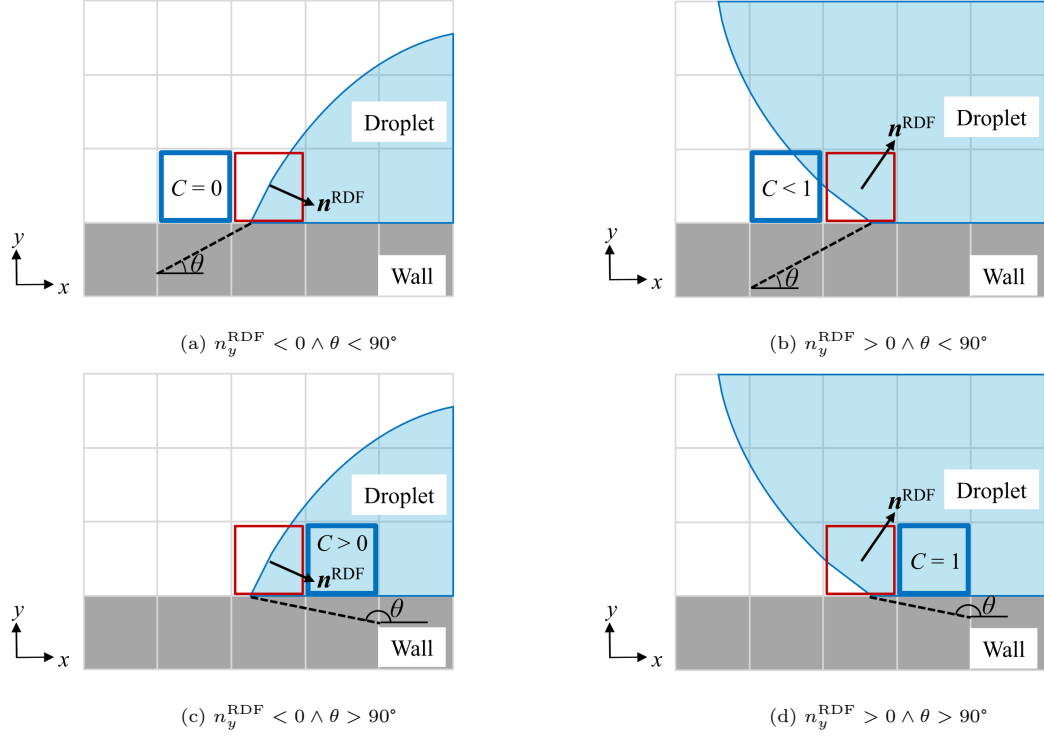


Figure 2: Arrangement of an adjacent cell indicated by the blue square just above the wall surface in 2D, referring to the y -component of the RDF-based interface-normal vector n_y^{RDF} and the contact angle θ . The black-colored dashed line beyond the wall surface indicates the extended interface, making the angle θ with the wall surface. Neighboring at least one contact-line cell indicated by the red square, the adjacent cell is placed on the opposite side of the droplet when $\theta < 90^\circ$ (corresponding to the cases (a) and (b)), while it is placed on the same side of the droplet when $\theta > 90^\circ$ (corresponding to the cases (c) and (d)). To achieve these arrangements, the adjacent cell must satisfy the condition related to the VOF function, which is written in the blue square in each case.

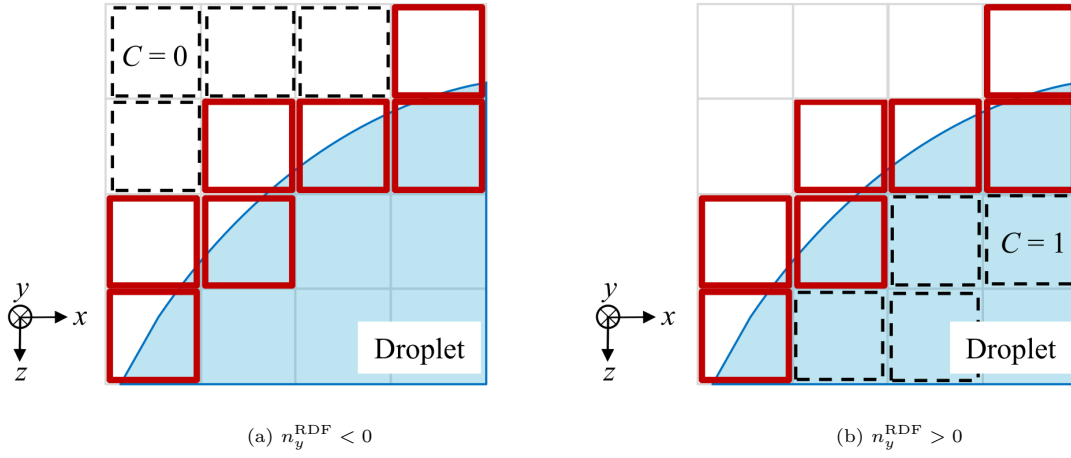


Figure 3: Arrangement of contact-line cells indicated by the red-colored solid squares just above the wall surface in 3D, referring to the y -component of the RDF-based interface-normal vector n_y^{RDF} . The contact-line cell is defined as the cell which satisfies the conditions that its VOF function C is between zero and one, and it neighbors at least one cell with $C = 0$ when n_y^{RDF} is negative (corresponding to the case (a)) or neighbors at least one cell with $C = 1$ when n_y^{RDF} is positive (corresponding to the case (b)). The cells neighboring the contact-line cell are indicated by the black dashed squares.

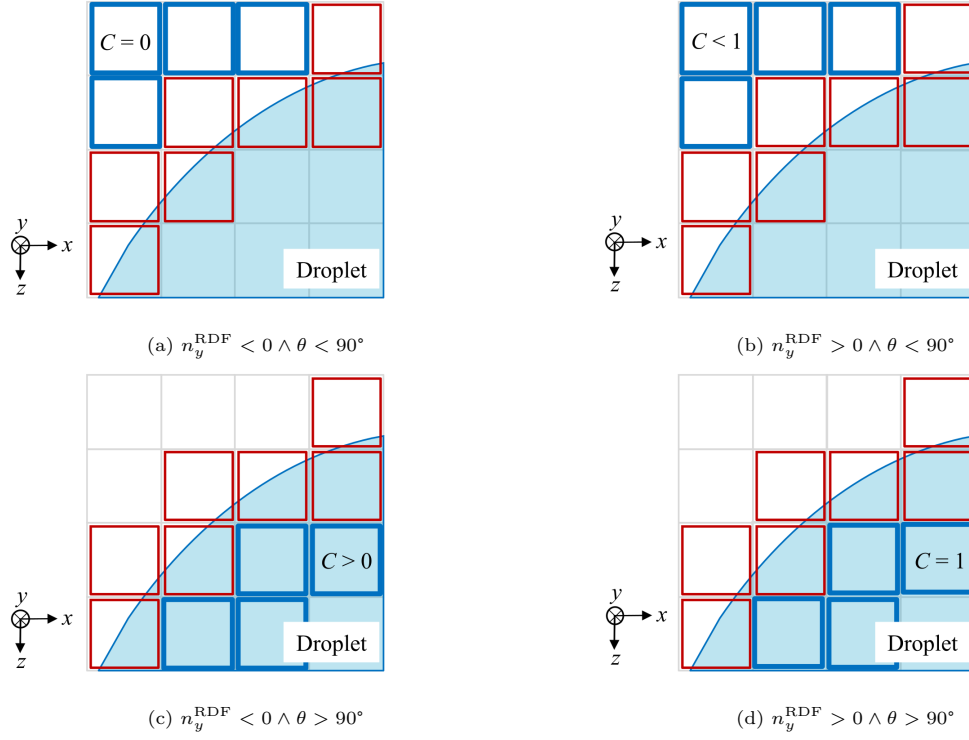


Figure 4: Arrangement of adjacent cells indicated by the blue squares just above the wall surface in 3D, referring to the y -component of the RDF-based interface-normal vector n_y^{RDF} and the contact angle θ . Neighboring at least one contact-line cell indicated by the red square, the adjacent cell is placed on the opposite side of the droplet when $\theta < 90^\circ$ (corresponding to the cases (a) and (b)), while it is placed on the same side of the droplet when $\theta > 90^\circ$ (corresponding to the cases (c) and (d)). To achieve these arrangements, the adjacent cell must satisfy the condition related to the VOF function, which is written in the blue square in each case.

