Research Report

Asymptotic Analysis of the Lattice Boltzmann Method and Its Applications

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ABSTRACT An asymptotic analysis of the lattice Boltzmann method is used to clarify the connection between the lattice Boltzmann algorithm and the partial differential equations to be analyzed. In the asymptotic analysis, a small value is chosen for the lattice spacing, and the distribution function and physical variables, such as the flow velocity and the fluid density, are all expanded as power series of this small parameter. The equations satisfied by the expansion coefficients are then investigated. In this article, a standard lattice Boltzmann equation is analyzed to show that the leading-order expansion coefficients solve the Navier–Stokes equations. A standard bounce-back rule at the boundaries is also examined, and the no-slip boundary condition is shown to be satisfied. The asymptotic analysis is useful for developing new lattice Boltzmann schemes that can capture a variety of physical models. Three schemes developed through asymptotic analysis are presented here: (i) a boundary scheme for modeling a pressure drop across a filter, (ii) an extension to the convection-diffusion equation in a curvilinear coordinate system, and (iii) a modification for capturing a boundary condition at a two-phase interface.

KEYWORDS Lattice Boltzmann Method, Asymptotic Analysis, Computational Fluid Dynamics, Navier–Stokes Equations, Convection-diffusion Equation

1. Introduction

Computational fluid dynamics (CFD) has played a very important role in research and development in the automotive industry, and now it is recognized as a fundamental technology for developing various parts in motor vehicles; for example, it is used in numerical analysis of the aerodynamics around car bodies, prediction of the combustion properties in engine cylinders, and simulations of a thermal management system exploiting a fluid. CFD consists of numerically solving fluid-dynamic-type equations, such as the Navier–Stokes equations. A numerical approach that has recently attracted attention is the lattice Boltzmann method (LBM).[1,2] Extensive studies of the LBM did not begin until after 1990, and thus it is a relatively new method, compared with the conventional finite-volume and finite-element methods. One of the main features of the LBM is an extremely simple algorithm for tracking the motions of virtual particles that are traveling over a lattice. This simplicity results in good compatibility with massively parallel computing and in an easy treatment of problems that include complex boundaries, and therefore the LBM is now considered to be one of the major numerical methods for flow simulations.

Since the algorithm is both intuitive and simple, creating computer programs for the LBM is straightforward. However, the theory behind the connection between the algorithm and the partial differential equations is complicated, in comparison with the conventional algorithms, which are obtained by directly discretizing the partial differential equations of interest. It is indeed possible to implement numerical analyses without going into the details of the theory if one uses the well-established LBM algorithm. When a new physical model is to be reflected in the partial differential equations or the boundary conditions, however, it is necessary to understand the theory in order to determine how to modify the LBM algorithm. In this article, we summarize a theoretical analysis that clearly explains the connection between the LBM algorithm and the partial differential equations that are to be solved numerically.

The most widely used method for analyzing the LBM is the so-called Chapman–Enskog expansion technique. However, we will employ a similar but essentially different technique, known as asymptotic analysis.[3-5] In both methods, it is necessary to choose a small parameter that corresponds to the lattice spacing; the velocity distribution function, a basic variable in the LBM, is then expanded as a power series in that

small parameter. One notable difference between these methods is that, in an asymptotic analysis, the unknown variables of the partial differential equations, as well as the velocity distribution function, are expanded in powers of that small parameter. Therefore, clear information about the structure of the numerical solution, including the approximation accuracy, is revealed.

In the next section, we will state the standard LBM algorithm, which was designed to numerically solve the Navier–Stokes equations. An asymptotic analysis of the lattice Boltzmann equation and a boundary treatment are outlined in Section 3. In Section 4, as examples of applications, we present three schemes that were developed through asymptotic analysis: Section 4. 1 shows, for the Navier–Stokes equations, a boundary condition that captures a pressure drop across a filter;[6] Section 4. 2 presents an extension to the convection-diffusion equation in curvilinear coordinate systems;[7] and in Section 4. 3, we show a new boundary scheme, which was recently developed for a boundary condition at a two-phase interface.[8]

2. Lattice Boltzmann Method

2. 1 Navier–Stokes Equations

In this article, we consider the LBM for the incompressible Navier–Stokes equations governing the flow velocity $\mathbf{v}(t, \mathbf{x})$ and the pressure $p(t, \mathbf{x})$:

$$\frac{\partial v_j}{\partial x_j} = 0, \tag{1}$$

$$\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 v_i}{\partial x_j^2}, \tag{2}$$

where $t \in [0, \mathcal{T}]$ is the time, $\mathbf{x} \in \mathbb{R}^d$ is the spatial coordinate in d-dimensional space, ρ_0 is the reference density of the fluid, and ν is the kinetic viscosity ($\nu = \mu/\rho_0$, where μ is the viscosity of the fluid). Throughout this article, the vector element in $\mathbb{R}^d$ is indicated by boldface letters, and we assign indices i, j, k to the components of the vectors. The summation convention for repeated indices is assumed.

