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# Linear and non-linear Robin boundary conditions for thermal lattice Boltzmann method: cases of convective and radiative heat transfer at interfaces

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ABSTRACT

Despite the wide applications of the linear and non-linear Robin boundary constraints in thermal simulations, not much works are reported on their implementation in lattice Boltzmann framework. In present work, counter-slip energy approach is employed to derive kinetic level equations, representing two particular cases of Robin boundary conditions; convection and combined convection and surface radiation. Loss of generality is avoided in the study and the terms accounting for boundary movement or viscous dissipation effects are incorporated, too. Utilizing a D2Q9 lattice structure, the derived equations are validated with 1D and 2D analytical solutions for conduction heat transfer problems in a square slab. Results of analysis show a first order rate of convergence for the convective boundary condition, while second order rate is found for combined convection and surface radiation constraint.



## 1. Introduction

Due to the convincing success of the lattice kinetic theory and most remarkably the lattice Boltzmann method (LBM) [1–5], much efforts has been made on its extension to more complex circumstances including those with more intricate geometries, turbulence conditions, non-isothermality and multiphase flows with interfacial dynamics. In the recent 20 years, a number of proposals have been made to answer the problem of non-isothermality (see for example [6–8]). In general the recommended schemes are classified into three categories; Multi-Speed (MS) approaches [9–11], double distribution function (DDF) models [12–15] and hybrid methods [16–18]. The previously proposed MS approaches mainly rely on the computation of the second velocity moments of particle distribution functions to extract thermal flux information. However, due to some unphysical mode-couplings [19], they suffer seriously from numerical instabilities. Prandtl (*Pr*) number limitations and narrow temperature range of applicability are other drawbacks of the method. Additionally, while the more recent hybrid methods may present better performance in low speed, velocity-energy decoupled flows, they still lack elegance, considering the non-kinetic foundations. In an attempt to redress the deficiencies of the aforementioned methods, DDF approaches are introduced based on the idea of doubling the degrees of freedom and employing two different distribution functions for energy and particle number density. The improvements are very interesting; higher numerical stability, adjustable fluid *Pr* number, capability to include viscous dissipation and compression work effects and fully kinetic foundation. The price to pay is the doubled computational costs.

The choice of accurate boundary condition is the other hot topic in today's thermal LBM research. Due to the essential similarities between the two evolution equations in DDF approach, extension of the advancements in hydrodynamic boundary treatment to thermal models has been regarded in a number of surveys. As a pioneering try, He et al. [14], modified the well-known rule of bounce back of non-equilibrium parts [20] to be employed with their thermal model. Although they simulated constant temperature (Dirichlet condition) case in their paper, but Tang et al. [21] showed that the method could be easily utilized for adiabatic conditions through a finite difference scheme. In another work by Tang et al. [22], and being highly inspired by the more general form of the rule introduced in [23,15], they employed a first order extrapolation scheme to approximate non-equilibrium distribution functions from the neighboring interior nodes. The authors reported that the approach successfully simulates Dirichlet and Neumann constraints; this occurred by means of a Dirichlet strategy. A few years later, Hiorth et al. [24] adopted the original bounce back of non-equilibrium parts rule but with an opposite sign for the

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adverse direction (the reader interested in reasoning behind the choice of *opposite sign* is referred to [25]) and by using Chapman–Enskog analysis derived expressions for linear Robin boundary condition in diffusion equation of NMR relaxation. They claimed that the method may be generalized to convective–diffusive problems if the velocity of the fluid could be ignored at the boundary. In another try, Liu et al. [26] extended the hydrodynamic boundary condition suggested in [27] and introduced Dirichlet and Neumann thermal boundary conditions by assuming unknown distributions being functions of local known energy distributions and an additional parameter called corrector. The results of their numerical simulations demonstrated the second order convergence accuracy of the scheme. The bounce back boundary condition [28] or its derivatives have also been widely extended to thermal LBM, despite the reports [29] claiming its erroneous nature in some thermal applications [30]. Chaabane et al. [31] tested several types of boundary conditions including Neumann, Dirichlet and convective heat transfer (linear Robin condition) constraints for a conduction problem in a square slab. Despite claiming the employment of bounce back concept in boundary treatments, neither detailed methodology nor any resulted equation is presented in their work. In an extensive work by Huang et al. [30], five different schemes including an extension of the regularized boundary method [32], simple extrapolation method, non-equilibrium extrapolation method, simple bounce-back method and an Equilibrium method were proposed. They concluded that the regularized boundary condition shows the best performance (second-order) in terms of spatial accuracy for first type or second type boundary constraints. Li et al. [33,34] has also used the bounce back concept but in combination with an interpolation scheme to impose Dirichlet, Neumann or linear Robin conditions on straight or curved boundaries. Considering an older research by Yoshida and Nagaoka [35], reveals that they [33,34] are highly inspired by the bounce back approach employed there. Note that both works claim that the idea leads to methods with a nearly second order convergence. In a more recent work, Zhang et al. [36] extended Ladd's [37] halfway bounce back scheme and the macroscopic gradient boundary conditions in [38] to find expressions for a convection–diffusion equation with arbitrary linear mixed-type constraints. Although they claim that their method can handle moving boundaries, but since they assume that non-equilibrium portions of distribution functions take opposite signs for adverse directions, Chen et al. [39] argued the applicability to non-static boundaries. Following the introduced method in [36], Chen et al. [40] improved the spatial resolution of the scheme by the employment of the midpoint bounce back technique [41] and an accurate form of finite difference method [42]. Their key idea is to make the calculations based upon the midpoint value of a boundary lattice link by an interpolation or extrapolation method. The reported results from simulation analysis reveal a geometry-depended order of accuracy, varying between unity and 2. As a more general framework on theoretical study of boundary conditions, Ginzburg [43] addressed a multi-reflection approach to model Dirichlet or Neumann time dependent constraints for advection and anisotropic dispersion equations for any arbitrary shaped surface. The presented idea is to tune the symmetric part of equilibrium functions to reach a second- or third-order of accuracy for Dirichlet boundary conditions, while employing the anti-symmetric part for normal flux specification.