2.4.2. Height-function construction in the horizontal direction

When estimating the curvature at the contact-line cells by derivating the height functions in the horizontal direction to the wall surface, the height function has to be constructed beyond the wall surface. Before going to 3D, the height-function construction in the horizontal direction in 2D is briefly explained. Fig.5 shows the height-function construction for the ghost cell beyond the contact-line cell in the x -direction in 2D. Consistent with a prior approach [16], the height function for the ghost cell $h_{i,-1}^x$ is estimated by the following equation, referring to the x -component of the RDF-based interface-normal vector $n_{x,i,0}^{\text{RDF}}$, the height function for the contact-line cell $h_{i,0}^x$, and the imposed contact angle θ .

$$h_{i,-1}^x = h_{i,0}^x - \text{sgn}(n_{x,i,0}^{\text{RDF}}) \Delta / \tan\theta. \quad (10)$$

In 3D, the curvature estimation at the contact-line cell requires height functions beyond the wall surface. For example, when the curvature is estimated for the contact-line cell $(i, 0, k)$ and n_x^{RDF} has its largest component in the x -direction, the height functions beyond the wall surface $h_{i,-1,k-1}^x$, $h_{i,-1,k}^x$, and $h_{i,-1,k+1}^x$ are required. Fig.6 shows the height-function construction for the ghost cell in the x -direction in 3D. The ghost cell is beyond the contact-line cell $(i, 0, k)$ indicated by the red-colored cube in Fig.6(a). The height-function for the ghost cell $h_{i,-1,k}^x$ can be constructed similarly to 2D. The only difference between 2D and 3D is that the interface-normal vector projected on the z - x plane $\mathbf{n}_{zx}^{\text{RDF}}$ can make an angle α with the considered stencil direction, as shown in Fig.6(b). In this case, the height function for the ghost cell $h_{i,-1,k}^x$ is calculated by the following equation as in [17, 18]. The height functions can also be constructed in the z -direction similarly.

$$h_{i,-1,k}^x = h_{i,0,k}^x - \text{sgn}(n_{x,i,0,k}^{\text{RDF}}) \Delta / (\tan\theta \cdot |\cos\alpha|). \quad (11)$$

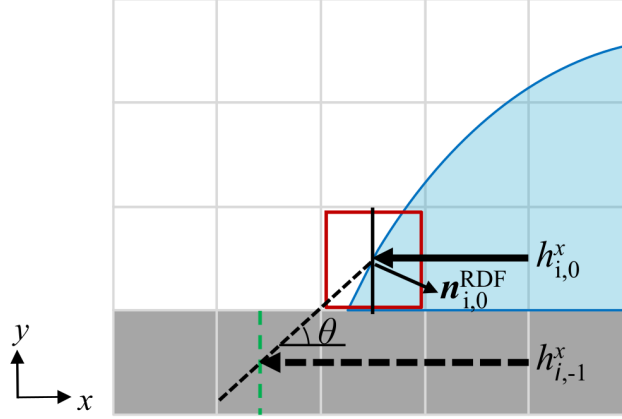


Figure 5: Schematic of the height-function construction for the ghost cell beyond the contact-line cell with a red-colored solid square in the horizontal direction to the wall surface in 2D, reflecting the contact angle. The black-colored dashed line beyond the wall surface indicates the extended interface, making the angle θ with the wall surface. The height function for the ghost cell in the x -direction $h_{i,-1}^x$ is estimated by the x -component of the RDF-based interface-normal vector $n_{x,i,0}^{RDF}$, the height function for the contact-line cell $h_{i,0}^x$ and the imposed contact angle θ . The dashed green line indicates the projected interface for estimating $h_{i,-1}^x$ at the ghost cell.

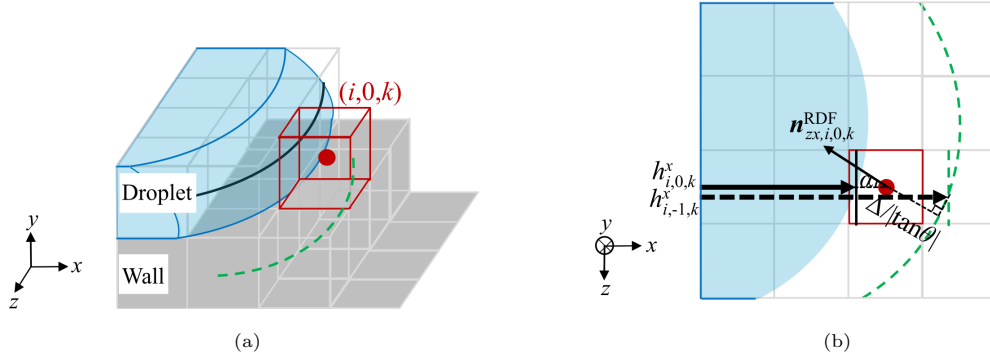


Figure 6: Schematic of the height-function construction for the ghost cell beyond the contact-line cell with a red-colored solid square in the horizontal direction to the wall surface in 3D. (a) The interfaces used to estimate the height-function at the contact-line cell $(i, 0, k)$ and ghost cell $(i, -1, k)$ are represented by a black-colored solid line and a green-colored dashed line, respectively. (b) The height function for the ghost cell beyond the surface in the x -direction $h_{i,-1,k}^x$ is estimated by the x -component of the RDF-based interface-normal vector $n_{x,i,0,k}^{RDF}$, the height function for the contact-line cell $h_{i,0,k}^x$, the imposed contact angle θ , and the angle α between the interface-normal vector projected on the z - x plane n_{zx}^{RDF} and the considered stencil direction.

2.4.3. Height-function construction in the vertical direction

185 When estimating the curvature at the contact-line cells using the derivatives of the height functions in the vertical direction to the wall surface, the height function is required for the adjacent cell whose arrangement is described in Section 2.4.1. For simplicity, the explanations below are limited to the condition of $n_y^{\text{RDF}} < 0$ and $\theta < 90^\circ$. On the other words, the contact-line and adjacent cells are arranged in 2D as in Fig.1(a) and Fig.2(a), respectively. In contrast, 190 they are arranged in 3D as in Fig.3(a) and Fig.4(a), respectively. As shown in Fig.7, the height function for the adjacent cell $(i-1, 0)$ with a blue-colored square is constructed in 2D by the following equation, reflecting the imposed contact angle. This method is similar to that in the previous work [16].

$$h_{i-1,0}^y = \begin{cases} h_{i,0}^y - \Delta \cdot \tan\theta & \text{if } \theta < 90^\circ, \\ h_{i,0}^y + \Delta \cdot \tan\theta & \text{if } \theta > 90^\circ. \end{cases} \quad (12)$$

Here, to calculate the height function at the contact-line cell $h_{i,0}^y$, a volume fraction must be 195 assigned to the ghost cell $(i, -1)$ beyond the wall surface, which requires the interface reconstruction there. As shown by a black-colored dashed line in Fig.7, the interface at the ghost cell is reconstructed by extending the interface segment from the contact-line cell to the ghost cell, and the volume fraction at the ghost cell is calculated within the framework using the PLIC scheme. The extension of the interface segment is performed so that the extended interface segment at 200 the ghost cell satisfies two conditions, e.g., it makes the imposed contact angle θ with the wall surface and connects to the interface segment for the contact-line cell. This extension can also be performed in 3D similarly.

In 3D, the method of the height-function construction in the vertical direction reflecting the contact angle has not yet been developed in previous works [17, 18] owing to the complexity of its 205 implementation, although this limitation results in poor applicability to wetting phenomena on super-hydrophilic and super-hydrophobic surfaces, corresponding to contact angles of $\theta < 45^\circ$ and $\theta > 135^\circ$. The proposed method includes constructing a height function in the vertical direction. The details are described as follows.

210 Fig.8 shows the height-function construction for the adjacent cell $(i+1, 0, k)$ in the vertical direction to the wall surface in 3D, reflecting the contact angle. First, as in 2D, the contact-line

cell must be defined, whose height function can be used to construct a height function for a neighboring adjacent cell. Because more than one contact-line cell can be found in the 3×3 stencil centered at the adjacent cell in 3D, the contact-line cell is selected among the ones to ensure that the following factor ξ is the largest, as in Fig.8(a).

$$\xi = |\mathbf{n}_{zx}^{\text{RDF}} \cdot \Delta \mathbf{x}|. \quad (13)$$

215 Here, ξ indicates the collinearity of the interface-normal vector at each contact-line cell $\mathbf{n}_{zx}^{\text{RDF}}$ and the translation vector from the adjacent cell to each contact-line cell $\Delta \mathbf{x}$.

After the contact-line cell is selected, the height function for the adjacent cell $h_{i+1,0,k}^y$ is estimated using the following equation, referring to the height function for the selected contact-line cell $h_{i,0,k}^y$, the imposed contact angle θ , and the angle α between $\mathbf{n}_{zx}^{\text{RDF}}$ and $\Delta \mathbf{x}$, as shown in
220 Fig.8(b).

$$h_{i+1,0,k}^y = \begin{cases} h_{i,0,k}^y - |\Delta \mathbf{x}| \cdot \tan \theta \cdot |\cos \alpha| & \text{if } \theta < 90^\circ, \\ h_{i,0,k}^y + |\Delta \mathbf{x}| \cdot \tan \theta \cdot |\cos \alpha| & \text{if } \theta > 90^\circ. \end{cases} \quad (14)$$

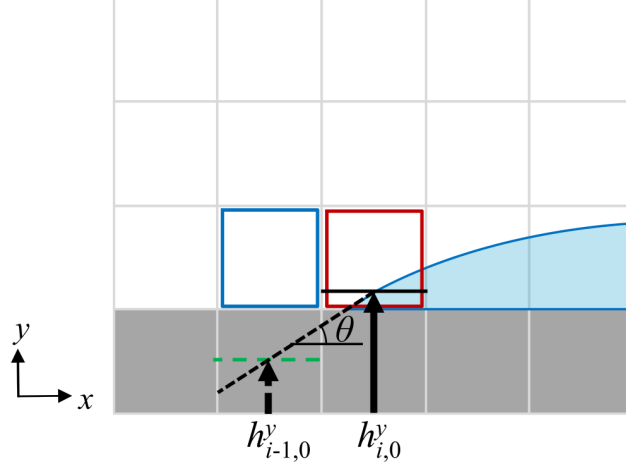


Figure 7: Schematic of the height-function construction for the contact-line cell with a red square and adjacent cell with a blue-colored square in the vertical direction to the wall surface in 3D, reflecting the contact angle. The height function for the contact-line cell $h_{i,0}^y$ is estimated by extending the interface segment from the contact-line cell to the ghost cell, as shown in the black-colored dashed line at the ghost cell, making the angle θ with the wall surface. The height function for the adjacent cell $h_{i-1,0}^y$ is estimated by the height function for the contact-line cell $h_{i,0}^y$ and the imposed contact angle θ . The dashed green line indicates the projected interface for estimating $h_{i-1,0}^y$ for the adjacent cell.