At the boundary between the fluid and the solid wall, the standard no-slip boundary condition is assumed:

$$v_j = 0, \text{ at boundary.} \tag{3}$$

2. 2 Lattice Boltzmann Equation

In this section, we formulate the LBM for solving Eqs. (1) and (2). The basic equation in the LBM is the lattice Boltzmann equation (LB equation), which governs the behavior of the velocity distribution function $f_\alpha(t, \mathbf{x})$, $\alpha = 0, 1, 2, ..., n$, where the value of n depends on the set of discrete velocities. The value of f_α indicates the fluid density distributed to $n + 1$ virtual particles, and the particles travel over the lattice with the assigned discrete velocities. The discrete velocities are defined in terms of $\mathbf{e}_\alpha$. There are different sets of $\mathbf{e}_\alpha$, depending on the spatial dimensions and on the type of partial differential equations to be solved. Here, we describe two sets that are widely used for solving the Navier–Stokes equations: one has fifteen velocities in three-dimensional space (D3Q15 model), and the other has nine velocities in two-dimensional space (D2Q9 model):

D3Q15 model:

$$[\mathbf{e}_0\ \mathbf{e}_1\ \mathbf{e}_2\ \mathbf{e}_3\ \mathbf{e}_4\ \mathbf{e}_5\ \mathbf{e}_6\ \mathbf{e}_7\ \mathbf{e}_8\ \mathbf{e}_9\ \mathbf{e}_{10}\ \mathbf{e}_{11}\ \mathbf{e}_{12}\ \mathbf{e}_{13}\ \mathbf{e}_{14}] = \begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \end{bmatrix}. \tag{4}$$

D2Q9 model:

$$[\mathbf{e}_0\ \mathbf{e}_1\ \mathbf{e}_2\ \mathbf{e}_3\ \mathbf{e}_4\ \mathbf{e}_5\ \mathbf{e}_6\ \mathbf{e}_7\ \mathbf{e}_8] = \begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}. \tag{5}$$

In this article, Greek subscripts are used to indicate the quantities corresponding to the directions of the discrete velocities, as f_α above, and the summation convention does not apply to these indices.

The summation of the velocity distribution function is related to the local density of the fluid through

$$\rho = \Sigma_\alpha f_\alpha, \tag{6}$$

where ρ is the local fluid density normalized by the reference density ρ_0. For an incompressible fluid, ρ should be close to unity, and the value of f_α approximates a discrete probability distribution function. Therefore, the average velocity of the virtual particles corresponds to the velocity of the fluid flow:

$$\mathbf{u} = \Sigma_\alpha C \mathbf{e}_\alpha f_\alpha, \tag{7}$$

where C is a measure of the particle velocity defined in terms of the time step Δt and the lattice spacing Δx as $C = \Delta x/\Delta t$. The LB equation governing the velocity distribution function is written as follows:

$$f_\alpha(t + \Delta t, \mathbf{x} + \mathbf{e}_\alpha \Delta x) = f_\alpha(t, \mathbf{x}) + Q_\alpha[f](t, \mathbf{x}). \tag{8}$$

Here, Q_α is the collision operator defined as

$$Q_\alpha[f] = \frac{1}{\tau}\,[f_\alpha^{\mathrm{eq}}(\rho(t, \mathbf{x}), \mathbf{u}(t, \mathbf{x}) - f_\alpha(t, \mathbf{x})], \tag{9}$$

where τ is the relaxation-time coefficient, which controls the relaxation speed of f_α toward f_α^{eq} during Δt. For stability, τ is required to be larger than 0.5. The equilibrium distribution function f_α^{eq} is defined in terms of the density ρ and the flow velocity $\mathbf{u}$ as

$$f_\alpha^{\mathrm{eq}}(\rho, \mathbf{u}) = \omega_\alpha[\rho + \frac{3}{C}\ u_j e_{j\alpha} + \frac{9}{2C^2}\,(u_j e_{j\alpha})^2 - \frac{3}{2C^2}\,u_j^2], \tag{10}$$

where ω_α is the weight coefficient, for which the values depend on the set of discrete velocities:

$$\text{D3Q15 model: } \omega_\alpha = \begin{cases} 2/9, & \alpha = 0 \\ 1/9, & \alpha = 1, \ldots, 6 \\ 1/72, & \alpha = 7, \ldots, 14. \end{cases} \tag{11}$$

$$\text{D2Q9 model: } \omega_\alpha = \begin{cases} 4/9, & \alpha = 0 \\ 1/9, & \alpha = 1, \ldots, 4 \\ 1/36, & \alpha = 5, \ldots, 8. \end{cases} \tag{12}$$

2. 3 Computational Procedure

Here, we present the procedure for implementing a numerical analysis using the LBM described in the previous subsection. We note that although the simplest choice of the initial distribution is $f_\alpha(0, \mathbf{x}) = f_\alpha^{\mathrm{eq}}(1, \mathbf{v}^{\mathrm{in}})$, if the initial transient behavior is important, then the initial distribution should be chosen more carefully.[4] Given the initial distribution $f_\alpha(t, \mathbf{x})$ with $t = 0$, the distribution function at $t + \Delta t$ is obtained in the following manner:

(i) Collision: the post-collision distribution, denoted by $\hat{f}_\alpha$, is given by

$$\hat{f}_\alpha(t, \mathbf{x}) = f_\alpha(t, \mathbf{x}) + Q_\alpha[f](t, \mathbf{x}). \tag{13}$$

(ii) Streaming: the post-collision value $\hat{f}_\alpha$ is moved to the neighboring node in the direction of $\mathbf{e}_\alpha$:

$$f_\alpha(t + \Delta t, \mathbf{x} + \mathbf{e}_\alpha \Delta x) = \hat{f}_\alpha(t, \mathbf{x}). \tag{14}$$

(iii) Macroscopic quantity: using the updated f_α, the values of ρ and $\mathbf{u}$ are computed from Eqs. (6) and (7).

(iv) If $t + \Delta t$ reaches $\mathcal{T}$, or if a specified convergence condition is satisfied in steady-state problems, then the computation is terminated; otherwise, processes (i) through (iii) are repeated.

In process (ii), if the node from which the post-collision value moves is outside the fluid domain, then Eq. (14) is replaced by

$$f_\alpha(t + \Delta t, \mathbf{x} + \mathbf{e}_\alpha \Delta x) = \hat{f}_\beta(t, \mathbf{x} + \mathbf{e}_\alpha \Delta x), \tag{15}$$

where (and in what follows) the index β indicates the direction opposite to α, i.e., $\mathbf{e}_\alpha = -\mathbf{e}_\beta$. The boundary scheme given in Eq. (15), which is often referred to as the bounce-back scheme, is the most widely used method to reproduce a no-slip boundary condition.

