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1 **Relevance of capillary interfaces simulation with the**
2 **Shan-Chen multiphase LB model**

3 **Z. Benseghier · O. Millet · P. Philippe · A.**
4 **Wautier · N. Younes · E. Liberge.**

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7 **Abstract** This paper presents a numerical study of capillary interfaces using the Single
8 Component Multi-phase Shan-Chen model, which is based on the lattice Boltzmann method.
9 Despite the simplicity of the model, it has been shown to be effective and the present study
10 aims to test its ability to correctly reproduce the physics of multiphase systems. To this
11 end, several benchmark simulations were carried out in the configurations of a drop on a
12 flat wall and then on a spherical surface to characterize the wetting behavior and relate
13 explicitly the contact angle to model parameters. In addition, the capillary forces induced
14 by a liquid bridge between two spherical particles were numerically calculated. We show
15 that the results obtained are in agreement with experimental and theoretical results from
16 the literature. The model is thus accurate in addressing the wetting behavior and capillary
17 interfaces in unsaturated granular soils despite the fact that surface tension and contact
18 angles are not explicit parameters of the model. To this respect, explicit relationships with
19 Shan-Chen parameters are provided.

20 **Keywords** capillary · contact angle · multi-phase · Lattice Boltzmann Method.

Z. Benseghier
LaSIE, UMR CNRS 7356, University of La Rochelle, 17042, La Rochelle Cedex 1, France.
E-mail: zeyd.benseghier@univ-lr.fr

O. Millet
LaSIE, UMR CNRS 7356, University of La Rochelle, 17042, La Rochelle Cedex 1, France.
E-mail: olivier.millet@univ-lr.fr

P. Philippe
INRAE, Aix Marseille Univ, RECOVER, 3275 route de Cézanne, 13100 Aix-en-Provence, France.
E-mail: pierre.philippe@inrae.fr

A. Wautier
INRAE, Aix Marseille Univ, RECOVER, 3275 route de Cézanne, 13100 Aix-en-Provence, France.
E-mail: antoine.wautier@inrae.fr

N. Younes
LaSIE, UMR CNRS 7356, University of La Rochelle, 17042, La Rochelle Cedex 1, France.
E-mail: nabil.younes@univ-lr.fr

E. Liberge
LaSIE, UMR CNRS 7356, University of La Rochelle, 17042, La Rochelle Cedex 1, France.
E-mail: erwan.liberge@univ-lr.fr

1 Introduction

Capillary effects play a fundamental role in the behavior of wet granular soils. When soil particles are subjected to humidity, capillary bridges occur and the induced adhesion forces lead to cohesion at the soil scale. The shape of such bridges is well described by Young-Laplace equation and ruled by the surface tension of the interfaces at stake. Consequently, a pressure difference will exist inside the capillary bridge, which in turn results in capillary forces between grains. In case capillary bridges merge or collapse (wetting or drying of the material), a progressive loss in cohesion may occur on a larger scale, such as in hydraulic earthworks (e.g. earth-dams, levees, and dikes), possibly with dramatic consequences on their mechanical stability. Therefore, it is crucial to first quantify accurately the capillary forces between solid grains in unsaturated media and next to perform reliable numerical computations at the scale of earthen structures.

Several numerical, experimental, and analytical studies have been carried out to quantify these forces. Mielniczuk et al. [19] have quantified capillary forces using an inverse problem technique for solving Young-Laplace equation when the capillary pressure is unknown. Their method was compared to experimental results and showed great similarities [19]. Recently, this approach has been extended to polydisperse particles, to capillary bridges between a sphere and a plane, or between two parallel planes [22, 23, 24, 25, 26, 27]. Duriez & Wan [8] have solved numerically the Young-Laplace equation in order to compute the attractive force between two grains when the capillary pressure is controlled and validated their strategy by comparing with experimental results.

Another way is to model all the phases before computing the capillary bridge directly from the simulation. Many works deal with gas-liquid-systems [6, 35], but only a few have focused on the calculation of the forces induced by capillary bridges. Miot *et al.* [20] used an energy minimization approach (with the open-source code Surface Evolver [3]) combined with the use of the virtual work principle to compute the shape of the capillary bridge and the corresponding forces transmitted to the grains. Even if the method can be applied to complex geometry and dynamic evolutions, it is limited to steady problems and the method relies on the use of well-chosen parameters to achieve the convergence of the results. Sun *et al.* [37] proposed a VOF-IB-DNS method, which combines Volume Of Fluid (VOF) to calculate the shape of the gas-liquid interface, Immersed Boundary (IB) to implement solid particles, and Finite Volume method to solve directly the Navier-Stokes (N-S) equations.

In this work, we propose to use the Lattice Boltzmann Method (LBM) to model wetting condition (contact angle) and capillary bridges between particles following the numerous advantages of this method in fluid dynamics, mainly in dealing with complex geometry. The LBM has been successfully developed for computational fluid dynamics since the 90's [2] and appears to be a suitable alternative numerical method. Based on the Boltzmann equation, the LBM considers the transport of the probability to find a particle according to time, space and velocity. Then, the macroscopic variables are obtained using momenta of the adapted distribution functions. The power of the LBM also lies in its simplicity and easy implementation on Graphic Processor Units (GPU) that considerably reduces the computation time [10].

There exists a considerable body of literature on modeling interface-tracking models with LBM, such as Cahn-Hilliard [38, 42, 44] or Allen-Cahn [9, 18] equations. These models have proved to be accurate when dealing with high-density ratios by solving, at the same time, the Navier-Stokes (N-S) equations as well as one of the interface-tracking equations indicated above. However, a primary problem of this strategy is the large computation and memory

68 costs, since two equations need to be solved simultaneously. Therefore, accurate computations
69 of capillary forces at the scale of a REV seem out of reach with these approaches.

70 A possible solution to address this issue would be to simulate capillary bridges and
71 compute the corresponding capillary forces based on a less accurate but more efficient
72 model, especially with the Shan-Chen model that accounts for multi-phase flows without
73 tracking the interface. This model relies on molecular interactions (pseudo-potential) between
74 phases, which leads to phase separation, and can be divided into two categories. The first
75 approach is Multi-Component Multi-Phase (MCMP), where two LB equations need to be
76 solved when the different fluids are made of different materials (two immiscible liquids for
77 instance). However, the maximum density ratio is of the order of $O(1)$, so that the method
78 cannot handle water/air interfaces in particular [15]. This approach was used for partially
79 saturated media [21, 28] and for studying the capillary forces between two particles [40]. The
80 second family of models is Single-Component Multi-Phase (SCMP), where only one LB
81 equation is required to solve N-S equations and a supplementary Equation Of State (EOS)
82 is introduced to simulate the coexistence between liquid and gaseous phase for the same
83 substance (for instance water liquid and water vapor). Some applications concern flows in
84 unsaturated porous materials [7, 14, 30, 36]. The density ratio is controlled by the EOS and
85 the maximum ratio that can be achieved is in the order $O(10^2)$ [15]. The latter is indeed
86 more efficient and will be described in more detail and implemented in the remainder of this
87 paper. While using this model for water, one has to keep in mind that the maximum density
88 ratio of $O(10^2)$ imposes to work at high temperature and high pressure.

89 The overall aim of this paper is to study the computational efficiency as well as the
90 accuracy of the SCMP model in dealing with contact angles for flat and convex solid
91 frontiers and in computing capillary forces. The plan of the paper is organized as follows. In
92 the first section, a brief introduction of LBM and the SCMP model is given in addition to
93 fluid-solid interaction with wetting conditions (contact angle). Afterward, several validation
94 benchmarks are performed to validate the model, including stationary spherical drop to verify
95 the Laplace equation and deduce the surface tension value, and drop on a flat and spherical
96 particle, to validate the contact angle implementation. Next, a section is devoted to capillary
97 bridges between two spherical grains and induced capillary forces with a comparison between
98 our results and experimental and theoretical ones from the literature [19, 29, 30]. Finally, the
99 last section provides a general conclusion opening up future prospects.

100 2 Implementation of LBM for multi-phase flows and wetting condition

101 2.1 Standard Lattice Boltzmann method

102 The Lattice Boltzmann method with Bhatnagar-Gross-Krook (BGK) collision operator and
103 a source term F_α can be written as follows:

$$f_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) = f_\alpha(\mathbf{x}, t) - \frac{1}{\tau} [f_\alpha(\mathbf{x}, t) - f_\alpha^{eq}(\mathbf{x}, t)] + F_\alpha(\mathbf{x}, t) \quad (1)$$

104 where f_α is the particle distribution function at a given lattice position \mathbf{x} , time t , and along a
105 direction α , restricted to a limited number of discrete velocities. The equilibrium distribution
106 function f_α^{eq} is given by

$$f_\alpha^{eq}(\rho, \mathbf{u}) = \rho w_\alpha \left[1 + \frac{\mathbf{u} \cdot \mathbf{c}_\alpha}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{c}_\alpha)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right] \quad (2)$$

107 where $c_s = c/\sqrt{3}$ is the lattice speed of sound with $c = \frac{\Delta x}{\Delta t}$ the lattice speed. Δx and Δt denote
 108 the lattice size and time steps, in general chosen equal to one in lattice units ($\Delta x = \Delta t = 1$ lu).
 109 The D3Q19 scheme (three dimensional configuration with nineteen velocities) is widely used
 110 in the literature for 3D simulation and implemented in this study, whose discrete velocities
 111 \mathbf{c}_α read

$$\mathbf{c}_\alpha = \begin{cases} (0, 0, 0) & \alpha = 0 \\ (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1), & \alpha = 1, 2, \dots, 6 \\ (\pm 1, \pm 1, 0), (\pm 1, 0, \pm 1), (0, \pm 1, \pm 1) & \alpha = 7, 8, \dots, 18 \end{cases} \quad (3)$$

112 with the corresponding weights $w_0 = 1/3$, $w_{1-6} = 1/18$, and $w_{7-18} = 1/36$.

113 The source term F_α in Eq. (1) can include external body force, fluid-fluid interaction
 114 force \mathbf{F}_{int} , and adhesive force \mathbf{F}_{ads} (i.e fluid-solid interaction force) which will be introduced
 115 in Sec. 2.3 ¹.