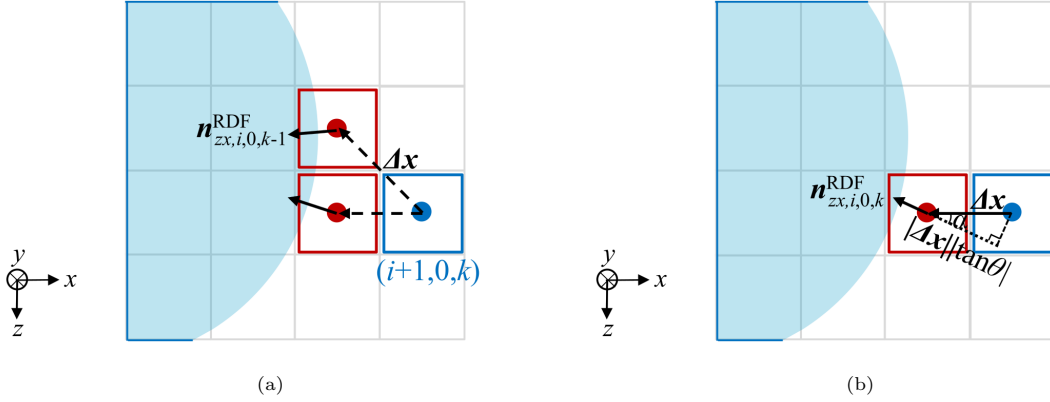


Figure 8: Schematic of the height-function construction for the adjacent cell with a blue square in the vertical direction to the wall surface in 3D, in the case of $\theta < 90^\circ$. (a) Based on the collinearity ξ of $\mathbf{n}_{zx,i,0,k-1}^{\text{RDF}}$ and $\Delta \mathbf{x}$, one contact-line cell is selected among the ones that neighbor the adjacent cell, indicated by the red square. (b) The height function for the adjacent cell is estimated considering the height function for the selected contact-line cell, the imposed contact angle θ , and the collinearity ξ .

2.5. Overall algorithm

The overall algorithm for computing interface curvatures, consistently applicable to wetting phenomena on super-hydrophilic and super-hydrophobic surfaces, is summarized as follows.

1. Arrange contact-line cells and adjacent cells
- 225 2. Calculate the VOF function for ghost cells beyond contact-line cells
3. Calculate the RDF-based interface-normal vectors
4. Evaluate height functions in the fluid region for each direction
 - (a) Evaluate height functions
 - (b) Check whether the height function construction is consistent
- 230 5. Evaluate height functions reflecting contact angle for each direction
 - (a) Evaluate height functions of ghost cells in the horizontal direction
 - (b) Evaluate height functions of adjacent cells in the vertical direction
6. Compute interface curvatures
 - (a) Determine a stencil direction based on the components of the normal vectors
 - 235 (b) If all height functions in the considered stencil are consistent, compute curvatures using Eq.(7)
 - (c) Otherwise, compute curvatures by Eq.(9) using the parabolic interface interpolation method

Firstly, when interactions with a solid wall are considered, contact-line and adjacent cells
240 must be arranged along the surface in Step 1, and the calculation of the volume fractions of ghost cells beyond the contact-line cells is required in Step 2. Then, referring to the RDF-based interface-normal vectors calculated in Step 3, the height functions in the fluid region are constructed in all coordinate directions in Step 4. Then, a contact angle boundary condition is imposed by constructing the height functions near the formed contact line in the horizontal
245 and vertical directions to the surface in Step 5. Finally, interface curvatures are computed in Step 6. In Step 6(a), the optimal direction for taking the derivative of the height functions, i.e., the stencil direction for computing curvatures, is determined based on the maximum component of the interface normal vector calculated in Step 3. If all height functions in the considered stencil are consistent, curvatures are computed in Step 6(b). Unless all height functions in

250 the considered stencil are consistent, the curvature is computed using the parabolic interface interpolation method in Step 6(c).

3. Results and discussion

3.1. Convergence of curvature estimation

A spherical droplet is considered in the convergence test. The droplet initially exhibits a diameter d of 0.5 and is stationary on a 1×1 wall surface where a boundary condition of a specific contact angle is imposed. The contact angle varies widely from 15° to 165° to confirm the applicability of the proposed height function method to wetting phenomena on super-hydrophilic and super-hydrophobic surfaces. The droplet and ambient gas have an identical value for the viscosity μ of 1 and density ρ of 4. The surface tension coefficient σ is set to be 0.357. The corresponding Ohnesorge number is $Oh = \mu/\sqrt{\sigma\rho d} = 1.18$. These settings of the physical properties correspond to the test case in the previous works [8, 17]. The initial velocity for the entire domain is zero, and the droplet is initially in an equilibrium state and should remain in this state.

Fig.9 shows the instantaneous iso-surfaces of the gas-liquid interface in the equilibrium state for cases with different contact angles. The gas-liquid interface is colored according to the direction of the height functions which are used to calculate the local interface curvature within the framework described in Section 2.5. For $\theta = 15^\circ, 30^\circ, 150^\circ$, and 165° , the interface along the contact line is colored in blue, which means that height functions in the vertical direction to the solid wall are used to calculate the local interface curvature. In contrast, for $\theta = 60^\circ, 90^\circ$, and 120° , the interface along the contact line is colored in light blue or yellow, implying that the height functions in the horizontal direction are used to calculate the curvatures. Therefore, the direction for taking the derivative of the height functions is optimally determined according to the local interface orientation within the framework described above, which ensures accuracy in the curvature estimation under the conditions of super-hydrophilic and super-hydrophobic surfaces.

Fig.10 shows the distribution of contact-line and adjacent cells along the contact line on the contact area at equilibrium for different contact angles. The red-colored contact-line cells are located referring to the green-colored line which is the iso-line of $C = 0.01$ and $C = 0.99$ for the cases with $\theta < 90^\circ$ and $\theta > 90^\circ$, respectively. On the other hand, the blue-colored adjacent cells are located outside the contact-line cells for $\theta < 90^\circ$, while they are located inside the contact-line cells for $\theta > 90^\circ$. Considering that the arrangement of the contact-line and adjacent cells is based on the local interface orientations and characterized by the contact angles, height functions can be constructed appropriately at the ghost cells beyond the contact-line cells and the adjacent

cells, reflecting the contact angle boundary conditions.

The accuracy of estimating the interface curvature by the proposed numerical framework is evaluated quantitatively. Fig.11 shows a comparison of the time variations of the L1 norm of the errors in estimated curvatures only at contact-line cells L_1^κ , calculated by the following equation.

$$L_1^\kappa = \sum_{i=1}^N |\kappa_{\text{exact}} - \kappa_{i,\text{approx.}}| \Delta_i^3. \quad (15)$$

Here, κ_{exact} and $\kappa_{i,\text{approx.}}$ are the exact curvatures of $4/d$ and the computed curvatures in an equilibrium state, respectively. In Fig.11(a), L_1^κ decreases over time for all cases with different
285 grid resolutions. In addition, L_1^κ converges with increasing the grid resolution although some fluctuations can be more or less observed for all cases. These fluctuations occur because the locations of the contact-line and adjacent cells change due to a slight shift of the gas-liquid interface even in an equilibrium state, introducing the fluctuation of the estimated curvature near the contact line. In Fig.11(b), L_1^κ decreases as time passes for the cases with contact angles
290 other than $\theta = 150^\circ$. In contrast, for $\theta = 150^\circ$, L_1^κ gradually increases after time of 5. For this benchmark case, with increasing a contact angle, the contact area becomes smaller despite of increase in the droplet volume. As a result, the droplet vibrates on the surface more easily due to the fluctuation of the estimated interface curvature observed in Fig.11(a), which makes it more difficult to get the convergence of L_1^κ under the condition of a higher contact angle. Fig.12
295 shows the grid convergence of L_1^κ at an equilibrium state. Here, the equilibrium state is defined as the state when a Courant number based on the maximum velocity magnitude becomes lower than a threshold. In this study, the threshold of the Courant number is set to be 2.5×10^{-6} , which corresponds to the velocity magnitude of 1×10^{-4} , 2×10^{-4} , and 4×10^{-4} , for the cases computed on different grids of $\Delta = 4 \times 10^{-3}$, 8×10^{-3} , and 16×10^{-3} , respectively. For each
300 contact angle, L_1^κ at equilibrium is obtained by taking the value at the identical time when the Courant number becomes lower than the threshold in all the cases with different grid resolutions. When compared among different contact angles, it is found that L_1^κ for $\theta = 90^\circ$ is much smaller than that for other contact angles, also observed in the previous work [17]. This is because for $\theta = 90^\circ$, the direction of the height functions used to calculate the interface curvature along the
305 contact line is horizontal to the wall surface, and the height functions at the ghost cells beyond the wall surface $h_{i,-1,k}$ whose calculation method is described in Section 2.4.2 are constructed as a symmetry boundary condition $h_{i,-1,k} = h_{i,0,k}$. Additionally, L_1^κ generally decreases with