In the following section, we prove by means of an asymptotic analysis that the procedure described above yields an approximate solution to the incompressible Navier–Stokes Eqs. (1) and (2).

3. Asymptotic Analysis

In this section, we conduct an asymptotic analysis to clarify the connection between the LBM algorithm and the Navier–Stokes equations. In Section 3. 2, we then show that the bounce-back scheme given in Eq. (15) realizes the no-slip boundary condition given in Eq. (3).

3. 1 Analysis of the Lattice Boltzmann Equation

Before starting the asymptotic analysis, we first rescale the time and spatial coordinates by introducing the following dimensionless variables:

$$\tilde{t} = \frac{U}{L}t,\ \ \tilde{\mathbf{x}} = \frac{1}{L}\mathbf{x},\ \ \tilde{\mathbf{u}} = \frac{1}{U}\mathbf{u}, \tag{16}$$

where L and U are the reference length and speed of the physical problem. Following the discussion in Refs. (3) and (4) we choose the value of U as

$$U = C\varepsilon,\ \ \varepsilon = \frac{\Delta x}{L}. \tag{17}$$

This definition indicates that the typical speed is much slower than the speed $C = \Delta x/\Delta t$ characterizing the virtual particle dynamics; this is consistent with the assumption that the Mach number is low in the incompressible regime. The small parameter ε defined in Eq. (17) is used as an expansion parameter in the asymptotic analysis, i.e., we investigate the behavior of the solution in the limit as $\varepsilon \to 0$.

Taking U as defined in Eq. (17) as the reference speed means that the reference time is $T = L/U = \Delta t/\varepsilon^2$. Then, the dimensionless time defined in Eq. (16) becomes $\tilde{t} = t\varepsilon^2/\Delta t$. Correspondingly, the dimensionless time step, defined as $\Delta\tilde{t} = \Delta t/T$, is expressed as $\Delta\tilde{t} = \varepsilon^2$. This means that $\Delta\tilde{t}/\varepsilon^2$ must be maintained as unity in the limit as $\varepsilon \to 0$.

Using these dimensionless variables, we rescale the Eq. (8) (LB equation) as follows:

$$f_\alpha(\tilde{t} + \varepsilon^2, \tilde{\mathbf{x}} + \mathbf{e}_\alpha\varepsilon) = f_\alpha(\tilde{t}, \tilde{\mathbf{x}}) + \tilde{Q}_\alpha[f](\tilde{t}, \tilde{\mathbf{x}}), \tag{18}$$

with

$$\tilde{Q}_\alpha[f] = \frac{1}{\tau}[\tilde{f}_\alpha^{\mathrm{eq}}(\rho(\tilde{t}, \tilde{\mathbf{x}}), \tilde{\mathbf{u}}(\tilde{t}, \tilde{\mathbf{x}})) - f_\alpha(\tilde{t}, \tilde{\mathbf{x}})], \tag{19}$$

where $\tilde{f}_\alpha^{\mathrm{eq}}$ is the equilibrium distribution function expressed using ρ and $\tilde{\mathbf{u}}$ as

$$\tilde{f}_\alpha^{\mathrm{eq}}(\rho, \tilde{\mathbf{u}}) = \omega_\alpha[\rho + 3\tilde{u}_j e_{j\alpha}\varepsilon + \frac{9}{2}(\tilde{u}_j e_{j\alpha})^2\varepsilon^2 - \frac{3}{2}\tilde{u}_j^2\varepsilon^2]. \tag{20}$$

We can express $\tilde{\mathbf{u}}$ in terms of f_α as

$$\tilde{\mathbf{u}} = \frac{1}{\varepsilon}\Sigma_\alpha \mathbf{e}_\alpha f_\alpha. \tag{21}$$

The scaling employed here is the so-called diffusive scaling, which was first developed by Sone[9] to explain the connection between the Boltzmann equation and fluid-dynamic systems,[10,11] and which was later applied to the LB equation by Inamuro et al.[12] to investigate the accuracy of the LB equation. Subsequently, Junk et al.[3] proposed a very general form of systematic asymptotic analysis that was based on diffusive scaling, and they proved the convergence of the numerical solution to the solution of the incompressible Navier–Stokes equation. Since then, this method has been extensively applied to various types of LB equations.[4,5,13]

The asymptotic analysis begins with expanding f_α in powers of ε:

$$f_\alpha = f_\alpha^{(0)} + f_\alpha^{(1)}\varepsilon + f_\alpha^{(2)}\varepsilon^2 + \cdots. \tag{22}$$

Correspondingly, we also expand ρ and $\tilde{u}$ as follows:

$$\rho = 1 + \rho^{(1)}\varepsilon + \rho^{(2)}\varepsilon^2 + \cdots, \tag{23}$$

$$\tilde{\mathbf{u}} = \tilde{\mathbf{u}}^{(1)} + \tilde{\mathbf{u}}^{(2)}\varepsilon + \tilde{\mathbf{u}}^{(3)}\varepsilon^2 + \cdots. \tag{24}$$

From Eqs. (6) and (21), the expressions of $\tilde{\rho}^{(m)}$ and $\tilde{\mathbf{u}}^{(m)}$ in terms of $f_\alpha^{(m)}$ are obtained as

$$\rho^{(m)} = \Sigma_\alpha f_\alpha^{(m)},\ \tilde{\mathbf{u}}^{(m)} = \Sigma_\alpha \mathbf{e}_\alpha f_\alpha^{(m)}. \tag{25}$$

