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Enhanced equilibrium distribution functions for simulating immiscible multiphase flows with variable density ratios in a class of lattice Boltzmann models

Sébastien Leclaire *, Nicolas Pellerin, Marcelo Reggio, Jean-Yves Trépanier

Department of Mechanical Engineering, École Polytechnique, 2500, chemin de Polytechnique, Montreal, Quebec H3T 1J4, Canada

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ABSTRACT

This research examines the behavior of a class of lattice Boltzmann (LB) models designed to simulate immiscible multiphase flows. There is some debate in the scientific literature as to whether or not the "color gradient" models, also known as the Rothman–Keller (RK) models, are able to simulate flow with density variation. In this paper, we show that it is possible, by modifying the original equilibrium distribution functions, to capture the discontinuity present in the analytical momentum profile of the two-layered Couette flow with variable density ratios. Investigations carried out earlier were not able to simulate such a flow correctly. Now, with the proposed approach, the new scheme is compatible with the analytical solution, and it is also possible to simulate the two-layered Couette flow with simultaneous density ratios of $O(1000)$ and viscosity ratios of $O(100)$. To test the model in a more complex flow situation, i.e. with non-zero surface tension and a curved interface, an unsteady simulation of an oscillating bubble with variable density ratio is undertaken. The numerical frequency of the bubble is compared to that of the analytical frequency. It is demonstrated that the proposed modification greatly increases the accuracy of the model compared to the original model, i.e. the error can be up to one order of magnitude lower with the proposed enhanced equilibrium distribution functions. The authors believe that this improvement can be made to other RK models as well, which will allow the range of validity of these models to be extended. This is, in fact, what the authors found for the method proposed in this article.

1. Introduction

Lattice Boltzmann models of multiphase flow can be classified in various categories. One possible classification could be the following:

- the RK from Rothman and Keller (1988);
- the SC from Shan and Chen (1993);
- the Free-Energy (FE) from Swift et al. (1996);
- the Mean-Field (MF) from He et al. (1998);
- the Field-Mediator (FM) from Santos et al. (2003).

It is worth noting that this classification is not universally adopted, and there are other models, not discussed in this work, that may be classified differently. Our goal here is to improve the RK category, and we begin by providing a short literature review of the RK lattice Boltzmann models.

The RK lattice Boltzmann model for simulating multiphase flow is derived from the lattice gas model of Rothman and Keller (1988). A couple of years later, Gunstensen et al. (1991) developed a lattice Boltzmann version of the RK model. Grunau et al. (1993) then modified the Gunstensen et al. model to accommodate variable density and viscosity ratios between the fluids in several test cases.

Tölke (2002) and Latva-Kokko and Rothman (2005) realized that the original recoloring step performed at the interface of the fluids in the above model was making the scheme unstable in some situations, or resulting in non-physical behavior such as lattice pinning. New recoloring schemes were developed in both studies and the authors of both agreed that the main problem with the original model was a very thin interface between the fluids. Tölke (2002) managed to achieve preliminary simulations that agreed well with experimental data.

Reis and Phillips (2007) changed the forcing scheme of the perturbation operator to induce the appropriate surface tension term in the macroscopic equations. Even without the newest recoloring operators, Reis and Phillips showed that their model could be used to simulate flow with large density ratios in some test cases. Leclaire et al. (2012a) adapted the recoloring operator of Latva-Kokko and Rothman for the Reis and Phillips model in the case of variable density ratios. This modification led researchers to conclude that numerical "noise" in the model could be substantially reduced.

* Corresponding author. Tel.: +1 514 340 5121.
E-mail address: sebastien.leclaire@polymtl.ca (S. Leclaire).

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Also, higher density ratios were tackled for the same Reis and Phillips test cases. However, as was the case in other studies (Rannou, 2008; Aidun and Clausen, 2010; Yang and Boek, 2013), the current RK model was not able to simulate flow with density variation for the multilayered Poiseuille or Couette flow test cases.

While some sought a cure for this problem, Leclaire et al. (2011) aimed to develop the RK model in order to increase precision in terms of simulating Laplace's law with isotropic discretization for the color gradient. Also, Liu et al. (2012) developed a three-dimensional version of the Reis and Phillips perturbation operator for the D3Q19 lattice. Satisfactory agreement with some experimental results was obtained in the Liu et al. research. Other efforts were also made by Leclaire et al. (2013) to develop an N-phase model. This latter study showed that the RK model was not able to capture the theoretical momentum discontinuity in the simple multilayered Couette flow. Our objective in the current research is to find a solution to this serious problem, which affects RK models in general.

