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# A simple and efficient curved boundary scheme of the lattice Boltzmann method for Robin boundary conditions of convection-diffusion equations

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### Abstract

This paper is concerned with boundary schemes of the lattice Boltzmann method for Robin boundary conditions of convection-diffusion equations on curved boundaries. For such boundary conditions, all the existing boundary schemes suffer from the possibility that the denominator in the scheme may become zero, which will lead to numerical instability. To avoid this possibility, we propose a boundary scheme by approximating the gradient along the outgoing discrete velocity at the boundary with the given Robin boundary condition and the gradient at the interior point next to the boundary. With this approximated gradient at the boundary, the classical bounce back scheme for Neumann-type boundary conditions is employed to obtain the unknown distribution function at the interior point. The scheme obtained has the first-order accuracy for curved boundaries and its advantages are: (1) the scheme is simple in form so that it can be easily implemented; (2) it avoids the denominator in the scheme to be zero, and (3) the scheme is single-node, *i.e.*, it only involves the information at the present point. Numerical examples demonstrate the designed accuracy and good stability of our scheme for complex boundaries.

*Keywords:* lattice Boltzmann method, convection-diffusion equations, Robin boundary condition, boundary scheme

## 1. Introduction

Convection-diffusion equations (CDEs) are widely used to describe the evolution of scalar quantities (*e.g.* mass and concentration) in natural phenomenon and engineering applications, such as ion transport in fuel cells [1, 2] and surface reactions in porous media [3, 4]. Due to the complexity and nonlinearity, CDEs usually have to be solved numerically. Traditional numerical methods for CDEs include finite difference, finite element, spectral methods, and so on ( see *e.g.* [5, 6, 7]). In this paper, we consider a relatively new method, the lattice Boltzmann method (LBM), for CDEs. Originally, the LBM is proposed as a mesoscopic method for fluid flow simulations [8, 9]. Thanks to its simple formulation and ability to treat complex boundaries, the LBM has also been adapted for CDEs [8, 9, 10, 11].

When using the LBM for CDEs, it is necessary to properly treat corresponding boundary conditions (BCs). The treatment of Dirichlet BCs of CDEs has been well established (see *e.g.* [12, 13, 14]). While for

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the Neumann or Robin BCs, the existing boundary schemes are not satisfactory and their efficient treatment is still the focus of current research [15, 16, 17, 18, 19, 20, 21]. In [15], a boundary scheme for straight boundaries is proposed by using the Neumann (or Robin) BCs to extrapolate the macroscopic quantity at the boundary. Then the classical boundary schemes for the Dirichlet BCs are employed to determine the unknown distribution functions. Unlike [15] using extrapolations, single-node schemes for Robin BCs are derived in [17] based on asymptotic analysis. The schemes have the first-order accuracy for curved boundaries and their second-order improvement is provided in [18]. In [16], the unknown distributions near the boundary are solved out by combining extrapolations, the anti-bounce back scheme, and the gradient expressed by distribution functions. Numerical results show that the convergence order of this scheme is between 1 and 1.5. Based on an expansion of distribution functions obtained by the Chapmann-Enskog analysis, boundary schemes for different types of BCs are constructed in [22]. However, the second-order accuracy of these schemes is demonstrated only via steady-state problems [22]. Besides, a first-order scheme for curved boundaries is formulated in [20], also with the aid of asymptotic analysis. More recently, a second-order curved boundary scheme of Neumann BCs is proposed by using extrapolations and the anti-bounce back scheme of Dirichlet BCs [19]. Similar ideas have also been used in [23] to deal with the reactive BCs. In [21], local second-order schemes for Dirichlet and Neumann BCs are derived by the extended method of moments [24]. These schemes are verified for straight boundaries. They enhance the existing ones with respect to locality, accuracy, and Péclet parametrization. The validity of the schemes relies on the inverse of a matrix, which may impose additional constraints on the convective velocity.

