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Mesoscopic modelling of local phase transitions and apparent-slip phenomena in microflows

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Abstract

The phenomenon of apparent slip in micro-channel flows is analyzed by means of a two-phase mesoscopic lattice Boltzmann model with non-ideal fluid–fluid and fluid–wall interactions. Analytical solutions of the weakly inhomogeneous hydrodynamic limit of this model are successfully compared with numerical simulations and show that the present mesoscopic approach is capable of filling the gap between the atomistic size of the interaction potential and the millimetric size of the slip length reported in microflow experiments. In the critical interplay between fluid–fluid and fluid–wall interactions, our approach indicates an exponential inflation of the slip length as a function of the ratio of potential to thermal energy.

Keywords: Mesoscopic modelling; Local phase transitions; Apparent-slip phenomena

The microscopic physics underlying fluid/solid interactions depends on a host of specific details of molecular interactions and geometrical/chemical details of the confining surfaces. However, on a macroscopic scale, these details can often be conveyed into synthetic statements regarding the nature of collective motion of the fluid relative the solid walls. The simplest such statement is the so-called "no-slip" boundary condition, which states the absence of any relative fluid–wall motion. This boundary condition forms the basis of mathematical treatments of bounded flows as continuum media [9]. Yet, from recent advances in microfluidics experiments [7,12], as well as numerical investigations [1,2,4,3], the evidence is that a large class of viscous flows *do* slip on the wall. Therefore, a general theoretical picture for the onset of slip motion is much needed. Among others, an increasingly popular explanation is that the flowing fluid would develop a lighter (less dense) phase and dynamically segregate it in the form of a thin film sticking to the wall [13,6]. This thin film would then offer a reduced resistance to the near-wall fluid flow, thus providing the basis for slip motion. Although appealing, this film picture is still in need of theoretical consolidation. This phenomenon of 'apparent slip' will be here addressed by means of numerical simulations as well as analytical solutions of the weakly inhomogeneous hydrodynamic equations with a non-ideal equation of state.

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For this purpose, we shall make use of the lattice Boltzmann model developed by Shan and Chen in [10] (hereafter SC). This reads as follows:

$$f_l(\boldsymbol{x}+\boldsymbol{c}_l, t+1) - f_l(\boldsymbol{x}, t) = -\frac{1}{\tau}(f_l(\boldsymbol{x}, t) - f_l^{(\mathrm{eq})}(\boldsymbol{x}, t)) + F_l \tag{1}$$

where $f_l(\boldsymbol{x}, t)$ is the probability density function associated to a mesoscopic velocity $\boldsymbol{c}_l$, τ a mean collision time, $f_l^{(\mathrm{eq})}(\boldsymbol{x}, t)$ the equilibrium distribution that corresponds to the Maxwellian distribution in the fully continuum limit and, finally, F_l is an external forcing associated with intermolecular interactions. The bulk interparticle interaction is controlled by a free parameter, G_b, entering the balance equation for the momentum change:

$$\frac{\mathrm{d}(\rho \boldsymbol{u})}{\mathrm{d}t} = G_\mathrm{b} \sum_l w_l \Psi[\rho(x)]\Psi[\rho(x+\boldsymbol{c}_l)]\boldsymbol{c}_l \tag{2}$$

where w_l is the equilibrium weights and Ψ is the potential describing non-ideal fluid–fluid interactions. By Taylor expanding Eq. (2) one recovers, in the hydrodynamic limit, the equation of motion for a non-ideal fluid with equation of state $P = c_\mathrm{s}^2(\rho - (1/2)G_\mathrm{b}\Psi^2(\rho))$, where c_s is the sound speed velocity. With the choice $\Psi(\rho) = 1 - \exp(-\rho/\rho_0)$ with $\rho_0 = 1$ a reference density, the model supports phase transitions whenever the control parameter exceeds the critical threshold $G_\mathrm{b} > G_\mathrm{b}^\mathrm{c}$. In our case, $G_\mathrm{b}^\mathrm{c} = 4$ for an averaged density $\langle\rho\rangle = \log(2)$.

