Numerical modelling of Super Hydrophobic Surfaces Using Lattice Boltzmann method

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Introduction

Super Hydrophobic Surfaces (SHS) have been of interest to researchers for many years, because of their ability to reduce drag and maintain the surface to be dry and clean, and a large variety of methods have been applied to study their phenomena. The lattice Boltzmann method, thanks to its mesoscopic nature is a suitable candidate to simulate the intermolecular interactions responsible for the interfacial flows in a microscale. In this contribution, we present a conservative, phase-field model for simulation of immiscible multiphase flows using an incompressible, velocity based Cascaded Lattice Boltzmann Method. As a study case, we present a simulation of a SHS.

How SHS works?

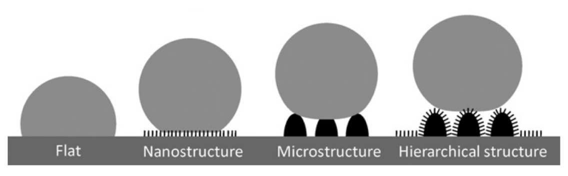

Figure 1: Surface structure

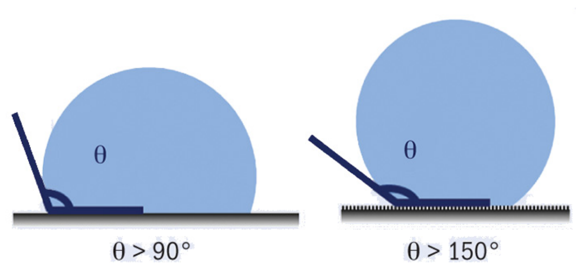

Figure 2: Coating vs structure

Generally, the super hydrophobic effect comes from both chemical interaction and surface shape in a microscale. The principle of work is based on the fact, that the tiny air-bubbles are entrapped into the microstructure of the surface being in the contact with fluids which is sliding on them. Unfortunately, usage of SHS depends on the flow condition. It may happen, that too fast flow or improper shape of the surface would cause the air-bubbles to wash out and to loose the desired properties. Chemical surface treatment can results in contact angles up to $120°$.Higher values observed in a macro scale can be achieved only by additional micro roughing of the surface.

How SHS looks like?

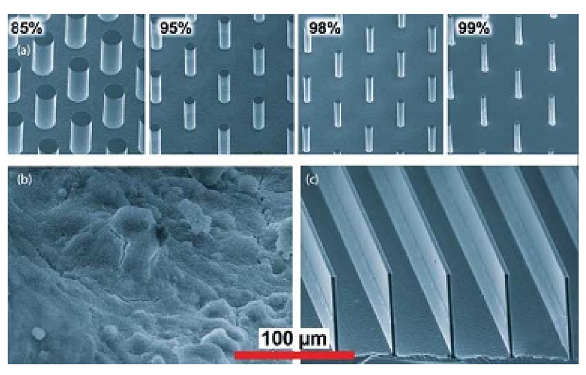

Figure 3: Manufactured

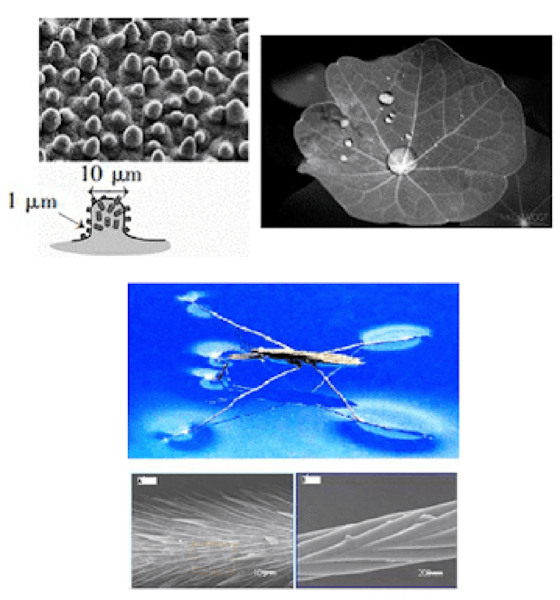

Figure 4: Natural

To support a thin layer of air, an array of posts or ridges is usually applied. Such symmetric structures are expensive to manufacture, fragile and not common in nature. However, experiments have shown that an unstructured, rough surface can work as well as regularly spaced arrays of ridges or posts.

Governing Equations

We simulate an incompressible, non-miscible, multiphase flow.