In summary, there have been various, either first- or second-order, boundary schemes of the LBM for Robin BCs of CDEs [15, 16, 17, 18, 19, 20, 23]. Though their effectiveness was validated numerically, a common problem for these schemes is that the denominators in the schemes may become zero, which will lead to numerical instability. For example, the scheme in [17] has a term $\tau - 1$ ($\tau$ is the relaxation time) in its denominator. If $\tau = 1$, the denominator will be zero and cause instability. This problem also exists in other schemes mentioned above [15, 16, 18, 19, 20, 23].

To address the above problem, we propose a curved boundary scheme for the Robin BCs neither by using the expansion of distribution functions nor by converting the BCs to Dirichlet type. Instead, we convert the curved boundary case to a straight boundary case. Specifically, we approximate the gradient along the outgoing discrete velocity at the boundary with the given Robin BC and the gradient at the interior point next to the boundary. With this approximated gradient at the boundary, the classical bounce back scheme for Neumann-type BCs on straight boundaries is employed to obtain the unknown distribution function at the interior point. The scheme obtained has the first-order accuracy for curved boundaries and its advantages are: (1) the construction idea of our scheme is easy to follow and the scheme is simple in form so that it can be easily implemented; (2) it avoids the denominator in the scheme to be zero, and (3) the scheme is single-node, *i.e.*, it only involves the information at the present point. Numerical experiments are conducted to test the accuracy and stability of our scheme. The computational results not only verify the designed accuracy of our scheme but also demonstrate its good stability.

The rest of the paper is organized as follows. Section 2 introduces the LBM for CDEs. In Section 3, we provide the construction of our boundary scheme. Numerical experiments are conducted in Section 4. Finally, some conclusions and remarks are given in Section 5.

## 2. LBM for CDEs

Consider a two-dimensional CDE with source term

$$\partial_t C + \nabla \cdot (C\boldsymbol{u}) = \nabla \cdot (D\nabla C) + F, \quad 0 < t < T, \boldsymbol{x} \in \Omega, \tag{2.1}$$

where $C := C(\boldsymbol{x}, t)$ is a scalar variable of spatial coordinate $\boldsymbol{x} \in \mathbb{R}^2$ and time $t$, $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x}, t)$ is the given velocity field, $D := D(\boldsymbol{x}, t)$ is the diffusion coefficient and $F := F(\boldsymbol{x}, t)$ is the source term. Assume that (2.1) is equipped with the Robin BC

$$\alpha_1 C + \alpha_2 \frac{\partial C}{\partial \boldsymbol{n}} = \alpha_3, \quad 0 < t < T, \boldsymbol{x} \in \partial\Omega, \tag{2.2}$$

where $\boldsymbol{n}$ is the unit normal vector to the boundary $\partial\Omega$, $\alpha_k, k = 1, 2, 3$ are given functions of $\boldsymbol{x}$ and $t$, and $\alpha_2 \neq 0$.

The D2Q5 (two dimensions and five discrete velocities) LBM for the CDE (2.1) reads as (see *e.g.* [17, 16])

$$g_i(\boldsymbol{x} + \boldsymbol{e}_i\delta_x, t + \delta_t) - g_i(\boldsymbol{x}, t) = -\frac{1}{\tau}(g_i(\boldsymbol{x}, t) - g_i^{(eq)}(\boldsymbol{x}, t)) + \delta_t\omega_i F, \quad i = 0, 1, 2, 3, 4. \tag{2.3}$$

Here $g_i := g_i(\boldsymbol{x}, t)$ is the $i$-th distribution function with discrete velocity $\boldsymbol{e}_i$ at position $\boldsymbol{x}$ and time $t$, $\delta_x$ is the lattice size, $\delta_t$ is the time step, $\tau$ denotes the dimensionless relaxation time, $g_i^{(eq)}$ is the equilibrium distribution function, and $\omega_i$ is the $i$-th weight. More specifically, $\boldsymbol{e}_0 = (0, 0), \boldsymbol{e}_1 = -\boldsymbol{e}_3 = (1, 0), \boldsymbol{e}_2 = -\boldsymbol{e}_4 = (0, 1)$, and $g_i^{(eq)}$ is given by

$$g_i^{(eq)}(\boldsymbol{x}, t) = \omega_i C(1 + \boldsymbol{c}_i \cdot \frac{\boldsymbol{u}}{c_s^2}), \tag{2.4}$$

