Large temperature difference heat dominated flow simulations using a pressure-based Lattice Boltzmann method with mass correction

Guanxiong WANG (王冠雄),¹ Lincheng XU (徐林程),¹ Eric SERRE,¹ and Pierre SAGAUT¹

Aix-Marseille University, CNRS, Centrale Marseille, M2P2, Marseille, France

(*Electronic mail: lincheng.XU@univ-amu.fr.)

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The paper addresses the simulation of heat dominated compressible flows in a closed cavity using a pressure-based lattice Boltzmann (LB) method in which the thermal effects are modelled by applying a pressure-featured zero-order moment of the distribution functions. A focus is made on the conservation of mass at boundary nodes, which is a challenging issue significantly complicated by the density-decoupled zero-order moment here. The mass leakage at boundary nodes is mathematically quantified, which enables an efficient local mass correction scheme. The performance of this solver is assessed by simulating buoyancy-driven flows in a closed differentially heated cavity with large temperature differences (non-Boussinesq) at Rayleigh numbers ranging from 10^3 to 10^7 . The simulations show that mass leakage at solid walls in such configurations is a critical issue to obtain reliable solutions, and that it eventually leads to simulations overflow when the cavity is inclined. The proposed mass correction scheme is however shown to be effective to control mass leakage and get accurate solutions. Thus, associated with the proposed mass conservation scheme, the pressure-based LB method becomes reliable to study natural convection dominated flows at large temperature differences in closed geometries with mesh aligned boundaries or not.

I. INTRODUCTION

Heat-dominated fluid dynamics is prevalent in both thermal sciences and engineering applications from low speed flow to high speed flow, such as the rising “thermals” used by soaring birds, various cooling systems for electronic devices, nuclear reactors, chemical processing equipment, cooling system in automotive vehicles and in turbomachinery. Despite that great progress has been made in understanding the relevant physics in different backgrounds, heat-dominated flow at high Raleigh numbers (e.g. $> 10^7$) still remains challenging for both experiments and numerical simulations. Mainly, the challenges can be attributed to the complex physics caused by the potential large temperature gradients^{1,2}.

As a typical heat-transfer scene, the natural thermal fluid convection driven by buoyancy force due to density and temperature variations has been intensively investigated both experimentally^{3,4} and numerically^{5–11}. In contrast to the numerical simulations, the thermal fluid experiments are more reliable, but are also much more expensive and difficult to manipulate fluid parameters and boundary conditions^{3,12}. However, many of the existed numerical schemes proposed to solve heat-dominated flows were mainly limited to solutions with small temperature variations where the Boussinesq approximation is reasonable to apply^{8,10}. Numerical methods adequate for thermal fluid dynamics with large temperature variations are of high demand, and are under faster developing^{13,14}. Especially, different from the traditional CFD methodologies, the relatively new lattice Boltzmann (LB) method using Cartesian grid is promising to provide efficient simulations for heat-dominated flows due to its advantages of simple parallel implementation, full compatibility with complex geometries, and high computational efficiency for unsteady flow¹⁵.

To date, the LB method has not only achieved a reputation in the weakly compressible isothermal flow region¹⁵, but also been extended to thermal compressible flow. First, under the low Mach number limit ($Ma < 0.2$), several pressure-based LB algorithms^{16–20} have been proposed with the energy equation either solved by another LB process (the well-known DDF method)^{18,21} or by the conventional finite difference (FD) method (known as the hybrid method)^{17,19,20,22}. These low Ma pressure-based LB methods have been successfully applied in different thermal flows, such as combustion^{19,20}, thermal flow with variable fluid properties²¹ and multi-physical flow²³. Second but more importantly, improved LB methods capable of thermal flow from low Ma to high Ma (e.g. $Ma = 1$) have been recently proposed, including the density-based LB method improved by Feng, Sagaut, and Tao¹³ and the pressure-based LB method developed by Farag *et al.*^{14,24}. Both

of these two methods adopted the hybrid strategy solving the energy equation using conventional finite difference schemes to maintain the high computational efficiency. The main difference is that Farag’s method includes the temperature in the LB framework by modifying the zeroth order moment of the distribution functions, while Feng’s method modifies the second order moment. Comparatively, Farag’s method exhibited superior capability for supersonic flow up to $Ma \approx 4^{24}$ while Feng’s method is up to $Ma \approx 1.5$. Since these two method remain within the classic LB framework, they are much more simple and efficient than the multi-speed (MS)^{25–27} approach which adopts enlarged discrete velocity set (e.g. D2Q27 and D3Q343) to restore the energy equation directly. The recent commercial solver ProLB adopting Farag’s pressure-based LB method has exhibited superior capability for subsonic and supersonic flows, and is promising to model complex thermal fluid dynamics with both low Ma and relatively high Ma involved. With the goal to address with a unique solver in ProLB complex industrial flow configurations with low and high Ma regions and improve the efficiency in terms of developments, support and use, we extend in this work its capability to deal with natural convection dominated flows at low speed and large temperature difference.