The studies on boundary treatment for a convection diffusion equation have not been restricted to those of thermal models. A quick survey in the literature shows that various models have also been proposed for solute transport and concentration dynamics at interfaces (see for example [25,36,40,44–47]). However it should be noticed that although the convection diffusion equation is very similar for both solute and energy transport cases, but since additional terms representing viscous dissipation and compressional work are also present in many energy models, their application (without further modification) to solute transport cases may result in mass conservation problems.

In addition to the aforementioned models, where generally are constructed based on common ideas like bounce back concept, non-equilibrium extrapolation, simple interpolation or extrapolation, or in a more generic framework the multi-reflection method, D'Orazio et al. [48–50] followed Inamuro et al. [51] counter-slip approach to formulate the first type and second type boundary constraints and they simulated for the first time a non-zero heat flux boundary condition in LBM. Note that since this approach guarantees the exact satisfaction of the specified temperature or heat flux at the boundary, it may be regarded as the most accurate one in terms of boundary node analysis [22]. On the other hand, compared to the previous methods, counter-temperature does not rely on any extrapolation, interpolation or differential method for flux and concentration derivation which may be important in some cases like modeling of nonlinear conditions. Based upon the foresaid facts and also considering the approach's capability to handle moving boundaries [52] and still it's clarity in accounting for viscous dissipation and compressional work sources, the authors are motivated to perfectly devote the current research to applications of this method in modeling of linear and nonlinear mixed type boundary constraints for flat surfaces. It should be stressed here that despite the recent proposals on linear Robin constraints for convection diffusion equation, the non-linear case which is very essential to problems like those of surface radiation or combined external convection and radiation (see [53]) still lacks enough research and to the best knowledge of the authors has been widely neglected so far from an LBM point of view. Accordingly the remainder of the article is organized as follows. In Section 2, the DDF model that the current work is constructed on, is explained and the basic equations are presented. In Sections 3.1 and 3.2 the convective boundary condition (linear Robin constraint) and combined surface radiation and convection boundary condition (non-linear Robin constraint) are discussed mathematically and a set of equations are derived for their representation in LBM scheme. Finally in Section 4, the proposed equations are validated with 2D and 1D analytical solutions.

## 2. Thermal model

Among the numerous DDF models, the widely accepted method proposed by He et al. [14] is regarded here. Note that although, a number of simplified versions [14,54,55] of the original approach are also available, but since they mainly neglect viscous dissipation or compressional work effects, the original scheme is adopted to avoid loss of generality. It is worth noting that a discussion on implementation of the model with Dirichlet or Neumann constraints is presented in previous papers [50,56] and the interested reader could refer to if necessary.

Letting $f$ being the particle number density distribution function, standard kinetic moment gives:

$$\rho(\vec{x},t) = \int f(\vec{x},\vec{\xi},t)d\vec{\xi} \tag{1}$$

$$\rho(\vec{x},t)\vec{U}(\vec{x},t) = \int \vec{\xi} f(\vec{x},\vec{\xi},t)d\vec{\xi} \tag{2}$$

And the continuous evolution equation for $f$ is defined by Boltzmann equation:

$$\partial_t f + (\vec{\xi}\cdot\nabla)f = \Omega(f) \tag{3}$$