116 The density ρ and velocity \mathbf{u} of the fluid, in lattice units, can be directly derived from
 117 the distribution functions as:

$$\rho = \sum_{\alpha} f_{\alpha} \quad (4)$$

$$\mathbf{u} = \frac{1}{\rho} \sum_{\alpha} f_{\alpha} \mathbf{c}_{\alpha}. \quad (5)$$

118 The relation between the relaxation time τ and the kinematic viscosity ν of the fluid
 119 classically reads ²:

$$\tau = \frac{\nu}{\Delta t c_s^2} + \frac{1}{2}. \quad (6)$$

120 2.2 SCMP Shan-Chen model

121 For single-component multi-phase system (SCMP) (e.g water and its vapor), we use the
 122 model proposed by Shan and Chen [32, 33], in which a fluid interaction force is introduced
 123 to induce phase separation. This interaction term reads

$$\mathbf{F}_{int}(\mathbf{x}) = -G\psi(\mathbf{x}) \sum_{\alpha} w_{\alpha} \psi(\mathbf{x} + \mathbf{c}_{\alpha} \Delta t) \mathbf{c}_{\alpha} \quad (7)$$

124 where $\psi(\mathbf{x})$ is the effective mass, which depends on the local density $\rho(\mathbf{x})$, and G is the
 125 interaction strength. w_{α} are the lattice weights as previously defined. Note that the sum runs
 126 over all neighboring fluid nodes.

127 The effective mass (also called the pseudopotential) proposed in the original work of
 128 Shan and Chen [32, 33] takes the following form:

$$\psi(\mathbf{x}) = \rho_0 \left[1 - \exp\left(-\frac{\rho}{\rho_0}\right) \right] \quad (8)$$

¹ Note that F_α can be linked to \mathbf{F} for instance following Guo et al. [12] through:

$$\mathbf{F}_\alpha = w_\alpha \left(\frac{\mathbf{c}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{c}_\alpha \cdot \mathbf{u}) \mathbf{c}_\alpha}{c_s^4} \right) \cdot \mathbf{F}.$$

² To recover Navier-Stokes equation with BGK collision operator.

129 where ρ_0 is a normalization constant which is usually chosen as 1 in lattice units. It was
 130 found however that using this form does not satisfy the thermodynamic consistency and may
 131 lead to high spurious currents [5, 41]. Therefore the expression of the effective density given
 132 in (8) can only be used to describe mixtures of liquid and gas with ratio of a maximum
 133 density of the order $O(10)$ [5].

134 In order to increase accessible density ratios and reduce spurious currents, we chose to
 135 implement a different Equation Of State (EOS), namely the Carnahan–Starling (C–S) one
 136 using the method developed in [41], where the effective mass reads

$$\psi(\rho) = \sqrt{\frac{2(P - \rho c_s^2)}{Gc_s^2}}. \quad (9)$$

137 The pressure P applied on a given node is expressed according to the following Equation Of
 138 State (EOS) ³

$$P = \rho RT \frac{1 + b\rho/4 + (b\rho/4)^2 - (b\rho/4)^3}{(1 - b\rho/4)^3} - a\rho^2 \quad (10)$$

139 where $a = 0.4963(RT_c)^2/P_c$, $b = 0.1873RT_c/P_c$, R is the perfect gas constant and T is
 140 the temperature, all expressed in lattice units. T_c and p_c denote the critical temperature and
 141 pressure, respectively (also expressed in lattice units). The expressions given for a and b
 142 consistently satisfy the conditions $(\partial P/\partial \rho)_T = (\partial^2 P/\partial^2 \rho)_T = 0$ at the critical point. Note
 143 that the parameter G no longer controls the interaction strength (as in Eq. (7)) but rather
 144 ensures that the term inside the square root in Eq. (9) is positive.

145 According to Yuan and Schaefer [41], these parameters are fixed at $a = 1$ lu, $b = 4$ lu
 146 and $R = 1$ lu. With these values, the interface thickness is approximately 5 lu for most T
 147 and τ values, and the simulation remains stable [15]. For water, the corresponding critical
 148 properties in lattice units are $T_c = 0.0943$ lu, $P_c = 0.00442$ lu, and $\rho_c = 0.1136$ lu [41]. The
 149 coexistence densities for C-S EOS can be deduced from the results of [41] and are shown in
 150 Figure 1.

151 In our simulations, the temperature is fixed to $T = 0.75T_c$, with the corresponding gas
 152 and liquid densities $\rho_g \approx 0.015$ lu and $\rho_l \approx 0.33$ lu, which are deduced from Fig. 1. In
 153 this work, it was found that by decreasing the temperature, the simulation becomes unstable.
 154 However, according to [13, 15], in this temperature range (for $T \geq 0.7T_c$), the thermodynamic
 155 consistency is satisfied with the C-S EOS.

156 The conversion from lattice units to physical units of the fluid properties can be done using
 157 the reduced properties concept [4, 41] based on the equivalence of some dimensional numbers
 158 between lattice and physical units (see the Appendix). Thus, the corresponding physical
 159 properties are temperature $T=212.17$ °C = 485.32 °K, water liquid density $\rho_l = 814.62$
 160 kg/m³, and water vapor density⁴ $\rho_g = 37.02$ kg/m³. It is important to quote that this choice
 161 of physical parameters T , P , and ρ (similar to other studies found in the literature) does
 162 not correspond to those used in experiments performed for comparison, but is mandatory
 163 to ensure the stability of the LBM simulations. However, as we will see in the application
 164 examples, this choice of parameters enables to recover the experimental values obtained
 165 for multi-phase systems, that proves its relevance which is not justified in literature to our
 166 knowledge.

³ Note that for an "ideal" or "perfect" gas laws, the pressure is $P(\rho) = \rho c_s^2$

⁴ The physical thermodynamic properties for water at the critical point are critical temperature $T_c=373.946$ °C = 647.096 °K, critical pressure $P_c=217.7$ atm = 220.6 bar = 22.06 MPa, and critical density $\rho_c=322$ kg/m³.

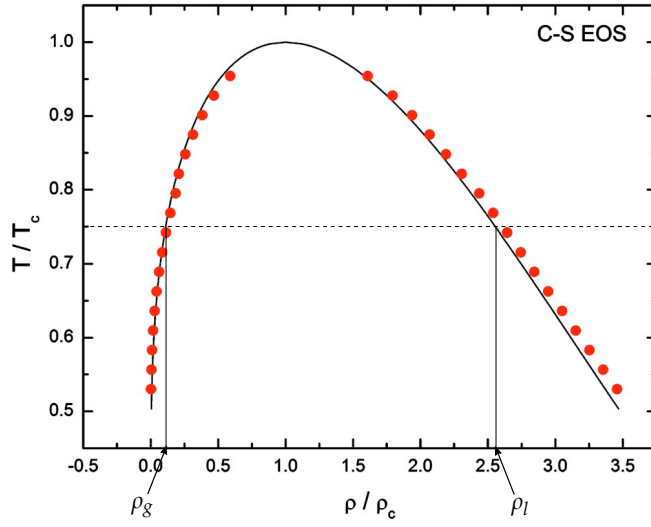


Fig. 1: Simulation (solid circles) and theoretical coexistence curves (solid line) for C-S EOS. The results and the figure are extracted from [41].

167 2.3 Fluid–solid interaction and contact angle

168 Modeling capillary bridges requires the introduction of a solid phase in addition to the two
 169 fluid phases presented in the previous section. The adhesion force between the fluids and the
 170 solid nodes takes a similar form as in Eq. (7) and reads according to [1]

$$\mathbf{F}_{ads}(\mathbf{x}) = -G\psi(\mathbf{x}) \sum_{\alpha} w_{\alpha}\psi(\rho_w)s(\mathbf{x} + \mathbf{c}_{\alpha}\Delta t)\mathbf{c}_{\alpha} \quad (11)$$

171 where s is the indicator function for the solid phase, equal to 1 for solid nodes and 0 for fluid
 172 nodes. The effective density, that is different from the real physical density, is denoted ρ_w .

173 The total force acting on a fluid node \mathbf{x} can be now written as:

$$\begin{aligned} \mathbf{F}(\mathbf{x}) &= \mathbf{F}_{int}(\mathbf{x}) + \mathbf{F}_{ads}(\mathbf{x}) \\ &= -\psi(\mathbf{x}) \left(-G \sum_{\alpha}^{fluid} w_{\alpha}\psi(\mathbf{x} + \mathbf{c}_{\alpha}\Delta t)\mathbf{c}_{\alpha} + G \sum_{\alpha}^{solid} w_{\alpha}\psi(\rho_w)\mathbf{c}_{\alpha} \right). \end{aligned} \quad (12)$$

174 To evaluate the effective density ρ_w , we use the method proposed by Li *et al.* [17], which
 175 is an improved version of the virtual-density scheme. ρ_w is a local quantity, instead of a
 176 constant value in the whole solid domain, defined as

$$\rho_w = \begin{cases} \varphi\rho_{ave}(\mathbf{x}), & \varphi \geq 1, \text{ For } \theta \leq 90^{\circ} \\ \rho_{ave}(\mathbf{x}) - \Delta\rho & \Delta\rho \geq 0, \text{ For } \theta \geq 90^{\circ}. \end{cases} \quad (13)$$

177 where φ and $\Delta\rho$ are constants to be tuned to achieve different contact angles θ . Moreover,
 178 the average fluid density ρ_{ave} reads

$$\rho_{ave}(\mathbf{x}) = \frac{\sum_{\alpha} w_{\alpha} \rho(\mathbf{x} + \mathbf{c}_{\alpha} \Delta t) (1 - s(\mathbf{x} + \mathbf{c}_{\alpha} \Delta t))}{\sum_{\alpha} w_{\alpha} (1 - s(\mathbf{x} + \mathbf{c}_{\alpha} \Delta t))}. \quad (14)$$

179 Note that in the definition given by (13), $\rho_w(\mathbf{x})$ is restricted to the range $\rho_g \leq \rho_w(\mathbf{x}) \leq \rho_l$.

180 To summarize, once the parameter φ or $\Delta\rho$ is set and ρ_w calculated from Eq. (13),
 181 the adhesive force between solid and fluid is evaluated by Eq. (11). As a consequence, a
 182 contact angle is implicitly obtained at equilibrium. It is important to notice that with this
 183 approach, the contact angle is a result of the LBM simulation at equilibrium, but is not a
 184 straightforward input data. As a result, the implicit relationship between the model parameters
 185 and the corresponding contact angle needs to be established to allow for an effective use of
 186 the model, which is one of the aims of the present study.

187 2.4 Numerical scheme

188 To specify the total force acting on the fluid \mathbf{F} , we chose to implement the velocity shift
 189 force scheme [32, 33]. In this scheme, the source term in Eq. (1) is set to 0 ($F_{\alpha} = 0$) and
 190 the force is incorporated in the velocity. More precisely, when calculating the equilibrium
 191 distribution function f^{eq} in Eq. (2), the following equilibrium velocity \mathbf{u}_{eq} is used instead
 192 of \mathbf{u} in Eq. (5):

$$\mathbf{u}_{eq} = \mathbf{u} + \frac{\tau}{\rho} \mathbf{F} \Delta t. \quad (15)$$

193 where $\mathbf{F}(\mathbf{x})$ is given by Eq. (12).

