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A New Boundary Condition for Three-Dimensional Lattice Boltzmann Simulations of Capillary Filling in Rough Micro-Channels

Alessandro De Maio[1,*], Silvia Palpacelli[1] and Sauro Succi[2,3]

[1] *Numidia s.r.l., via Berna 31, 00144 Roma, Italy.*
[2] *Istituto Applicazioni Calcolo, CNR, via dei Taurini 19, 00185 Roma, Italy.*
[3] *Freiburg Institute for Advanced Studies, School of Soft Matter Research, Albertstr. 19, 79104 Freiburg im Breisgau, Freiburg, Germany.*

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Abstract. A new boundary condition, aimed at inhibiting near-wall condensation effects in lattice Boltzmann simulations of capillary flows in micro-corrugated channels, is introduced. The new boundary condition is validated against analytical solutions for smooth channels and demonstrated for the case of three-dimensional microflows over randomly corrugated walls.

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Key words: Microfluidics, capillary flows, lattice Boltzmann simulation.

1 Introduction

The Lattice Boltzmann method was devised as a computational alternative to the solution of the Navier-Stokes equations for the numerical simulation of macroscopic flows [1]. For the last few years, however, an intense activity has been directed by many groups towards the application of LB techniques to microscopic and nanoscopic flows [2–7]. The somewhat unanticipated success of LB beyond the macroscopic context is probably due to the existence of a large body of microfluidic problems, in fact larger than textbook indications, for which continuum hydrodynamics is violated, but somehow mildly, i.e., in a way which can be mended without necessarily resorting to atomistic simulations (molecular dynamics). This statement can be made a little more precise as follows. The breakdown of hydrodynamics in microfluidic problems is often signalled by the appearance of infinities/singularities in the corresponding solutions. Moving contact lines, droplet

*Corresponding author. *Email addresses:* demaio.a@gmail.com (A. De Maio), silviapalpacelli@gmail.com (S. Palpacelli), succi@iac.rm.cnr.it (S. Succi)

break-up and coalescence, are just but a few examples in point [8–10]. It is generally understood that such infinities are regulated by an atomistic cutoff. Nevertheless, going all the way down to atomistic simulation proves unpractical for want of compute power. This no-fly zone offers in principle a rich hunting ground for mesoscopic/kinetic methods. However, achieving quantitative accuracy is by no means a given, and depends on a careful application of these methods in the appropriate parameter regime. In this paper we shall discuss a few aspects related to the specific case of capillary front-propagation in rough geometries.

2 The method

We use the LB method with the standard Shan-Chen (SC) [11] pseudo-potential forcing. The corresponding lattice Boltzmann equation takes the following form:

$$f_i(\vec{r}+\vec{c}_i\Delta t,t+\Delta t)-f_i(\vec{r},t)=\frac{\Delta t}{\tau}\left(f_i^{eq}(\vec{r},t)-f_i(\vec{r},t)\right), \tag{2.1}$$

where $f_i(\vec{r},t)$ represents the probability of finding a particle at time t on the lattice site $\vec{r}$, moving with velocity $\vec{c}_i$. The left-hand-side represents the particle free-streaming, while the right hand side encodes particle collisions in the form of a relaxation on a time scale τ to the local equilibrium f_i^{eq}. The latter is given by a Maxwell-Boltzmann distribution truncated to second order in the local Mach number, and reads as follows:

$$f_i^{eq}(\vec{r},t)=\rho w_i\left(1+\frac{\vec{u'}\cdot\vec{c}_i}{c_s^2}+\frac{\vec{u'}\vec{u'}:\vec{\vec{Q}}_i}{2c_s^4}\right), \tag{2.2}$$

where w_i are the standard weights for the 19-speed 3d lattice considered in this work, and $\vec{\vec{Q}}=\vec{c}_i\vec{c}_i-c_s^2 I$ is the quadrupole projector upon the i-the direction, $c_s^2=\sum_i w_i c_{ix}^2$, being the lattice sound speed. In the above, $\rho=\sum_i f_i$ is the local fluid density and $\vec{u'}=(\sum_i f_i\vec{c}_i+\vec{F}\tau)/\rho$ is the local fluid speed, including the contribution of the interparticle-interaction force

$$\vec{F}=-G\Psi(\vec{r};t)\sum_i w_i\Psi(\vec{r}+\vec{c}_i\Delta t)\vec{c}_i. \tag{2.3}$$

In the above, G is the coupling strength, and Ψ is the usual density-dependent pseudo-potential $\Psi(\rho)=(1-e^{-\rho})$. As is well known, the SC method provides the two basic features of non-ideal fluid behavior, namely a non-ideal equation of state $p=\rho c_s^2+Gc_s^2\Psi^2/2$, and a non-zero surface tension

$$\gamma\propto-\frac{G}{2}c_s^4\int(\nabla\Psi)^2dy,$$

where y runs across the interface. It is readily shown that for $G<-4$, the above equation of state generates coexisting liquid and vapor phases.