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Regularized lattice Boltzmann multicomponent models for low capillary and Reynolds microfluidics flows

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ABSTRACT

We present a regularized version of the color gradient lattice Boltzmann (LB) scheme for the simulation of droplet formation in microfluidic devices of experimental relevance. The regularized version is shown to provide computationally efficient access to capillary number regimes relevant to droplet generation via microfluidic devices, such as flow-focusers and the more recent microfluidic step emulsifier devices.

1. Introduction

In the last two decades, microfluidic devices have gained a prominent role in several fields of research, from basic fluid dynamics to material science, biomedicine, as well as industrial applications [1–3]. In the early 2000s, several pioneering works showed the potential of such devices for generating droplets at the microscale with unprecedented degree of uniformity and rational design, thereby establishing the basis of the lab-on-a-chip concept [4–7]. Nowadays, many publications show that the drops microfluidics has surged well beyond the proof-of-concept paradigm, proving the viability of the new approach through substantial contributions to chemistry, biology, medicine, 3d-printing, to name but a few [8–12]. Due to their ease of fabrication via soft lithography methods [13,14], microfluidic devices are intensely exploited for the study and manipulation of fluids at the submillimeter length scale. In particular, microfluidic devices have been successfully employed for producing porous scaffolding materials with an accurate control over scaffold specifications, such as pore size, shape, distribution and interconnectivity [15,16].

In such context, droplet generation units are the main components to produce emulsion templating porous materials by means of microfluidic devices. Several droplet-based microfluidic chips include at least one droplet generation unit within different geometries, alongside with droplet splitting/merging units (e.g., flow focusing, coflow, T-, X-, and Y-junctions). Although, experiments have driven many of the advances in the field, many quantities of design interest lie still beyond experimental reach, thereby precluding a complete understanding of the basic physics of droplet generation by experimental means and thus holding back further progress in the operation and optimization of microfluidic devices.

Models and simulations may provide valuable insights into basic microfluidic mechanisms and, more specifically, computational studies can help to elucidate the nature of optimal flow conditions in terms of geometrical and physico–chemical properties, thus facilitating a rational design of the final product.

Over a decade ago, different numerical methods focused on the breakup mechanisms [17,18], characterizing droplet formation in terms of the relevant dimensionless parameters [19,20]. In particular, it was noted that by varying volume flow rates of the dispersed and continuous phases, and therefore changing the Reynolds and capillary numbers, three distinct regimes of formation of droplets can be identified: *squeezing, dripping and jetting*, three regimes which have been found to be consistent with experimental observations [4,21,22]. Among other, the lattice Boltzmann (LB) method has played a major role in the simulation of droplet formation across a wide variety of microfluidic cross-junctions [20,23–26].

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The LB method is known to experience stability and efficiency limitations at both low and high viscosities [27]; low viscosities threaten numerical stability, while large ones undermine the very hydrodynamic limit of the LB scheme, due to the onset of strong non-equilibrium effects.

Different strategies can be employed to mitigate the above constraints: the multirelaxation-time (MRT) method [28], and a regularized version (REG) of the standard single-relaxation-time (SRT) LB scheme [29,30], also known as Regularized lattice Bhatnagar–Gross–Krook model, as well as the entropic version of the LB method [31].

In this paper, we investigate and demonstrate the benefits of the regularization procedures, as applied to the color gradient model [32,33], for the simulation of microfluidic devices.

The main idea behind the REG approach is to filter out the non-hydrodynamic modes, also known as ghost-modes, originating from non-equilibrium effects stemming from free molecular motion between two subsequent collisions [30,34–36], which proves particularly useful for microfluidic applications characterized by low capillary numbers.

The paper is organized as follows. In Section 2 the lattice Boltzmann equation with the BGK collisional operator is described, together with the color gradient model and the regularization algorithm for simulating multicomponent fluids . In Section 3 the regularization algorithm is commented and its benefits for LB simulation in microfluidics context are highlighted, while in Section 4 we present the results of flow-focusing simulations in two spatial dimensions, as well as preliminary three-dimensional simulations of the newly proposed step emulsification volcano micro devices. Finally, a summary is provided in Section 5.

2. Methods

The LB immiscible multicomponent model is based on the following lattice Bhatnagar–Gross–Krook (BGK) equation:

$$f_i^k(\vec{x}+\vec{c}_i\Delta t,\, t+\Delta t) = f_i^k(\vec{x},\, t) + \Omega_i^k(f_i^k(\vec{x},\, t)), \tag{1}$$

where f_i^k is the discrete distribution function, representing the probability of finding a particle of the kth component at position $\vec{x}$ and time t with discrete velocity $\vec{c}_i$. The lattice time step is taken equal to 1, and i the index spans the lattice discrete directions $i = 0, \ldots, b$, where $b = 8$ for a two dimensional nine speed lattice (D2Q9). The density ρ^k of the kth fluid component is given by the zeroth order moment of the distribution functions

$$\rho^k(\vec{x},\, t) = \sum_i f_i^k(\vec{x},\, t), \tag{2}$$

while the total momentum $\rho\vec{u}$ is defined by the first order moment:

$$\rho\vec{u} = \sum_i \sum_k f_i^k(\vec{x},\, t)\vec{c}_i. \tag{3}$$

The collision operator Ω_i^k results from the combination of three sub-operators, namely [33,37]

$$\Omega_i^k = \left(\Omega_i^k\right)^{(3)}\left[\left(\Omega_i^k\right)^{(1)} + \left(\Omega_i^k\right)^{(2)}\right]. \tag{4}$$