After inserting the expansion (22) into Eq. (18), the Taylor expansion is applied to $f_\alpha(\tilde{t} + \varepsilon^2, \tilde{\mathbf{x}} + \mathbf{e}_\alpha\varepsilon)$. Then, we equate the coefficients of the same power of ε in order to obtain the following sequence of equations:

$$order\ \varepsilon^0\colon\ 0 = \frac{1}{\tau}(\tilde{f}_\alpha^{\mathrm{eq}(0)} - f_\alpha^{(0)}), \tag{26}$$

$$order\ \varepsilon^1\colon\ \frac{\partial e_j f_\alpha^{(0)}}{\partial \tilde{x}_j} = \frac{1}{\tau}(\tilde{f}_\alpha^{\mathrm{eq}(1)} - f_\alpha^{(1)}), \tag{27}$$

$$order\ \varepsilon^2\colon\ \frac{\partial f_\alpha^{(0)}}{\partial \tilde{t}} + \frac{\partial e_j f_\alpha^{(1)}}{\partial \tilde{x}_j} + \frac{1}{2}\frac{\partial^2 e_i e_j f_\alpha^{(0)}}{\partial \tilde{x}_i \partial \tilde{x}_j}\frac{1}{\tau}(\tilde{f}_\alpha^{\mathrm{eq}(2)} - f_\alpha^{(2)}), \tag{28}$$

$$order\ \varepsilon^3\colon\ \frac{\partial f_\alpha^{(1)}}{\partial \tilde{t}} + \frac{\partial e_j f_\alpha^{(2)}}{\partial \tilde{x}_j} + \frac{1}{2}\frac{\partial^2 e_i e_j f_\alpha^{(1)}}{\partial \tilde{x}_i \partial \tilde{x}_j} + \frac{1}{6}\frac{\partial^3 e_i e_j e_k f_\alpha^{(0)}}{\partial \tilde{x}_i \partial \tilde{x}_j \partial \tilde{x}_k} = \frac{1}{\tau}(\tilde{f}_\alpha^{\mathrm{eq}(3)} - f_\alpha^{(3)}), \tag{29}$$

where $\tilde{f}_\alpha^{\mathrm{eq}(m)}$ is the coefficient of ε^m in the expansion of $\tilde{f}_\alpha^{\mathrm{eq}}$. The specific expression of $\tilde{f}_\alpha^{\mathrm{eq}(m)}$ is obtained by substituting Eqs. (22) through (24) into Eq. (20) and equating the coefficients for the same powers of ε:

$$f_\alpha^{\mathrm{eq}(0)} = \omega_\alpha, \tag{30}$$

$$f_\alpha^{\mathrm{eq}(1)} = \omega_\alpha\rho^{(1)} + 3\omega_\alpha e_{i\alpha}\tilde{u}_i^{(1)}, \tag{31}$$

$$f_\alpha^{\mathrm{eq}(2)} = \omega_\alpha\rho^{(2)} + 3\omega_\alpha e_{i\alpha}\tilde{u}_i^{(2)} + \frac{9\omega_\alpha}{2}(\tilde{u}_j^{(1)}e_{j\alpha})^2 - \frac{3\omega_\alpha}{2}(\tilde{u}_j^{(1)})^2, \tag{32}$$

$\cdots$.

Equations (26) through (29) are regarded as equations for $f_\alpha^{(m)}$, and they are thus solved successively from the lowest order. Here, for the inhomogeneous linear Eqs. (28) and (29) to be solved for $f_\alpha^{(2)}$ and $f_\alpha^{(3)}$, certain solvability conditions for the inhomogeneous terms must be satisfied. The specific conditions are obtained by multiplying them by $\mathbf{e}_\alpha$ or unity and then taking summations with respect to α. These solvability conditions form partial differential equations for $\rho^{(m)}$ and $\tilde{\mathbf{u}}^{(m)}$:

$$\frac{\partial \tilde{u}_j^{(1)}}{\partial \tilde{x}_j} = 0, \tag{33}$$

$$\frac{\partial \tilde{u}_i^{(1)}}{\partial \tilde{t}} + \tilde{u}_j^{(1)} \frac{\partial \tilde{u}_i^{(1)}}{\partial \tilde{x}_j} = -\frac{1}{3}\frac{\partial \rho^{(2)}}{\partial \tilde{x}_i} + \frac{1}{3}\left(\tau - \frac{1}{2}\right)\frac{\partial^2 \tilde{u}_i^{(1)}}{\partial \tilde{x}_j^2}, \tag{34}$$

where Eq. (33) is obtained from Eq. (28) multiplied by unity, and Eq. (34) is obtained from Eq. (29) multiplied by $\mathbf{e}_\alpha$. Apart from these conditions, $\rho^{(1)}$ is revealed to be constant by multiplying Eq. (28) by $\mathbf{e}_\alpha$ and taking summation with α. The set of partial differential equations described above shows that the quantities obtained using the LBM approximate the solution of the incompressible Navier–Stokes Eqs. (1) and (2), if we set the following relations:

$$p = C_S^2 \rho_0 \rho = C_S^2 \rho_0 (1 + \rho^{(1)}\varepsilon + \rho^{(2)}\varepsilon^2 + \cdots), \tag{35}$$

$$\mathbf{v} = \mathbf{u} = \varepsilon C(\tilde{\mathbf{u}}^{(1)} + \tilde{\mathbf{u}}^{(2)}\varepsilon + \cdots), \tag{36}$$

$$\nu = \frac{1}{3}\left(\tau - \frac{1}{2}\right)\frac{\Delta x^2}{\Delta t}, \tag{37}$$

where $C_S = C/\sqrt{3}$ is a quantity that is often referred to in the LBM as the pseudo-sound speed.

If we proceed to the higher-order conditions, we see that $\tilde{\mathbf{u}}^{(2)}$ and $\tilde{\rho}^{(3)}$ must satisfy linear homogeneous equations. (Since the analysis proceeds in parallel, we omit a detailed description of the higher-order analysis.) As will be shown in the following subsection, the corresponding boundary condition is also linear and homogeneous, and therefore $\tilde{\mathbf{u}}^{(2)}$ and $\rho^{(3)}$ only have trivial solutions (or they are zero). Hence, from Eq. (36), the approximation accuracy of the LBM for solving the Navier–Stokes equation is found to be second order with respect to ε.

The specific forms of the solutions of Eqs. (26) through (29) are obtained in a straightforward manner using Eqs. (30) through (32), as follows:

$$f_\alpha^{(0)} = \omega_\alpha, \tag{38}$$

$$f_\alpha^{(1)} = \omega_\alpha \rho^{(1)} + 3\omega_\alpha e_{i\alpha} \tilde{u}_i^{(1)}, \tag{39}$$

$$f_\alpha^{(2)} = \omega_\alpha \rho^{(2)} + 3\omega_\alpha e_{i\alpha} \tilde{u}_i^{(2)} + \frac{9\omega_\alpha}{2}(\tilde{u}_j^{(1)} e_{j\alpha})^2 - \frac{3\omega_\alpha}{2}(\tilde{u}_j^{(1)})^2 - 3\tau\omega_\alpha e_{j\alpha} e_{k\alpha} \frac{\partial \tilde{u}_k^{(1)}}{\partial \tilde{x}_j}. \tag{40}$$

3. 2 Analysis of the Bounce-back Scheme

We next analyze the boundary scheme shown in Eq. (15) using an expansion technique similar to that described in the previous subsection. In the course of the analysis, we use the explicit expressions of the asymptotic solutions (38) through (40) in order to rewrite the conditions for the distribution function into conditions for the physical quantities, such as the flow velocity and the density. Here, we assume that the boundary is located at the midpoint between two lattice points, and the expansion is performed around the point on the boundary $\tilde{\mathbf{x}}_B = \tilde{\mathbf{x}} - \mathbf{e}_\alpha\varepsilon/2 = \tilde{\mathbf{x}} + \mathbf{e}_\beta\varepsilon/2$ ($\mathbf{e}_\beta = -\mathbf{e}_\alpha$). Equation (15) can be rewritten in terms of $\tilde{\mathbf{x}}_B$ as follows:

$$f_\alpha(\tilde{t} + \varepsilon^2, \tilde{\mathbf{x}}_B + \mathbf{e}_\alpha\varepsilon/2) = f_\beta(\tilde{t}, \tilde{\mathbf{x}}_B - \mathbf{e}_\beta\varepsilon/2) + \frac{1}{\tau}[\tilde{f}_\beta^{\mathrm{eq}} - f_\beta](\tilde{t}, \tilde{\mathbf{x}}_B - \mathbf{e}_\beta\varepsilon/2). \tag{41}$$

After substituting the expansions (22) and (30) through (32) into the above equation, we apply the Taylor expansion around $(\tilde{t}, \tilde{\mathbf{x}}_B)$. Then, equating the coefficients of ε results in the conditions satisfied by $f_\alpha^{(m)}$ on the boundary. These conditions can be rewritten in terms of $\tilde{\mathbf{u}}^{(m)}$ and $\rho^{(m)}$ by using the solutions (38) and (39) obtained in the asymptotic analysis.

In the leading-order analysis, we obtain the condition $f_\alpha^{(0)} = f_\beta^{(0)}$, which is automatically satisfied because $f_\alpha^{(0)} = \omega_\alpha$ (Eq. (38)) and $\omega_\alpha = \omega_\beta$.

Proceeding to the first order in ε, we obtain a similar condition: $f_\alpha^{(1)} = f_\beta^{(1)}$. By substituting the asymptotic solution (39), this is transformed into the following condition for $\tilde{\mathbf{u}}^{(1)}$:

$$e_{j\alpha}\tilde{u}_j^{(1)} = 0. \tag{42}$$

In deriving the above equation, we used the relations $\mathbf{e}_\beta = -\mathbf{e}_\alpha$ and $\omega_\alpha = \omega_\beta$. The condition (42) corresponds to the no-slip boundary condition (3), because $\mathbf{e}_\alpha \neq 0$

for $\alpha > 0$.

Similarly, the condition in the second order in ε is obtained as follows:

$$3e_{j\alpha}\tilde{u}_j^{(2)} + \frac{1}{2}e_{j\alpha}\frac{\partial \rho^{(1)}}{\partial \tilde{x}_j} = 0. \quad (43)$$

Since the asymptotc solution of $\rho^{(1)}$ is constant as mentioned below Eq. (34), the above equation results in $\tilde{\mathbf{u}}^{(2)} = 0$.

4. Applications of the Asymptotic Analysis

In the previous section, by means of an asymptotic analysis, the leading-order coefficient of the expansion of the flow velocity $\tilde{\mathbf{u}}^{(1)}$ was shown to satisfy Eqs. (33) and (34), and the next-order coefficient $\tilde{\mathbf{u}}^{(2)}$ was shown to vanish. This means that the quantity $\mathbf{u}$ obtained in the LBM through Eq. (7) approximates the solution of the Navier–Stokes equations with second-order accuracy with respect to Δx (= $L\varepsilon$). As has been demonstrated, a careful analysis is required to understand the theory behind the connection between the LBM algorithm and the target partial differential equations. Once we understand this connection, however, it is easy to modify the LBM algorithm for a new model on the partial differential equations or on the boundary conditions. In this section, we present three schemes developed by modifying the LBM algorithm through the asymptotic analysis.

4. 1 Pressure Drop Across a Filter

Simulating gas flow in particulate air filters, such as the intake filters of automobile engines and diesel particulate filters, is difficult because of two different length scales included in the systems, namely, the larger scale representing the overall flows and the smaller scale of the pore size of the filter materials. Resolving both length scales requires enormous computational resources, with long CPU times and large memory overheads. One solution to this problem is to coarse-grain the microscopic structure of the filter material and to incorporate its effects into the overall flow analysis. However, filters are usually very thin, and it is still necessary to prepare a computational grid that is sufficiently fine to resolve the thin material in order to apply the coarse-grained model. If the effect of the filter material can be incorporated as a boundary condition rather than as a bulk property, the computational efficiency is greatly improved.

As a promising method for simulating such filter problems, we proposed in Ref. (6) a permeable bounce-back scheme, in which a fraction of the distribution function is bounced back, and the remainder transmits through a filter. Since in this scheme only part of the momentum is transported to the neighboring nodes, a pressure drop due to a momentum loss is reproduced. More specifically, in the streaming process of the LBM, Eq. (14) is replaced by the following scheme when the distribution function moves across a filter boundary:

$$f_\alpha(t + \Delta t, \mathbf{x}) = \theta \hat{f}_\beta(t, \mathbf{x}) + (1 - \theta)\hat{f}_\alpha(t, \mathbf{x} - \mathbf{e}_\alpha \Delta x), \quad (44)$$

where the coefficient $\theta \in (0, 1)$ determines the permeability of the porous filter. In Ref. (6), by using an asymptotic analysis, the relation between the pressure variation Δp at the filter boundary and the parameter θ was clarified:

$$\frac{\Delta p}{\Delta x |\mathbf{e}_\alpha|} = -\frac{2\theta}{1-\theta}\frac{\rho_0}{\Delta t} n_j^\alpha u_j, \quad (45)$$

where $\mathbf{n}^\alpha$ is a unit vector in the direction of $\mathbf{e}_\alpha$. In order to numerically validate the theoretical result (45), flows through a filter were simulated using the algorithm described in Eq. (44), for various values of θ. **Figure 1** shows the numerical results along with the analytical prediction, which confirms the validity of Eq. (45). We note that applicability of the same algorithm to simulating the Brinkman model, which describes the flows through porous media, is examined in detail in Ref. (6).

4. 2 The Convection-diffusion Equation in Curvilinear Coordinate Systems

The LBM is normally restricted to uniform grids, but in this section, we extend it to general curvilinear coordinate systems by utilizing a multiple-relaxation-time collision operator.[7]

While the LBM was developed as a numerical scheme for solving the Navier–Stokes equations, a natural extension for solving the convection-diffusion equation (CDE) has recently been presented.[14-19] The LBM is used not only to solve physical problems that are primarily governed by the CDE,[20,21] but also to support simulating thermal flows[22,23] and to capture the interface of multiphase flows.[24,25]

Originally, the LBM was based on lattice points that were uniformly distributed in the computational domain, and in most cases, a square (cubic) lattice was used. A number of attempts have been made to remove this limitation in order to widen its applicability. One strategy by which to remove the limitation is to transform the LB equation into its differential form;[26-29] however, in so doing, the locality of the scheme, which is one of the important features of the LBM, is sacrificed. Another method is to evaluate the value of the distribution function on the nonuniform lattice by means of an interpolation procedure using the values of the distribution function that propagate uniformly in the directions of the Cartesian coordinates.[30,31] The problem with this method is that the interpolation procedure causes unphysical numerical viscosities, as discussed in Ref. (32).

In Ref. (7), we proposed an LBM for the CDE in curvilinear coordinate systems; this method does not require an interpolation procedure, and thus it maintains the algorithmic simplicity of the original lattice Boltzmann scheme. In this method, nonuniform grids are used, but the LBM is actually implemented on a uniform grid by using a coordinate transformation. The apparent anisotropy of diffusion caused by the coordinate transformation is handled using the multiple-relaxation-time technique that was proposed in Ref. (5). It was proven in Ref. (7) that the proposed algorithm correctly approximates the solution of the CDE in curvilinear coordinate systems, and several numerical experiments have been carried out for specific problems in order to numerically validate the method.

As a numerical example, we show the results of simulations of ion diffusion onto an axisymmetric microelectrode. An oblate hemispherical electrode with the major and minor axes a_0 and b_0, respectively, is placed as shown in **Fig. 2**, and an inert plane spanning in the x-y space is located at $z = 0$. The domain $z > 0$ is filled with an electrolyte solution, and the concentration of the solute, denoted by c, is initially maintained uniformly at C_0. If a negative

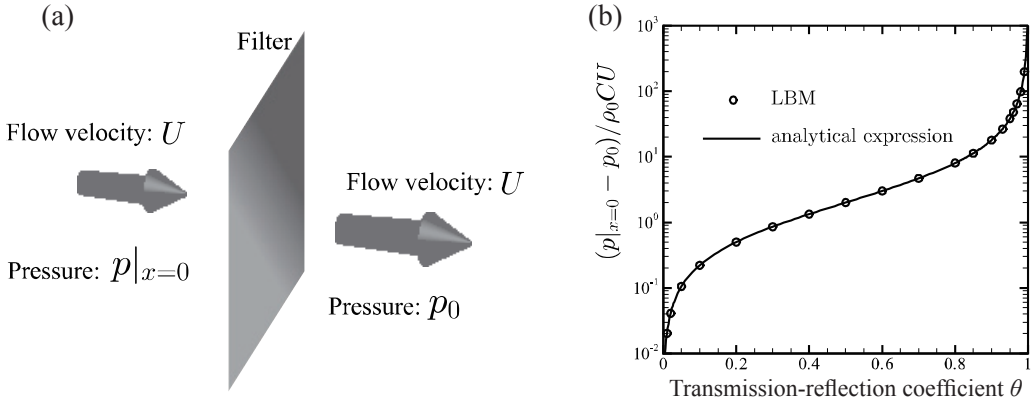

Fig. 1 (a) Flow through a filter. (b) Pressure difference as a function of the transmission-reflection coefficient θ. The open circles indicate the numerical values of $(p|_{x=0} - p_0)/p_0CU$ obtained using the LB simulation, and the solid line indicates the analytical counterpart $2\theta/(1 - \theta)$ (Eq. (45)).