where the weight coefficients are $\omega_0 = 1/3$, $\omega_{1,2,3,4} = 1/6$, $\boldsymbol{c}_i = c\boldsymbol{e}_i$ with $c := \delta_x/\delta_t$, $c_s := c/\sqrt{3}$, and the macroscopic quantity $C$ is defined by $g_i$ as

$$C = \sum_i g_i. \tag{2.5}$$

Under the diffusive scaling $\delta_x = h, \quad \delta_t = ah^2$ ($a$ is an adjustable parameter), one can recover the CDE (2.1) with $D = c_s^2(\tau - 0.5)\delta_t$. Moreover, the gradient of $C$ can be approximated with second-order accuracy by (see *e.g.* [12, 16])

$$\nabla C \approx -\frac{1}{c_s^2\tau\delta t}\left(\sum_i \boldsymbol{c}_i g_i - \boldsymbol{u}C\right). \tag{2.6}$$

## 3. Boundary scheme for Robin BCs

In this section, we construct a boundary scheme for the Robin BC (2.2) on curved boundaries. As illustrated in Fig. 1, our aim is to obtain the distribution function $g_i(\boldsymbol{x}_f, t + \delta_t)$ by using the BC and the information at the interior points.

Suppose we are given the relation

$$\beta = -(\boldsymbol{e}_i \cdot \boldsymbol{u})C(\boldsymbol{x}_b, t) + D\frac{\partial C(\boldsymbol{x}_b, t)}{\partial \boldsymbol{e}_i} \tag{3.7}$$

at the boundary point $\boldsymbol{x}_b$ (see Fig. 1), where $\beta = \beta(\boldsymbol{x}_b, t)$ is a given function. Then according to [12, 17], the following bounce back scheme can be used to determine $g_i(\boldsymbol{x}_f, t + \delta_t)$:

$$g_i(\boldsymbol{x}_f, t + \delta_t) = g'_{\bar{i}}(\boldsymbol{x}_f, t) - \frac{\beta\delta_t}{h}. \tag{3.8}$$

Here $\boldsymbol{x}_f$ is the interior point next to the boundary (see Fig. 1), $\bar{i}$ is defined such that $\boldsymbol{e}_{\bar{i}} = -\boldsymbol{e}_i$, and $g'_{\bar{i}} := g'_{\bar{i}}(\boldsymbol{x}_f, t)$ is the post-collision distribution function

$$g'_{\bar{i}}(\boldsymbol{x}_f, t) = g_{\bar{i}}(\boldsymbol{x}_f, t) - \frac{1}{\tau}(g_{\bar{i}}(\boldsymbol{x}_f, t) - g_{\bar{i}}^{(eq)}(\boldsymbol{x}_f, t)) + \delta_t\omega_{\bar{i}}F. \tag{3.9}$$

The scheme (3.8) has second-order accuracy if $\boldsymbol{x}_b$ is a middle point, namely, $\boldsymbol{x}_b = \boldsymbol{x}_f - \frac{1}{2}\delta_x\boldsymbol{e}_i$, and otherwise it is first-order accurate [12].

Next we turn to compute $\beta$ defined in (3.7). Once $\beta$ is obtained, (3.8) can be used for the treatment of BC (2.2). To do this, we approximate $C(\boldsymbol{x}_b, t)$ as