194 The actual physical fluid velocity, which will be used in section 4 for stress calculation,
 195 is defined as [33]:

$$\mathbf{u}_p = \mathbf{u} + \frac{1}{2\rho} \mathbf{F} \Delta t. \quad (16)$$

196 The algorithm adopted to solve the Lattice Boltzmann equation with the BGK collision
 197 model Eq. (1) is presented in Fig. 2. The collision step is expressed as follows

$$f_{\alpha}^*(\mathbf{x}, t) = f_{\alpha}(\mathbf{x}, t) - \frac{1}{\tau} [f_{\alpha}(\mathbf{x}, t) - f_{\alpha}^{eq}(\mathbf{x}, t)] \quad (17)$$

198 whereas the streaming step reads

$$f_{\alpha}(\mathbf{x} + \mathbf{c}_{\alpha} \Delta t, t + \Delta t) = f_{\alpha}^*(\mathbf{x}, t). \quad (18)$$

199 The non-slip boundary condition at the solid frontier relies on the halfway bounce-back
 200 scheme [43], in which the unknown distribution functions at the boundary fluid node \mathbf{x}_b ,
 201 next to the solid, are replaced by the ones in the opposite directions

$$f_{\bar{\alpha}}(\mathbf{x}_b, t + \Delta t) = f_{\alpha}^*(\mathbf{x}_b, t) \quad (19)$$

202 where $\bar{\alpha}$ stands for the opposite direction of α and f_{α}^* is the post collision distribution
 203 function. Figure 3 shows an illustration of the position of fluid, fluid boundary, and solid
 204 nodes.

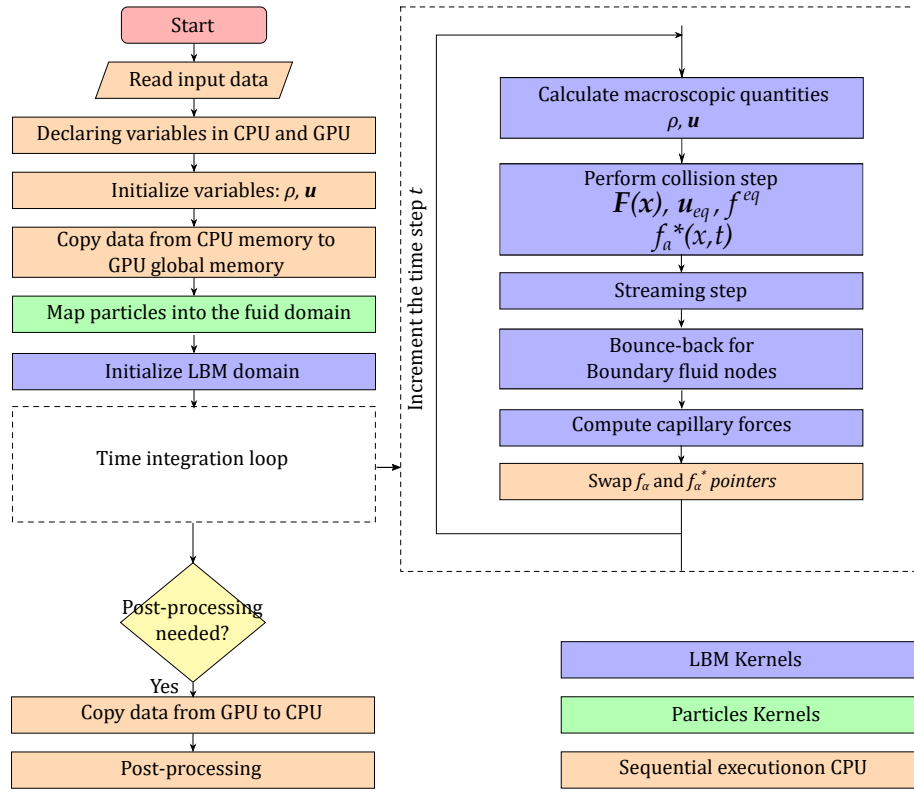


Fig. 2: Algorithm for LBM resolution with GPU implementation. Kernels are GPU functions that are executed in parallel by different GPU threads.

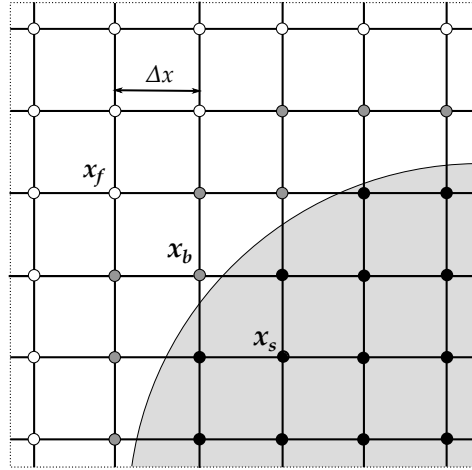
205 3 Benchmark simulations

206 In this section three benchmark configurations are considered: a drop of water i) with
 207 no contacts, ii) lying on a solid plane or iii) lying on a solid sphere. These benchmark
 208 simulations will be used to derive the explicit relationship between the model parameters
 209 and the corresponding surface tension and contact angle.

210 3.1 Surface tension deduced from the simulation of a stationary spherical drop

211 In order to bridge the gap between the model parameters describing the shape of the solid
 212 gas interface and more physically relevant quantities, as surface tension and contact angle,
 213 a series of numerical simulations are performed to compute the equilibrium of an initially
 214 spherical water drop of radius r_0 . In this simple configuration, the Laplace equation must be
 215 satisfied. For a spherical drop of radius r , this equation reads

$$\Delta P = P_{in} - P_{out} = \frac{2\gamma}{r} \quad (20)$$



- Fluid node, ◐ Boundary Fluid node
- Solid node

Fig. 3: Representation of fluid, boundary fluid, and solid nodes.

216 where P_{in} and P_{out} are the pressure inside and outside the drop far away from the interface,
 217 γ is the surface tension, and r is the droplet radius at equilibrium. More precisely, r
 218 is calculated as the distance between the center of the droplet and the middle position of the
 219 interface: $r = (r_{in} + r_{out})/2$, where r_{in} and r_{out} are the inner and outer radius of the fluid/gas
 220 interface. Far from the interface, $\rho = \rho_l$ in the fluid and $\rho = \rho_g$ in the gas. Note that in LBM
 221 multi-phase simulations, the interface has a thickness that may not be neglected, and depends
 222 on the mesh resolution. Moreover, with the approach used here, the interface thickness cannot
 223 be imposed but it is a result of the thermodynamic equilibrium that actually follows the EOS
 224 (10).

225 A series of simulations was conducted by varying the initial drop radius r_0 . The drop is
 226 placed in the middle of the domain of size $N_x \times N_y \times N_z = 256 \times 256 \times 256$, with N_x , N_y ,
 227 and N_z the domain size in x , y , and z direction, respectively. Periodic boundary conditions
 228 are applied in all directions. The temperature ratio is fixed at $T/T_c = 0.75$, the relaxation
 229 time $\tau = 1$ lu, and gas and liquid densities are fixed at $\rho_g = 0.015$ lu and $\rho_l = 0.33$ lu,
 230 respectively.

231 Figure 4b shows pressure distribution along the x -axis for an initial drop radius $r_0 = 30$
 232 lu. It can be seen that the pressure is almost constant inside and outside the drop. There is
 233 a positive and negative tips inside the interface, which is due to the strong non-linearity of
 234 C-S EOS (Eq. 10).

235 Figure 5 shows the pressure drop ΔP versus $2/r$ for two different resolutions. The fact
 236 that the relationship is linear is fully consistent with the existence of a surface tension
 237 corresponding to the slope of the curve. The comparison between the two mesh resolutions
 238 highlights that γ is not mesh dependent. The slopes represent indeed the surface tension with
 239 a value $\gamma = 0.0111$ lu ($R^2 = 0.99968$) for the resolution $256 \times 256 \times 256$ and $\gamma = 0.0114$ lu
 240 ($R^2 = 0.99953$) for the resolution $384 \times 384 \times 384$. Note that a very similar value of 0.01025
 241 was reported in a previous work using the same model parameters [13].

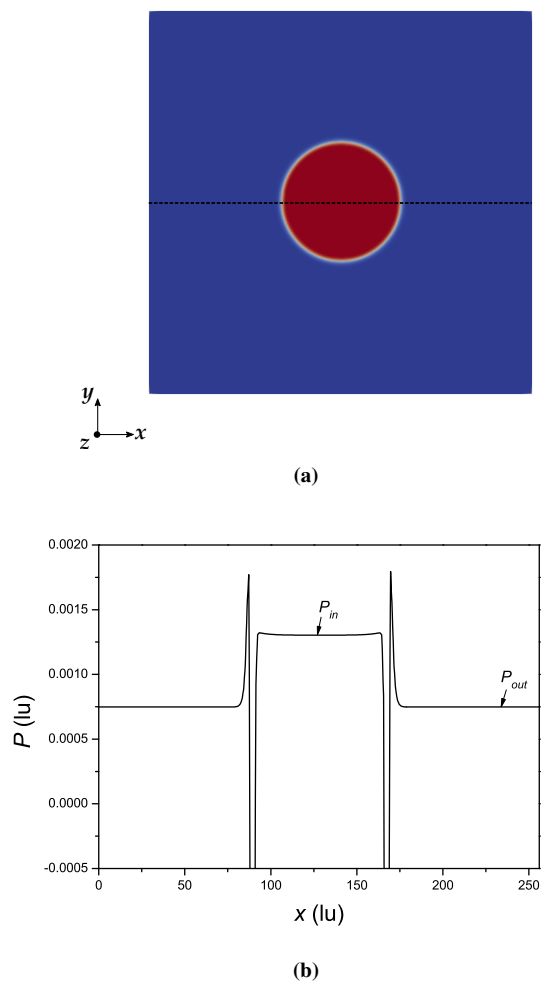


Fig. 4: (a) Density contours at equilibrium state for initial drop radius $r_0 = 30$ lu. (b) Pressure distribution along the horizontal axis that passes through the center of the domain.