Although the above mentioned thermal LB method is theoretically able to model thermal flow, the reported validations were all based on aligned boundaries. Actually, mass conservation (or mass leakage) along non-aligned boundaries is a substantial challenge to extend the LB method to heat-dominated simulations, and this is especially true for the Farag’s pressure-based method. The mass leakage (ML) problem has been noticed and reported since a long time^{28–30}. It has been theoretically proved very recently by Xu *et al.*³¹ to be inevitable for general LB methods using boundary treatments of at least second-order accuracy at general boundaries. Moreover, it was pointed out³¹ that the ML problem could be more serious for flow featuring significant compressible effect, which is a prominent in heat-dominated flow at high Rayleigh numbers, because fluid compressibility is a direct source of the mass leakage. For the Farag’s method, the implementation of mass conservation is supposed to be significantly complicated because the redefinition of the zeroth order moment of the LB distribution functions is decoupled from the fluid density. Therefore, it is critical to identify the mass leakage and to implement mass correction to apply the Farag’s pressure-based LB method to heat-dominated flows simulations.

Based on the above analysis, in this paper, we focus on extending Farag’s pressure-based LB method using mass correction to simulate heat-dominated flow with aligned and non-aligned boundaries. The rest of this paper is organized as follows: Firstly fundamentals of Farag’s

pressure-based LB model are briefed in §II. Then the mass leakage at boundary nodes is theoretically identified in §III. Based on that, the pressure-based LB method using mass correction is used to simulate heat dominated flow with aligned and inclined boundaries at a wide range of Rayleigh numbers in §V. Finally, some critical conclusions are drawn in §VI.

II. FUNDAMENTALS OF FARAG'S PRESSURE-BASED LB METHOD

Farag's pressure-based LB method¹⁴ solves the full Navier-Stokes equations with the mass and momentum equations solved within the LB framework and the energy equation computed by using traditional finite difference (FD) schemes. The two processes are thoroughly coupled. The fluid density and velocity resolved in the LB process is directly used to conduct the thermal convective behaviors in the conventional CFD process. In turn the conventionally resolved thermal variable is directly included in the definition of the zeroth order moment of the distribution functions during the LB collision process (see Appendix B). Details of the FD schemes solving the energy equation is provided in Appendix C.

Here, we concentrate on the LB part with an emphasis on the mass conversation issue. For sake of simplicity but without loss of generality, the classical BGK model is used to demonstrated the basic characteristics, i.e.,

$$f_i(t + \Delta t, \mathbf{x} + \mathbf{e}_i \Delta t) - f_i(t, \mathbf{x}) = -\frac{1}{\tau}(f_i - f_i^{eq}) + \frac{\Delta t}{2} F_i \quad (1)$$

where f_i is the i^{th} distribution function, t is time, Δt is the time step, $\mathbf{x}$ is the Eulerian coordinate vector of a lattice node, $\mathbf{e}_i$ is the i^{th} discrete velocity, τ is the relaxation parameter determined as $\tau = 1/2 + \mu/(\rho c_s^2 \Delta t)$ with c_s being the sound speed and μ being the fluid dynamic viscosity, f_i^{eq} is the equilibrium part of f_i , and F_i is the i^{th} external force term according to Guo's model³². The LB equation (1) is usually solved by directly decomposing it into a linear stream process (the left-hand side) and a local non-linear collision process (the right-hand side). f_i is the distribution function after the stream process, and f_i^{col} will be used to denote that after the collision process.

In Farag's pressure-based method, the temperature is directly included in the definition of f_i^{eq} to model thermal and compressible effects, i.e.,

$$f_i^{eq} = \omega_i \left[\rho \theta + \frac{e_{i\alpha}}{c_s^2} \rho u_\alpha + \frac{e_{i\alpha} e_{i\beta} - c_s^2 \delta_{\alpha\beta}}{2c_s^4} : \rho u_\alpha u_\beta + \frac{e_{i\alpha} e_{i\beta} e_{i\gamma} - c_s^2 [e_i \delta]_{\alpha\beta\gamma}}{6c_s^6} : \rho u_\alpha u_\beta u_\gamma \right] \quad (2)$$

where the Einstein summation convention is applied, ω_i is the i^{th} weight factor, ρ is the fluid density, $\theta = T/T_{ref}$ is the normalized temperature, u_α is the α^{th} velocity component with α, β, γ

being coordinate indices, and $[e_i \delta]_{\alpha\beta\gamma} = e_{i\alpha} \delta_{\beta\gamma} + e_{i\beta} \delta_{\alpha\gamma} + e_{i\gamma} \delta_{\alpha\beta}$. Consistently, the first three moments of the distribution functions can be expressed as

$$\sum f_i^{col} = p/c_s^2 = \rho \theta, \quad \sum f_i e_i = \sum f_i^{col} e_i = \rho \mathbf{u}, \quad \sum f_i e_i e_i = \sum f_i^{col} e_i e_i = \rho \mathbf{u} \mathbf{u} + p \mathbf{I} \quad (3)$$

where $\sum$ represents summation over the whole discrete velocity set, p is the pressure, and $\mathbf{I}$ is the identity matrix. Noticeably, the zeroth order moment of f_i is not given above because it is significantly complicated by the implementation of mass conservation and will be demonstrated in the followed paragraphs.

As illustrated in Eq. (3), the main difference compared to the classical LB method is that the zeroth order moment is directly related to the pressure instead of the usually used density (i.e., $\sum f_i^{eq} = \rho$). Due to this modification, on one hand the compressible Navier-Stokes momentum equation is fully restored within the LB conception, on the other hand the summation of f_i is no longer directly related the mass conservation, and hence the mass equation cannot directly restored from the stream and collision processes.

Alternatively, the mass conservation equation is enforced in a way combining the LB and the traditional FD conceptions. Similar to the classical LB method, the mass flux can be properly approximated during stream process since it directly depends on the first-order moment, i.e.,

$$\begin{aligned} \nabla(\rho \mathbf{u}) &= - \sum \frac{f_i(t + \Delta t, \mathbf{x}) - f_i^{col}(t, \mathbf{x})}{\Delta t} = - \sum \frac{f_i(t, \mathbf{x} - \mathbf{e}_i \Delta t) - f_i^{col}(t, \mathbf{x})}{\Delta t} \\ &= \nabla \sum \mathbf{e}_i f_i^{col}(t, \mathbf{x}) + O(\Delta t) \end{aligned} \quad (4)$$

Accordingly, the mass equation can be discretized as

$$\frac{\rho(t + \Delta t, \mathbf{x}) - \rho(t, \mathbf{x})}{\Delta t} = -\nabla(\rho \mathbf{u}) + O(\Delta t) = \sum \frac{f_i(t + \Delta t, \mathbf{x}) - f_i^{col}(t, \mathbf{x})}{\Delta t} \quad (5)$$

It should be noticed that, to this step, the discretization scheme in Eq. (5) is still shared by Farag's pressure-based and the classical density-based LB methods. According to the widely applied Chapman-Enskog analysis³³, this scheme is actually of second order accuracy because the first-order error term in the left-hand side is implicitly resolved to second-order accuracy in the stream process in the right-hand side.

By substituting the zeroth order moment of f_i^{col} (see (3)) into Eq. (5), the density is consistently updated as

$$\rho(t + \Delta t, \mathbf{x}) = \rho(t, \mathbf{x}) + \sum f_i(t + \Delta t, \mathbf{x}) - (\rho \theta)(t, \mathbf{x}) \quad (6)$$

Clearly, the zeroth order moment of f_i is apparently distinguished from that of f_i^{col} or f_i^{eq} by including the time derivative of ρ , which significantly complicated the relationship between the distribution functions and the mass conservation.

From the above description, we can conclude that by incorporating the conventionally solved temperature into the definition of the zeroth order of the LB distribution functions and applying a consistently modified implementation of mass conservation, Farag’s pressured-based LB method successfully recovers the mass and compressible momentum equations to second order accuracy. In this way, the weakly compressible limitation is removed with most of the favorable characteristics of the LB method maintained. However, since the physical meaning of the distribution functions is significantly complicated and cannot be solely expressed by their moments, the boundary treatments directly focusing on reconstructing the unknown distribution functions cannot be used within the pressure-based LB method without significant adjustment. In contrast, the existing immersed boundary methods focusing on reconstructing macroscopic variables (e.g. the interpolation-based IB method implemented in ProLB) can be directly extended in the pressure-based LB method.

III. MASS LEAKAGE QUANTIFICATION

In this section, mass leakage (ML) within Farag’s pressure-based LB framework is measured by adopting the bounce-back (BB) conception widely used in the classic density-based LB method. The main challenge to complete this ML measurement is that the physical definition of the zeroth order moment of the distribution functions varies during the stream and collision processes, and its expression of macroscopic variables could be rather complex for ML analysis (see §II). Whereas, the mass leakage is conceptually a non-physical mass flux through the boundaries during the convective stream process, which is mainly determined by the first-order moment of the distribution functions, e.g. $\rho \mathbf{u} = \sum f_i \mathbf{e}_i$. Since $\rho \mathbf{u} = \sum f_i \mathbf{e}_i = \sum f_i^{col} \mathbf{e}_i$ is shared throughout both Farag’s method and the classic LB method, the mass leakage analysis achieved in the classic LB frame can be definitely extended to its pressure-based counterpart. In the rest of this paper, only static boundaries are considered.

For the classic density-based LB method, the widely accepted definition of mass leakage is the

net loss of distribution functions during the stream process at boundary nodes (see Fig. III), i.e.,

$$E(\mathbf{x}) = \frac{\Delta x}{\Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left[f_i^{col}(\mathbf{x}) - f_{\bar{i}}^{col}(\mathbf{x} + \mathbf{e}_i \Delta t) \right] \quad (7)$$

where S represents the non-fluid area, Δx is the grid spacing, and Δt is the time step, and $\mathbf{e}_i$ is the i^{th} discrete velocity with its components taking values among 0 and $\pm \Delta x / \Delta t$. Actually, E in Eq. (7) is an approximation of the local mass flux cross the boundary, i.e.,

$$\begin{aligned} E(\mathbf{x}) &= \frac{\Delta x}{\Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left[f_i^{col}(\mathbf{x}) - f_{\bar{i}}^{col}(\mathbf{x} + \mathbf{e}_i \Delta t) \right] \\ &\approx \sum f_{i,w} \text{Sign}(\mathbf{e}_i \cdot \mathbf{n}) \approx \sum f_{i,w} \mathbf{e}_i \cdot \mathbf{n} = \rho \mathbf{u}_w \cdot \mathbf{n} = 0 \end{aligned} \quad (8)$$

where the sub-index w represents the involved wall boundary, $\mathbf{e}_{\bar{i}} = -\mathbf{e}_i$, and $\mathbf{n}$ is the local normal vector at the boundary. The relationship (8) is of first-order accuracy for aligned boundaries, otherwise is of zero-order accuracy³¹. Despite the perturbations of the approximation to the conventional mass flux, E has been demonstrated as an effective and accurate measurement of the mass leakage within the classic LB framework. For example, the well-known BB scheme, directly assigning the distribution functions streaming towards non-fluid areas to those associated with the reversed velocity directions yielding $E = 0$ at every node, is the only known boundary treatment satisfying the mass conversation well. In addition, Eq. (8) clearly demonstrates that the reasonability of E in Eq. (7) stems from the first-order moment definition of f_i as mentioned above.

However, Eq. (7) cannot be directly applied within Farag's pressure-based LB method in a clean way (e.g. the classic BB scheme) due to the complicated relationship between f_i and ρ . To avoid this complexity, it is appealing to express the ML definition in Eq. (7) from a macroscopic viewpoint before going to the pressure-based framework. This can be achieved by including the distribution functions streaming from the neighbouring fluid nodes and boundary nodes (see Fig. III) into Eq. (7), i.e.,

$$\begin{aligned} E(\mathbf{x}) &= \frac{\Delta x}{\Delta t} \left[\sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} f_i^{col}(\mathbf{x}) + \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in F} f_i^{col}(\mathbf{x} + \mathbf{e}_i \Delta t) \right] \\ &\quad - \frac{\Delta x}{\Delta t} \left[\sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} f_{\bar{i}}^{col}(\mathbf{x} + \mathbf{e}_i \Delta t) + \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in F} f_{\bar{i}}^{col}(\mathbf{x} + \mathbf{e}_i \Delta t) \right] \\ &= \frac{\Delta x}{\Delta t} [\rho^{BB}(\mathbf{x}) - \rho(\mathbf{x})] \end{aligned} \quad (9)$$

FIG. 1. Sketches of the streaming process at boundary nodes considering a D2Q9 lattice. Nodes in the solid area, e.g. G_1 , are not necessary.

where F represents the fluid domain, ρ^{BB} is the density applying the BB strategy satisfying $E = 0$ at every boundary node, and ρ is the density reconstructed by specific boundary treatments. Clearly, Eq. (9) is now independent of the zero-moment definition of f_i , and thus can be used to measure the mass leakage for both the LB methods. The remained problem is to construct ρ^{BB} properly within Farag's pressure-based LB framework.

Considering that the distribution functions in Eq. (9) are actually the post-stream distribution functions at $\mathbf{x}$, the required ρ^{BB} can be determined by the mass conservation equation (6) as

$$\rho^{BB}(t + \Delta t, \mathbf{x}) = \rho(t, \mathbf{x}) + \left[\sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} f_i^{col}(t, \mathbf{x}) + \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in F} f_i^{col}(t, \mathbf{x} + \mathbf{e}_i \Delta t) \right] - \rho(t, \mathbf{x}) \theta(t, \mathbf{x}) \quad (10)$$

Similarly, the other distribution functions in Eq. (9) is implicitly included in $\rho(t + \Delta t, \mathbf{x})$. Therefore, by substituting Eq. (10) into Eq. (9), the mass leakage within Farag's pressure-based LB framework can be formulated as

$$E(t + \Delta t, \mathbf{x}) = \frac{\Delta x}{\Delta t} \left[\rho(t, \mathbf{x}) + \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} f_i^{col}(t, \mathbf{x}) + \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in F} f_i^{col}(t, \mathbf{x} + \mathbf{e}_i \Delta t) - \rho(t, \mathbf{x}) \theta(t, \mathbf{x}) - \rho(t + \Delta t, \mathbf{x}) \right] \quad (11)$$

Consequently, the local density correction can be expressed as

$$\begin{aligned}
\Delta\rho(t+\Delta t, \mathbf{x}) &= \frac{\Delta t}{\Delta x} E(t+\Delta t, \mathbf{x}) \\
&= \rho(t, \mathbf{x}) + \left[\sum_{\mathbf{x}+\mathbf{e}_i\Delta t \in S} f_i^{col}(t, \mathbf{x}) + \sum_{\mathbf{x}+\mathbf{e}_i\Delta t \in F} f_i^{col}(t, \mathbf{x} + \mathbf{e}_i\Delta t) \right] \\
&\quad - \rho(t, \mathbf{x})\theta(t, \mathbf{x}) - \rho(t+\Delta t, \mathbf{x})
\end{aligned} \tag{12}$$

Similar to the local mass correction methods used by Bao, Yuan, and Schaefer²⁹, in the rest of this paper, $\Delta\rho$ in Eq. (12) will be directly used to correct the density at boundary nodes, i.e., $\rho(\mathbf{x}) = \rho^{BB}$.

IV. PHYSICAL CONFIGURATION AND NUMERICAL SETUP

The canonical natural convection flow in a heated square cavity is considered in this paper to assess Farag's pressure-based LB method using mass correction in simulating heat-dominated flow. The method based on the D3Q19 model (see Appendix A) is implemented in the commercial solver ProLB with the energy equation conventionally solved (see Appendix C). The recursively regularized technique^{34,35} is adopted to facilitate stable solutions. A cut-cell immersed boundary (IB) method is used to implement the boundary conditions³⁶ for both the LB process and the FD procedure (see Appendix D). In this IB method, the macroscopic variables (e.g. the density, velocity and temperature) at the boundary nodes are interpolated from their surrounding fluid nodes and nearest boundary points so that the equilibrium distribution functions can be reconstructed. Meanwhile, the non-equilibrium distributions are reconstructed from the derivatives of the macroscopic variables generated during the macroscopic interpolations. For the simulations conducted in this paper, uniform grid strategy is applied over the whole fluid domain (see Fig. 2).