$$C(\boldsymbol{x}_b, t) \approx C(\boldsymbol{x}_f, t). \tag{3.10}$$

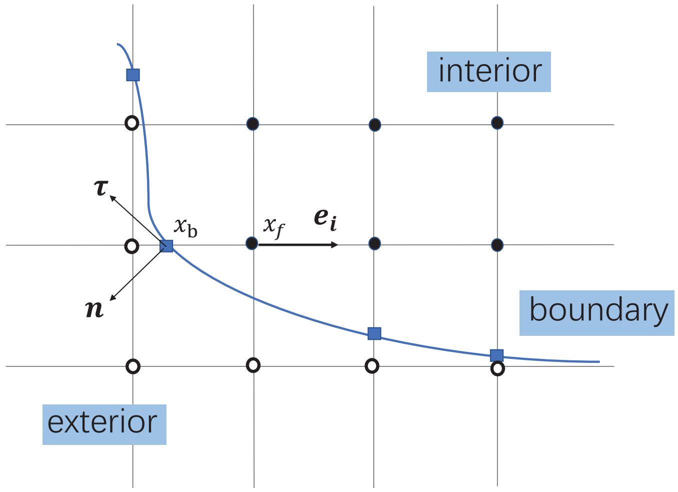


Figure 1: Schematic depiction of the lattice and a curved boundary. Black circles: interior points; White circles: exterior points; Blue squares: boundary points.

To approximate $\frac{\partial C(\boldsymbol{x}_b,t)}{\partial \boldsymbol{e}_i}$, we employee the decomposition

$$\frac{\partial C(\boldsymbol{x}_b,t)}{\partial \boldsymbol{e}_i} = \boldsymbol{e}_i \cdot \nabla C(\boldsymbol{x}_b,t) = (\boldsymbol{e}_i \cdot \boldsymbol{n})(\boldsymbol{n} \cdot \nabla) C(\boldsymbol{x}_b,t) + (\boldsymbol{e}_i \cdot \boldsymbol{\tau})(\boldsymbol{\tau} \cdot \nabla) C(\boldsymbol{x}_b,t), \tag{3.11}$$

where $\boldsymbol{\tau}$ is the unit tangential vector to the boundary $\partial\Omega$. Then we need to compute the two terms on the right side of the above equation. For the first term, it follows from the BC (2.2) and (3.10) that

$$(\boldsymbol{e}_i \cdot \boldsymbol{n})(\boldsymbol{n} \cdot \nabla) C(\boldsymbol{x}_b,t) \approx (\boldsymbol{e}_i \cdot \boldsymbol{n}) \frac{\alpha_3 - \alpha_1 C(\boldsymbol{x}_f,t)}{\alpha_2}. \tag{3.12}$$

For the second term, we approximate it as

$$(\boldsymbol{e}_i \cdot \boldsymbol{\tau})(\boldsymbol{\tau} \cdot \nabla) C(\boldsymbol{x}_b,t) \approx (\boldsymbol{e}_i \cdot \boldsymbol{\tau}) \boldsymbol{\tau} \cdot \nabla C(\boldsymbol{x}_f,t), \tag{3.13}$$

where $\nabla C(\boldsymbol{x}_f,t)$ is computed by (2.6). Combing (3.10) and (3.11)–(3.13) gives

$$\beta = -(\boldsymbol{u} \cdot \boldsymbol{e}_i) C(\boldsymbol{x}_f,t) + D \left[ (\boldsymbol{e}_i \cdot \boldsymbol{n}) \frac{\alpha_3 - \alpha_1 C(\boldsymbol{x}_f,t)}{\alpha_2} + (\boldsymbol{e}_i \cdot \boldsymbol{\tau}) \boldsymbol{\tau} \cdot \nabla C(\boldsymbol{x}_f,t) \right]. \tag{3.14}$$

With this $\beta$, (3.8) becomes a scheme for (2.2). This is our scheme for curved boundaries.

**Remark 3.1.** *Our scheme is simple in form so that it can be implemented easily. Since $\alpha_2 \neq 0$ in Robin BCs, our scheme avoids zero denominator thoroughly. Additionally, the scheme is single-node, i.e., it only involves the information at the present point $\boldsymbol{x}_f$, and thus it is very suitable for complex boundaries. Furthermore, we would like to point out that our scheme can also be used for the Neumann BCs with $\alpha_1 = 0$ and $\alpha_2 = 1$.*

**Remark 3.2.** *Since the approximation* (3.10) *is first-order accurate and the boundary point $\boldsymbol{x}_b$ is not necessary the middle point $\boldsymbol{x}_f - \frac{1}{2}\delta_x \boldsymbol{e}_i$, our scheme only has first-order accuracy. It may be improved to be second-order accurate by replacing* (3.10) *with a two-point extrapolation (see e.g. [23]) and extrapolating $\beta$ at the middle point. We have implemented this idea and find that it is successful for straight boundaries but will cause instability for curved ones.*