Here, $\left(\Omega_i^k\right)^{(1)}$ is the standard BGK operator for the kth component, accounting for relaxation towards a local equilibrium

$$\left(\Omega_i^k\right)^{(1)} f_i^k(\vec{x},\, t) = f_i^k(\vec{x},\, t) - \omega_k\left(f_i^k(\vec{x},\, t) - f_i^{k,eq}(\vec{x},\, t)\right), \tag{5}$$

where ω_k is the relaxation rate, and $f_i^{k,eq}(\vec{x},\, t)$ denotes local equilibria, defined by

$$f_i^{k,eq}(\vec{x},\, t) = \rho^k\left[\phi_i^k + w_i\left(\frac{\vec{c}_i\cdot\vec{u}}{c_s^2} + \frac{(\vec{c}_i\cdot\vec{u})^2}{2c_s^4} - \frac{(\vec{u})^2}{2c_s^2}\right)\right]. \tag{6}$$

Here, w_i are weights of the discrete equilibrium distribution functions, c_s is the lattice sound speed, and ϕ_i^k takes values in D2Q9 lattice

$$\phi_i^k = \begin{cases} \alpha_k, & i = 0, \\ (1-\alpha_k)/5, & i = 1,2,3,4, \\ (1-\alpha_k)/20, & i = 5,6,7,8, \end{cases} \tag{7}$$

where we number $i = 1,2,3,4$ the nearest-neighbor lattice displacements, and $i = 5,6,7,8$ the diagonal ones. In the above expression, α_k is a free parameter, modulating the density ratio γ_k of the kth component with respect to the others [38], as well as tuning its relative pressure

$$p^k = \frac{3\rho^k(1-\alpha_k)}{5}. \tag{8}$$

In this work, $\alpha_k = 4/9$ for both components, so that both components have the same density and speed of sound $c_s = 1/\sqrt{3}$.

In this model, $\left(\Omega_i^k\right)^{(2)}$ is a perturbation operator, modeling the surface tension of the kth component. Denoting by $\vec{F}$ the color gradient in terms of the color difference (see below), this term reads

$$\left(\Omega_i^k\right)^{(2)} f_i^k(\vec{x},\, t) = f_i^k(\vec{x},\, t) + \frac{A_k}{2}|\vec{F}|\left[w_i\frac{(\vec{F}\cdot\vec{c}_i)^2}{|\vec{F}|^2} - B_i\right], \tag{9}$$

with the free parameters A_k modeling the surface tension, and B_k a parameter depending on the chosen lattice [38,39]. The above operator models the surface tension, but it does not guarantee the immiscibility between different components. In order to minimize the mixing of the fluids, a recoloring operator $\left(\Omega_i^k\right)^{(3)}$ is introduced. Following the approach in Ref. [38], being ζ and ξ two immiscible fluids, the recoloring operators for the two fluids read as follows

$$\begin{aligned} \left(\Omega_i^\zeta\right)^{(3)} &= \frac{\rho^\zeta}{\rho}f_i + \beta\frac{\rho^\zeta\rho^\xi}{\rho^2}\cos(\phi_i)\sum_{k=\zeta,\xi} f_i^{k,eq}(\rho^k, 0) \\ \left(\Omega_i^\xi\right)^{(3)} &= \frac{\rho^\xi}{\rho}f_i - \beta\frac{\rho^\zeta\rho^\xi}{\rho^2}\cos(\phi_i)\sum_{k=\zeta,\xi} f_i^{k,eq}(\rho^k, 0) \end{aligned} \tag{10}$$

where β is a free parameter and $\cos(\phi_i)$ is the cosine of the angle between the color gradient $\vec{F}$ and the lattice direction $\vec{c}_i$. It is worth mentioning that, in this work, we implemented the color gradient as:

$$\nabla(\rho_\zeta - \rho_\xi)/(\rho_\zeta + \rho_\xi) \tag{11}$$

Note that $f_i^{k,eq}(\rho^k, 0)$ stands for the set of equilibrium distributions of kth fluid evaluated setting the macroscopic velocity to zero. In the above equation, $f_i = \sum_k f_i^k$. The LB color gradient model has been enriched with the so called regularization procedure [29,34,36], namely a discrete Hermite projection of the post-collisional set of distribution functions onto a proper set of Hermite basis. The main idea is to introduce a set of pre-collision distribution functions which are defined only in terms of the macroscopic hydrodynamic moments. All the higher-order non-equilibrium information, often referred to as *ghosts* [28], is discarded.In equations, the regularized LB reads as follows:

$$f_i^k(x_i + c_i\Delta t, t+\Delta t) = \mathcal{R}f_i^{k,neq}(x,t) \equiv f_i^{k,eq} - \Delta t\omega_k(f_i^{k,reg} - f_i^{k,eq}) \tag{12}$$

where $f_i^{k,reg}$ is the hydrodynamic component of the full distribution f_i^k (see [29]) for the kth color, and $\mathcal{R}$ is the regularization operator. The above equation shows that the post-collision distribution, of a 4th-order isotropic lattice, is defined only in terms of the conserved and the transport hydrodynamic modes, namely density ρ, current $\rho\vec{u}$ and momentum–flux tensor $\mathbf{\Pi} = \sum_i f_i\vec{c}_i\vec{c}_i$.