242 3.2 Contact angle of a drop on a flat solid surface

243 3.2.1 Method for contact angle evaluation

244 Here, the simulation of a liquid drop spread on a flat surface is addressed. We study in
 245 particular the influence of the model parameter φ on the contact angle θ without gravity. As
 246 a starting configuration of the simulation, the domain is initialized with the gas density ρ_g ,
 247 except a drop region of radius r_0 (see Fig. 7) where prevails the liquid density ρ_l . The center
 248 of the drop is initially located at $(N_x/2, r_0, N_z/2)$. Periodic boundary conditions (BC) are
 249 imposed in both horizontal and front-back directions, whereas wall BC are applied at the
 250 top and at the bottom of the domain. Note that for the wall, we implemented the improved

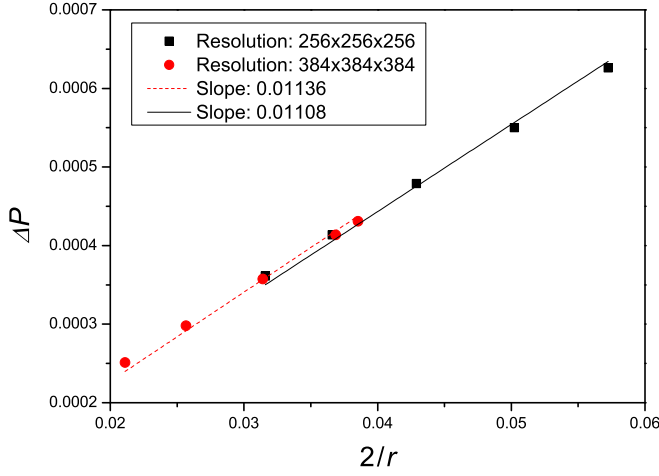


Fig. 5: Pressure drop between inside and outside the droplet versus $2/r$. The solid and dashed lines represent a linear fit with zero intercept consistent with the Laplace equation (20).

251 virtual density scheme (see Sec. 2.3), which ensures the wetting condition implicitly (contact
252 angle). Then, the simulation is launched until a final equilibrium situation is reached.

253 The contact angle is evaluated geometrically using Eq. (21) given below, with the as-
254 sumption that the shape of the drop is spherical, which is the case in the absence of gravity:

$$\theta = \begin{cases} 2 \tan^{-1}(\frac{2h}{b}) & \text{For } \theta \leq 90^\circ \\ \arcsin \frac{h-r}{r} + \frac{\pi}{2} & \text{For } \theta > 90^\circ. \end{cases} \quad (21)$$

255 Figure 6 shows the geometric parameters, namely h , r , and b , required to perform the contact
256 angle calculation in Equation (21).

257 Figure 7 illustrates a drop on a plane surface with the boundary conditions used for
258 the simulation and the shape of the drop at initial state and final state, once equilibrium is
259 reached.

260 3.2.2 Sensitivity to the mesh resolution

261 We first analyze the mesh sensitivity on the value of the contact angle. For all meshes, the
262 ratio $r_0/(N_x - 1)$ is kept fixed, where N_x is the number of lattices nodes in x-direction (r_0
263 is thus constant in physical units).

264 The values of parameter φ and contact angle θ are shown in Table 1. By comparison to
265 a reference value chosen as the one given by the finest resolution available, we first observe
266 that the relative error decreases as the mesh resolution increases. It is to note also that the
267 error tends to roughly decrease with φ .

268 In the following, all the LBM simulations will be performed with the second mesh
269 resolution, since the latter gives accurate results within reasonable calculation time.

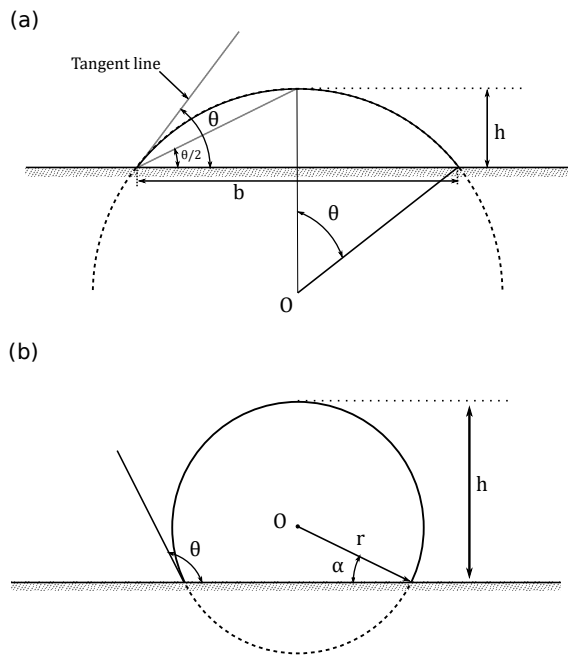


Fig. 6: Definitions of several geometric parameters needed for the contact angle θ calculation for: (a) $\theta < 90^\circ$ and (b) $\theta > 90^\circ$.

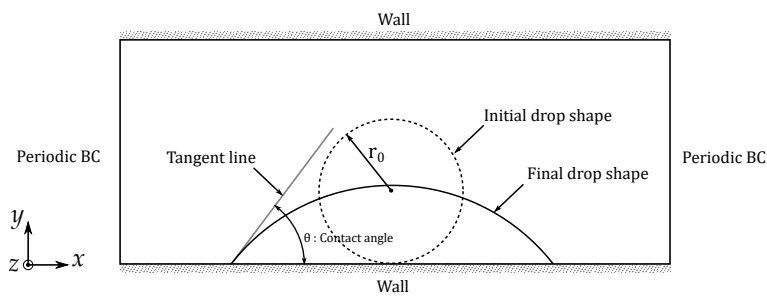


Fig. 7: Diagram illustrating a drop on a flat surface and the boundary conditions used for the simulation.

Resolution: ($N_x \times N_y \times N_z$)	$128 \times 128 \times 128$		$256 \times 128 \times 256$		$384 \times 128 \times 384$	
r_0 (lu)	10		20		30	
φ	θ ($^\circ$)	error (%)	θ ($^\circ$)	error (%)	θ ($^\circ$)	error (%)
0.8	91.87	0.66	91.11	0.17	91.27	-
1.0	72.43	1.98	71.22	0.27	71.03	-
1.2	60.44	1.85	59.57	0.38	59.34	-
1.4	50.17	2.87	50.92	1.41	51.65	-
1.6	42.95	1.76	43.51	0.49	43.72	-
1.8	35.15	4.2	36.29	1.08	36.69	-
2.0	26.33	8.63	27.82	3.48	28.82	-

Table 1: Values obtained for the contact angle θ versus φ for different mesh resolutions. The errors are calculated based on the finest resolution values.

3.2.3 Influence of the initial drop volume on the contact angle

In line with the previous finding on the influence of the parameter φ on the contact angle, a parametric study was performed by varying now the initial drop radius r_0 (corresponding to the initial drop volume) to verify that the observed contact angle (which is a response parameter of the LBM scheme) is not problem dependent.

Figure 8 shows the evolution of the contact angle θ versus φ for different initial drop radius r_0 . It can be concluded that, with the virtual density scheme implemented here, the initial drop volume does not influence significantly the contact angle in the absence of gravity. This is consistent with the fact that the contact angle is indeed a material property. This implicit definition of the contact angle in the numerical scheme is consequently physically sounded, at least when considering a drop on a plane.

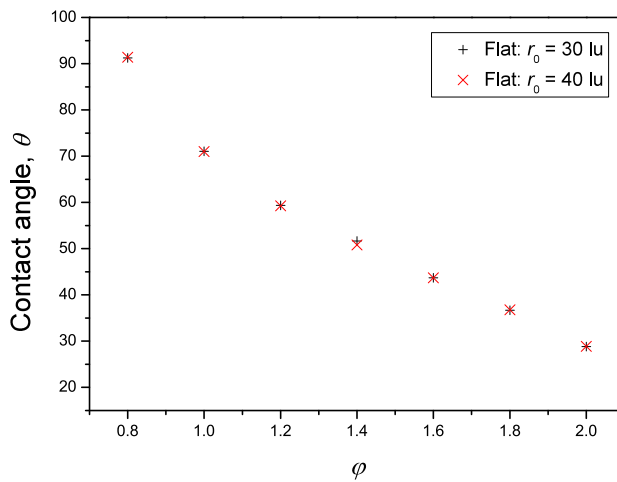


Fig. 8: Values obtained for the contact angle θ versus the parameter φ for different initial drop radii r_0 for a drop on a flat surface.

280

3.3 Contact angle of a drop on a convex solid surface

3.3.1 Method for contact angle and drop volume evaluation

In this second configuration, we now consider a liquid drop on a convex solid surface, namely a spherical cap. Yet again, the drop is placed exactly at the top of the solid surface as sketched in Figure 9(a). Here, the objective is to confirm that the contact angle does not depend on the curvature of the solid surface. Periodic BC are applied in both horizontal and front-back directions as well as top-bottom limits. We apply the improved virtual density scheme at the solid boundary to ensure the wetting condition (contact angle) while the bounce-back scheme is implemented for the probability distribution function f .

289

290 To evaluate the contact angle, we use image processing tools to identify the drop and
 291 solid disk in its vertical median plane at the end of the simulation, as sketched in Figure 9(b).
 292 Once both discs have been identified, we measure the geometric parameters R , r , and d . The
 293 contact angle is then calculated using the generalized Pythagorean theorem

$$\cos \theta = \frac{R^2 + r^2 - d^2}{2rR}. \quad (22)$$

294 We can also determine the so-called apparent contact angle $\theta' = \theta + \alpha$ (see Fig. 9).

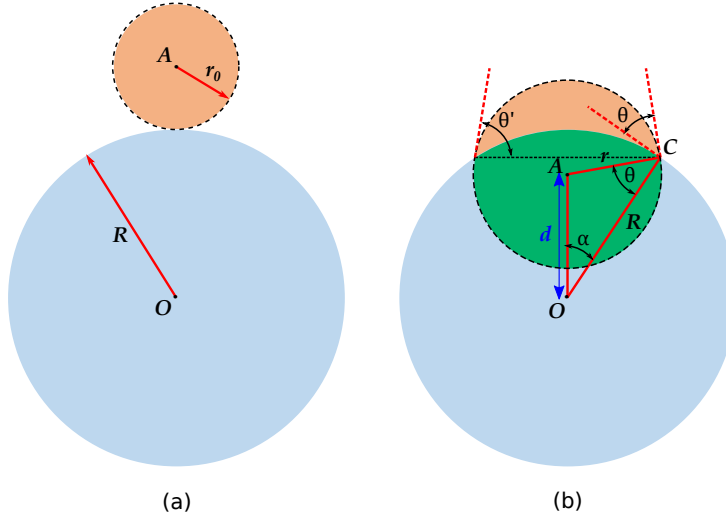


Fig. 9: Scheme illustrating the geometric parameters required to calculate the contact angle θ on a sphere: (a) initial condition, (b) equilibrium condition.