Hydrodynamics

The continuity and momentum equations are,

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \\ \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \nabla\cdot(\mu[\nabla\mathbf{u} + (\nabla\mathbf{u})^\top]) + \mathbf{F}_s + \mathbf{F}_b. \end{cases}$$

Forcing terms are given as,

$$\boldsymbol{F}_s = \mu_\phi \nabla\phi \quad ; \quad \boldsymbol{F}_b = [G_X, G_Y]^\top.$$

Phase-field

Interface tracking is realized using the phase-field approach,

$$\frac{\partial\phi}{\partial t} + \nabla\cdot\phi\mathbf{u} = \nabla\cdot M\left(\nabla\phi - \frac{\nabla\phi}{|\nabla\phi|}\frac{[1-4(\phi-\phi_0)^2]}{\gamma}\right).$$

The interface is located in $\phi_0 = (\phi_H + \phi_L)/2$.
Density is a linear interpolation between ρ_H and ρ_L,

$$\rho = \rho_L + \frac{\phi - \phi_L}{\phi_H - \phi_L}(\rho_H - \rho_L).$$

'Advection - Diffusion' of ϕ is solved on a separate D2Q9 lattice.

Lattice Boltzmann Method - Algorithm

The raw moments and central moments are defined as,

$$\Upsilon_{mn} = \sum_\alpha (e_{\alpha x})^m (e_{\alpha y})^n f_\alpha$$

$$\tilde{\Upsilon}_{mn} = \sum_\alpha (e_{\alpha x} - u_x)^m (e_{\alpha y} - u_y)^n f_\alpha$$

Pressure and velocity are interpreted as zeroth and first moment respectively,

$$p^* = \Upsilon_{00} = \sum_\alpha f_\alpha,$$

$$\mathbf{u} = [u_x, u_y]^\top = [\Upsilon_{10}, \Upsilon_{01}]^\top = \sum_\alpha f_\alpha \mathbf{e}_\alpha + \frac{\mathbf{F}}{2\rho}\delta t.$$

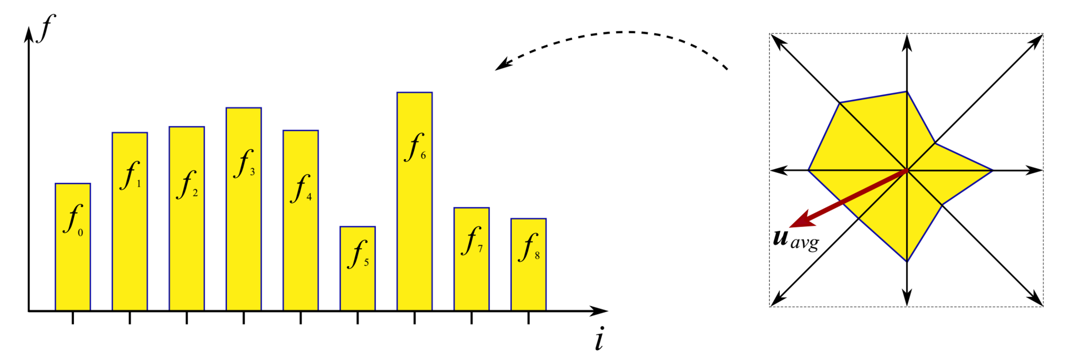

Figure 5: Concept of lattice velocities

We introduce improvements to the LB equations for interface tracking and incompressible hydrodynamics, by transforming the operations into the central moment space. The relaxation of central moments is defined in a reference frame moving with the fluid. As a consequence, Galilean invariance and stability of the method is improved.

Hydrodynamics

1 Initialize $\boldsymbol{f}(\mathbf{x}, t)$,

2 Compute $\mathbf{u} = [u_x, u_y]^\top = [k_{10}, k_{01}]^\top = \sum_\alpha f_\alpha \mathbf{e}_\alpha + \frac{\mathbf{F}}{2\rho}\delta t$,

3 Compute
$\tilde{\boldsymbol{\Upsilon}}(\mathbf{x}, t) = \mathbb{N}\mathbb{M}\mathbf{f}(\mathbf{x}, t)$, $\quad \tilde{\boldsymbol{\Upsilon}}^{eq}(\mathbf{x}, t) = ...$, $\quad \tilde{\mathbf{F}}(\mathbf{x}, t) = ...$,

4 Collision
$\tilde{\boldsymbol{\Upsilon}}^*(\mathbf{x}, t) = (\mathbb{1} - \mathbb{S})\tilde{\boldsymbol{\Upsilon}} + \mathbb{S}\tilde{\boldsymbol{\Upsilon}}^{eq} + (\mathbb{1} - \mathbb{S}/2)\tilde{\mathbf{F}}$,

5 Streaming
$\boldsymbol{f}(\mathbf{x} + \mathbf{e}\delta t, t + \delta t) = \mathbb{M}^{-1}\mathbb{N}^{-1}\tilde{\boldsymbol{\Upsilon}}^*(\mathbf{x}, t)$.