increasing the grid resolutions and is the smallest for a grid of $\Delta = 4 \times 10^{-3}$ for all contact angle conditions. Furthermore, for all cases with θ ranging from 15° to 165° , the accuracy order of the interface curvature is approximately one or two because the height functions in the horizontal and vertical directions at the contact line are constructed using linear extrapolation in Eqs.(11) and (14), respectively. Here, the accuracy order for $\theta = 15^\circ$ is slightly smaller than other cases. This is because, for this benchmark case with such a low contact angle, the resolution of a droplet on the surface tends to be insufficient, which makes it difficult to obtain the result with good accuracy, especially for the case with $\Delta = 16 \times 10^{-3}$.

Additionally, the prediction accuracy is evaluated in terms of the spurious currents which can potentially be induced by poorly accurate curvature estimation. Fig.13 shows the time variations of the L-infinity norm of spurious currents L_∞^u , calculated using the following equation.

$$L_\infty^u = \max \sqrt{u^2 + v^2 + w^2}. \quad (16)$$

Here, u , v , and w are the x -, y -, and z -components of the velocity vector, respectively. In Fig.13(a), L_∞^u decreases as time passes for all cases with different grid resolutions at equilibrium though some fluctuations corresponding to those in Fig.11(a) are observed. In Fig.13(b), L_∞^u decreases over time for all cases with different contact angles.

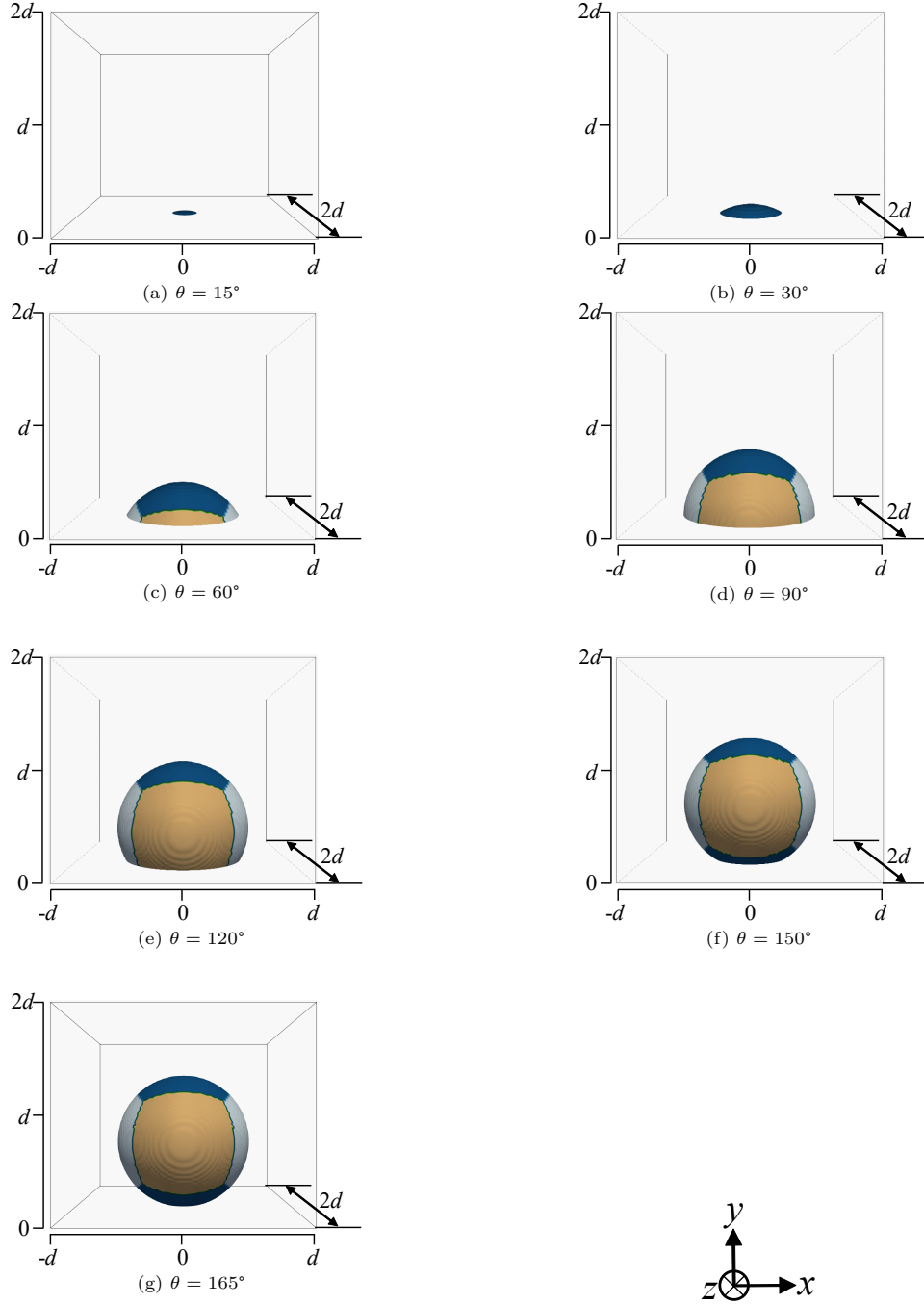


Figure 9: Snapshots of the instantaneous iso-surface of the VOF function $C = 0.5$ at $t = 20$ in an equilibrium state in the cases with contact angles of (a) 15° , (b) 30° , (c) 60° , (d) 90° , (e) 120° , (f) 150° , and (g) 165° computed on a grid of $\Delta = 8 \times 10^{-3}$. The iso-surfaces where the local interface curvature is calculated using the height functions in the x -, y -, and z -directions are colored in light blue, blue, and yellow, respectively.

