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A lifting relation from macroscopic variables to mesoscopic variables in lattice Boltzmann method: Derivation, numerical assessments and coupling computations validation

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ABSTRACT

In this paper, analytic relations between the macroscopic variables and the mesoscopic variables are derived for lattice Boltzmann methods (LBMs). The analytic relations are achieved by two different methods for the exchange from velocity fields of finite-type methods to the single particle distribution functions of LBM. The numerical errors of reconstructing the single particle distribution functions and the non-equilibrium distribution function by macroscopic fields are investigated. Results show that their accuracy is better than the existing ones. The proposed reconstruction operator has been used to implement the coupling computations of LBM and macro-numerical methods of FVM. The lid-driven cavity flow is chosen to carry out the coupling computations based on the numerical strategies of domain decomposition methods (DDMs). The numerical results show that the proposed lifting relations are accurate and robust.

1. Introduction

In the past decades, LBM has been widely used to simulate fluid flow problems [1,2], including complex turbulent fluid flows [3,4] and multiscale modeling [5,6]. This method is based on the Boltzmann kinetic equation which is used to describe a number of interacting populations of particles. As described in [7], "The LBE could potentially play a twofold function-as a telescope for the atomistic scale and a microscope for the macroscopic scale". In [8] dense fluids flow past and through a carbon nano tube (CNT) was studied by a hybrid model coupling LBM and MDS. The authors pointed out that replacing the finite volume solver by a LBM aims to take advantage of the mesoscopic modeling inherent in LB simulations. Thus LBM is a mesoscopic method in nature is a widely-accepted understanding in the literature. The macroscopic parameters such as fluid density, velocity and pressure can be obtained via some averages of the mesoscopic variable which conform the basic conservation laws of mass and momentum [2]. In practical applications of LBM to simulate a macroscopic problem, a crucial problem is confronted, that is, a reasonable initial meso-field must be specified to start the evolution process. The first initializing method was proposed in [9] in 1993. Recently, several methods have been proposed to improve the accuracy of numerical results and reduce the initial layers (oscillation layers) [10,11]. Such oscillations have a numerical origin and are due to the artificial compressibility of LBM. Here, "initial layer" refers to such a computational stage within which the macroscopic parameters are oscillating. When the initial data is not well-prepared, there is an initial layer during which the solution adapts itself to match the profile dictated by the environment. For the LBM, the existence of the initial layers is a common phenomenon [10]. In this paper, we will derive the lifting relations between the macroscopic variables and the mesoscopic variables in LBM by two ways. According to the authors' knowledge, the proposed lifting relations in this paper are different from those in the existing literature [9–15]. The proposed relations will offer us some new views about the reconstruction of nonequilibrium distribution functions in LBM.

Challenging multiscale phenomena or processes are widely existed in material science, chemical engineering process, energy and power engineering, and other engineering fields. Generally speaking, for a multiscale problem, we often must use different methods to numerically model the processes at different geometric sub-regions and exchange solution information at interface [16–19]. Such coupling computations are widely adopted in the present-day multiscale simulation. As indicated above LBM is a kind of mesoscopic method, which is a candidate to implement the meso–macro or micro–meso coupling computations in

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engineering applications [7]. So, the proposed method not only can be used to obtain a better initial field for LBM, but also can be adopted in the multi-scale computation. For example in [7] the possibility of coupling LBM with molecular dynamics simulation (MDS) was investigated and found that with proper time and geometric scales the two numerical methods can be coupled. And in [8] such coupling simulation was conducted. In the existing literatures the coupling of finite difference method (FDM, which is a macrosopic method) with LBM was adopted in [19–21], but the proposed coupling method is similar to a multigrid method and a simple regularization formula is used in their computations. The regularization formula in [19] only considers the first-order approximation of the single particle distribution function and the coupling formula in [20] is only used to deal with the one-dimensional reaction–diffusion system. In [8] the coupling between LBM and MDS was implemented by exchange of velocity and velocity gradient at the interface region. In this paper, the proposed meso–macro (or micro–meso) coupling is expected to be used for domain decomposition methods, in which LBM and macro-type numerical method (or micro-type numerical method and LBM) are adopted in different sub-domain and information is exchanged at the interface. We believe that our proposed relation is more useful method for engineering multiscale computations. In addition, the proposed coupling method can also be used to carry out the multigrid computations and equation-free multiscale (EFM) computations [22]. It is well-known that LBM is very powerfull for the parallel computing on a low cost [23,24]. So, the proposed relation can be used in the parallel simulations for multiscale simulations of complex fluid flows based on the refinement strategies.

To the authors' understanding the glossary "lifting relation" means that macroscopic variables in a lower degree-of-freedom (DoF) system are upscaled to meso/microscopic variables in a higher DoF system. Generally, it is difficult to establish the one-to-one map from a lower DoF system to a higher DoF system, although the lower DoF system can be seemed to be an approximate or approaching form of a higher DoF system in some referred scales. This situation happens when numerical results of different scales are coupled at the same location. For example when MDS and continuum method are coupled, reference [25] indicated that it is straightforward to obtain the continuum quantities (such as velocity, pressure) from the particle description by averaging over the local region and over time, but the reverse problem, generating meso/microscopic particle configuration from known macroscopic quantities is non-trivial and must necessarily be non-unique. The glossary "lifting relation" in the title of this paper is proposed based on the concept of the DoF of the governing equations.