Phase-field

1 Initialize $\boldsymbol{h}(\mathbf{x}, t)$,

2 Compute $\phi = \sum_\alpha h_\alpha(\mathbf{x}, t)$

3 Compute
$\tilde{\boldsymbol{\Upsilon}}^\phi(\mathbf{x}, t) = \mathbb{N}\mathbb{M}\mathbf{h}(\mathbf{x}, t)$, $\quad \tilde{\boldsymbol{\Upsilon}}^{\phi,eq}(\mathbf{x}, t) = ...$, $\quad \tilde{\mathbf{F}}^\phi(\mathbf{x}, t) = ...$,

4 Collision
$\tilde{\boldsymbol{\Upsilon}}^{\phi,*}(\mathbf{x}, t) = (\mathbb{1} - \mathbb{S}^\phi)\tilde{\boldsymbol{\Upsilon}}^\phi + \mathbb{S}^\phi\tilde{\boldsymbol{\Upsilon}}^{\phi,eq} + (\mathbb{1} - \mathbb{S}^\phi/2)\tilde{\mathbf{F}}^\phi$,

5 Streaming
$\boldsymbol{h}(\mathbf{x} + \mathbf{e}\delta t, t + \delta t) = \mathbb{M}^{-1}\mathbb{N}^{-1}\tilde{\boldsymbol{\Upsilon}}^{\phi,*}(\mathbf{x}, t)$.

Benchmarks

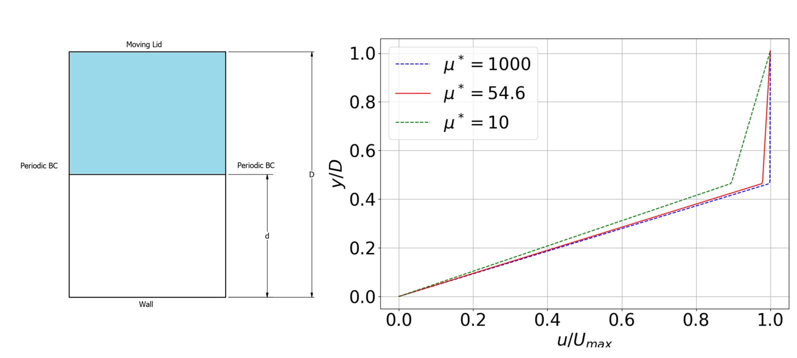

Figure 6: Two phase Coutte flow:
influence of μ^* on velocity slip between phases

In fig. 6 we can observe that for $\mu^* = 1000$ the velocity profile resembles a perfect slip condition. In the case of a water-air interface, $\mu^*_{water-air} = 54.6$, thus the common simplification of the interface by a slip BC seems to be justified with $\sim 2\%$ error.

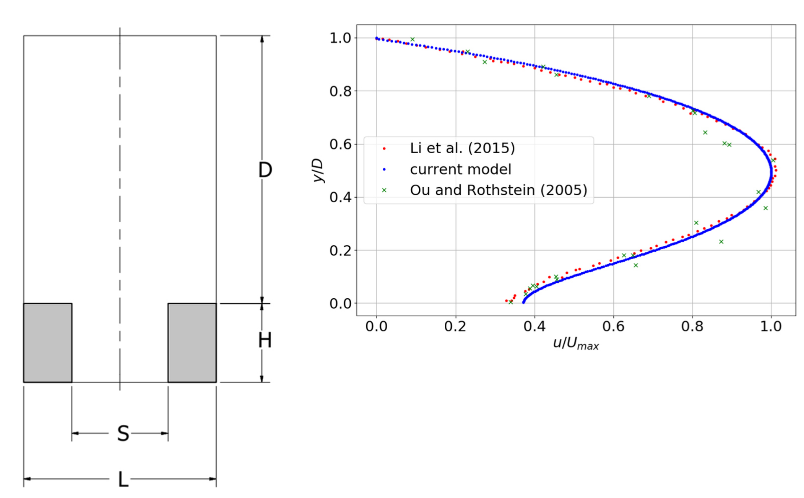

Figure 7: Dimensionless velocity profile at the center of the air pocket $\rho^* = \mu^* = 54 : 6$

A typical geometry of a simple, periodic super hydrophobic surface is shown in fig. 7. Gentle filling of the geometry with water keeps the air bubble entrapped between solid posts (grey). Finally, the flow can be driven by gravity or a pressure difference. Having compared the velocity profiles above the entrapped air, we conclude that our results are in agreement with the ones obtained by other researchers.

Summary

In this work, a phase-field LBM was proposed with an implementation of the collision routine in the central moment space, which improves the model performance in terms of both Galilean invariance and discretization errors. Presented model have been successfully validated against both analytical and experimental benchmarks. Additionally, the LBM is relatively easy in implementation and able to handle complex geometries such as porous media or rough surface. Computations are performed locally, thus the algorithm can be parallelized in a straightforward manner.

Treatment of an air-water interface

Common simplifications

- rigid surface
- perfect slip
- seek of an ideal SHS may leads to a trivial solution - two phase Coutte flow

What we achieved

- simulations of a deformable air-water interface at micro scale
- applicable to fluids having high density ratio
- able to capture complex geometry