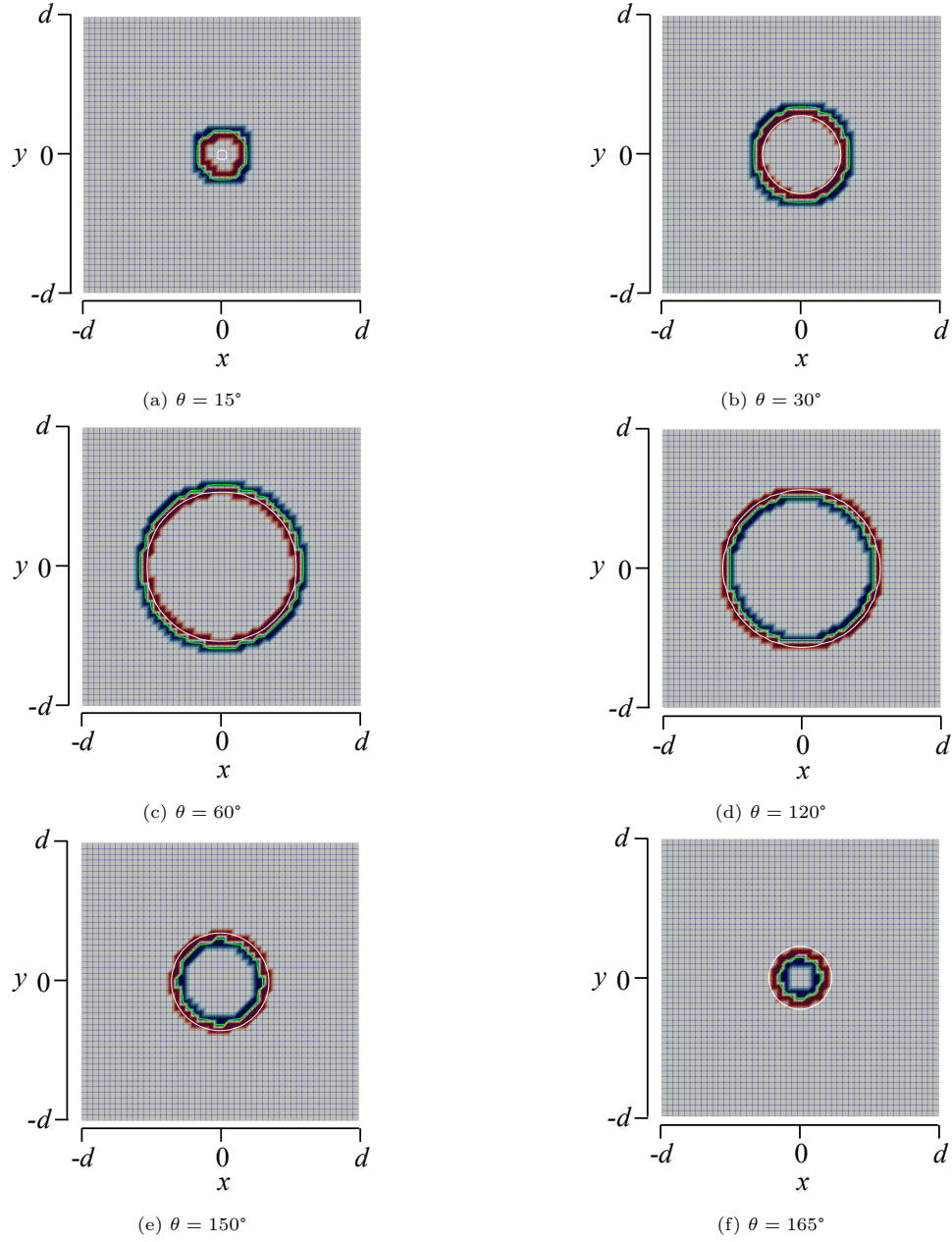


Figure 10: Instantaneous distributions of the contact-line cells and adjacent cells along the contact line on the contact area, which are colored in red and blue, respectively, at $t = 20$ in an equilibrium state in the cases with contact angles of (a) 15° , (b) 30° , (c) 60° , (d) 120° , (e) 150° , and (f) 165° computed on a grid of $\Delta = 16 \times 10^{-3}$. The gas-liquid interface is represented by the white iso-line of $C = 0.5$. The green line is the line used for arranging contact-line cells, which is the iso-line of $C = 0.01$ and $C = 0.99$ for the cases with $\theta < 90^\circ$ (corresponding to the cases (a)-(c)) and $\theta > 90^\circ$ (corresponding to the cases (d)-(f)), respectively.

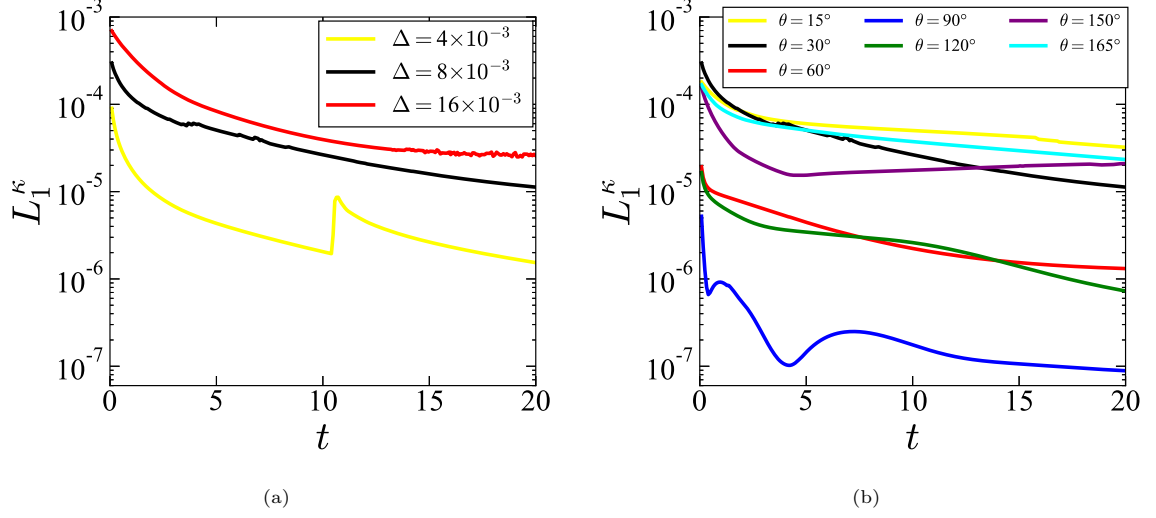


Figure 11: Time variations of the L1 norms of errors in estimated curvatures only in contact-line cells L_1^κ in the cases with (a) contact angle $\theta = 30^\circ$ computed on different grids of $\Delta = 4 \times 10^{-3}$, 8×10^{-3} , and 16×10^{-3} and (b) $\theta = 15^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ, 150^\circ$, and 165° computed on a grid of $\Delta = 8 \times 10^{-3}$.

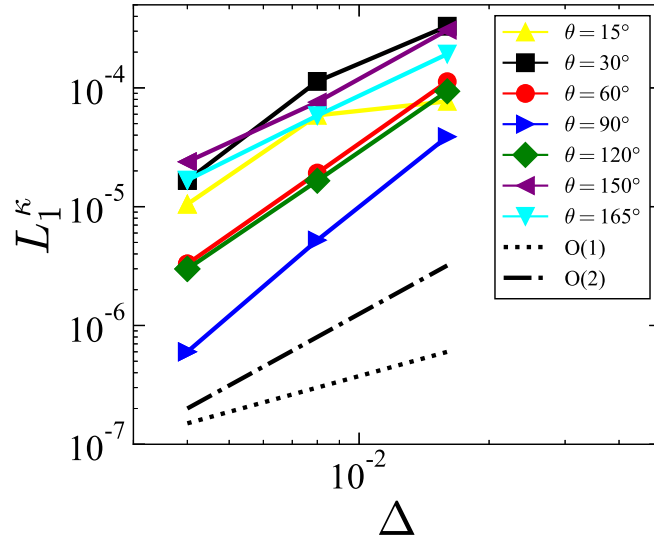


Figure 12: Grid convergence of the L1 norms of the errors in the interface curvature at the contact-line cells L_1^κ at equilibrium with different contact angles of $\theta = 15^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ, 150^\circ$, and 165° .

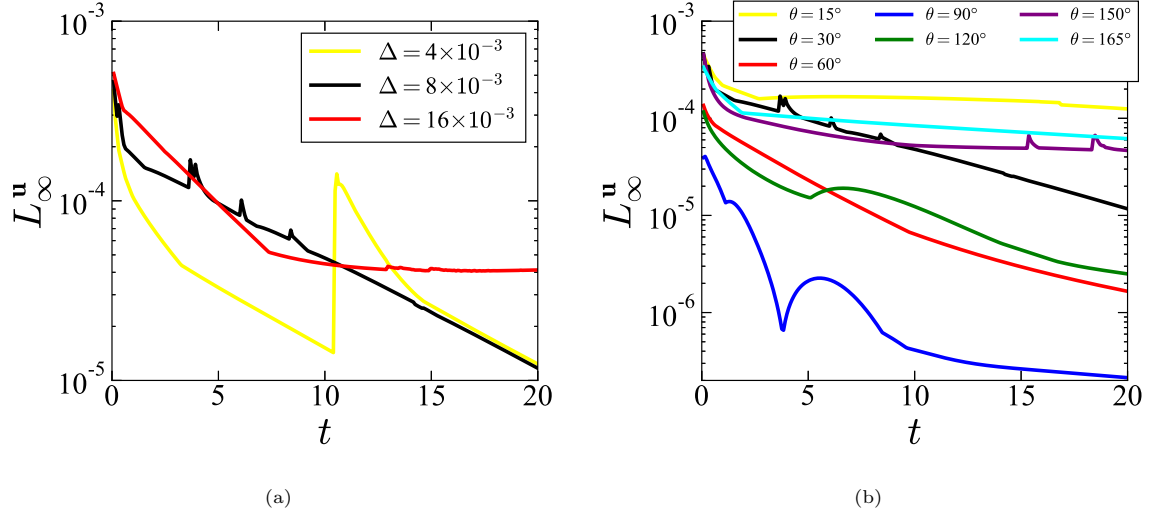


Figure 13: Time variations of the L-infinity norms of the spurious currents L_∞^u in the cases with (a) contact angle $\theta = 30^\circ$ computed on different grids of $\Delta = 4 \times 10^{-3}$, 8×10^{-3} , and 16×10^{-3} and (b) $\theta = 15^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ, 150^\circ,$ and 165° computed on a grid of $\Delta = 8 \times 10^{-3}$.

3.2. Surface tension-driven droplet spreading

The present simulations consider a semi-spherical droplet placed on a wall surface, implying that the contact angle is initially 90° . Table.1 lists the parameters determined by referring to [17]. Subsequently, a contact angle different from the initial value of 90° is suddenly imposed. Owing to this sudden change, the droplet spreads or retracts toward the desired equilibrium state corresponding to the imposed contact angle.

Table 1: Parameters for simulations of surface tension-driven droplet spreading.

Liquid density, ρ_l	800
Liquid viscosity, μ_l	7.52×10^{-2}
Gas density, ρ_g	1
Gas viscosity, μ_g	7.52×10^{-4}
Liquid-gas surface tension coefficient, σ	0.1
Initial droplet diameter, d_0	0.5
Droplet Ohnesorge number, Oh	1.33×10^{-2}

Figs.14 and 15 show the time variations of the gas-liquid interface of droplets. Owing to the sudden change in the contact angle, the droplet changes its shape to reach a new equilibrium state. Additionally, the color of the gas-liquid interface changes while the droplet reaches the equilibrium state, indicating that the direction of the height functions used to calculate the local interface curvature is optimally determined, as shown in Fig.9. Fig.16 shows the time variations of the reference direction of the height functions to calculate the interface curvature. It can be confirmed that the reference direction can be chosen based on the local interface orientation, only in the vicinity of the interface. In addition, the curvatures at red-colored cells are estimated by the parabolic interface interpolation method. Furthermore, when looking at the contact line indicated by the white iso-line, it is found that the contact area maintains its axisymmetric shape during the droplet spread.