In this paper, we will give two methods to establish the relations between variables of the Navier–Stokes equations and variables of LBM. Numerical tests demonstrate that the proposed methods of computing non-equilibrium distribution functions are effective and accurate.

The rest of the paper is organized as follows. In Section 2, the details of multi-scale derivation of non-equilibrium distribution functions is given. In Section 3, the non-equilibrium distribution functions are obtained by Boltzmann–BGK equations. In Section 4, the performances of the proposed relations to reconstruct non-equilibrium distribution functions are demonstrated by numerical tests. Finally, some conclusions are given.

2. Lattice Boltzmann hydrodynamics and multiscale approach

In this section, we will review LBM and the corresponding macroscopic equation. Based on this review, we will derive a relation for lifting macroscopic variables to microscopic variables by multiscale approach.

2.1. Lattice Boltzmann hydrodynamics

We now introduce the lattice Boltzmann–BGK model as a solver for the weakly-compressible Navier–Stokes equations. LBM is built up from the lattice gas cellular automata models [2]. The numerical scheme of LBM is established based on a finite discrete-velocity model of the Boltzmann–BGK equation and can be expressed as follows

$$f_i(\mathrm{x}+\delta t\mathrm{c}_i, t+\delta t) - f(\mathrm{x}, t) = \Omega_i, \tag{1}$$

where f_i represents the single-particle distribution function along the direction c_i ($i = 0, \ldots, n$), c_i is the element of the discrete velocity set $\mathcal{V} = \{\mathrm{c}_0, \ldots, \mathrm{c}_n\}$. Ω_i denotes the collision operator which is non-dimensional. The macroscopic variables, the density ρ and the velocity u, are defined locally by the distribution functions as follows

$$\rho(\mathrm{x}, t) = \sum_{i=0}^{n} f_i(\mathrm{x}, t) = \sum_{i=0}^{n} f_i^{\mathrm{eq}}(\mathrm{x}, t), \tag{2}$$

$$\mathrm{u}(\mathrm{x}, t) = \frac{1}{\rho}\sum_{\mathrm{c}_i\in\mathcal{V}} \mathrm{c}_i f_i(\mathrm{x}, t) = \frac{1}{\rho}\sum_{\mathrm{c}_i\in\mathcal{V}} \mathrm{c}_i f_i^{(\mathrm{eq})}(\mathrm{x}, t). \tag{3}$$

For the standard LBM, the collision operator is defined by the so-called BGK collision

$$\Omega_i^{\mathrm{BGK}} = -\frac{1}{\tau_{\mathrm{lbm}}}[f_i(\mathrm{x}, t) - f_i^{(\mathrm{eq})}(\mathrm{x}, t)]. \tag{4}$$

For the convenience of comparison, from here, we use the similar notations in [26]. The local equilibrium distribution $f_i^{(\mathrm{eq})}$ is defined by

$$f_i^{(\mathrm{eq})}(\mathrm{x}, t) = f_i^{\mathrm{L}(\mathrm{eq})}(\mathrm{x}, t) + f_i^{\mathrm{Q}(\mathrm{eq})}(\mathrm{x}, t), \tag{5}$$

where $f_i^{\mathrm{L}(\mathrm{eq})}(\mathrm{x}, t)$ and $f_i^{\mathrm{Q}(\mathrm{eq})}(\mathrm{x}, t)$ denote the linear part and the quadratic part of the equilibrium distribution, respectively. The linear part is given by

$$f_i^{\mathrm{L}(\mathrm{eq})}(\mathrm{x}, t) = \omega_i\rho\left(1 + \frac{1}{c_s^2}\mathrm{c}_i\cdot\mathrm{u}(\mathrm{x}, t)\right), \tag{6}$$

and the quadratic part is expressed by

$$f_i^{\mathrm{Q}(\mathrm{eq})}(\mathrm{x}, t) = \omega_i\frac{1}{2c_s^4}\rho(\mathrm{u}(\mathrm{x}, t)\mathrm{u}(\mathrm{x}, t)) : \Sigma_i, \tag{7}$$

where c_s is the lattice sound speed of the model, ω_i denotes the weight and Σ_i is a second-order tensor defined by

$$\Sigma_{i\alpha\beta} = c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta}. \tag{8}$$

The tensor product definition between two first order tensors **a** and **b** is given as follows

$$(\mathbf{ab})_{\alpha\beta} = \mathbf{a}_\alpha\mathbf{b}_\beta, \tag{9}$$

and the corresponding second-order tensor :-product between **A** and **B** is given by

$$\mathbf{A} : \mathbf{B} = \sum_{\alpha,\beta=1}^{d} \mathbf{A}_{\alpha\beta}\mathbf{B}_{\alpha\beta}, \tag{10}$$

where d denotes the spatial dimension.

In this paper, we mainly focus on the standard LBM. By the Chapman–Enskog expansion, under the small Ma number restriction ($Ma \leqslant 0.2$), we can recover the Navier–Stokes equations as follows

$$\partial_t\rho + \partial_\alpha(\rho u_\alpha) + \mathbf{O}(\delta t^2) = 0, \tag{11}$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p + \nu\partial_\beta(\rho(\partial_\alpha u_\beta + \partial_\beta u_\alpha)) + \mathbf{O}(\delta t^2) + \mathbf{O}(\delta t u^3), \tag{12}$$