295 Additionally, the volume of the drop can be calculated. Indeed, in all our simulations,
 296 the final volume of the drop at equilibrium is not equal to its initial value due to the exchange
 297 of matter between the two fluid phases of the same component (water and its vapor). The
 298 calculation of the final drop volume requires the introduction of the two heights h_1 and h_2
 299 as defined in Figure 10. From there, the volume of the drop is given by the difference between
 300 the volume of the sphere of radius r and the intersection volume V_{int} as colored in green in
 301 Fig. 9. This volume V_{int} is simply the sum of two spherical caps of radii R and r , and heights
 302 h_1 and h_2 , respectively. From the formula of the volume of a spherical cap ⁵, one gets:

$$\begin{aligned} V_{int} &= V(R, h_1) + V(r, h_2) \\ &= \frac{\pi(R+r-d)^2(d^2 + 2dr - 3r^2 + 2dR + 6rR - 3R^2)}{12d} \end{aligned} \quad (23)$$

303 with

$$h_1 = \frac{(r-R+d)(r+R-d)}{2d} \quad (24)$$

⁵ The volume of a spherical cap of height h and radius R is $V_{cap}(R, h) = \frac{1}{3}\pi h^2(3R-h)$

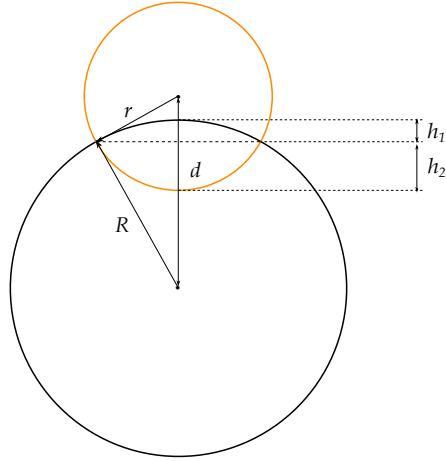


Fig. 10: Schematic defining the heights h_1 and h_2 used to calculate.

$$h_2 = \frac{(R - r + d)(R + r - d)}{2d}. \quad (25)$$

304 The volume of the drop is consequently equal to:

$$V = \frac{4}{3}\pi r^3 - V_{int}. \quad (26)$$

305 3.3.2 Sensitivity to the mesh resolution

306 Figure 11 shows the equilibrium state by the end of the simulation for different mesh
 307 resolutions. The data obtained for the contact angle as a function of φ are shown in Table 2.

308 Using as a reference value the one obtained with the finest resolution, we observe that
 309 the error decreases as the mesh size decreases. Here again, we will use the second mesh
 310 resolution to speed-up the calculation time as the error compared with the finest case remains
 311 limited to a few percents.

Resolution: ($N_x \times N_y \times N_z$)	128 × 128 × 128		256 × 256 × 256		320 × 320 × 320	
R (lu)	24		48		60	
r_0 (lu)	14		30		37	
φ	θ (°)	error (%)	θ (°)	error (%)	θ (°)	error (%)
0.8	87.96	2.98	91.6	1.05	90.65	-
1.0	67.7	3.4	69.65	0.62	70.09	-
1.2	54.25	7.21	55.71	4.71	58.46	-
1.4	46.04	2.55	48.13	1.88	47.24	-
1.6	38.95	3.85	39.25	3.11	40.51	-
1.8	33.47	2.98	32.16	1.06	32.5	-
2.0	19.85	14.72	22.25	4.38	23.27	-

Table 2: Values obtained for the contact angle θ versus φ for different mesh resolutions of a drop on a sphere. The errors are calculated based on the finest resolution.

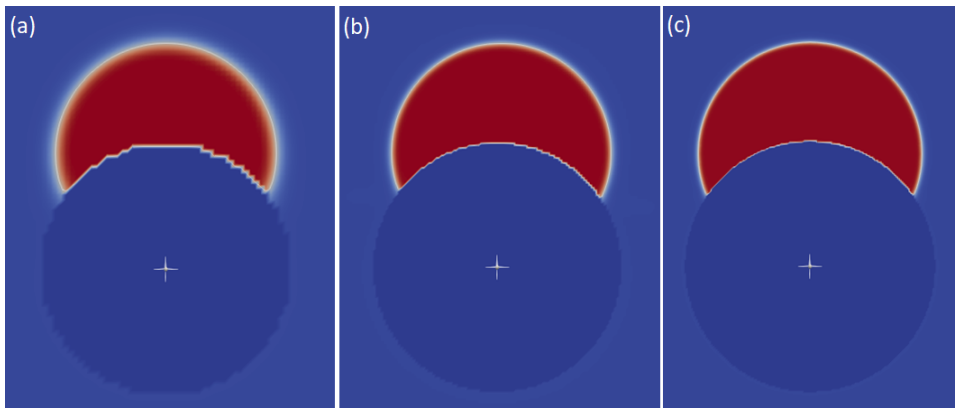


Fig. 11: Equilibrium state obtained for different mesh resolutions with $\varphi = 1.2$: a) $N_x \times N_y \times N_z = 128 \times 128 \times 128$, b) $N_x \times N_y \times N_z = 256 \times 256 \times 256$, (c) $N_x \times N_y \times N_z = 320 \times 320 \times 320$.

312 3.3.3 Influence of the solid surface curvature radius

313 The influence of the solid curvature radius R on the contact angle calculation is first studied.
 314 The initial drop radius is fixed at $r_0 = 30$ lu, while $R = 48, 64,$ and 72 lu.

315 The corresponding data of the contact angle versus φ is plotted in Figure 12. It can be
 316 seen that the results almost collapse on a unique curve, showing that the curvature radius
 317 of the solid surface has merely no influence on the contact angle, which is, here again,
 318 consistent with the fact that the contact angle is a material property independent from the
 319 problem geometry.

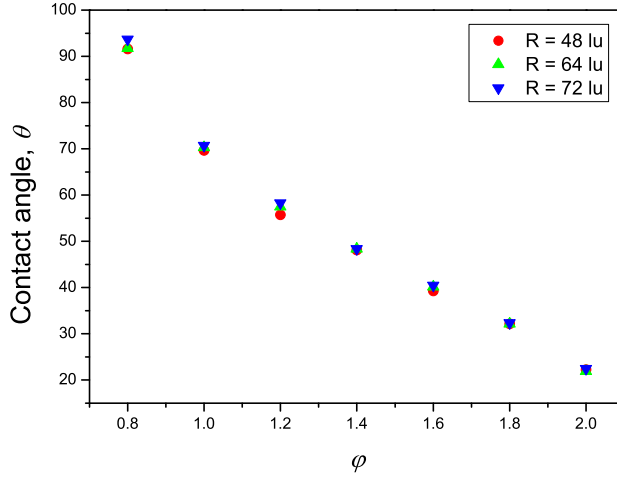


Fig. 12: Values obtained for the contact angle versus φ with a fixed initial drop radius $r_0 = 30$ lu and three different solid radii for a drop on a sphere. The mesh resolution is $256 \times 256 \times 256$.

3.3.4 Influence of the initial drop volume

Similarly to section 3.3.3, we now examine the potential impact of the initial drop radius. To this end, Figure 13 shows the contact angle as a function of φ for different initial drop radii r_0 . The previous data of a drop on a flat surface are added for comparison. It can be seen that the data are almost all identical, especially for small values of φ ($\varphi < 1.4$ or $\theta > 50^\circ$)⁶. In the same way, we can conclude that the impact of the drop volume is negligible, confirming again that the contact angle can be definitely considered as a material property depending only on the model parameter φ .

It can be noted that based on the simulation data, the parameter φ can be approximated by a polynomial of degree four in θ as shown in Fig. 14 and given in Eq. (27). Then, for any value of the contact angle θ in radians, this empirical interpolation enables to prescribe the parameter φ to be used in the LBM simulation to recover the target value of θ . Note finally that for a fixed value of θ corresponds a unique value of φ for $\theta \leq 90^\circ$.

$$\varphi = 1.655 + 3.216\theta - 8.048\theta^2 + 5.697\theta^3 - 1.330\theta^4. \quad (27)$$

Finally, Figure 15 shows the dimensionless drop volume at equilibrium V/R^3 versus φ . We see that the method for calculating the volume, from (26), gives the same results and collapse with the LBM simulations, except for the larger volume where a small gap appears (of the order of 4%). Moreover, we can conclude that the final volume of the drop does not depend on φ and therefore on the contact angle θ . Equivalently, for an imposed volume V_0 , the final volume at equilibrium does not depend on θ , that is physically consistent.

⁶ For small values of θ , the improved virtual-density scheme [17] appears less accurate for a drop on convex solid surfaces than on flat surfaces due to the discretization of the surface.

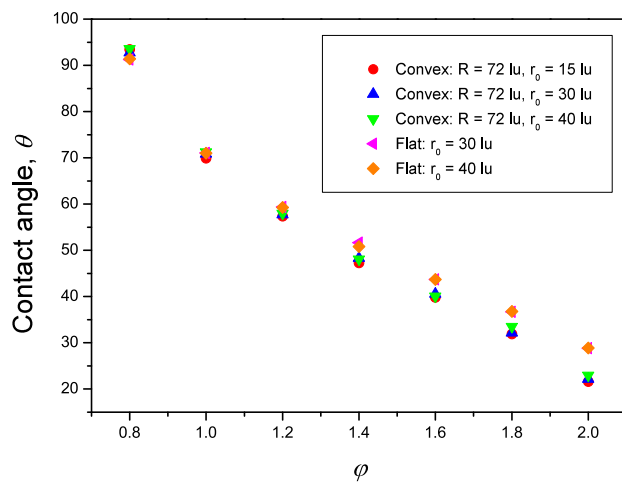


Fig. 13: Values obtained for the contact angle versus ϕ for three different initial drop radii r_0 and a fixed solid radius $R = 72$ lu. The data of a drop on a flat surface are added.