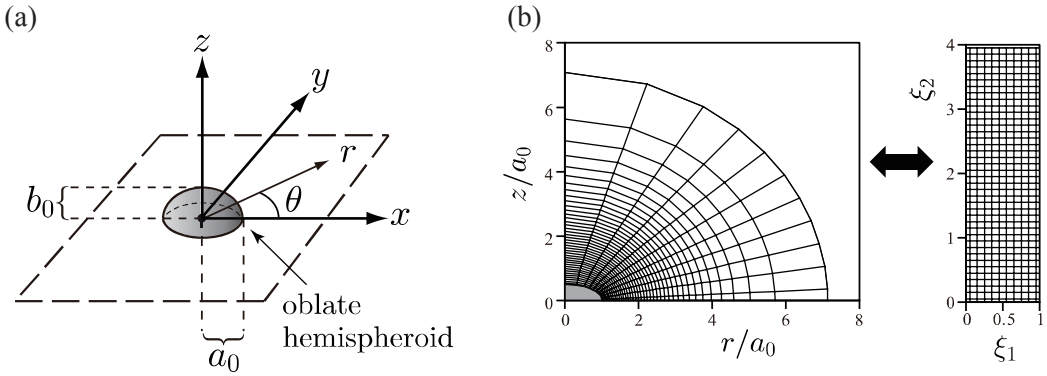

Fig. 2 (a) Oblate hemispherical electrode. (b) Computational grids in (ξ_1, ξ_2) space and (r, z) space.

voltage is applied to the electrode at $t = 0$, the solute is consumed on the surface, and the concentration is maintained at $c = 0$ for $t > 0$. The behavior of c is then investigated on the basis of the diffusion equation. Since the problem is symmetric about the z axis, the diffusion equation is written in terms of the coordinates $r = (x^2 + y^2)^{1/2}$ and z. We then introduce the curvilinear coordinates (ξ_1, ξ_2) in order to deal with the curved surface of the hemispherical electrode in a simple manner. The coordinate systems (r, z) and (ξ_1, ξ_2) are analytically related, and the transformation of grids is depicted in Fig. 2, where the lattice points distributed uniformly in (ξ_1, ξ_2) space are mapped onto the nonuniformly distributed points in the (r, z) space. The algorithm described in Ref. (7) enables using such a nonuniform grid while maintaining the algorithmic simplicity of the original LBM. **Figure 3** shows the time evolution of the normalized current $I/4FDC_0a_0$ onto the electrode, for various values of b_0/a_0, along with the analytical solution and existing numerical results. Here, F and D are the Faraday constant and diffusion coefficient, respectively. For all the values of b_0/a_0, the LBM results agree well with the results in the literature, which confirms the validity of the present method.

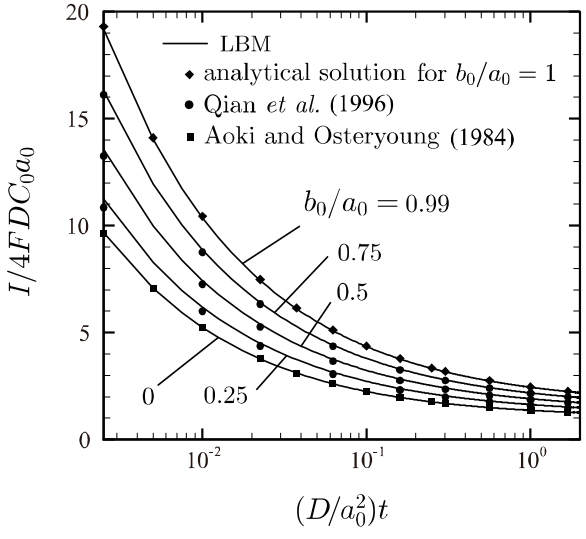

Fig. 3 Time evolution of the diffusion-limited current for various values of b_0/a_0. The solid line indicates the LBM results, the symbol ♦ indicates the exact solution in the case of $b_0/a_0 = 1$, the symbol • indicates the numerical results of Qian et al.,[33] and the symbol ■ indicates the analytical approximation of Aoki and Osteryoung.[34]

4. 3 Boundary Condition at a Two-phase Interface

As mentioned in the previous subsection, the LBM has been studied as a powerful tool for numerically solving the CDE. Boundary treatments other than the standard bounce-back rule have also been investigated in order to apply the LBM to various types of boundary conditions.[35-37] However, difficulties remain when dealing with the interface between two phases with different transport properties, and most of the lattice Boltzmann algorithms that capture the interfaces are restricted to a steady-state analysis.[38,39] Developing a scheme that correctly satisfies the interface boundary condition is very important, since such an interface is encountered frequently in practical engineering problems, e.g., heat conduction between different materials and ion transport between media with different porosities.

In order to clarify the problem, we specify the boundary conditions at the interface. The CDE is written in the following form:

$$\lambda\frac{\partial\phi}{\partial t} + \lambda\frac{\partial}{\partial x_j}(\phi v_j) = K\frac{\partial^2\phi}{\partial x_j^2}, \tag{46}$$

where ϕ is the physical quantity governed by the CDE, t is the time, K is the conductivity, and x_j and v_j are the jth components of the spatial vector $\mathbf{x}$ and the velocity of the fluid $\mathbf{v}$, respectively. The coefficient λ controls the relaxation speed, corresponding to the volumetric specific heat in the heat-conduction problem. If the media is homogeneous and is characterized by a single set of λ and K, Eq. (46) is often divided by λ and the diffusivity $D = K/\lambda$ is used as a parameter. On the other hand, if there is an interface between two phases of different properties, the coefficient λ and the conductivity K appear in the boundary condition in the following form:[40]

$$\phi^A = \phi^B, \tag{47}$$

$$\left(-K^A\frac{\partial\phi^A}{\partial x_j} + \lambda^A v_j\phi^A\right)n_j = \left(-K^B\frac{\partial\phi^B}{\partial x_j} + \lambda^B v_j\phi^B\right)n_j, \tag{48}$$

where n_j is the normal unit vector on the interface, and the superscripts A and B are the indices distinguishing the values in the different phases. Eq. (47) indicates the continuity of the scalar variable, and Eq. (48) indicates the continuity of the flux. In this case, we

need to specify the values of both λ and K. Since the relation $D = K/\lambda$ is usually used in the LBM, most of the existing schemes that satisfy the conditions specified by Eqs. (47) and (48) are restricted to the analysis of steady states.[20,38,39,41]