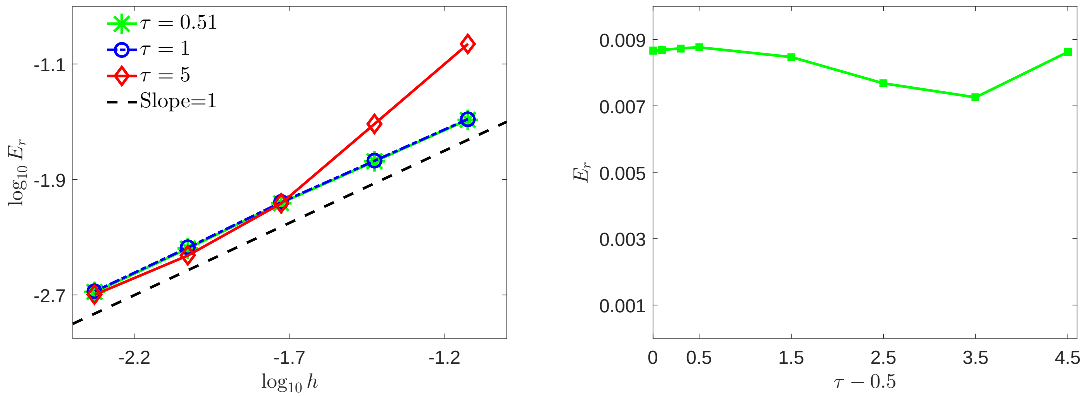


Figure 2: Example 4.1. Left:$L^2$-error versus the lattice size $h$; Right:$L^2$-error versus the relaxation time $\tau$ with fixed $h = 3/160$.

## 4. Numerical validations

In this section, we validate our boundary scheme via several numerical examples. In each example, we specify the diffusion coefficient $D$, the relaxation time $\tau$ and the mesh size $h$. Then all the other parameters can be determined: $\delta_t = ah^2$, $c = 1/ah$ and $a = (\tau-0.5)/3D$. To evaluate the accuracy, we define the $L^2$-error as

$$E_r = \frac{\sqrt{\sum_{\boldsymbol{x}}(C(\boldsymbol{x},T)-C^*(\boldsymbol{x},T))^2}}{\sqrt{\sum_{\boldsymbol{x}} C(\boldsymbol{x},T)^2}}, \tag{4.15}$$

where $T$ is the terminal time, which is set to be 0.5 in all the examples, $C(\boldsymbol{x},T)$ denotes the LBM solution, $C^*(\boldsymbol{x},T)$ is the analytical solution, and the summation is taken over all the points in computational domain.

*4.1. Example 1*

We first take $D = 1, \boldsymbol{u} = (0,1)^T$ and set the analytical solution as $C(\boldsymbol{x},t) = sin(txy)$. The corresponding source term is $F = cos(txy)(xy+tx)+Dsin(txy)(x^2+y^2)t^2$. We consider a circular domain $\Omega := \{(x,y)|(x-0.5)^2+(y-0.5)^2 \le r^2, r = 1.35\}$ with the Robin BC

$$C + \frac{\partial C}{\partial \boldsymbol{n}} = \alpha_3, \quad (x,y)\in\partial\Omega, \quad t>0, \tag{4.16}$$

where $\alpha_3 = sin(txy) + (n_x y + n_y x)tcos(txy)$ with $n_x, n_y$ being the $x$- and $y$-component of the unit normal vector $\boldsymbol{n}$, respectively.

Fig. 2 (left) plots the errors of our scheme for $h = 3/40, 3/80, 3/160, 3/320, 3/640$. It can be seen that standard first-order convergence is achieved for $\tau = 0.51, 1, 5$ as $h$ decreases.

Furthermore, we test the stability of our scheme in terms of the relaxation time $\tau$. We fix $h = 3/160$ and search for an interval of $\tau$ in which the LBM solutions are convergent. Here by convergence we mean that the $L^2$-error defined in (4.15) is less than $10^{-2}$. To avoid too much computation time (for small $\tau$) or too large $\delta_t$ (for large $\tau$), we only test $\tau$ in the interval [0.5005,5]. With a number of numerical experiments, we find that our scheme is stable for all $\tau$ in [0.5005,5]. Additionally, as shown in Fig. 2 (right), the error of our scheme is not sensitive to $\tau$. These results indicate the excellent stability of our scheme.

