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A unified coupling scheme between lattice Boltzmann method and finite volume method for unsteady fluid flow and heat transfer

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ABSTRACT

In this paper, a unified coupling scheme between the lattice Boltzmann method (LBM) and the finite volume method (FVM) is proposed for the unsteady fluid flow and heat transfer problems. Three improvements are achieved comparing to the existing coupling methods. Firstly, a generalized form of the reconstruction operator (RO) is derived for the information transfer from macroscopic parameters to LBM distribution functions. The existing RO for various LBM can all be derived from this generalized form. Secondly, an RO corresponding to the incompressible LBM is derived to deal with the incompressible flow, which can prevent the inconsistency between the incompressible FVM and the density change in the LBM. Thirdly, the time coupling scheme between LBM and FVM is proposed for the unsteady simulations. The LBM and FVM are solving sequentially and the information is transferred between the two methods at the intervals. The coupling scheme is validated by three numerical examples: the convection–diffusion of a Gaussian pulse, the unsteady flow past a circular cylinder and the start-up process of the natural convection in a square cavity. The numerical results agree well with the existing researches. The flow past a porous medium is also simulated to show the application of the coupling method. This method can give the detailed flow information and save the computational time. The proposed coupling scheme improves and expands the coupling scheme between LBM and FVM. It has the flexibility to simulate unsteady multiscale processes.

1. Introduction

Many physical processes are multiscale in nature, such as the mass transfer in a fuel cell [1], the chemical vapor deposition on a thin film [2], the CO_2 sequestration [3] and the heat transfer in silica aerogel composite insulating materials [4]. In these "multiscale processes", the overall behaviors are dominated by several strongly coupled sub-processes which occur in different length and time scales and are always described by different governing equations [5]. The numerical simulations are efficient ways to study these complex problems and direct the experiments. However, since the traditional numerical methods always model the problems from a single scale, they are not suitable for the multiscale simulations. A numerical simulation from the large scale ignores the detailed local information which is often mostly concerned, while the large computational time consuming of a simulation from the small scale is also unacceptable [6]. Therefore, the new numerical methods are needed and the multiscale simulation methods are proposed.

The "Solving problems regionally and coupling at the interface [7]" is a widely used multiscale strategy, where the computational domain is divided into different sub-regions in which the most proper numerical methods are adopted as shown in Fig. 1. An overlapping region where both methods are adopted is located between the sub-regions for information transfer. A compression operator (CO) is employed at the macroscopic boundary for the information transfer from the micro/mesoscale to the macroscale and a reconstruction operator (RO) is adopted at the micro/mesoscopic boundary for the inverse information transfer [7]. Based on this strategy, many coupling methods between different numerical models have been proposed for various multiscale problems, such as molecular dynamic (MD)-continuum [8–13], direct simulation of Monte Carlo (DSMC)-continuum [14,15], and lattice Boltzmann method (LBM)-finite volume method (FVM) [16–21].

The research in this paper is focused on the coupling between the LBM and the FVM. The LBM has been developed into a useful method for multi-physical and multi-component problems [22,23]. It can be adopted to obtain the detailed information in the

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complex boundaries due to its flexibility [24] and the FVM can be adopted in the free area to speed up the computation [5]. This kind of coupling method has been used to simulate the lid-driven cavity flow [5], the natural convection [16], the flow around a circular cylinder, an airfoil, a porous medium [17] and the fluid flow and mass transfer in a proton exchange membrane fuel cell [18,19].

However, there are three shortages in the existing coupling methods.

Firstly, the ROs of different lattice Boltzmann (LB) models are derived separately. For example, the ROs for the density–velocity distribution functions and the concentration/temperature distribution functions have been derived separately in Refs. [16,18,19]. The applications of these ROs are limited because there are many other different LB models used in the numerical simulations and the new operators are needed. Meanwhile, the derivation procedures are not well summarized in the existing researches, so the derivations of the new operators may be complicated. Therefore, a generalized form of the RO is needed.

Secondly, in the LBM region, the lattice Boltzmann BGK (LBGK) model [24] is used to simulate the velocity field. Since the macroscopic equations recovered by the LBGK model are actually compressible [25,26], they are inconsistent with the incompressible equations used in the FVM. This leads to some troubles in the coupling. For example, the recovered compressible momentum equation introduces into the RO a term including the density gradient, although the density in the FVM region remains constant [16–21]. Consequently, the gradient of the pressure in the FVM region is used as a substitute since the pressure in the LBGK model is in proportion to the density [20]. The application of an incompressible LBM can resolve this mismatch.