Fortunately, a review of the scientific literature has revealed that models have been developed with demonstrable ability to simulate the multilayered Couette or Poiseuille flow. Lishchuk et al. (2008), for example, developed a multicomponent LB method for fluids with density contrast, which was shown to recover the multilayered Couette flow with a density ratio different from 1. It is not clear, however, how their idea could be used to apply a simple fix to the RK models that were previously not working (Grunau et al., 1993; Tölke, 2002; Reis and Phillips, 2007; Rannou, 2008; Leclaire et al., 2012a, 2011; Liu et al., 2012). Although this basic flow was successfully simulated in the work of Knutson et al. (2009), the authors clearly state that their method, as presented, is not suitable for more complicated flow configurations, and a great deal of effort is still needed to generalize their method to solving general complex flows. One reason why an attempt is being made to incorporate the level-set method into the lattice Boltzmann method is that the level-set method is better at preserving the volume of the various phases than the lattice Boltzmann method. A volume preserving approach for the multiphase lattice Boltzmann method was studied in the work of Reis and Dellar (2011). Yiotis et al. (2007) show that their model can simulate the multilayered Poiseuille flow with density ratios; nevertheless, considerable effort would be required to adapt their ideas to the current RK formulation, as their model use a new pressure distribution function. Recently, a new approach to resolving the discontinuity problem of the RK model, using source terms, has been published by Huang et al. (2013). This approach is interesting, but different from the one that we are proposing.

Holdych et al. (1998) modified the equilibrium stress tensor of the free energy model of Swift et al. (1996), in order to recover the analytical solution of the multilayered Couette flow with variable density ratios. In fact, we show here that their approach can be readily and easily adapted to the RK model to correctly recover the Navier–Stokes equations in the single phase region with a weak pressure gradient and within the limits of small Mach and Knudsen numbers. Moreover, our method does allow the current RK model to correctly simulate the multilayered Couette flow, even in the case of simultaneous high density $O(1000)$ and high viscosity $O(100)$ ratios. Also, the proposed enhanced equilibrium distribution greatly increases the accuracy of the model with a variable density ratio in a more complex flow situation. This will be illustrated with an unsteady oscillating bubble with a density ratio of $O(100)$, where the numerical frequency of the bubble is compared to its analytical frequency, and much better results are achieved with the proposed modification.

This simple fix can also be applied in a straightforward manner to the following RK model (Grunau et al., 1993; Tölke, 2002; Reis and Phillips, 2007; Rannou, 2008; Leclaire et al., 2012a, 2011; Liu et al., 2012), and perhaps to other LB models with similar issues (Rannou, 2008).

2. Lattice Boltzmann immiscible multiphase model

The current LB approach follows the two-phase model of Reis and Phillips (2007), along with the improvements presented by Leclaire et al. (2012a, 2011, 2013) for the recoloring operator, the isotropic color gradient, and the model generalization to N-phase flows. For this 2D LB model, there are N sets of distribution functions, one for each fluid, moving on a D2Q9 lattice with the velocity vectors $\vec{c}_i$. With $\theta_i = \frac{\pi}{4}(4-i)$, these velocity vectors are defined as:

$$\vec{c}_i = \begin{cases} (0,0), & i=1 \\ [\sin(\theta_i),\cos(\theta_i)]c, & i=2,4,6,8 \\ [\sin(\theta_i),\cos(\theta_i)]\sqrt{2}c, & i=3,5,7,9 \end{cases} \tag{1}$$

where $c = \Delta x/\Delta t$, $\Delta y = \Delta x$, Δx is the lattice spacing, and Δt is the time step.

The distribution functions for a fluid of color k (e.g. $k = r$ for red, $k = g$ for green, and $k = b$ for blue) are noted $N_i^k(\vec{x},t)$, while $N_i(\vec{x},t) = \sum_k N_i^k(\vec{x},t)$ is used for the color-blind distribution function. The algorithm uses the following evolution equation:

$$N_i^k(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = N_i^k(\vec{x},t) + \Omega_i^k\left(N_i^k(\vec{x},t)\right) \tag{2}$$

where the collision operator Ω_i^k is the result of the combination of three sub operators (similar to Tölke (2002)):

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

These original operators are rewritten in such a way that the evolution equation is solved in four steps with operator splitting, as follows:

1. Single phase collision operator:
$$N_i^k(\vec{x},t_*) = \left(\Omega_i^k\right)^{(1)}\left(N_i^k(\vec{x},t)\right)$$
2. Multiphase collision operator (perturbation):
$$N_i^k(\vec{x},t_{**}) = \left(\Omega_i^k\right)^{(2)}\left(N_i^k(\vec{x},t_*)\right)$$
3. Multiphase collision operator (recoloring):
$$N_i^k(\vec{x},t_{***}) = \left(\Omega_i^k\right)^{(3)}\left(N_i^k(\vec{x},t_{**})\right)$$
4. Streaming operator:
$$N_i^k(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = N_i^k(\vec{x},t_{***})$$

The model presented with the evolution Eq. (2) suggests the use of one set of distribution functions for each fluid. Leclaire et al. (2013) explains how the number of distribution functions necessary for the simulation of N-phase flows can be reduced. Conceptually, only the distribution functions of the color-blind fluid and each density field are required to implement the model, although it is much easier to describe the theoretical model using one set of distribution functions for each fluid.

2.1. Original single phase collision operator

The first sub operator, $\left(\Omega_i^k\right)^{(1)}$, is the standard BGK operator of the single phase LB model, where the distribution functions are relaxed towards a local equilibrium, in which ω_{eff} denotes the effective relaxation factor: