

Bergische Universität Wuppertal

Fakultät für Mathematik und Naturwissenschaften

Institute of Mathematical Modelling, Analysis and Computational Mathematics (IMACM)

Preprint BUW-IMACM 20/60

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December 20, 2020

http://www.imacm.uni-wuppertal.de

A Non-Equilibrium Bounce-Back Boundary Condition for thermal multispeed LBM

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Abstract

High-order lattice Boltzmann methods provide an elegant and systematic way to incorporate thermal and compressible effects and represent a promising approach for the study of beyond-hydrodynamics regimes characterized by finite Knudsen numbers. However, the presence of multiple layers makes the definition of boundary conditions non-trivial, since one needs to define the missing information for particle distributions across several boundary layers. In this work we present a thermal extension of a recently proposed non-equilibrium bounce-back boundary condition and compare it against established algorithms by simulating standard benchmarks with wall-bounded flows.

Keywords: Lattice Boltzmann Method, Thermal Boundary Conditions, High Order Multispeed Models, Non Equilibrium Bounce Back Boundary Conditions, D2Q17, D2Q37

1. Introduction

Over the last few decades, the Lattice Boltzmann Method (LBM) has emerged as a computationally efficient tool for solving the Navier Stokes equations [1, 2]. Continuous efforts are being made to broaden the range of applicability of the LBM and tackle problems such as thermal compressible flows, for which a macroscopic description is provided by the laws of Navier-Stokes-Fourier. There are currently two main approaches to thermal LBM present

Preprint submitted to Journal of Computational Science

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in the literature: i) the double distribution approach, where a second set of populations is used to evolve the temperature field and ii) the multispeed approach, where the velocity space is discretized using high order quadrature rules, which imply the adoption of larger velocity sets defined over several layers.

The former approach tends to be more popular, since it supports a variable Prandtl number and allows using standard lattices. On the other hand, multispeed models offer a natural coupling between the evolution of velocity and temperature, with viscous dissipation and compression work naturally emerging from kinetic theory. There are also indications that higher order models based on multispeed stencils contribute to enhanced numerical stability [3]. Finally, in a more general perspective, it is certainly valuable to have alternative approaches available.

The presence of multiple boundary layers clearly makes the formulation of Boundary Conditions (BC) for multispeed stencils more complex. Proper BCs are thus even more important in this setting, since naive formulations may cancel the gains in terms of stability obtained when employing higher order models.

In spite of this, not much work has been devoted to the development of boundary conditions for thermal multispeed LBM. In this article, we introduce an extension to thermal models for a recently proposed Non-Equilibrium Bounce-Back (NEBB) BC [4], originally developed for isothermal multispeed LBM. We evaluate and benchmark several different implementations of the NEBB BC, comparing its performance against the established diffusive BC [5, 6] for a few selected standard benchmarks of wall-bounded thermal flows. This article is organized as follows: in section 2 we provide a brief description of the thermal LBM used in this work. In section 3 we provide the mathematical formulation of the thermal NEBB BC, which are then numerically evaluated in section 4. Concluding remarks and future directions are then given in section 5.

2. Thermal Lattice Boltzmann Model

In this section, we provide a brief introduction of the thermal LBM adopted in this work, which correctly reproduces the equation of state of a perfect gas $(p = \rho T)$. The model takes root from a minimal version of the Boltzmann equation, in which the momentum space is discretized on a regular lattice. The lattice description is based on a set of discrete probability distribution functions $f_i(\mathbf{x}, t)$, to which we will refer to as lattice populations. Each population is associated with a given lattice velocity c_i , $i = 1, \ldots, q$. It is customary to distinguish between LBM models following the DdQq nomenclature, in which d indicates the number of spatial dimensions, and q the number of discrete velocities forming the stencil. The discrete velocities c_i can be defined as the abscissa of a Gauss-Hermite quadrature rule $\{(\omega_i, c_i) : i = 1, \ldots, q\}$, which allows for the exact calculation of the first N moments of the particle distribution function. It has been shown that



Figure 1: Two-dimensional high-order velocity sets: (left) D2Q17, third order, and (right) D2Q37, fourth order

quadratures with an degree of precision of a least nine are the minimum requirement to recover the Navier-Stokes-Fourier equations, since they allow correct capturing of momentum, temperature and their fluxes [7]. Minimal on-lattice quadrature rules satisfying this requirement that make only use of integer valued velocity components with absolute value less or equal to three consist of q = 37 velocities in two spatial dimensions and q = 103 velocities in three spatial dimensions [8, 9]. These stencils are referred to as D2Q37 and D3Q103 respectively. When dealing with mildly compressible flows, or in cases where the contribute of the heat flux is known to be negligible, it could be sufficient to employ models based on a seventh order quadrature. Minimum velocity sets in this case are given by the D2Q17 and D3Q39 models, which offer a trade-off between computational cost and numerical accuracy. In what follows, we will focus our analysis to the 2-dimensional case, thus adopting the 17 and 37 velocities configurations depicted in Fig. 1. We adopt the single relaxation time collisional operator provided by the Bhatnagar-Gross-Krook (BGK) model. The discrete lattice Boltzmann equa-

tion, describing the time evolution of each population f_i is given by

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{\Delta t}{\tau} \big(f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t) \big), \qquad (1)$$

where τ is the relaxation time and f_i^{eq} is the (discrete) equilibrium distribution function for which we make use of a fourth order Hermite-expansion of the Maxwell-Boltzmann distribution:

$$\begin{split} f_i^{\rm eq}(\rho,\mathbf{u},T) &= \omega_i \rho \bigg(1 + \mathbf{u} \cdot \mathbf{c} + \frac{1}{2c_s^2} \big[(\mathbf{u} \cdot \mathbf{c})^2 - u^2 + (T-1)(c^2 - d) \big] \\ &+ \frac{\mathbf{u} \cdot \mathbf{c}}{6c_s^4} \big[(\mathbf{u} \cdot \mathbf{c})^2 - 3u^2 + 3(T-1)(c^2 - d - 2) \big] \\ &+ \frac{1}{24c_s^6} \bigg[(\mathbf{u} \cdot \mathbf{c})^4 - 6(\mathbf{u} \cdot \mathbf{c})^2 u^2 + 3u^4 \\ &+ 6(T-1)\big((\mathbf{u} \cdot \mathbf{c})^2 (c^2 - d - 2) + |\mathbf{u}|^2 (2 + d - c^2) \big) \\ &+ 3(T-1)^2 (c^4 - 2(d+2)c^2 + d(d+2)) \bigg] \bigg), \end{split}$$

where c_s denotes the lattice speed of sound.

The time evolution of Eq. 1 follows a stream and collide paradigm, in which the streaming step moves the populations to neighboring nodes along the directions defined by the stencil, while the collision step performs all the mathematical operations needed to update the distributions and the macroscopic quantities at each grid point.

The macroscopic quantities of interest, such as density ρ , velocity \boldsymbol{u} and temperature T are given by the moments of the particle distribution function, which—thanks to the quadrature rule—can be expressed in terms of discrete

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summations over the lattice populations:

$$\rho = \sum_{i=1}^{q} f_i,\tag{2}$$

$$\rho \mathbf{u} = \sum_{i=1}^{q} f_i \mathbf{c}_i,\tag{3}$$

$$d\rho T = \sum_{i=1}^{q} f_i |\mathbf{c}_i - \mathbf{u}|^2.$$
(4)

In order to incorporate external forces into the algorithm, we follow the approach given in [10], where the equilibrium f^{eq} is calculated with respect to a shift in the velocity and temperature fields:

$$\bar{\mathbf{u}} = \mathbf{u} + \tau \mathbf{g}, \quad \bar{T} = T + \frac{\tau(\Delta t - \tau)|\mathbf{g}|^2}{d}.$$

It can be then shown via a Chapman-Enskog expansion that the hydrodynamic quantities governed by Navier-Stokes-Fourier equation can be obtained from the lattice formulation as follows:

$$\rho^{(H)} := \rho, \quad \mathbf{u}^{(H)} := \mathbf{u} + \frac{\Delta t}{2} \mathbf{g}, \quad T^{(H)} := T + \frac{(\Delta t)^2 |\mathbf{g}|^2}{4d}$$

Notice, we use the superscript (H) to indicate these hydrodynamic quantities.

3. Non-Equilibrium Bounce-Back Boundary Condition

Unless working in fully periodic domains, the streaming step generally leaves several populations undefined, since boundary nodes do not have fluid neighbors to draw the corresponding populating from. The task of any boundary condition is to specify these unknown populations. Let us label the different boundary layers with the index l, where l = 1 denotes the outermost boundary layer. Furthermore, let $U^{(l)}$ denote the set of indices of unknown post-streaming populations in the boundary layer l.

In a hydrodynamic description, one typically wants to define BC in terms of macroscopic fields rather than particle distributions. Since there are in general more unknown populations than macroscopic quantities, one needs to define a suitable ansatz to define a closed system of equations to work out the expressions for the unknown populations. One possible choice is to follow the Zou-He BC [11], in which a bounce-back condition is assumed to be valid on the non-equilibrium part of the boundary nodes:

$$f_i - f_i^{\text{eq}} = f_{\overline{i}} - f_{\overline{i}}^{\text{eq}}, \quad i \in U^{(l)},$$
(5)

where \bar{i} represent the opposite direction with respect to the one present in the $U^{(l)}$ ensemble (i.e., $c_{\bar{i}} = -c_i$). The ansatz in Eq. 5 is commonly employed to define BCs for standard single-speed LBM models. Its generalization to multi-speed models have been recently introduced by Lee et al. [4]. The general idea is to define a closed system of equations by introducing further momentum-correction terms in Eq. 5.

By following the same approach, we propose the following ansatz for unknown populations in the boundary layer l:

$$f_{i} = f_{i}^{\text{eq}} + f_{\bar{i}} - f_{\bar{i}}^{\text{eq}} + M_{i} \left(\sum_{k=1}^{d} c_{i}^{k} Q_{k} + c_{i}^{2} Q_{t} \right), \quad i \in U^{(l)}, \tag{6}$$

where Q_k denotes the momentum correction for the k-th vector component, and Q_t denotes a scalar temperature correction. The expression M_i can be chosen to be either one or ω_i , i.e., the lattice weight corresponding to the unknown population. While the former (unscaled model) might seem to be the more natural choice, the latter (scaled model) has been reported to allow for a lower attainable viscosity [4], potentially a very welcome feature given the fact that the stability range for NEBB based BC is in general more narrow when compared to other BC schemes [12].

Regardless of the chosen velocity stencil, the d+1 equations Eq. 3 and Eq. 4, combined with the ansatz in Eq. 6, deliver a closed system which can be solved for the d+1 correction terms, yielding a Dirichlet BC. The authors



Figure 2: Internal and external population replacement strategy for a bottom boundary and the D2Q37 velocity stencil. In the internal treatment (left panel), only the unknown post-streaming populations are set. In the external treatment (right panel), all boundary layers share the same set of unknown populations.

in [4] distinguish between the internal and external boundary treatment. In the internal treatment, only the missing populations are assigned in each boundary layer (Fig. 2, left), which results in a different system of equations per boundary layer. Here, the macroscopic quantities to be imposed at inner boundary layers can simply be the same as at the outermost layer. Alternatively, said values may be obtained by interpolation between the outermost boundary layer – where certain macroscopic values are explicitly imposed – and the first full fluid layer.

Conversely, in the external treatment all boundary nodes are subjected to identical macroscopic values, and missing populations are all handled alike, meaning that the missing populations from the outermost layer are to be replaced in all remaining layers, regardless how they interact with the inner nodes (Fig. 2 right).

Now, it is possible to combine and implement four different NEBB BC schemes: i) unscaled-internal (UI) ii) scaled-internal (SI), iii) unscaled-external (UE), iv) scaled-external (SE). In Appendix A, we provide an example with the analytic expressions for the UE case applied to the D2Q17 model.