Figs.17 and 18 show the time variations of the L1 and L-infinity norms of the velocities, respectively, for different grid resolutions and contact angles. Note that the results for the contact angle of 150° are not presented in all of the following investigations because the droplet bounces out of the domain in this condition as shown in Fig.15(b), which disables the quantitative

calculations. Whereas the L-infinity norm L_∞^u is calculated using Eq.(16), the L1 norm of the velocities L_1^u is calculated as follows.

$$L_1^u = \sum_{i=1}^N \sqrt{u^2 + v^2 + w^2} \Delta_i^3. \quad (17)$$

It is found that for all cases, the velocity magnitude decreases with oscillation as the droplet reaches a new equilibrium state. Additionally, with decreasing a grid spacing, L_1^u and L_∞^u generally decrease in Figs.17(a) and 18(a), respectively, though some fluctuations can be observed in 18(a). Furthermore, the oscillation is marked in the cases with higher contact angles in Figs.17(b) and 18(b). This is because, for this benchmark case, the contact area in the new equilibrium state becomes smaller with a higher contact angle, which makes the droplet unstable.

The proposed height function method is quantitatively evaluated using the values of the L1 and L-infinity norms of errors in the volume fractions, calculated as follows.

$$L_1^C = \sum_{i=1}^N |C_{\text{exact}} - C_{i,\text{approx.}}| \Delta_i^3, \quad (18)$$

$$L_\infty^C = \max |C_{\text{exact}} - C_{i,\text{approx.}}|. \quad (19)$$

Here, C_{exact} is the volume fraction in the expected equilibrium state defined by the initial droplet volume and imposed contact angle, while $C_{i,\text{approx.}}$ is the time-dependent volume fraction obtained by the simulations. Figs.19 and 20 show the comparison of the temporal evolutions of L_1^C and L_∞^C , respectively. For all cases, both L_1^C and L_∞^C decrease as a droplet reaches a new equilibrium state and show the same tendency of the oscillation as in Figs.17 and 18. Table.2 shows the grid convergence of L_1^C and L_∞^C for cases with a contact angle of $\theta = 30^\circ$. It is found that L_1^C decreases with increasing the grid resolution, but L_∞^C is the smallest for a grid of $\Delta = 8 \times 10^{-3}$. Additionally, L_∞^C is below 0.1 even for the case computed on the coarsest grid $\Delta = 16 \times 10^{-3}$, indicating that the gas-liquid interface in the equilibrium state is obtained with good accuracy even on the coarsest grid.

Based on the above results, the proposed height function method indicates that the grid convergence behavior in the estimation of the interface curvature of the sessile droplet on the solid wall for contact angles from 15° to 165° can be achieved by constructing the height functions not only in the horizontal direction but also in the vertical direction to the wall surface, and

taking the derivatives of such height functions in the direction determined according to the local
360 interface orientation. In summary, the method can be applied with good accuracy to the wetting
phenomena on super-hydrophilic and super-hydrophobic surfaces. Additionally, although the
details of the proposed height function method are explained only for the case wherein the wall
lies at the bottom and its surface is perpendicular to the y -direction in Section 2.4, the proposed
method can be extended for cases with any other wall orientations and applied to more complex
365 solid surfaces.

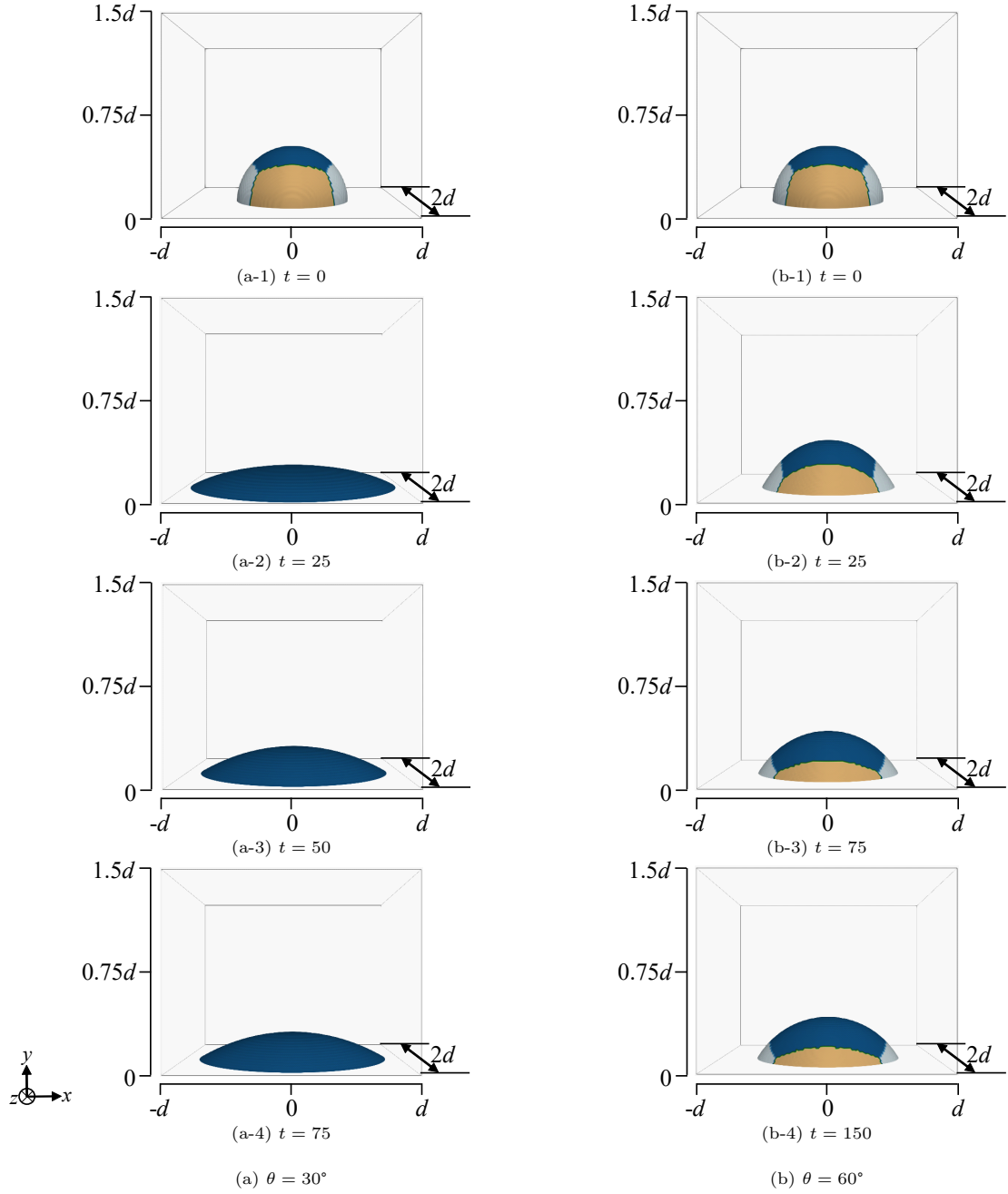


Figure 14: Time variations of the instantaneous iso-surface of the VOF function $C=0.5$ in the cases with contact angles of (a) 30° and (b) 60° , computed on a grid of $\Delta = 8 \times 10^{-3}$. The iso-surfaces where the local interface curvature is calculated using the height functions in the x -, y -, and z -directions are colored in light blue, blue, and yellow, respectively.