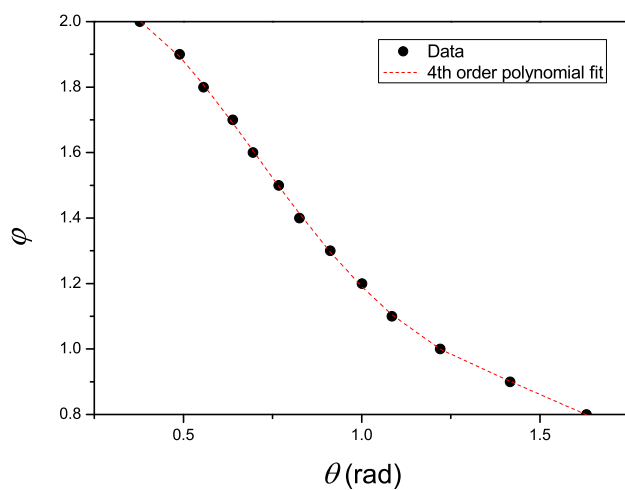


Fig. 14: Empirical calibration of ϕ versus θ with a 4th order polynomial approximation. The data correspond to the situation of an initial drop radius $r_0 = 15$ lu and a convex surface with a fixed radius of curvature $R = 72$ lu.

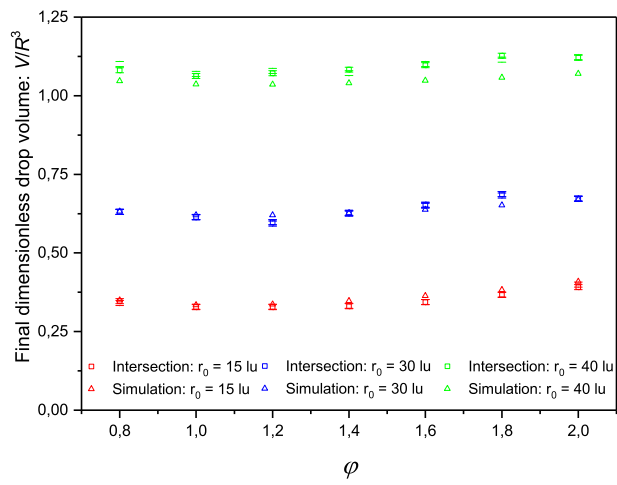


Fig. 15: Values obtained for the dimensionless drop volume at equilibrium V/R^3 versus φ for different initial drop volumes V_0 and a fixed radius of curvature of the solid surface $R = 72$ lu.

339 3.3.5 Comparison to experiments

340 To validate our results, we simulate the same experiments as in [39], where water drops of
 341 different volumes were deposited on a spherical PC (polycarbonate) surface with a radius of
 342 curvature $R = 6.35$ mm. The measured value of the contact angle was $\theta = 89^\circ$. Based on
 343 the proposed empirical relation (27), the wetting parameter is fixed at $\varphi = 0.769$ giving a
 344 contact angle equal to the experimental value.

345 Figure 16 shows a comparison of the apparent contact angle $\theta' = \theta + \alpha$ (Fig. 9) between
 346 the experimental data of [39] and the values obtained with our simulation as a function of the
 347 reduced volume V/R^3 , with R the radius of curvature of the solid surface. The agreement is
 348 rather satisfactory, even if we observe a small deviation in the simulation results. This may be
 349 due to the solid surface which is not perfectly spherical in the simulation as it is represented
 350 through a stair-case approximation which may cause small errors in the measurement of the
 351 apparent contact angle.

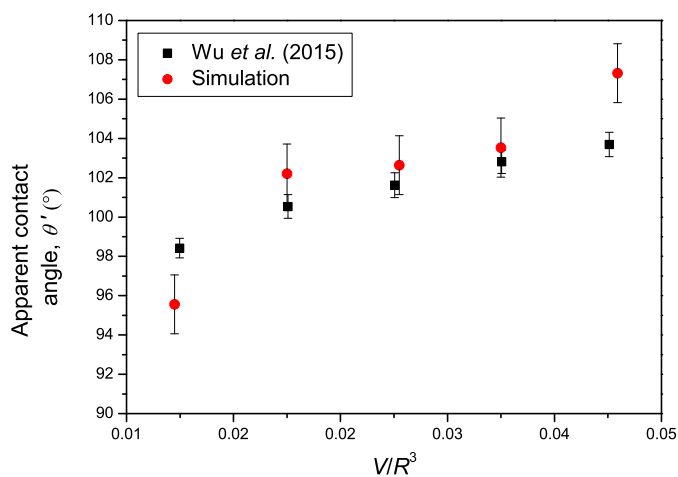


Fig. 16: Values obtained for the apparent contact angle θ' versus dimensionless drop volume V/R^3 for a radius of curvature of the solid surface $R = 6.35$ mm. The experimental results of [39] are included for water drops on PC surface ($\theta = 89^\circ$). The error bar in the simulation is induced by the mesh resolution with a one-pixel uncertainty in the calculation of the different geometric quantities.

352 4 Capillary forces induced by a liquid bridge between two spherical particles

353 As already explained in the introduction, the aim of this work is to develop an efficient LBM
 354 method, fast and accurate enough, to simulate capillary interfaces between several solid
 355 particles and to compute the resulting capillary forces.

356 The last study being addressed in the present work therefore concerns the calculation of
 357 the capillary force between two solid spheres connected by a liquid bridge. To this end, two
 358 solid particles with the same radius $R = 102 \text{ lu}$ ($R = 8 \text{ mm}$) are placed in the domain and
 359 separated with a dimensionless separation distance $D^* = D/R = 0.2$. The parameter φ was
 360 fixed at 2.0 which corresponds to a contact angle $\theta = 21.4^\circ$ from Eq. (27).

361 The lattice size in physical units is fixed at $\Delta x_{phy} = L_c/(N_x - 1)$, where $L_c = 0.03 \text{ m}$ is
 362 the domain length in x-direction. Snapshots of the liquid bridge shape during the simulation
 363 is shown in Figure 17, corresponding to condensation phenomenon.

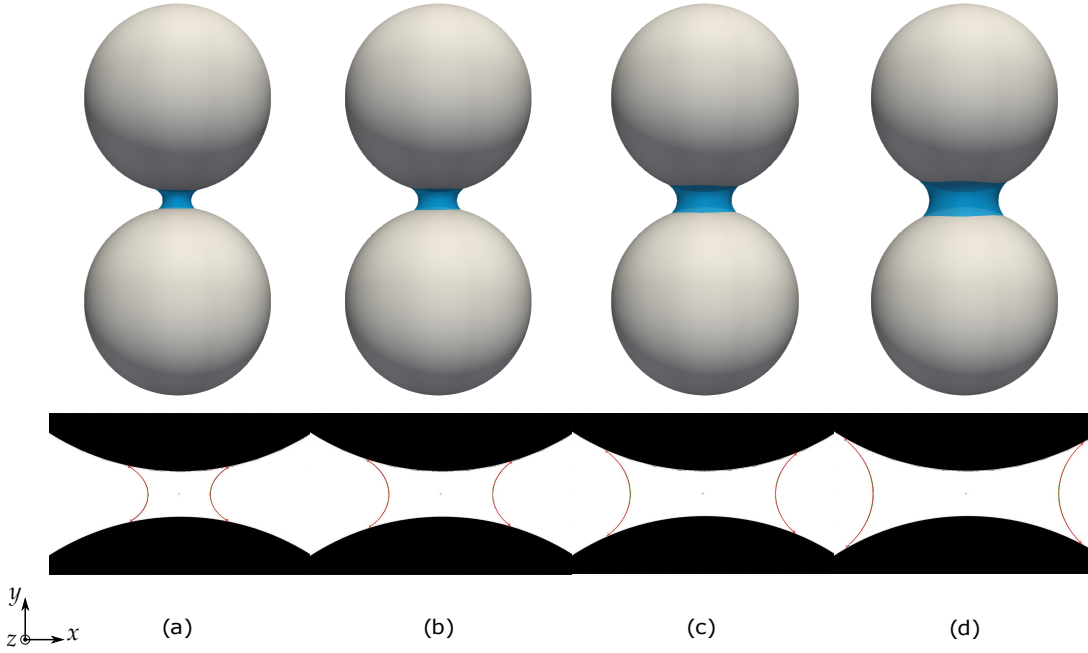


Fig. 17: The numerical (top) and theoretical (bottom) shapes of the liquid capillary bridge profiles during the simulation for different dimensionless volumes ($V^* = V/R$): (a) $V^* = 0.016$, (b) $V^* = 0.041$, (c) $V^* = 0.085$, and (d) $V^* = 0.15$.

364 4.1 Brief reminder on capillary bridges modelling and associated forces

365 Let us recall that the shape of a capillary bridges between two spherical particles is axisym-
 366 metric of revolution along the x-axis connecting the centers of the two particles. It is given
 367 by a solution of the Young-Laplace equation:

$$\frac{y''(x)}{(1 + y'^2(x))^{3/2}} - \frac{1}{y(x)\sqrt{1 + y'^2(x)}} = -\frac{\Delta P}{\gamma} = H \quad (28)$$

368 where $H = -\frac{\Delta P}{\gamma}$ denotes the mean curvature which is constant in all the capillary bridges,
 369 while $\Delta P = P_{in} - P_{out}$ stands for the pressure difference between inside and outside of the

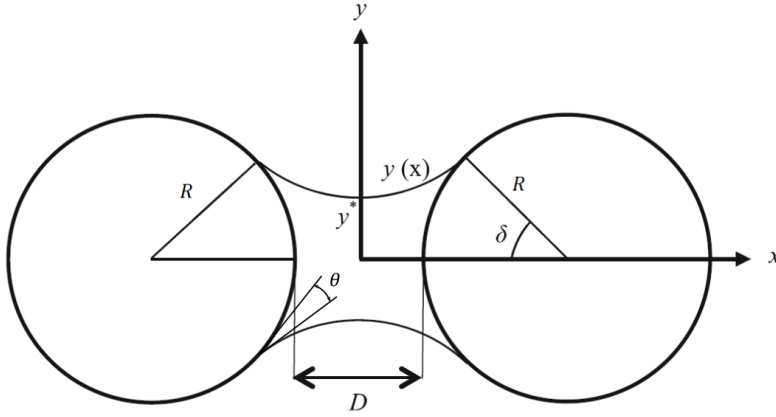


Fig. 18: Illustration of a capillary bridge between two identical spherical particles. δ and θ are the filling and contact angle, respectively. Figure extracted from [11].

370 liquid bridge, and γ is the surface tension of the fluid. In Figure 18, δ denotes the filling
 371 angle, y^* the gorge radius, and θ the wetting angle. D is the separation distance between the
 372 particles. At static equilibrium, the capillary force is a first integral of the Young–Laplace
 373 equation [11, 19] and can be calculated at the gorge radius y^* as

$$F_{cap} = \pi\gamma H y^{*2} + 2\pi\gamma y^* \quad (29)$$

374 or at the contact line following

$$F_{cap} = \pi\gamma H R^2 \sin^2 \delta + 2\pi\gamma R \sin \delta \sin (\delta + \theta). \quad (30)$$

375 Therefore, the capillary force classically includes two contributions: the first one results from
 376 the pressure difference inside and outside of the bridge (Laplace pressure) and the second
 377 contribution is due to surface tension along the wetted interfaces.