We need to remark that the BC as originally formulated by Lee et al. [4] do not ensure mass conservation. Since this is generally a desirable feature of LBM, we here introduce a procedure to reinforce mass conservation by keeping track of the outflowing mass entering the calculation of ρ . We start by defining at each boundary node the quantity

$$\Delta m = \sum_{i \in U^{(l)}} f_i - \sum_{i \in O^{(l)}} f_i^\star.$$

In the above, $O^{(l)}$ denotes the set of populations pointing out of the computational domain in boundary layer l and f_i^* are pre-streaming populations. Then, Δm is added to the rest population, i.e., $f_0 = f_0 + \Delta m$.

4. Numerical Results

In this section, we analyze the accuracy of the BC schemes introduced in the previous section, testing them with standard numerical benchmarks. We consider three well-known wall-bounded flows in d = 2 spatial dimensions within a rectangular computational domain: Poiseuille flow, Couette flow, and Rayleigh-Bénard convection. For all benchmark cases, we have implemented the different NEBB-BC schemes to impose the desired macroscopic values at the upper and lower plates, while periodic boundary conditions are used for the lateral boundaries. For simplicity, we impose the same macroscopic values at all boundary layers in the internal treatment of the NEBB-BC. We also compare the numerical accuracy of the NEBB-BC against that provided by an implementation of diffusive boundary conditions for multispeed models [6].

Important control parameters for the simulations behavior are the Reynolds, Mach and Knudsen numbers:

$$\operatorname{Re} = \frac{\operatorname{U}_0 \cdot \operatorname{L}}{\nu}, \quad \operatorname{Ma} = \frac{\operatorname{U}_0}{\operatorname{c}_s}, \quad \operatorname{Kn} \sim \frac{\operatorname{Ma}}{\operatorname{Re}},$$

where, in lattice units, L is the grid resolution, U_0 the characteristic flow velocity, and ν the kinematic velocity

$$\nu = \rho_0 T_0 (\tau - \frac{1}{2}) c_s^2, \tag{7}$$

with ρ_0 and T_0 respectively a reference density and reference temperature values.

In order to compare the BCs, we keep the Reynolds number fixed when varying grid resolutions. This can be realized by modifying either the value of U_0 or of ν , as long as the assigned parameter values are within the range of applicability of the LBM. More precisely, the velocity must remain in the low Mach number regime and the viscosity cannot be chosen arbitrarily close to zero. Moreover, the Knudsen number has to be sufficiently small to justify a hydrodynamic approach.

Further relevant parameters used in simulations are the Prandtl and Eckert numbers

$$\Pr = \frac{\nu}{\alpha}, \quad \operatorname{Ec} = \frac{U_0^2}{c_p \,\Delta T}$$

with thermal diffusivity α , specific heat at constant pressure $c_p = \frac{d}{2} + 1$ and temperature difference between top and bottom plate ΔT . In this work we will restrict ourself to flows at $\Pr = 1$.

In order to quantify the accuracy of the different BC schemes, we introduce the relative L2-error for a generic macroscopic quantity A, calculated with respect to the the exact solution A^{ex} along a vertical slice through the center of the computational domain:

$$e_{A} = \sqrt{\frac{\sum_{j=1}^{L} \left(A^{sim}(x_{i}, y_{j}) - A^{ex}(y_{j})\right)^{2}}{\sum_{j=1}^{L} \left(A^{ex}(y_{j})\right)^{2}}}$$

4.1. Thermal Poiseuille flow

We consider a fluid between two stationary horizontal plates placed at a distance H. The top plate is heated, i.e., $T_{\text{top}} > T_{\text{bot}}$, and a constant acceleration acts along the *x*-axis. The analytic steady state solutions [13] for velocity and reduced temperature $\hat{T} = \left(\frac{T-T_{\text{bot}}}{\Delta T}\right)$ read as

$$u_x^{\text{ex}}(y) = \frac{g \cdot y}{2\bar{\nu}}(H - y) \qquad u_y^{\text{ex}} \equiv 0,$$
$$\hat{T}^{\text{ex}}(y) = \frac{y}{H} + \frac{\Pr \cdot \text{Ec}}{3} \left(1 - \left(1 - \frac{2y}{H}\right)^4\right).$$

In the above, $\bar{\nu} = \rho_0 T_0 \nu$, where ρ_0 and T_0 denote the system averaged density and temperature respectively; g denotes a constant external acceleration acting along the x-axis. Unless stated otherwise, the simulations were conducted using Re = 100, Ec = 1, Ma = 0.05 and $T_{\text{bot}} = 1$; this directly determines the values for g, ν and T_{top} .

In Fig. 3, we show a few examples for the steady state profiles of velocity and temperature.

A grid-convergence study is presented in Fig. 4, where we compare the different implementation of the NEBB BC using both the D2Q17 and the D2Q37 models. Looking at the overall picture, we observe that the convergence speed and accuracy of NEBB is found to be very similar to that of diffusive BC for most of the settings taken into account.

While diffusive BC ensure stability for the D2Q17 even at the most coarse grid resolutions, the external NEBB suffer from instabilities due to low viscosity values. These instabilities are cured when using finer grids, or higher order models; indeed the D2Q37 proves stable over all the parametric range explored in the present analysis.

When results are not affected by stability issues, the convergence rate is approximately of the second order. An interesting exception is given by the



Figure 3: Steady state profiles for a thermal Poiseuille flow. Top: Velocity profiles obtained using the different BC with the D2Q37 stencil at Ec = 1. Inlet: Zoom in the proximity of the top plate. The internal NEBB BC cause a small overshoot. Scaled versions have been omitted since they perform very similar to their unscaled counterparts. Bottom: Temperature profiles at different Eckert numbers for both the D2Q17 and D2Q37 models, obtained with the NEBB-UE BC. All simulations have been performed on a L = 512 grid, with Re = 100, Ma = 0.05 and $T_{bot} = 1$.



Figure 4: Grid convergence test for the thermal Poiseuille flow, comparing different BC models. Top panels show the comparison with respect to the error in the velocity profiles, while at bottom panels the error is computed with respect to the temperature profile. On the left panels we report results for the D2Q17 model, while on the right we report results obtained using the D2Q37 model. All simulations have been performed with Re = 100, Ma = 0.05, Ec = 1 and $T_{bot} = 1$.

external NEBB, which on one hand presents a first order convergence speed for what concerns the error in the velocity profile, but—on the other hand offers significantly lower error levels than all the other BC over the grid sizes considered.

Finally, if we consider the errors in the velocity profiles we do not observe relevant differences comparing the accuracy of the scaled NEBB BC against that offered by their corresponding unscaled version, consistently with the findings in [4]; on the other hand, scaled NEBB seem to offer slightly more accurate results when inspecting the temperature profiles.

4.2. Thermal Couette flow

In this setup, we consider a fluid between two horizontal plates at a distance H. The heated top plate is moving horizontally with constant velocity U_0 and is kept at a fixed temperature T_{top} , whereas the bottom plate is kept at temperature $T_{\text{bot}} < T_{\text{top}}$ and remains stationary. The benchmark admits an



Figure 5: Steady state temperature profiles for a thermal Poiseuille flow, simulated using the D2Q37 model with the NEBB-UE BC, for a few selected Eckert numbers. All simulations have been performed with a spatial resolution of L = 512 points, Re = 100, Ma = 0.05 and $T_{\rm bot} = 1$.

analytic steady-state solution, here reported for the velocity, reduced tem-

perature and density [14]:

$$u_x^{\text{ex}}(y) = U\frac{y}{H}, \qquad u_y^{\text{ex}} \equiv 0,$$
$$\hat{T}^{\text{ex}}(y) = \frac{y}{H} + \frac{\Pr \cdot \text{Ec}}{2} \frac{y}{H} \left(1 - \frac{y}{H}\right),$$
$$\rho^{\text{ex}}(y) = \frac{\rho_0 T_0}{T^{\text{ex}}(y)} \left(1 + \frac{\Pr \text{Ma}_e^2}{3}\right),$$

where $Ma_e = \frac{U_0}{\sqrt{c_p T_0}}$ is a lattice-specific Mach number. In Fig. 5, we show a



Figure 6: Grid convergence test for the thermal Couette flow, comparing different BC models. Shown are L2-Errors with respect to the exact solutions for velocity (top-left), reduced temperature (top-right) and density (bottom). All simulations have been performed with Re = 100, Ma = 0.05, Ec = 1 and $T_{\rm bot} = 1$.

few examples of steady state temperature profiles at different Eckert numbers. Like in the previous section, we perform a grid-convergence study, for which we report results in Fig. 6. This time we have restricted the analysis to the D2Q37 model. We have considered simulations with $T_{\rm bot} = 1$ and $T_{\rm top}$ and ν tuned in order to keep fixed values Re = 100, Ec = 1, Ma = 0.05. The

results are consistent with the analysis reported for the thermal Poiseuille flow: again, we observe approximately second order convergence for the error in both velocity, temperature and density profiles. An exception is given by the external NEBB BC which exhibits significantly lower errors than the other BC over all grid sizes considered, at the price of a lower convergence speed.

Comparing the scaled and unscaled version of the different NEEB BC, we do not observe differences for the internal case, while looking at the external case the scaled version seems to offer a systematic advantage in terms of accuracy.

4.3. Rayleigh Bénard convection



Figure 7: Example for the temperature fields in the Rayleigh Bénard convection. Left: Stratified temperature field in the steady conductive state for low Ra. Right: Steady convective state near the critical Rayleigh number. White lines represent the velocity streamlines.

The third and last benchmark considered in this section is the Rayleigh Bénard convection, a classic example of natural convection occurring in a fluid subjected to the gravity force and heated from below.

The numerical setup consists of two horizontal walls placed at a distance H, kept at a fixed temperature, respectively T_{top} and T_{bot} , with $T_{\text{top}} < T_{\text{bot}}$. The gravity-like force acting along the y axis induces an acceleration $\boldsymbol{g} = (0, -g)^T$. The dynamic behavior of the system can be characterized by the Rayleigh number, defined as

$$Ra = \Pr \frac{\Delta T}{T_0} \frac{gH^3}{\nu_0^2},\tag{8}$$

where the kinematic viscosity ν_0 is evaluated at the reference temperature T_0 and reference density ρ_0 .

For flows at low Ra (Fig. 7-left), the system is stationary and exhibits a constant temperature gradient between the hot and the cold plates. When the Rayleigh number is increased above a critical value Ra_{crit} the system becomes unstable and convective rolls start to appear (Fig. 7-right).

By performing a linear stability analysis, it is possible to show that for a incompressible fluid $\operatorname{Ra}_{\operatorname{crit}} \approx 1707$. This case is arguably the most commonly studied convection configuration, and is often used to benchmark numerical methods withing the Boussinesq limit (see e.g. [15, 16, 17] for a few examples based on LBM solvers). In our case, we will instead work outside the Boussinesq regime, in order to test the accuracy of our BC scheme in the presence of seizable compressibility effects. Once again, it is possible to provide analytical estimates for the critical Rayleigh number, which for the compressible regime is found to be a function of two main parameters, respectively the non-dimensional temperature jump $\Delta T/T_0$ and the polytropic index $m = g \frac{H}{\Delta T}$ [18, 19].

We consider the same setup described in [20] and limit ourselves to the study of the specific case $\Delta T/T_0 = 0.6$, m = 0.98, for which the analytic prediction of the critical Rayleigh number is $\text{Ra}_{\text{crit}} \approx 1604$, and attempt to get a numerical estimate of Ra_{crit} from simulations testing the different implementation of the NEBB-BC described in the previous section.

Table 1: Numerical estimate of the critical Rayleigh number in a non-Boussinesq regime with $\Delta T/T_0 = 0.6$, m = 0.98. The analytic result from a linear stability analysis predicts $Ra_{crit} \approx 1604$.

Grid	Diffusive	NEBB-UE	NEBB-SE	NEBB-UI	NEBB-SI
101×50	1617	1591	1599	-	-
202×100	1610	1602	1602	1575	1586
404×200	1603	1608	1607	1568	1568

In order to obtain an estimate of $\operatorname{Ra}_{\operatorname{crit}}$, we perform simulations at various Rayleigh numbers by tuning g and ν and track the time evolution of the average kinetic energy $E_{\operatorname{kin}}^{\operatorname{avg}}$ along a central slice of the domain; this quantity grows in time for supercritical Rayleigh numbers, decreasing instead at subcritical Rayleigh numbers. We perform a linear fit to extrapolate $\operatorname{Ra}_{\operatorname{crit}}$ in correspondence of the Rayleigh number that would exhibit a zero growth rate.

The estimate obtained for the different BC schemes and for different grid resolutions are reported in Tab. 1. We observe that the external NEBB BC, both in the scaled and unscaled version, performs similarly to the diffusive BC, giving results consistent with theoretical predictions. The internal treatment, on the other other hand, suffers from stability issues at coarse grid resolutions, which most likely still partly hampers the quality of the estimates obtained, even for the finer grid sizes taken into account in our analysis. We have found that working with slightly smaller values of the polytropic index m = 0.95, which in turn translates in larger values of the kinematic viscosity, makes simulation stable and in general improves the accuracy of the estimates; for example, using the internal-unscaled NEBB BC on a 404×200 grid, leads in this case to Ra_{crit} ≈ 1599 .

5. Conclusion

In this work, we have presented a NEBB BC for thermal LBM based on multispeed models, extending previous works which specialized to the isothermal case. We have implemented two schemes, which differ in the way the boundary layers are handled from a macroscopic point of view, namely an internal and external approach. The internal approach allows for replacing only the unknown populations at each boundary layer, but might require interpolation in order to define the macroscopic fields in the fluid nodes adjacent to the boundary. Conversely, the external approach treats all the boundary layers is a unified way, hiding much of the complexities introduced by multispeed models. From this point of view, the external NEBB BC represents a promising approach to handle boundary layers, allowing the use of high order multispeed models even in the presence of complex geometries. We have compared the NEBB BC considering well known examples of thermal flows bounded between parallel walls, such as the Poiseuille, Couette flows and Rayleigh-Bénard convections, comparing against the results obtained employing diffusive boundary conditions. In terms of accuracy and convergence speed NEBB BC are found to be comparable to diffusive boundary conditions. Interestingly, the external NEBB scheme is at times producing superior results, specially for relatively coarse grid resolutions.

We shall remark that although we have restricted our analysis to the two dimensional case, the procedure for constructing this class of BC can be easily extended to three dimensional models, and to stencils formed by even larger velocity sets (at the price of cumbersome analytic expressions which would require employing metaprogramming techniques).

Finally, although a more thorough analysis of the stability properties induced

by the NEBB BC will be object of future works, our analysis hints to the fact that this class of BC supports a more narrow range of numerical parameters when compared to the diffusive BC. In a future extended version of the present work we plan to consider more complex geometries, and to analyze the stability of the NEBB BC by considering turbulent flows in both 2 and 3 dimensions.

Appendix A. Analytical Expression for NEBB-UE correction terms

Here, we report an example for the correction terms used in the definition of the BC (Eq. 6), for the specific case of the NEBB-UE BC. We consider the D2Q17 model, in the configuration shown in Fig. 1, and a south boundary layer. The expressions for other boundaries and other stencils can be obtained in a similar form following the procedure described in the main text. For convenience, we label the discrete component of the stencil as for Table A.2.

Table A.2: Discrete velocities forming the D2Q17 stencil. Each Group forms a fully symmetric set of discrete velocities that are assigned the Indices in lexicographic order, i. e. f_1 corresponds to the rest population and $f_2 = (-1, -1), f_3 = (-1, 1), f_4 = (1, -1), f_5 = (1, 1).$