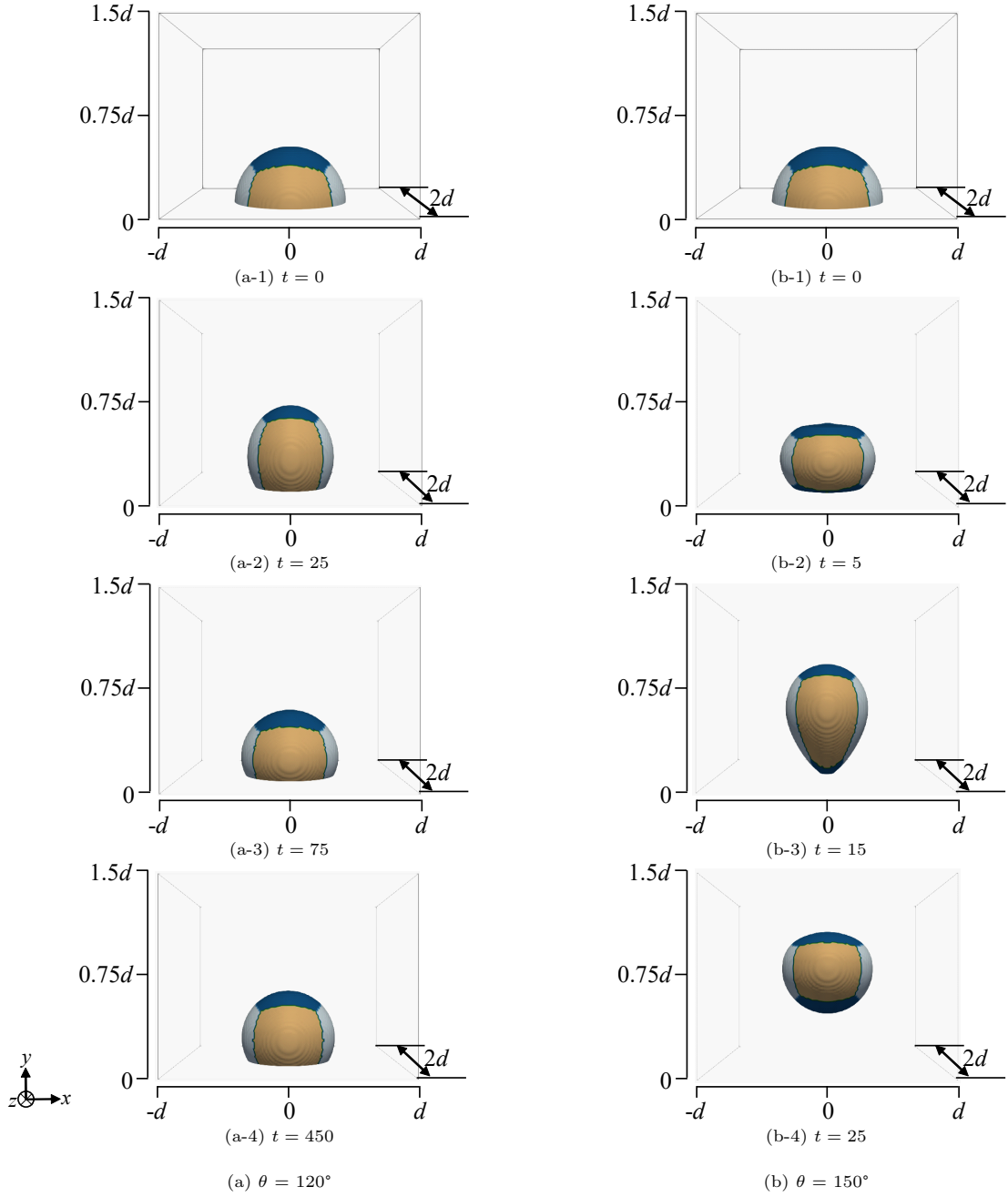


Figure 15: Time variations of the instantaneous iso-surface of the VOF function $C = 0.5$ in the cases with contact angles of (a) 120° and (b) 150° , computed on a grid of $\Delta = 8 \times 10^{-3}$. The iso-surfaces where the local interface curvature is calculated using the height functions in the x -, y -, and z -directions are colored in light blue, blue, and yellow, respectively.

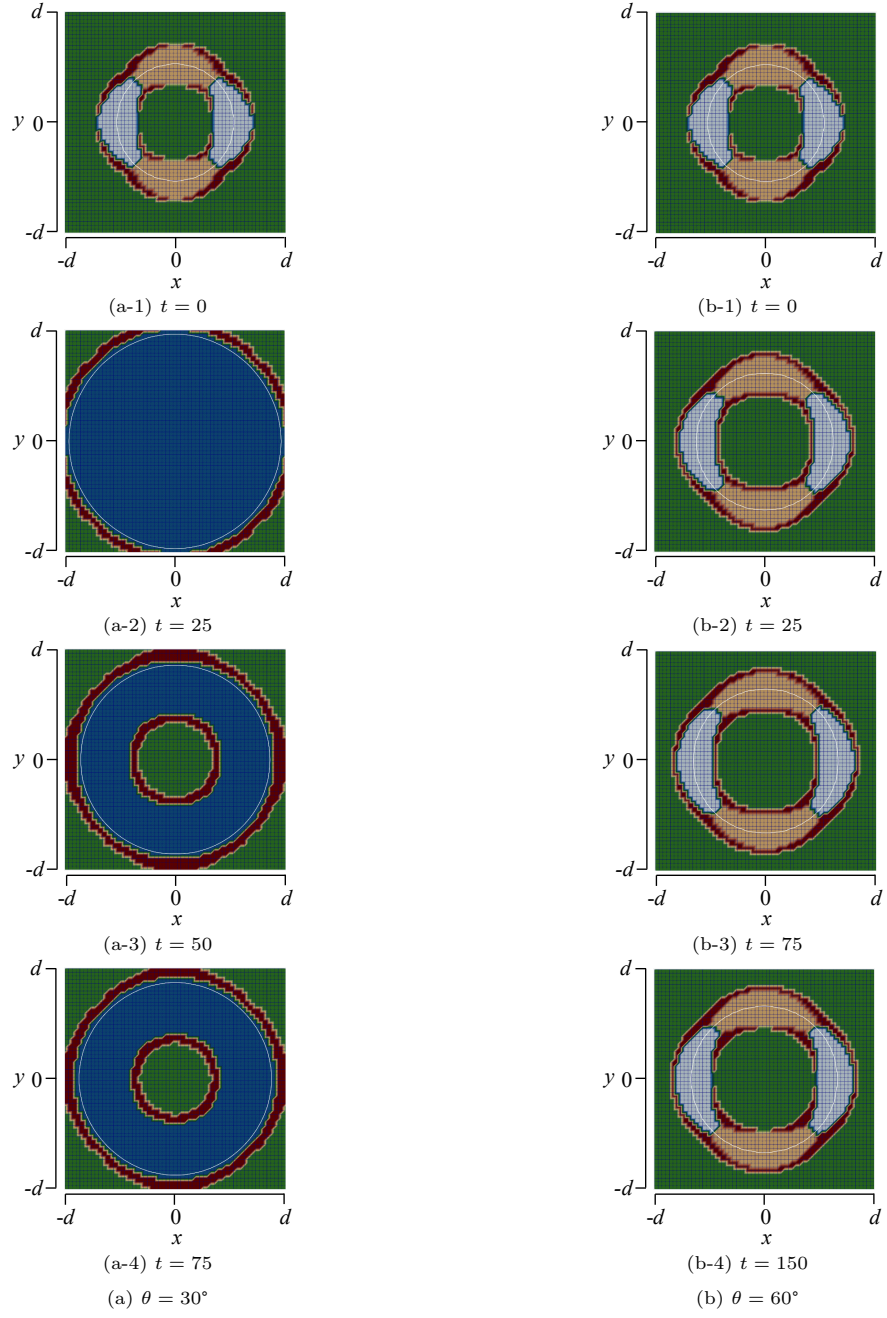


Figure 16: Time variations of the reference direction for the interface curvature calculation on the contact area in the cases with contact angles of (a) 30° and (b) 60° , computed on a grid of $\Delta = 16 \times 10^{-3}$. The cells where the local interface curvature is calculated using the height functions in the x -, y -, and z -directions or the parabolic interface interpolation method are colored in light blue, blue, yellow, and red, respectively. The gas-liquid interface is represented by the white iso-line of $C = 0.5$.

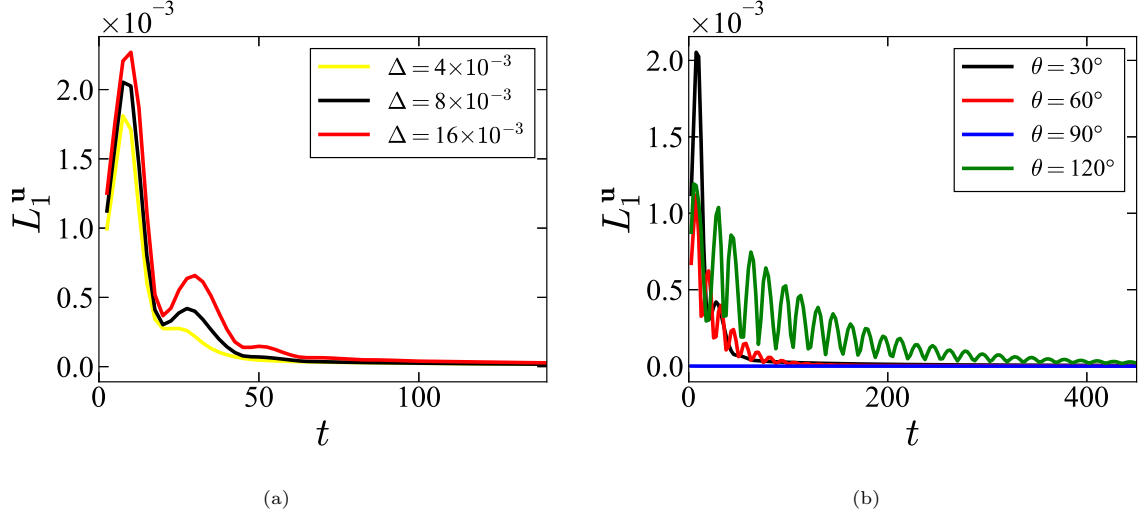


Figure 17: Time variations of the L1 norms of the velocities L_1^u in the cases with (a) contact angle $\theta = 30^\circ$ computed on different grids of $\Delta = 4 \times 10^{-3}$, 8×10^{-3} , and 16×10^{-3} and (b) $\theta = 30^\circ$, 60° , 90° , and 120° computed on a grid of $\Delta = 8 \times 10^{-3}$.