*4.2. Example 2*

Next we test our scheme with an example from [17], which contains a quite irregular domain $\Omega = \{(x,y)|P(x,y) \le 0\}$ with $P(x,y) = x^4 - 5x^2 - 3x + 2y^4 - 6y^3 - y - 1$ (see Fig. 3 (left)) [1]. As in

[1]For a general curved boundary $f(x,y) = 0$, the unit normal and tangential vectors can be computed as $(f_x/(\sqrt{f_x^2+f_y^2}), f_y/(\sqrt{f_x^2+f_y^2}))$ and $(-f_y/(\sqrt{f_x^2+f_y^2}), f_x/(\sqrt{f_x^2+f_y^2}))$, respectively.

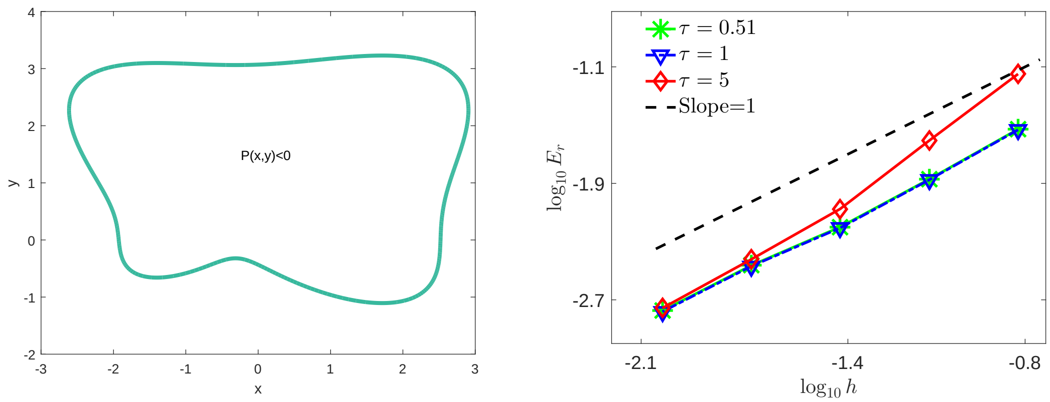


Figure 3: Example 4.2. Left: Schematic depiction for the irregular boundary; Right: $L^2$-error versus the lattice size $h$.

[17], we take $D = 1, \boldsymbol{u} = (1,0)^T$ and $C(x,y,t) = (x^3 + y^2)sin(t)$. The BC is given as (4.16) with $\alpha_3 = (x^3 + y^2 + 3n_x x^2 + 2n_y y)sin(t)$. With a set of lattice sizes $h = 6/40, 6/80, 6/160, 6/320, 6/640$, the convergence behavior is shown in Fig. 3 (right). It is clear that designed first-order accuracy is obtained again for such a complex boundary.

## 5. Conclusions and remarks

In this paper, we propose a curved boundary scheme of the LBM for Robin BCs of CDEs. The scheme is constructed by approximating the gradient along the outgoing discrete velocity at the boundary with the given Robin boundary condition and the gradient at the interior point next to the boundary. With this approximated gradient at the boundary, the classical bounce back scheme for Neumann-type boundary conditions is employed to obtain the unknown distribution function at the interior point. The scheme obtained has the first-order accuracy for curved boundaries and its advantages are: (1) the scheme is simple in form so that it can be easily implemented; (2) it avoids the denominator in the scheme to be zero, and (3) the scheme is single-node, *i.e.*, it only involves the information at the present point. Several numerical experiments are conducted to test the accuracy and stability of our scheme. The numerical results not only verify the designed accuracy of our scheme but also demonstrate its good stability. We would like to point out that our scheme can also be used for the Neumann BCs. Additionally, it can be used for the D2Q9 model as well and its extension to the D3Q7 model is straightforward.

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