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Boundary conditions of the lattice Boltzmann method for convection–diffusion equations

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ABSTRACT

In this paper, we employ an asymptotic analysis technique and construct two boundary schemes accompanying the lattice Boltzmann method for convection–diffusion equations with general Robin boundary conditions. One scheme is for straight boundaries, with the boundary points locating at any distance from the lattice nodes, and has second-order accuracy. The other is for curved boundaries, has only first-order accuracy and is much simpler than the existing schemes. Unlike those in the literature, our schemes involve only the current lattice node. Such a "single-node" boundary schemes are highly desirable for problems with complex geometries. The two schemes are validated numerically with a number of examples. The numerical results show the utility of the constructed schemes and very well support our theoretical predications.

1. Introduction

Heat and mass transfers coupled with fluid flows are prevalent physical phenomena and possess wide applications in energy and environmental sciences, chemical engineering, geology, and so on. Mathematically, these phenomena are usually described by convection–diffusion equations together with the Navier–Stokes equation. On the other hand, for many applications including ion transport in fuel cells and secondary batteries [1–3] and surface reactions in porous media [4–6], the diffusion phenomena often occur in a physical domain with extremely complex geometries. In those situations, boundary or interfacial interactions play critical roles. Due to the complex geometries, it is quite difficult to investigate the problems with traditional numerical methods.

In the past two decades, the lattice Boltzmann method (LBM) has become an effective and viable tool for simulating various fluid flow problems [7–11]. This method has a clear physical interpretation, is simple in formulation and easy for parallelization, and can deal effectively with complex boundaries [12–15]. These advantages suggest that the LBM could be a convenient and efficient tool in studying the diffusion problems above. Indeed, the LBM has been widely used to solve the convection–diffusion problems in recent years and most of the existing works treat Dirichlet and/or Neumann boundary conditions on straight boundaries only. The interested reader is referred to [16–18] for detailed reviews about the works.

However, general Robin boundary conditions on complex boundaries do arise in many applications, such as chemical engineering and geology, and therefore have attracted a lot of attentions [16–21]. Among these works, Refs. [16,19–21] treated straight boundaries only. In [16,17,21], the key idea is to simply replace the normal derivative in the Robin conditions with finite differences. Such replacements seem not natural and can increase the computational cost, especially in modeling

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transport processes in porous media. By using interpolation of the distribution functions, the authors of [18] constructed second-order accurate boundary schemes for both Dirichlet and Neumann boundary conditions on straight boundaries. Moreover, they established a general framework to treat Robin boundary conditions on curved boundaries. We remark that all the schemes above for Robin boundary conditions always involve other lattice nodes rather than the current one and those in [17,18] are first-order accurate in the curved boundary situations. In addition, other works known to us for curved boundaries are [22] and [23] for Dirichlet and Neumann boundary conditions.

In this work, with the aid of the asymptotic analysis technique developed in [24–26], we construct two boundary schemes accompanying the lattice Boltzmann method for 2-dimensional convection–diffusion equations with general Robin boundary conditions. One scheme is for straight boundaries, with the boundary points locating at any distance from the lattice nodes, and has second-order accuracy. Our motivation to construct such a non-halfway scheme is similar to that in [18], namely, to develop efficient boundary schemes for general curved boundaries. The other scheme is for curved boundaries, has only first-order accuracy and is much simpler than the existing schemes [17,18]. Unlike the aforementioned schemes, ours involve only the current lattice node. Such "single-node" boundary schemes are highly desirable to deal with problems with complex geometries, like those in porous media [11].

The two schemes are numerically tested with a number of examples. These examples are (i) one-D transient convection–diffusion with Robin boundary conditions, (ii) Helmholtz equation in a square domain, (iii) steady heat conduction inside a ring, (iv) steady heat conduction inside a circle with Dirichlet and Neumann boundary conditions, and (v) two-D time-dependent convection–diffusion problem in a quite irregular domain. The numerical results show the utility of the constructed schemes and very well support our theoretical predications on the accuracy thereof.

Let us mention that although our boundary schemes are for a 2-dimensional BGK model, the construction can be directly generalized to 3-dimensional cases or multiple-relaxation-time (MRT) models [26]. Moreover, the ideas in this paper seem promising to develop second-order accurate boundary schemes accompanying the D2Q9 model for curved boundaries. We hope to report our progress in the near future.

The paper is organized as follows. In Section 2 we specify the convection–diffusion equations together with Robin boundary conditions, present the lattice Boltzmann method, and review the asymptotic analysis technique. Section 3 contains our main idea and two boundary schemes together with some remarks, while the detailed derivation of these schemes are given in Appendix A. Numerical experiments are reported in Section 4. Some concluding remarks are given in Section 5.

2. Preliminaries

Consider a convection–diffusion equation (CDE) for a physical quantity (concentration, temperature, etc.) $C = C(t, \boldsymbol{x})$ defined for $\boldsymbol{x} \in \Omega$:

$$\frac{\partial C}{\partial t} + \nabla \cdot (\boldsymbol{u} C) = D\nabla^2 C + S(C, t, \boldsymbol{x}), \quad 0 < t < T, \boldsymbol{x} \in \Omega, \tag{1}$$

with initial condition

$$C(0, \boldsymbol{x}) = C_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega.$$

Here $\boldsymbol{u} = \boldsymbol{u}(t, \boldsymbol{x})$ is a given velocity field, D is a diffusion coefficient, $S = S(C, t, \boldsymbol{x})$ is a source term depending on the unknown C, and T is a pre-specified time. On the boundary $\partial\Omega$, a Robin (or called third-type) boundary condition is prescribed:

$$\alpha_1 C + \alpha_2 \frac{\partial C}{\partial \boldsymbol{n}} = \alpha_3, \quad 0 < t < T, \boldsymbol{x} \in \partial\Omega. \tag{2}$$

Here $\boldsymbol{n}$ is the outward unit normal vector to the boundary $\partial\Omega$, and α_k $(k = 1, 2, 3)$ are given functions of t and $\boldsymbol{x}$.

2.1. Lattice Boltzmann method

The main purpose of this paper is to derive novel boundary schemes for the general Robin boundary condition (2). In order to present our idea clearly, we work only with the simple two-dimensional five-velocity (D2Q5) BGK model due to Yoshida and Nagaoka [26], while the idea can be directly extended to general cases (e.g. MRT models) but with tedious calculations. In that model, the five discrete velocities are

$$\boldsymbol{c}_i = \begin{cases} (0, 0), & i = 1, \\ (\cos[(i-2)\pi/2], \sin[(i-2)\pi/2]), & i = 2, 3, 4, 5. \end{cases}$$

The evolution equation for the i-th distribution function $g_i = g_i(t, \boldsymbol{x})$ reads as

$$g_i(t + \delta_t, \boldsymbol{x} + c\delta_t \boldsymbol{c}_i) - g_i(t, \boldsymbol{x}) = -\frac{1}{\tau}(g_i(t, \boldsymbol{x}) - g_i^{(eq)}(t, \boldsymbol{x})) + \omega_i \delta_t S(C, t, \boldsymbol{x}) \tag{3}$$

for $i = 1, 2, \cdots, 5$. Here δ_t is a time step, $c = h/\delta_t$ is the lattice speed with h the lattice size, τ is the dimensionless relaxation time given by