378 Note that equation (28) can be also solved analytically using a cylindrical approximation
 379 [29] leading to a direct and convenient relationship between the dimensionless capillary
 380 forces $F_{cap}^* = F_{cap}/(2\pi\gamma R)$, the dimensionless inter-particles distance $D^* = D/R$, and the
 381 dimensionless volume $V^* = V/R^3$:

$$F_{cap}^* = \cos \theta \left(1 - \frac{1}{\sqrt{1 + \frac{2V^*}{\pi D^{*2}}}} \right). \quad (31)$$

382 This relationship is however only valid for small volumes, typically for $V^* < 0.01$. Richefeu
 383 et al. [31] further proposed the following empirical relation for the capillary force based on
 384 fitting the numerical solution of Laplace-Young equation for two particles of same diameter:

$$F_{cap}^* = \cos \theta \exp \left(\frac{-D^*}{0.9\sqrt{V^*}} \right). \quad (32)$$

385 These two approximate expressions of capillary force will be used in section 4.3 to validate
 386 our LBM numerical simulations of capillary bridges.

4.2 Numerical calculation of the capillary forces

The total force exerted by the fluid on the solid can be calculated based on the integration of the fluid stress tensor σ on a surface Ω close to the solid particle as illustrated in Figure 19:

$$\mathbf{F}_t = \int_{\Omega} \sigma \cdot \mathbf{n} dA \quad (33)$$

where \mathbf{n} is the outer unit normal vector to the surface Ω and dA stands for an elementary area element. For viscous Newtonian fluids, the fluid stress tensor is given by

$$\sigma_{ij} = -P\delta_{ij} + \tau_{ij}. \quad (34)$$

In expression (34), P is the fluid pressure given by Eq. (10) whereas the viscous stress tensor τ_{ij} , reads

$$\tau_{ij} = \mu(\partial_j u_i + \partial_i u_j) \quad (35)$$

where μ is the dynamic fluid viscosity ($\mu = \rho\nu$).

Note that we follow almost the same integration technique as in [34] but with different stress tensor formula, since they use a free-energy method to model two-phase liquid–vapor flows which are different than the shan-chen model.

The discretized form of Eq. (33), that will be used for LBM numerical calculations reads

$$\mathbf{F}_t = \sum_{x_{\Omega}} \sigma \cdot \mathbf{n} dA \quad (36)$$

where x_{Ω} accounts for all lattice points located on the voxelized surface Ω , as shown in the zoom of Fig. 19. The area element dA is equal to 1 in lattice units. Note that the center of the cubes of the voxelized surface Ω are considered to be located at the lattice points to avoid interpolation of fluid quantities. The viscous stress tensor τ_{ij} is calculated from the LBM simulation using finite difference method applied to Eq. (35).

It is important to stress that Eqs. (33) or (36) do not include the surface tension term that is present in expression (29) or (30) of capillary forces. However since the interface has a finite thickness in the LBM computation (Fig. 4b), we will prove through the LBM simulations that the surface tension term is implicitly included in the contribution of the stress in the interface.

Before concluding on this point, we will check the mesh dependency of the capillary force measurement. To do so, the capillary forces will be computed at two different distances ε away from the solid particle for three different resolutions, as indicated in Table. 3 and Fig. 19. Note that ε is constant in physical units (mm) but varies in lattice units (lu) according to the chosen mesh resolution. The reason for using a strictly positive epsilon is to get rid of non physical phases junction of the fluid pressure on the solid/fluid interface.

The capillary forces calculated with the three mesh resolutions and the two values of ε are displayed in Figure 20 versus the dimensionless volume V^* of the water bridge and for $D^* = 0.2$. As can be seen, the resolution has a limited effect on the capillary force, especially for the smallest epsilon value. Therefore, the simulations and calculations of the associated capillary forces will be done with the finest mesh $384 \times 450 \times 384$ in the following to minimize the error on the wetting angle. The GPU simulation time was about 100 min for this resolution using a GPU card Quadro RTX 5000.

⁷ The capillary force at this position was linearly interpolated between 7th and 8th lattice.

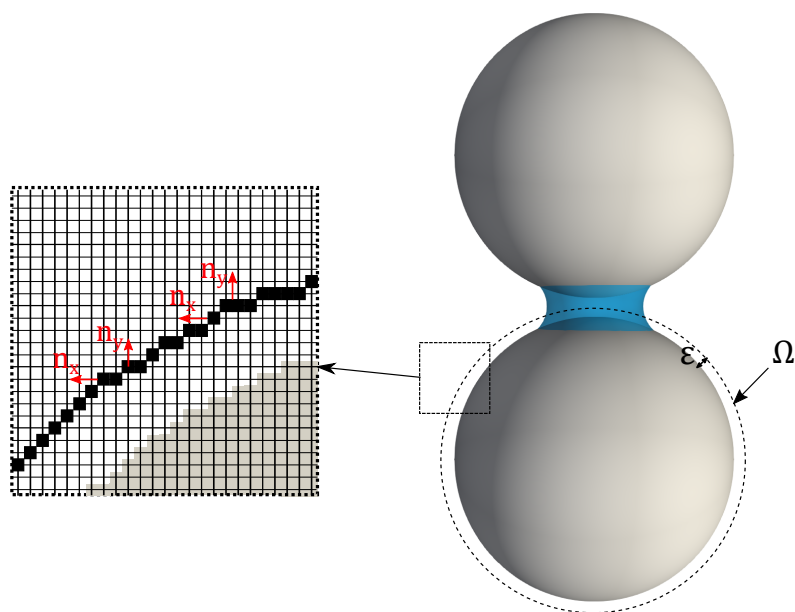


Fig. 19: Snapshot of a simulation of a liquid bridge between two spherical particles. Ω is the integration surface. In this example, the dimensionless separation distance is $D^* = D/R = 0.2$ and the reduced liquid volume is $V^* = V/R^3 = 0.18$.

Resolution: ($N_x \times N_y \times N_z$)	256 × 384 × 256	320 × 380 × 320	384 × 450 × 384
ε (mm)	ε (lu)		
0.471	4	5	6
0.706	6	7.5 ⁷	9

Table 3: Distance of integration ε in physical (mm) and lattice (lu) units for three different mesh resolutions.

422 The stress integration results are given in Figure 21. As a general trend, it can be observed
 423 that the capillary forces increase as the volume increases in the range $0 \leq V^* \leq 0.4$. Also, the
 424 capillary forces increase with the distance ε from the solid surface where they are calculated.
 425 It thus appears that the choice of the integration surface Ω is particularly crucial. The reason
 426 why the integration surface Ω is shifted at some distance ε from the solid particles is that a
 427 thin liquid film is created near the outer solid surface due to the implementation of the wetting
 428 condition as shown in Figure 22 where the density profile is plotted versus the distance from
 429 the solid surface. Therefore, ε should be chosen higher than or equal to 5 lu ($\varepsilon \geq 5$ lu). In
 430 the sequel, for the comparison between the capillary force calculated with LBM simulation
 431 and the existing results from the literature, we will consider $\varepsilon = 5$ lu.

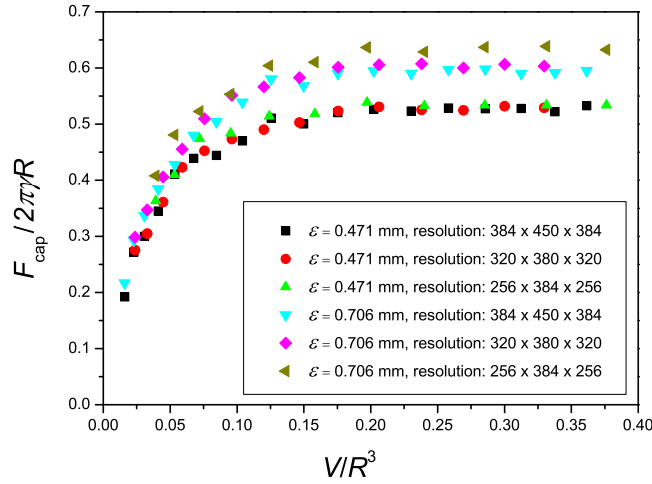


Fig. 20: Normalized capillary forces versus normalized volume for three different resolutions at two distances of integration $\varepsilon = 0.471$ mm and $\varepsilon = 0.706$ mm.

432 4.3 Comparison with the literature

433 In Figure 23, we compare the results obtained with our LBM simulations using $\varepsilon = 5$ lu
 434 during the condensation of the liquid bridge with the two theoretical expressions of capillary
 435 force given by Eq. (29) and (30), and with the approximations given by Eq. (31) and (32).
 436 The experimental data of [19] are also added. It can be observed that the LBM simulations
 437 with $\varepsilon = 5$ lu give values of the capillary force very close to the gorge radius expression (29)
 438 and in good agreement with the contact line expression (30), the cylindrical approximation
 439 of Eq. (31), and the experiments of [19]. **Based on the founding, we can conclude that the**
 440 **capillary force is a result of the integration of the pressure and the viscous part, and the**
 441 **fluid velocity does not tend toward zero at equilibrium, which is specific to the shan-chen**
 442 **model with the velocity shift force scheme. In other words the viscous part contribute to the**
 443 **capillary force, even when the capillary bridge is at equilibrium.**

444 To finish, Figure 24 shows the dimensionless mean curvature $H^* = H \times R$, with $H =$
 445 $-\Delta P/\gamma$, versus $V^* = V/R^3$, where ΔP is deduced from the LBM simulation results. Two
 446 different shapes are encountered: nodoid shape, which corresponds to $H > 0$, and unduloid
 447 shape for $H < 0$, as described in detail in [11]. **The theoretical H values are determined**
 448 **using inverse problem technique to solve Young-Laplace equation, the same image processing**
 449 **in-house code as in [11] is used.**

450 The effect of the wetting angle on the capillary force is shown in Fig. 25 . The stress
 451 integration method is used with $\varepsilon = 5$ lu. We see that the forces decreases as the wetting
 452 angle increases.

