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An improved multiphase lattice Boltzmann flux solver for three-dimensional flows with large density ratio and high Reynolds number

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ABSTRACT

An improved multiphase lattice Boltzmann flux solver (MLBFS) is proposed in this work for effective simulation of three-dimensional (3D) multiphase flows with large density ratio and high Reynolds number. As a finite volume scheme, the MLBFS originally proposed in [27] applies the finite volume method to solve for macroscopic flow variables directly. The fluxes are reconstructed locally at each cell interface by using the standard LBM solutions. Due to the modeling error of the standard LBM, the reconstructed fluxes deviate from those in the Navier–Stokes equations; and to compensate this error, a complex tensor is introduced in the original MLBFS. However, the computation of the tensor introduces additional complexity and usually needs a relatively thicker interface thickness to maintain numerical stability, which makes the solver be complex and inefficient in the 3D case. To remove this drawback, in this work, a theoretical analysis to the formulations obtained from the Chapman–Enskog expansion is conducted. It is shown that the modeling error can be effectively removed by modifying the computation of the equilibrium density distribution function. With this improvement, the proposed 3D MLBFS not only avoids the calculation of the compensation tensor but also is able to maintain numerical stability with very thin interface thickness. Several benchmark cases, including the challenging droplet impacting on a dry surface, head-on collisions of binary droplets and droplet splashing on a thin film with density ratio 1000 and Reynolds number up to 3000, are studied to validate the proposed solver. The obtained results agree well with the published data.

1. Introduction

Multiphase flows have wide applications in many essential areas [1–4], such as ink jet printing, combustion in an engine and interactions of bubbles in a chemical reactor. To effectively simulate such flows, both the continuum Navier–Stokes (N–S) solver [5–8] and the kinetic lattice Boltzmann method (LBM) [9,10] have been proposed. The N–S solver solves the mass and momentum equations directly for macroscopic flow properties while the LBM solves discrete kinetic equations in both spatial and velocity spaces for the particle distribution functions (PDFs). As compared with the N–S solver, the LBM is proven to be more efficient and has a simpler solution process. In addition, the intrinsic kinetic nature makes the LBM

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particularly suitable for multiphase flows. Due to these attractive features, the LBM is becoming more and more popular for simulating complex multiphase flows [11–17].

Existing multiphase LB models can be roughly classified into three categories, i.e., the color-gradient model [11,18], the pseudo-potential model [12,16,19,20] and the free-energy model [13–15]. In the development of these models, a critical issue is the structural problem caused by the sharp change of fluid density across the interface. Consequently, the linear relationship between the fluid density ρ and pressure p, i.e., the equation of state, $p = \rho c_s^2$ (c_s is the sound speed), which is commonly applied in singe-phase LB models, does not exist. This is because across the interface, the density has a sharp change but the pressure is smooth. To effectively resolve this problem, one way is to introduce more realistic equation of state for pressure, which is able to describe the relationship between the pressure and density physically [17]. External forcing terms are also introduced to guarantee the mechanical stability condition thermodynamically so that the effect of pressure and surface tension in the momentum equations can be accurately realized. This strategy is mostly applied in the pseudo-potential model [21–23]. Another way is to introduce an incompressible transformation by changing the equilibrium particle distribution function (PDF) originally for density and velocity to that for pressure and velocity [14]. This transformation is able to consider the effect of pressure with a second order of accuracy. Since the standard LBE with the transformed PDF generates obvious errors in the recovered macroscopic equations, external forcing terms are also introduced for compensation. This approach has been readily applied in many free-energy models [15,24–27].

Although the structural problem is properly resolved, the LB model still faces a great challenge in simulating multiphase flows with large density ratio and high Reynolds number. For large-density-ratio flows, the large gradient of density at fluid interfaces easily spoils the numerical stability through the generation of unphysical spurious currents and strong convection. For high-Reynolds-number flows, it usually requires more lattices in a characteristic length and/or a relatively larger characteristic velocity to obtain a suitable value for the relaxation time parameter. The former requirement obviously increases the computational effort while the later may introduce numerical stability. Nevertheless, several works [15,16,27–32] have been carried out in this area. Inamuro et al. [16] proposed a projection-like pseudo-potential LB model to suppress the spurious currents and successfully applied it to binary flows with density ratio of 1000. Lee and Lin [15] proposed a stable free-energy model by introducing the upwind concept into the discretization of convective terms in the LBE.. Yu and Zhao [28] and Li et al. [30] also devised MRT pseudo-potential LB models independently. It is noticed that the interface thickness applied in some models [16,25] are usually quite thick for large-density-ratio flows, which spread the fluid interface on about 8 to 9 lattices. Although this helps the LB model to maintain numerical stability, the accuracy is also sacrificed [33]. Since the LB model restricts its ability in capturing interfacial structures equal to or less than the interface thickness, the LB model with thick interface thickness may need much more grid points or even fail to study 3D multiphase flows with complex topology changes [34,35], such as droplet splashing on a thin film.

Recently, a multiphase lattice Boltzmann flux solver (MLBFS) [26,27] was proposed based on the free-energy LB model and transformed equilibrium PDF. Unlike the conventional multiphase LB model, which solves for the PDFs, the MLBFS directly applies the finite volume method to solve for the macroscopic flow variables while the fluxes at cell interface are reconstructed locally through the standard lattice Boltzmann solutions. Through the Chapman–Enskog analysis, it was found that the fluxes reconstructed by the standard LBM are not able to match the correct fluxes in the momentum equations and an error tensor is generated. After compensating this error term, the MLBFS is successfully applied on both uniform and non-uniform grids for simulating multiphase flows with large density ratio. In addition, the application of high order upwind scheme for capturing the fluid interface makes the MLBFS quite stable even if very thin interface thinness is used. Due to these features, the MLBFS seems to have a high potential for simulating very challenging multiphase flows in practical three dimensions.

However, it is noticed that a compensated error tensor is introduced in original MLBFS, which involves complex gradient terms of density. The presence of the error tensor at each cell interface makes the reconstruction of the fluxes rather complicated. Moreover, inappropriate discretization of the gradient term of the density may also cause numerical instability. To eliminate these drawbacks, an improved MLBFS is proposed in this work. Since the error term is generated as a viscous term, an analysis to the formulations obtained from the Chapman–Enskog analysis is conducted. It will be shown that the error term can be completely removed by modifying the computation of equilibrium PDF. As a consequence, the discretization of the compensation term is not necessary. With this improvement, the reconstruction of the fluxes at each interface can be greatly simplified, which essentially follows the same procedure as that in the LBFS for single phase flows [36,37]. Another contribution of this work is to systematically demonstrate the capability of the improved MLBFS in simulating a variety of complex 3D multiphase flows with large density ratio and high Reynolds number. Essential examples include droplet impacting on a dry surface, head-on collisions of binary droplet and droplet splashing on a thin film with density ratio 1000 and Reynolds number up to 3000, which involves complex interfacial interactions and requires thin interface in numerical simulations.