Let us now consider the central point of this work, namely the critical interplay between bulk physics and wall effects. In fact, in order to make contact with experiments and MD simulations, it is important to include fluid–wall interactions, and notably a parametric form of mesoscopic interactions capable of mimicking wettability properties as described by contact angles between droplets and the solid wall [5]. This effect can be achieved by assuming that the interaction with the wall is represented as an external force F_w normal to the wall and decaying exponentially [14,11], i.e.

$$F_\mathrm{w}(\boldsymbol{x}) = G_\mathrm{w}\rho(\boldsymbol{x})\,\mathrm{e}^{-|\boldsymbol{x}-\boldsymbol{x}_\mathrm{w}|/\xi} \tag{3}$$

where $\boldsymbol{x}_\mathrm{w}$ is a vector running along the wall location and ξ is the typical length-scale of the fluid–wall interaction. Here, we aim at studying the effects of G_w when the thermodynamically stable bulk physics is governed by a single phase. The main result is that the presence of the wall may trigger a local phase coexistence, inducing the formation of a less dense phase in the vicinity of the walls and an apparent slip of the bulk fluid velocity profile extrapolated at the wall location.

With the flow driven by a constant pressure gradient in the x (streamwise) direction, $F_i = \delta_{i,x}\,\partial_x P_0$, and the walls located at $y = 0$ and L_y, Eqs. (1)–(3) have been numerically solved in two dimensions. No-slip boundary conditions are used at the boundary and G_w is such that a repulsive force for the liquid at the wall is introduced. The *macroscopic* limit of our model reads then as follows:

$$\begin{aligned} &\partial_t\rho + \partial_i(u_i\rho) = 0 \\ &\rho[\partial_t u_i + (u_j\,\partial_j)u_i] = -\partial_i P + \nu\,\partial_j(\rho\,\partial_i u_j + \rho\,\partial_j u_i) + F_i \end{aligned} \tag{4}$$

where subscripts i and j run over the two spatial dimensions, $\nu = c_\mathrm{s}^2(\tau - 1/2)$ and $P = c_\mathrm{s}^2\rho - V_\mathrm{eff}(\rho, y)$ is the total pressure consisting of an ideal-gas contribution ($c_\mathrm{s}^2\rho$) plus the so-called excess pressure, V_eff, due to potential–energy interactions. The expression of V_eff in terms of both G_b and G_w reads:

$$V_\mathrm{eff}(\rho, y) = \frac{c_\mathrm{s}^2}{2}G_\mathrm{b}(1-\exp(-\rho))^2 + G_\mathrm{w}\int_0^y \mathrm{d}s\rho(s)\,\exp\left(-\frac{s}{\xi}\right).$$

For steady states ($\partial_t = 0$) and under the assumption of homogeneity ($\partial_x = 0$), the spanwise (y) momentum balance equation reduces to:

$$\partial_y P(\rho) = c_s^2\,\partial_y\rho - 2G_\mathrm{b}c_\mathrm{s}^2(1-\mathrm{e}^{-\rho})\,\mathrm{e}^{-\rho}\partial_y\rho - G_\mathrm{w}\rho\,\mathrm{e}^{-y/\xi} = 0 \tag{5}$$

whose solution delivers the density profile. The corresponding velocity profile is then obtained by the momentum equation along the streamwise coordinate $\nu\,\partial_y(\rho\,\partial_y u_x) = -\partial_x P_0$. With density variations concentrated in a thin layer of thickness δ near the wall, the mass flow rate Q_{eff} for small δ can be estimated as follows:

$$\frac{Q_{\mathrm{eff}}}{Q_{\mathrm{pois}}} = 1 + \frac{3}{2}\frac{\Delta\rho_{\mathrm{w}}}{\rho_{\mathrm{w}}}\frac{\delta}{H} \tag{6}$$

