Computers and Mathematics with Applications 72 (2016) 48–63

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Lattice Boltzmann flux scheme for the convection–diffusion equation and its applications

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ARTICLE INFO

Article history:
Received 29 August 2015
Received in revised form 14 April 2016
Accepted 22 April 2016
Available online 11 May 2016

Keywords:
Lattice Boltzmann flux scheme
Convection–diffusion equation
Multiple relaxation time
Finite volume method
Anisotropic diffusion

ABSTRACT

In this work a lattice Boltzmann flux scheme for the convection–diffusion equation (CDE) is proposed. In this scheme, the fluxes across the cell interface are calculated by using the local solution of the multiple-relaxation-time lattice Boltzmann equation for CDE. The present method is suitable for simulating both isotopic and anisotropic diffusion processes. Meanwhile, through applying the midpoint time integration technique, the present method relaxes the time step constraint in the original lattice Boltzmann flux scheme. Four convection–diffusion problems are simulated to validate the present scheme. The obtained results agree well with the analytical or previous published solutions.

1. Introduction

Transport phenomenon is widely encountered in many engineering fields. These transport processes usually can be described using the convection–diffusion equation (CDE). Traditionally, people applied the finite-difference, finite-volume and finite-element numerical methods to solve the CDE. However, these methods are difficult to treat the transport problems with complex interfaces efficiently.

In the past two decades, lattice Boltzmann method (LBM) has proven to be a powerful computational technique to study complex physical systems, such as multicomponent/multiphase flows [1,2], turbulence [3,4], microflows [5,6], fluid–solid interactions [7–10]. Compared with the conventional methods, the treatment of boundary conditions is very easy in LBM when involving the complex geometries. Moreover, LBM code is easily implemented in parallel due to its particle-based feature. LBM has also extended to solve the CDE. A representative example is the LB models for thermal flows [11–14]. In addition to these thermal LB models, many other models which are designed for generalized convection–diffusion have been developed. Van der Sman and Ernst proposed a LB scheme for CDE on irregular lattices [15]. They asserted that the LB scheme has little numerical diffusion compared with conventional Lax–Wendroff scheme. Ginzburg extended two different LB models (Equilibrium-type and link-type) to advection and anisotropic-dispersion equation [16]. Because the mass conservation is taken into consideration, the accuracy and stability of the isotropic convection–diffusion LB models are enhanced. Furthermore, Shi and Guo developed a LBGK model for nonlinear CDE. In this model, both real and complex-valued distribution function are considered [17]. Note that many existing LB models for CDE have a common defect. The additional deviation term exists in the recovered macroscopic equations. To eliminate the unwanted terms, Chopard et al.

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http://dx.doi.org/10.1016/j.camwa.2016.04.032
0898-1221/

introduced a source term in the LB evolution equation [18]. However, the time-derivative and space-derivative are included in the source term. As a result, these correction terms cannot computed locally. Through designing the new equilibrium distribution function and the discrete source term, Chai and Zhao constructed a LBGK model for CDE [19]. In this model, both collision process and fluxes calculation can be implemented locally. It should be noted that the above LB models are designed only for the isotropic diffusion processes. Yoshida and Nagaoka presented a multiple-relaxation-time LB model for the convection and anisotropic diffusion equation [20]. Through introducing the off-diagonal components of the relaxation matrix, the anisotropic diffusion-coefficient tensor can be obtained. The asymptotic analysis indicates that their MRT LB model has first- and second-order accuracy in time and space, respectively. Huang and Wu gave a modified MRT-LBM for convection–anisotropic equation [21]. Their model can recover the corresponding CDE with anisotropic diffusion coefficient with no deviation term.

Although LBM has many notable merits, it also suffers from some drawbacks. As pointed out by Wang et al. [22–24], standard LBM can only applied on a regular mesh. The time step is tied up with the mesh spacing in LBM. Furthermore,the discrete lattice effects of the source term and boundary condition must be considered. To avoid these drawbacks, Wang et al. proposed a lattice Boltzmann flux scheme [22–24]. Like the gas kinetic scheme, the fluxes across the cell interface are evaluated by the solution of the discrete lattice BGK equation. The distribution function can be reconstructed using the first order Chapman–Enskog expansion. As a result, the memory overhead in this method is much less than the LBM. As a finite volume method, this method can be applied on an irregular mesh conveniently. The treatment methods of the source term and boundary conditions are same as those in the conventional finite volume method.