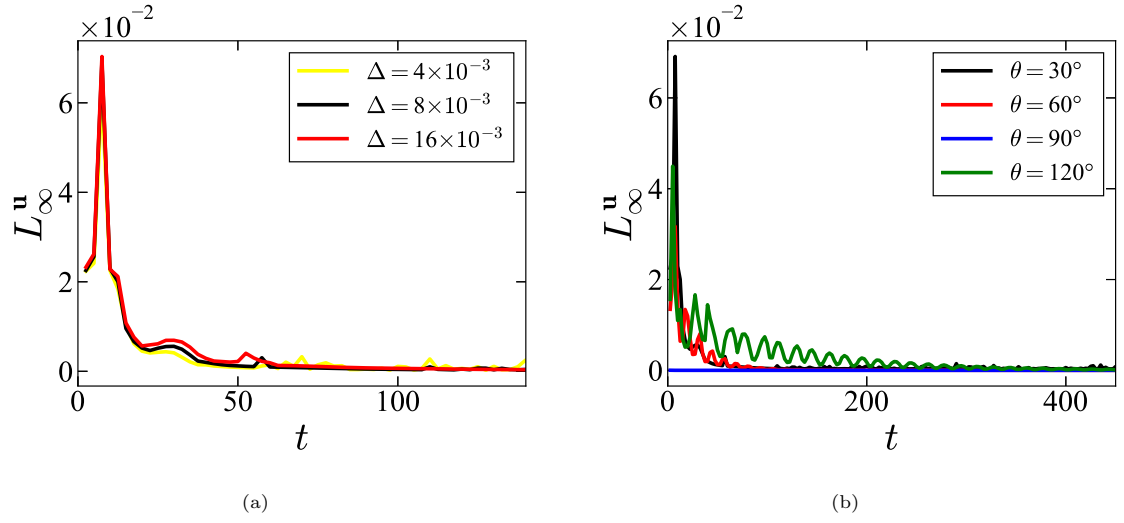


Figure 18: Time variations of the L-infinity norms of the velocities L_∞^u in the cases with (a) contact angle $\theta = 30^\circ$ computed on different grids of $\Delta = 4 \times 10^{-3}$, 8×10^{-3} , and 16×10^{-3} and (b) $\theta = 30^\circ$, 60° , 90° , and 120° computed on a grid of $\Delta = 8 \times 10^{-3}$.

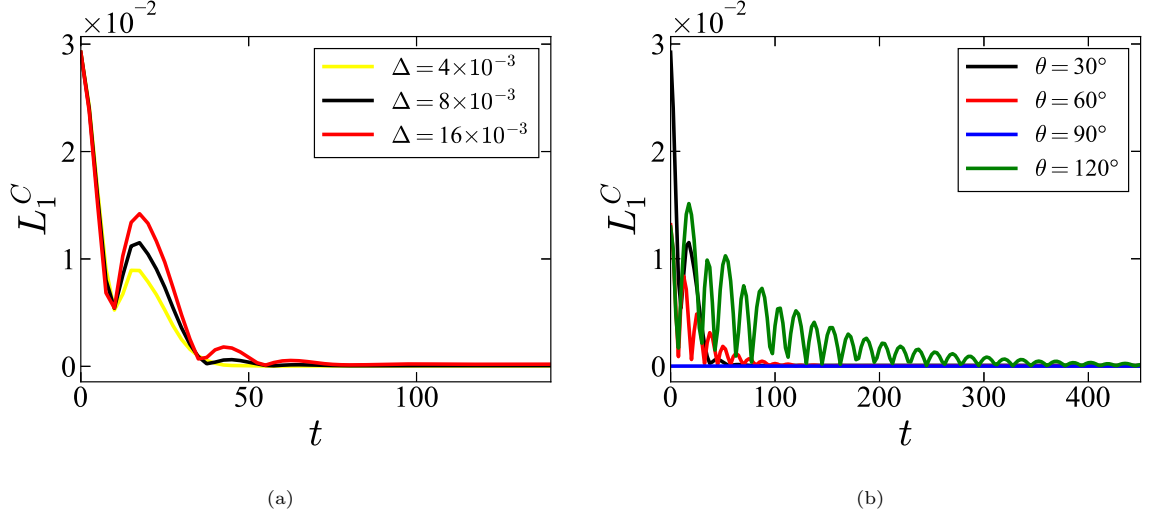


Figure 19: Time variations of the L1 norms of errors in volume fractions L_1^C in the cases with (a) contact angle $\theta = 30^\circ$ computed on different grids of $\Delta = 4 \times 10^{-3}$, 8×10^{-3} , and 16×10^{-3} and (b) $\theta = 30^\circ$, 60° , 90° , and 120° computed on a grid of $\Delta = 8 \times 10^{-3}$.

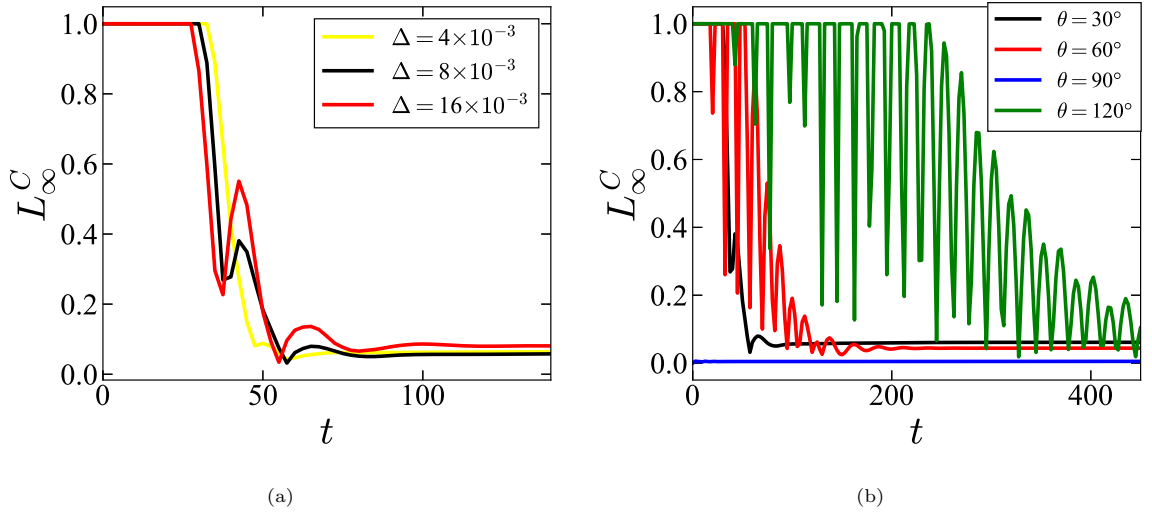


Figure 20: Time variations of the L-infinity norms of errors in volume fractions L_∞^C in the cases with (a) contact angle $\theta = 30^\circ$ computed on different grids of $\Delta = 4 \times 10^{-3}$, 8×10^{-3} , and 16×10^{-3} and (b) $\theta = 30^\circ$, 60° , 90° , and 120° computed on a grid of $\Delta = 8 \times 10^{-3}$.

Table 2: Grid convergence of the L1 and L-infinity norms of the errors in volume fractions at equilibrium with a contact angle of $\theta = 30^\circ$.

Δ	L_1^C	L_∞^C
4×10^{-3}	3.93×10^{-5}	6.38×10^{-2}
8×10^{-3}	6.72×10^{-5}	5.80×10^{-2}
16×10^{-3}	2.01×10^{-4}	8.07×10^{-2}

4. Conclusions

In this study, an extended height function method that can be consistently utilized for 3D VOF simulations of wetting phenomena on super-hydrophilic and super-hydrophobic surfaces, was proposed. First, contact-line and adjacent cells were arranged along the contact line such that the contact angle boundary condition could be imposed at the contact line within the framework of the height function method. After the arrangement, the height functions were constructed in the horizontal and vertical directions of the wall, reflecting the contact angle boundary conditions. These height functions were used to calculate the local interface curvatures. When the interface was under-resolved, the interface curvature was estimated using a parabolic interface interpolation method.

The proposed method was first verified by performing a convergence test of the curvature estimation for a sessile droplet. The contact-line and adjacent cells were appropriately arranged with respect to the imposed contact angle. Additionally, whether the direction of the height functions used to calculate the local interface curvature is horizontal or vertical to the wall surface was determined optimally. Furthermore, the proposed height function method showed approximately first- or second-order convergence of the curvature at a contact line for a contact angle ranging from 15° to 165° , corresponding to the conditions of super-hydrophilic and super-hydrophobic surfaces. In addition, the error in the estimated curvature and the spurious currents introduced by the inaccurate curvature estimation decayed over time under a wide range of contact angle conditions. The proposed method was then applied to the surface tension-driven droplet spreading. Investigations of the velocities and errors in the volume fractions indicated that the proposed method can reasonably reproduce the behavior of a droplet reaching an equilibrium state defined by an imposed contact angle.

Acknowledgments

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Data Availability Statement

The data that support the findings of this study are available from the corresponding author
395 upon reasonable request.

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