where Q_{pois} corresponds to the Poiseuille rate $2\,\partial_x P_0 H^3/3\nu$ valid for incompressible flows with no-slip boundary conditions. In Eq. (6), the quantity $\Delta\rho_{\mathrm{w}}$ is defined as the difference between ρ computed in the center of the channel and ρ_{w} computed at the wall. The effective slip length, usually defined in terms of the increment in the mass flow rate, reads [8]:

$$\lambda_{\mathrm{s}} \sim \delta\frac{\Delta\rho_{\mathrm{w}}}{\rho_{\mathrm{w}}}. \tag{7}$$

This is the best one can obtain using a continuum approach. The added value of the mesoscopic approach rests with the possibility to directly compute the density profile, and its dependency on the underlying wall–fluid and fluid–fluid physics.

We now turn our attention to the non-trivial interference between bulk and wall interactions whenever $G_{\mathrm{b}} > 0$. To this purpose, we define the bulk pressure as: $P_{\mathrm{b}} = c_{\mathrm{s}}^2\rho - (c_{\mathrm{s}}^2/2)G_{\mathrm{b}}(1-\exp(-\rho))^2$. For the case $G_{\mathrm{b}} = 0$, one readily obtains $\Delta\rho_{\mathrm{w}} = \rho_{\mathrm{w}}(\exp(\xi G_{\mathrm{w}}/c_{\mathrm{s}}^2) - 1)$ and, using (7), the effective slip-length as follows:

$$\lambda_{\mathrm{s}} \sim \xi\,\mathrm{e}^{\xi G_{\mathrm{w}}/c_{\mathrm{s}}^2} \quad [G_{\mathrm{b}} = 0]. \tag{8}$$

This shows that the slip length grows exponentially with the ratio of potential to kinetic energy $\phi \equiv G_{\mathrm{w}}\xi/c_{\mathrm{s}}^2$. For the most general case, we can rewrite Eq. (5) to highlight its physical content as follows:

$$\log\left(\frac{\rho(y)}{\rho_{\mathrm{w}}}\right) = \frac{\xi G_{\mathrm{w}}(1-\mathrm{e}^{-y/\xi})}{\overline{\partial P_{\mathrm{b}}/\partial\rho}} \tag{9}$$

where the bulk effects appear only through the term

$$\overline{\frac{\partial P_{\mathrm{b}}}{\partial\rho}} \equiv \frac{1}{\log(\rho(y)/\rho_{\mathrm{w}})}\int_0^y \frac{\partial P_{\mathrm{b}}}{\partial\rho}\frac{\mathrm{d}\rho}{\rho}.$$

Eq. (9) highlights two results. First, the effect of the bulk can always be interpreted as a renormalization of the wall–fluid interaction by

$$G_{\mathrm{w}}^{\mathrm{R}} \equiv \frac{G_{\mathrm{w}}}{\overline{\partial P_{\mathrm{b}}/\partial\rho}}. \tag{10}$$

Second, as it is evident from (10), one notices that near the bulk critical point, where $\partial P_{\mathrm{b}}/\partial\rho \to 0$, the renormalizing effect can drive the effective coupling to extremely large values, thus triggering a sort of local phase transition with no counterpart in an unbounded fluid. Consequently, while $G_{\mathrm{b}} \to G_{\mathrm{c}} = 4$ and the rarefaction effect grows (see inset of Fig. 1), the mass flow rate increases as shown in Fig. 1.

What we showed here is that the combined actions of G_{w} and $G_{\mathrm{b}} \to G_{\mathrm{b}}^{\mathrm{c}}$ may strongly increase the formation of this less dense region in the proximity of the surface. For a more quantitative check, we have numerically integrated our streamwise momentum equation for a given value $\langle\rho\rangle = \log(2)$. The analytical estimate for ρu_x is compared with the numerical results in Fig. 2. This is a stringent test for our analytical interpretation. The result is that the analytical estimate is able to capture the deviations from a pure parabolic profile at approaching the wall region, where rarefaction effects are present.