In this paper, a lattice Boltzmann flux scheme for CDE is proposed. In Ref. [23], Wang et al. considered a thermal lattice Boltzmann scheme based on single-relaxation-time LB model for incompressible thermal flows. However, only isotropic heat diffusion can be treated using their methods. Different from the previous works [22–24,27], the multiple-relaxation-time discrete lattice Boltzmann equation is used to evaluate the fluxes across the cell interface. In this study, the multiple-relaxation-time LB model for CDE which is proposed by Yoshida and Nagaoka is applied [20]. The local solution of this multiple-relaxation-time model is used to compute both convective and diffusive fluxes. Both isotropic and anisotropic diffusion processes can be captured. Furthermore, the midpoint time integration rule is used, which relaxes the time step limit in the original method [22]. Four convection–diffusion problems are simulated to validate the present scheme. The computational results are in good agreement with the analytical or numerical solutions reported in the previous literatures.

2. Numerical methodology

We consider the following convection–diffusion equation

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \nabla \cdot (\mathbf{D}\nabla\phi), \tag{1}$$

where ϕ is a scalar function of time and space. $\mathbf{u}$ is the velocity and usually governed by incompressible Navier–Stokes equation. $\mathbf{D}$ denotes the diffusion coefficient matrix. In this paper only the two-dimensional case is studied. It should be noted that the present method can be extended to solve three-dimensional CDE directly. In fact, three types of diffusion coefficient matrices are considered. The first type of diffusion-coefficient matrix has full anisotropy with non-zero off-diagonal components

$$\mathbf{D} = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix}. \tag{2}$$

Note that $\mathbf{D}$ must be symmetric and positive definite to ensure the physical reality. If $D_{12} = D_{21} = 0$, the diffusion coefficient matrix $\mathbf{D} = diag(D_{11}, D_{22})$ is diagonally anisotropic. The third type is the isotropic diffusion matrix, i.e. $D_{11} = D_{22}$ and $D_{12} = D_{21} = 0$.

Different from the work in Ref. [23], the multiple-relaxation-time (MRT) LBM is employed to construct the present algorithm [20,21,25]. The evolution equation can be expressed as

$$\mathbf{g}(\mathbf{x} + \mathbf{e}_\alpha \Delta t, t + \Delta t) - \mathbf{g}(\mathbf{x}, t) = -\mathbf{\Lambda}(\mathbf{g}(\mathbf{x}, t) - \mathbf{g}^{eq}(\mathbf{x}, t)) = -\mathbf{M}^{-1}\mathbf{S}_g(\mathbf{m}(\mathbf{x}, t) - \mathbf{m}^{eq}(\mathbf{x}, t)), \tag{3}$$

where the above nations denote

$$\mathbf{g}(\mathbf{x}, t) = (g_0(\mathbf{x}, t), g_1(\mathbf{x}, t), \ldots, g_8(\mathbf{x}, t))^T, \tag{4}$$

$$\mathbf{m}(\mathbf{x}, t) = \mathbf{M}\mathbf{g} = (m_0(\mathbf{x}, t), m_1(\mathbf{x}, t), \ldots, m_8(\mathbf{x}, t))^T, \tag{5}$$

$$\mathbf{m}^{eq}(\mathbf{x}, t) = (m_0^{eq}(\mathbf{x}, t), m_1^{eq}(\mathbf{x}, t), \ldots, m_8^{eq}(\mathbf{x}, t))^T. \tag{6}$$

Here $g_\alpha(\mathbf{x}, t)$ is the distribution function for the discrete velocity $\mathbf{e}_\alpha$. Δt is the time step. $\mathbf{\Lambda} = \mathbf{M}^{-1}\mathbf{S}_g\mathbf{M}$ is the relaxation matrix in the velocity space. The scalar variable ϕ can be computed as:

$$\phi = \sum_\alpha g_\alpha = \sum_\alpha g_\alpha^{eq}. \tag{7}$$