In order to apply the LBM to problems that include such interfaces, in Ref. (8), we proposed an alternative boundary scheme for the LBM that correctly satisfies the boundary conditions (47) and (48). This scheme is based on two simple modifications in the original LBM algorithm, one for the collision process and the other for the streaming process: (i) In each phase, a different value is assigned to the weight coefficient included in the collision term. (ii) The velocity distribution function in the LBM is multiplied (or divided) by a factor γ when it passes through the interface. These modifications result in new boundary conditions at the interface controlled by the ratio of the weight coefficients and the value of γ. Appropriate definitions of the values of these parameters enable the boundary conditions (47) and (48) to be satisfied simultaneously.

In Ref. (8), the proposed algorithm was proven to satisfy Eqs. (47) and (48) by means of an asymptotic analysis, and it was verified numerically for several specific problems. In **Fig. 4**, the numerical results are presented for the diffusion process in a core-shell sphere with an interface between the core and the shell (Fig. 4(a)). Initially, the value of ϕ is uniform in the sphere ($\phi = \phi^{\text{in}}$ at $t = 0$), and the surface of the sphere ($r = R^B$) is maintained at $\phi = 0$ for $t > 0$. The internal boundary condition at $r = R^A$ is described by Eqs. (47) and (48) without the background velocity $\mathbf{v}$. In Fig. 4(b), we show the time evolution of the profiles of ϕ in the case of ϕ, in the case of $\lambda_B/\lambda_A = 0.5$, $K^B/K^A = 0.5^{3/2}$, and $R^B/R^A = 2$. The LBM results correctly capture the behavior of the exact solution, and this demonstrates the applicability of the proposed scheme to the two-phase boundary condition. In addition to the comparison with the exact solution, the accuracy of the numerical scheme and the influence of the curved boundary are also discussed in detail in Ref. (8).

5. Concluding Remarks

In this article, we outlined an asymptotic analysis of the LBM, and thus we clarified the theoretical connection between the LBM algorithm and the partial differential equations that are to be solved numerically. More specifically, we expanded the flow velocity $\mathbf{u}$ obtained via Eq. (7) as in Eq. (24), and we proved that the leading-order coefficient $\tilde{\mathbf{u}}^{(1)}$ satisfies Eqs. (33) and (34). In addition, the next-order coefficient $\tilde{\mathbf{u}}^{(2)}$ was shown to vanish, and this certifies the second-order accuracy of the LBM with respect to the lattice spacing Δx ($= L\varepsilon$) when numerically solving the Navier–Stokes equations.

Although the algorithm of the LBM is simple to implement, an understanding of its connection with the target partial differential equations (here, the Navier–Stokes equations) requires careful theoretical investigation. Once the connection is clarified, however, one can easily modify the LBM algorithm as desired. As presented in Section 4, when we wish to reflect a new model for the partial differential equations or

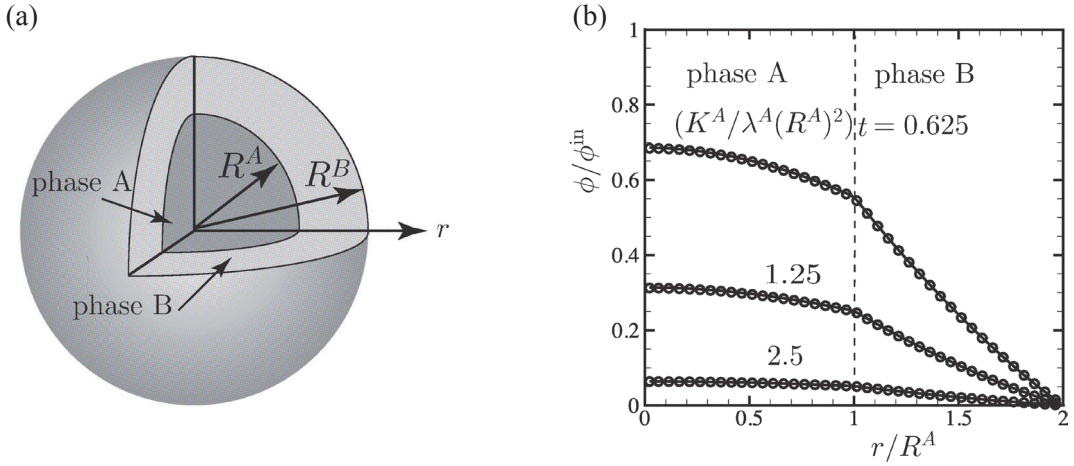

Fig. 4 (a) Core-shell sphere with two phases. (b) Profiles of ϕ along the radial distance in the core-shell sphere, in the case of $\lambda^B/\lambda^A = 0.5$ and $K^B/K^A = 0.5^{3/2}$. The symbol indicates the LBM results, and the solid line indicates the exact solution.[8]

for the boundary conditions on the LBM, a promising strategy for developing a new scheme is to follow an asymptotic analysis. We hope that the information in this review contributes to future development of innovative numerical methods associated with the LBM.

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