Thirdly, all the above coupling methods between the LBM and the FVM are proposed for the steady problems and few researches have been published for the unsteady coupling method. This limits the application of these coupling methods since many problems are unsteady, not only the problems in the start-up stage or with time-variant boundary conditions, but also the problems at high Reynolds number (Re) such as the von Karman vortex street behind a circular cylinder when $Re > 40$ [27]. Therefore, the Re in the existing papers is relatively low [5]. The steady coupling method also causes an inconvenience in deriving the RO. The key point for the derivation of the RO is to calculate the distribution functions of the LBM by the values and the gradients of the macroscopic parameters. The unsteady nature of the LBM will inherently bring the time derivatives into the RO. However, since the time is not clearly defined in the steady coupling method, the time derivatives are replaced by the spatial derivatives according to the conservation equations [5,16–21]. This expedient inevitably complicates the derivation and elongates the expressions of the RO. A clear definition of the time in the coupling methods may preclude this inconvenience. Consequently, an unsteady coupling method between LBM and FVM is needed.

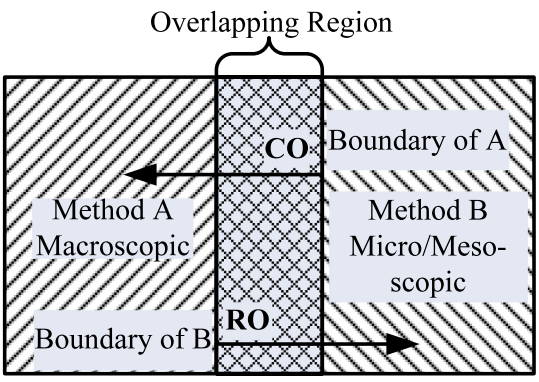

Fig. 1. Sketch of the computational domain of the coupling strategy "Solving problems regionally and coupling at the interfaces". CO is the compression operator and RO is the reconstruction operator.

As for the first problem, the derivation procedures of the RO can be divided into two parts. First part includes the common procedures which do not depend on the models, such as the Chapman–Enskog expansions and the chain rule of derivatives. The other part includes the procedures depend on the models such as the macroscopic equations at different scale and the partial derivatives of the distribution functions. In the existing derivations, the two parts are mixed. If we rearrange the derivations and carry out all the independent procedures before the dependent ones, the generalized form of the RO may be established.

The solution for the second problem is easy because the incompressible LBM already exists [25,26]. Once the generalized RO is obtained, the RO for the incompressible LBM will be derived without difficulty.

The third problem is more challenging because the boundary conditions vary with time at the boundaries of the overlapping region during the simulation. Some helpful references can be found in the coupling between the MD and the continuum methods. The MD simulates the motions of the individual molecules and calculates the macroscopic values by the time averages. It is also an unsteady method in nature which is similar to the LBM. Two types of the time coupling strategies are described by Delgado-Buscalioni and Coveney: the synchronized and sequential coupling [28]. The synchronized-coupling is a parallel strategy in which the two methods advance separately and exchange information at certain moments. In the sequential-coupling strategy, the MD firstly advances for a time interval Δt_c equal to that of the continuum method. Then the continuum method advances for Δt_c with the boundary conditions given by the above MD interval. The new solution of the continuum method is used as the boundary condition of the MD, and the above procedures are repeated. The sequential-coupling strategy is employed in many researches [11–13,29]. Therefore, a similar time coupling strategy will be used in the present work to deal with the unsteady problems.

The rest of the paper is organized as follows. In Section 2, the incompressible LBM and FVM are briefly described. Then, the generalized RO is derived in Section 3 and the existing ROs are also derived from this generalized form. In Section 4, the RO for the incompressible LBM is derived and the unsteady coupling scheme is described. Finally, the numerical examples are simulated in Section 5 and some conclusions are given in Section 6.

2. Brief introduction of the FVM and the incompressible LBM

2.1. Finite volume method

The macroscopic conservation equations are the bases of the FVM. In the present work, the fluid is assumed to be incompressible and the thermal diffusivity and viscosity are constants. The conservations of mass and momentum are given by

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla P + \nu \nabla^2 \mathbf{u} \tag{2}$$

and the energy conservation is given by

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u}T) = \alpha \nabla^2 T \tag{3}$$

Here $\mathbf{u}$ is the velocity, t is the time, P is the kinematic pressure, T is the temperature, ν is the kinematic viscosity and α is the thermal diffusivity.

In this paper, The SIMPLE algorithm [30,31] is used to solve these equations. The fully implicit scheme is used for the time