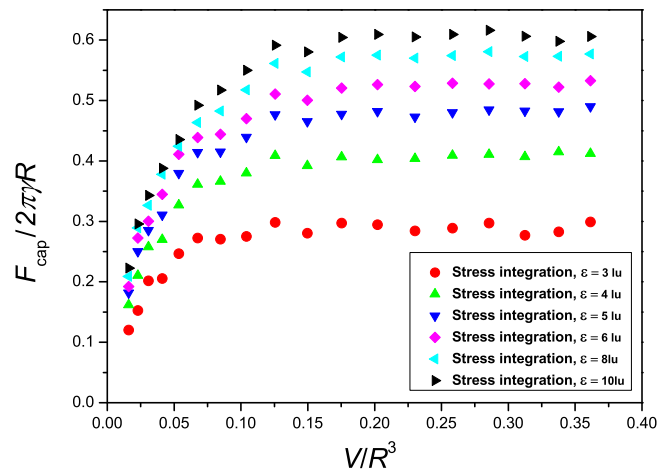


Fig. 21: Normalized capillary force versus normalized volume during the condensation of a liquid bridge between two spherical particles of same radius R at different distances ε .

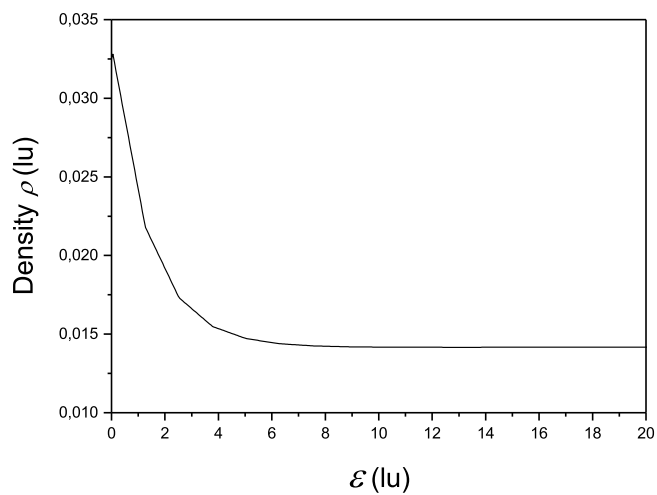


Fig. 22: Density profile versus the distance ε from the solid surface out of the capillary bridge region, where $\rho_g = 0.015$ lu corresponds to the gas phase. The density of the liquid phase $\rho_l = 0.333$ lu.

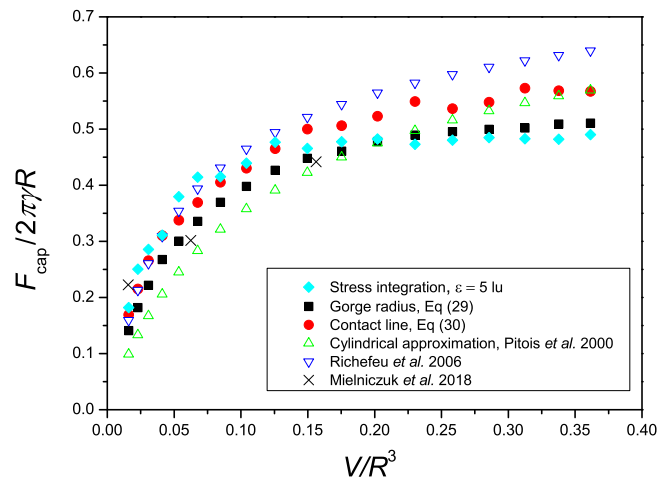


Fig. 23: Comparison of normalized capillary force versus normalized volume calculated using stress integration method with $\varepsilon = 5$ lu, gorge radius (Eq. (29)), contact line (Eq. (30)), cylindrical approximation (Eq. (31)), approximation given by Richefeu (Eq. (32)), and experimental data of [19].

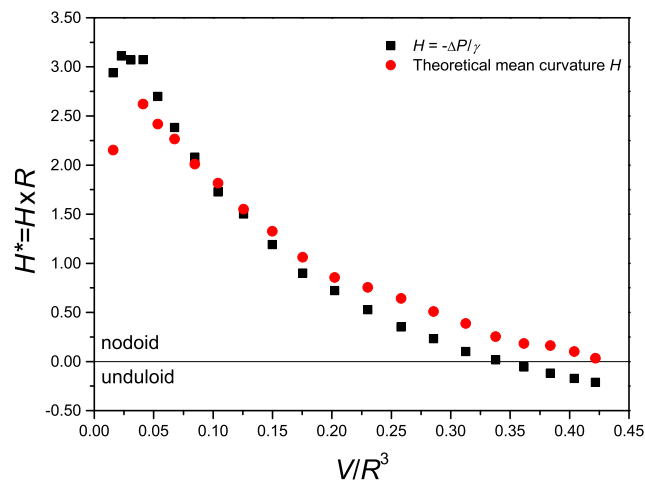


Fig. 24: Variation of the dimensionless mean curvature $H^* = H \times R$ of the capillary bridge between two spheres versus dimensionless volume. $H > 0$ corresponds to a nodoid shape and $H < 0$ corresponds to a unduloid shape.

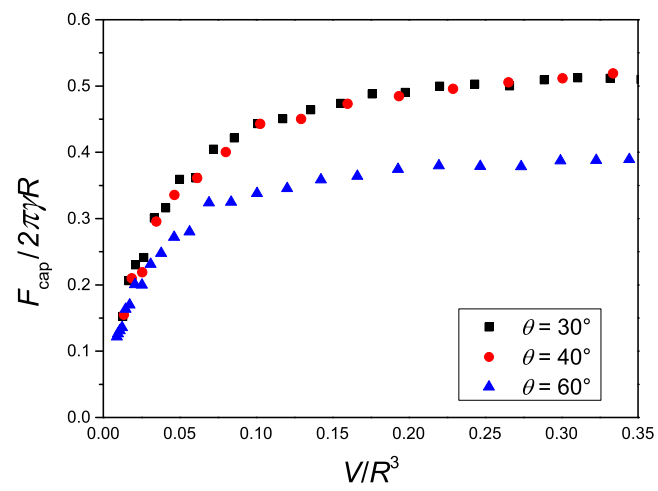


Fig. 25: Normalized capillary force versus normalized volume for different contact angles.

5 Conclusion

In this paper, we have studied the Single Component Multi-Phase (SCMP) Shan-Chen model for simulating capillary interfaces in various configurations and for calculating the induced capillary forces. The SCMP model was implemented in 3D and solved using GPU. The relevance of the model was verified by performing several benchmarks, such as drop on flat and spherical walls and stationary spherical drops. Regarding the latter, results found for the surface tension and the contact angle are consistent. Moreover, we have highlighted a direct relation between the parameters of the virtual density scheme and the induced wetting angle θ that enables to easily adjust the parameters to directly determine the desired value of θ . Next, we have considered capillary bridges between two spherical particles and analyzed in details the capillary interface, and then calculated the associated capillary force. Although we have revealed some limitations of the SCMP Shan-Chen model (high values of temperature and pressure to guarantee the numerical stability which do not correspond to classical experimental values, difficulty to control the interface thickness), we have proved however that the computation of the capillary forces at some distance from the solid grain, provides results quite close to analytical expressions existing in literature and to experiments performed in similar conditions while avoiding spurious terms in the calculation. This way, we can justify the values of the parameters usually used in LBM SCMP model in literature, which are given in lattice units and never compared to usual values encountered in lab experiments or in natural conditions. Therefore, accounting for the very small computation time needed to stabilize the capillary interface, this approach may be considered promising to simulate the behavior of a partially saturated granular assembly containing a large number of particles. Also, this approach is suited for time evolution problems, such as partially saturated granular media subjected to condensation/evaporation cycles for instance.

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Appendix: Conversion between physical and lattice units

The LBM simulations with Shan-Chen model involve four dimensional quantities: time, length, mass and temperature. The conversion between lattice units and physical units is done with use of the reduced properties concept [4, 41] for the fluid properties (namely density ρ , pressure P , and temperature T) and with one additional conversion factors for length.

$$\rho_R = \frac{\rho}{\rho_c}, \quad P_R = \frac{P}{P_c}, \quad T_R = \frac{T}{T_c}, \quad (37)$$

where the subscript "R" and "c" are the reduced and critical properties, respectively. According to this concept, the reduced properties in lattice and physical units should be equal. As an example, we have $\rho_R^{lu} = \rho_R^{phy}$, leading to $\rho^{phy} = \rho^{lu} \rho_c^{phy} / \rho_c^{lu}$. The other properties can be obtained in a similar manner.

The conversion factors for length, time and density are respectively $C_l = \Delta x_{phy} / \Delta x_{lu}$, $C_t = \Delta t_{phy} / \Delta t_{lu}$, and $C_\rho = \rho_{phy} / \rho_{lu} = \rho_c^{phy} / \rho_c^{phy}$. The conversion factor for force can be deduced as $C_f = C_\rho C_l^4 / C_t^2$.

494 To get the value in physical units, the corresponding value in lattice units is multiplied by the conversion factor
495 that has the same physical units. For example, for length we have $L_{phy} = L_{lu} \times C_l$.

496 For capillary interfaces with no flow, where the Reynolds number is no longer relevant, the time scale is
497 not given by viscosity ⁸. The conversion between surface tension γ in lattice and physical units reads

$$\gamma^{phy} = \gamma^{lu} C_\rho \frac{C_l^3}{C_t^2} \quad (38)$$

498 In the presence of gravity, the conversion between gravity in lattice and physical units is given as

$$g^{phy} = g^{lu} \frac{C_l}{C_t^2} \quad (39)$$

499 Alternatively, physical units can be related to lattice units through dimensionless numbers (e.g. the Bond
500 number (Bo)) instead of using the conversion factors. As an example, the dimensionless Bond number is
501 defined as

$$Bo = \frac{(\rho_l - \rho_g)gr^2}{\gamma} \quad (40)$$

502 where g is the gravity, γ is the surface tension and r is the length scale (e.g. drop radius in the case studied
503 in section 3.2). By setting $Bo_{lattice} = Bo_{physical}$, the conversion leads to

$$\frac{(\rho_l^{phy} - \rho_g^{phy})g^{phy}(r^{phy})^2}{\gamma^{phy}} = \frac{(\rho_l^{lu} - \rho_g^{lu})g^{lu}(r^{lu})^2}{\gamma^{lu}}. \quad (41)$$

504 Expression (41) enables to fix the gravity in lattice units g^{lu} that can be used in LBM simulation when taking
505 it into account.

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⁸ The time scale for flows that are controlled by Reynolds number is classically given by: $\Delta t_{phy} = c_s^2 (\tau - \frac{1}{2}) \Delta x_{phy}^2 / \nu_{phy}$, where c_s and τ in lattice units [16].

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