Group	(0,0)	(1, 1)	(2,2)	(3,3)	(3, 0)
Indices	1	2 - 5	6 - 9	10 - 13	14 - 17

The external treatment allows a unified description of the different boundary layers. This translates in specifying the same set of unknown populations at each boundary layer, i.e., $U^{(l)} = U$ for l = 1, 2, 3. The indices of unknown populations to be set for our specific case are

$$U = \{u_1, \ldots, u_7\} = \{3, 5, 7, 9, 12, 15, 17\}$$

The solution of the system of equations formed by Eq. 5 and Eq. 6 reads as

follows:

$$\begin{split} \rho &= -\frac{f_1 + 2Z_1 + 2Z_2 + Z_3 + +2Z_4 + 65Qt + 15Qy}{A_0} \\ Qx &= \frac{A_2(691f_1 + 2(1051f_{11} + 1411Z_4 + 3(257Z_1 + 337Z_2))) + A_3f_{10} - A_4f_{13}}{28A_1} \\ Qy &= -\frac{2(A_{10}Z_4 + 3(A_7Z_1 + A_8Z_2)) + A_6f_1 + A_9Z_3}{4A_5} \\ Qt &= \frac{A_{12}f_1 + 2(A_{13}Z_1 + A_{14}Z_2 + A_{16}Z_4) + A_{15}Z_3}{4A_{11}} \end{split}$$

where the auxiliary variables Z_i are given in terms of known post-streaming populations as

$$\begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \\ Z_4 \end{pmatrix} = \begin{pmatrix} f_2 + f_4 \\ f_6 + f_8 \\ f_{10} + 2f_{11} + f_{13} \\ f_{14} + f_{16} \end{pmatrix}.$$

The further auxiliary variables A_i are given in terms of $\alpha_j = f_i^{\text{eq}} - f_{\bar{i}}^{\text{eq}}$, with $i \in U$, and depend on the imposed macroscopic velocity **u** and temperature T. We report the most general expression, which would significantly simplify for the case of a stationary wall:

$$\vec{A} = M\vec{\alpha} + \vec{\omega},$$

with
$$\vec{A} = (A_0, \dots, A_{16})^{\top}$$
 and $\vec{\alpha} = (\alpha_1, \dots, \alpha_7)^{\top}$,

	/ 1	1	1	1	1	1	1
	-306	-306	-81	-81	344	-16	-16
	1	-1	2	-2	0	3	-3
	133	-1969	1859	-2345	1032	3105	-3201
	-1969	133	-2345	1859	1032	-3201	3105
	-306	-306	-81	-81	344	-16	-16
	523	523	362	362	1056	-483	-483
	245	245	148	148	336	-177	-177
M =	457	457	230	230	288	-225	-225
	1477	1477	731	731	840	-699	-699
	2431	2431	1100	1100	624	-915	-915
	-306	-306	-81	-81	344	-16	-16
	97	97	46	46	180	-153	-153
	141	141	60	60	164	-169	-169
	273	273	102	102	116	-217	-217
	295	295	109	109	108	-225	-225
	\ 493	493	172	172	36	-297	-297 /

and

$$\vec{\omega} = \begin{pmatrix} 1\\ 80c_s^2T + 40u_x^2 + 40u_y^2 - 465u_y + 691\\ u_x\\ 240c_s^2T + 120u_x^2 + 1051u_x + 120u_y^2 - 1395u_y + 2073\\ 240c_s^2T + 120u_x^2 - 1051u_x + 120u_y^2 - 1395u_y + 2073\\ 80c_s^2T + 40u_x^2 + 40u_y^2 - 465u_y + 691\\ 342c_s^2T + 171u_x^2 + 171u_y^2 - 865u_y\\ 114c_s^2T + 57u_x^2 + 57u_y^2 - 245u_y - 114\\ 114c_s^2T + 57u_x^2 + 57u_y^2 - 115u_y - 456\\ 342c_s^2T + 171u_x^2 + 171u_y^2 - 280u_y - 1539\\ 342c_s^2T + 171u_x^2 + 171u_y^2 - 305u_y - 3078\\ 80c_s^2T + 40u_x^2 + 40u_y^2 - 465u_y + 691\\ 74c_s^2T + 37u_x^2 + 37u_y^2 - 171u_y\\ 74c_s^2T + 37u_x^2 + 37u_y^2 - 141u_y - 74\\ 74c_s^2T + 37u_x^2 + 37u_y^2 - 51u_y - 296\\ 74c_s^2T + 37u_x^2 + 37u_y^2 - 36u_y - 333\\ 74c_s^2T + 37u_x^2 + 37u_y^2 + 99u_y - 666 \end{pmatrix}$$

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