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Lattice Boltzmann Models with Mid-Range Interactions

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Abstract. An extension of the standard Shan-Chen model for non ideal-fluids, catering for mid-range, soft-core and hard-core repulsion, is investigated. It is shown that the inclusion of such mid-range interactions does not yield any visible enhancement of the density jump across the dense and light phases. Such an enhancement can however be obtained by tuning the exponents of the effective interaction. The results also indicate that the inclusion of soft-core repulsion can prevent the coalescence of neighborhood bubbles, thereby opening the possibility of tailoring the size of multi-droplet configurations, such as sprays and related phase-separating fluids.

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1 Introduction

The Lattice-Boltzmann (LB) approach has proven to represent a powerful mesoscopic alternative to classical macroscopic methods for computational hydrodynamics [1,2]. The pseudopotential method put forward a decade ago by Shan-Chen to endow Lattice Boltzmann (LB) models with potential energy interactions, is one of the most successful outgrowth of basic LB theory [3,4]. The Shan-Chen (SC) model is based on the idea of representing intermolecular interactions at the mesoscopic scale via a density-dependent

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nearest-neighbor pseudopotential $\psi(\rho)$. Despite its highly simplified character, the SC model provides the essential ingredients of non-ideal (dense) fluid behavior, that is i) a non-ideal equation of state, ii) surface tension effects at phase interfaces. Because of its remarkable computational simplicity, the SC method is being used for a wide and growing body of complex flows applications, such as multiphase flows in chemical, manufacturing and geophysical problems.

In spite of its undeniable success, the SC method has made the object of intense criticism. In particular, i) lack of thermodynamic consistency, ii) spurious currents at interfaces and iii) surface tension tied-down to the equation of state. Problem i) refers to the fact that there is only one functional form, namely $\psi(\rho)\propto\rho$, securing compatibility between mechanical stability of the interface and equilibrium thermodynamics, i.e., Maxwell's area law in the Van der Walls loop of the non-ideal equation of state. However, recent studies [6] have clearly shown that the use of suitable pseudopotentials such that $\psi(\rho)\to\rho$ in the limit of zero density, makes this problem largely irrelevant to any practical purposes. Problem ii) is in general held responsible for setting a sharp limit on the density jumps across the dense/rarefied fluid interface to values around ten or less. This is a rather severe limitation for many practical applications, in which two-three orders of magnitude density jumps are often encountered (typically 1:1000 for air-water interfaces). Recent studies indicate that the density ratio can be drastically enhanced by resorting to different types of equations of state (EOS) other than the original one derived by Shan-Chen [7]. These new EOS are parametric variants of Van der Walls (VdW) equation of state, hence they include both hard-core short-range repulsion (absent in the SC model) and soft-core long-range attraction. Short-range repulsion is known to represent a potential danger for numerical stability, since it implies intense and localized interactions which may disrupt the numerical time-marching scheme. Hence, it is reasonable to wonder whether higher density ratios may be achieved by augmenting the original SC pseudopotentials with additional soft-core interactions and, more in general, which are the effects of such inclusion. This is precisely the route explored in this work.

2 Shan-Chen model with mid-range interactions

We consider the standard lattice Boltzmann (LB) equation with pseudopotentials

$$f_i(\vec{r}+\vec{c}_i,t+1)-f_i(\vec{r},t)=-\omega(f_i-f_i^{eq})+F_i. \tag{2.1}$$

In the above, all symbols are standard, except for the pseudo-force F_i, as discussed below. We consider generalized pseudoforces of the following form

$$\vec{F}(\vec{r})=\sum_{j=1}^{2}c_s^2G_j\psi_j^{n(j)}(\rho(\vec{r}))\sum_{i=1}^{b_j}p_{ij}\vec{c}_{ij}\psi_j^{n(j)}(\rho(\vec{r}+\vec{c}_{ij})). \tag{2.2}$$

In the above, the index j labels the Seitz-Wigner cell (*belt* for simplicity) defined by the condition $|\vec{r'}-\vec{r}|^2\le 2j^2$, whereas $\vec{c_{ij}}$ denotes the set of discrete speeds belonging to the j-th