Most of the results shown here share the same physical picture emerging by MD numerical simulations [1,2,4,3]. Anyway, in our case, the use of explicit fluid–wall potentials in LB simulations might be questioned on account of the fact that the range of the fluid–wall potential, ξ, is a genuinely atomistic quantity, of the order of the nanometer or so. As a result, consistent simulations with $\Delta x \sim \xi$ would – in principle – require millions of grid points to cover the millimetric distances relevant to microflow experiments. This criticism can be, at least partially, offset by appealing to universality: as long as the relevant physics is governed by dimensionless numbers, rather than by the actual value of physical quantities, a mesoscopic approach appears to be fully justified.

In summary, we have shown that a suitable form of the lattice Boltzmann equation with non-ideal interactions provides a valuable numerical *and* conceptual framework for the interpretation of the apparent-slip phenomenon in

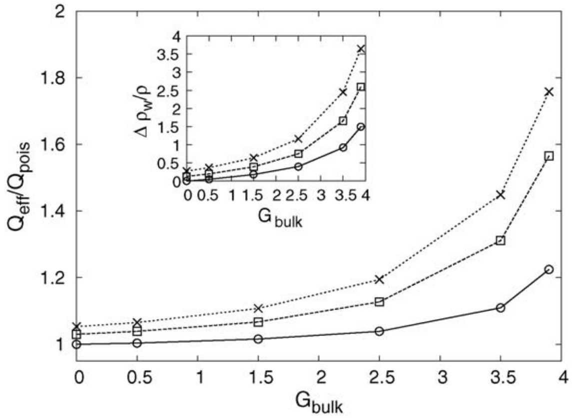

Fig. 1. Increase of the mass flow rate with the coupling strength G_b of fluid–fluid bulk interactions. Fixing the wall correlation function $\xi = 2$, we plot the mass flow rate (Q_{eff}) normalized to its Poiseuille value (Q_{pois}) as a function of G_b for different values of G_{wall}: $G_{wall} = 0.0$ (◯), $G_{wall} = 0.04$ (□), $G_{wall} = 0.08$ (×). (Inset) Same as the main figure for $\Delta\rho_w/\rho$.

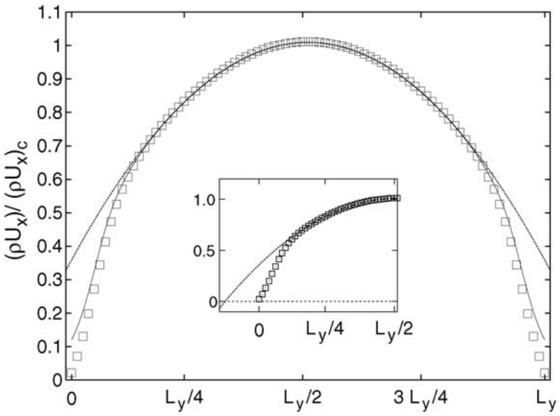

Fig. 2. We plot the momentum profile (ρu_x) normalized to its center channel value (($\rho u_x)_c$) as a function of the normalized distance from the wall. The results of numerical simulations (□) with $G_b = 3.5$, $G_w = 0.08$ and $\xi = 2$ are compared with the analytical estimate (continuous line). The parabolic fit in the center channel region (dotted line) is also plotted. (Inset) Estimate of the apparent slip length in the channel obtained the same parabolic fit as in the main figure.

microflows. The advantage over the continuum approach is that slip boundary conditions arise spontaneously because, close to the wall, a "gas" layer is formed as a consequence of the intermolecular interactions. The major result of our analysis is that the synergistic combination of fluid–wall and fluid–fluid interactions can trigger local phase transitions in the vicinity of the wall thus providing large slip effects.

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