The physical configuration of the heated square cavity is shown in Fig. 2. The air modeled as a perfect gas satisfying $P = \rho RT$ (R is the gas constant) is considered in the fluid domain. Sutherland's law is utilized to compute the dynamic viscosity $\mu(T) = \mu^* * (\frac{T}{T^*})^{3/2} * \frac{T^*+S}{T+S}$ with $T^* = 273K$, $S = 110.5K$, and $\mu^* = 1.68 * 10^{-5} kgm^{-1}s^{-1}$. The thermal conductivity is calculated by $\lambda(T) = \frac{\mu(T)C_p}{Pr}$ with C_p being the specific heat capacity of air and $Pr = 0.71$. For the wall boundaries, as shown in Fig. 2, isothermal conditions are assigned to the left and right walls with the temperature fixed at T_1 and T_2 , respectively, while the top and bottom walls are set to be adiabatic (i.e., $\partial T / \partial n = 0$). Meanwhile, $\partial p / \partial n = 0$ is applied to all the boundaries, and an external gravity is imposed on the fluid. Consequently, the flow is resulted from the interaction

among the implied gravity, the buoyancy force caused by thermal effect, and the fluid viscosity. Accordingly, the Rayleigh number, the ratio between the buoyancy force and viscous force, is the main characteristic parameter, i.e.,

$$Ra = \frac{g\rho_0^2\Delta TL^3Pr}{T_0\mu_0^2} \quad (13)$$

where g is the gravity acceleration, $\rho_0, T_0 = (T_1 + T_2)/2$ and μ_0 is the reference density, mean temperature and the fluid dynamic viscosity, respectively, $\Delta T = T_2 - T_1$, Pr is the Prandtl number, and L is the length of the cavity serving as a free parameter to change the Rayleigh number. Besides, the normalized temperature gap (i.e., $\varepsilon = \frac{T_1 - T_2}{T_1 + T_2}$), indicating the variation amplitude of the temperature, is another important characteristic parameter for the heat-dominated flow.

In the concerned numerical assessment, heat-dominated flow with $T_1 = 240K$, $T_2 = 960K$ and thus a large $\varepsilon = 0.6$ (the Boussinesq assumption requires $\varepsilon < 0.1$) is simulated over a wide range of Ra , i.e., $10^3 \leq Ra \leq 10^7$. Moreover, cavities inclined at different angles from 0° to 45° (see Fig. 2(b)) are included to verify the capability for non-aligned boundaries.

FIG. 2. Aligned (a) and inclined (b) heated square cavities with uniform Cartesian grid $\Delta x/L = 0.02$.

To facilitate quantitative analysis in the rest of this paper, some critical physical measurements are introduced here. Firstly, following Vierendeels, Merci, and Dick¹¹, the Nusselt number Nu measuring heat flux across the vertical walls as well as its averaged value $\overline{Nu}$ is defined as:

$$Nu(y) = \frac{L}{\lambda_0 \Delta T} \lambda \frac{\partial T}{\partial x} \Big|_{wall} \quad \overline{Nu} = \frac{1}{L} \int_{y=0}^{y=L} Nu(y) dy \quad (14)$$

Secondly, mass leakage in the cavity simulations is measured by the overall mass loss normalized as

$$ML = \frac{\sum_V \rho^n - \sum_V \rho_0}{\sum_V \rho_0} \quad (15)$$

where V represents the whole fluid domain. In addition, $U_{ref} = \frac{Ra^{0.5} \mu(T_0)}{\rho_0 L}$ is used as the reference velocity¹¹ in the rest of this paper.

V. RESULTS AND DISCUSSION

The assessment of Farag's pressure-based LB method using mass correction in heat-dominated flow over $10^3 \leq Ra \leq 10^7$ is conducted using the ProLB software in this section. Firstly, the mass leakage as well as the caused problems are analyzed in §V A. Then, performance of the mass correction equipped method for non-aligned boundaries is assessed in §V B. Finally, performance of the method over the considered Rayleigh number range is assessed in §V C.

A. Mass leakage quantification and its effect on thermal simulations

The mass leakage in thermal simulations using Farag's pressure-based LB method as well as its influence on the solutions (e.g. the heat flux estimation) is investigated here. $Ra = 10^7$ is used in the simulations as it is supposed to be associated with the most complex thermal physics for the considered range of Rayleigh numbers, $10^3 \leq Ra \leq 10^7$. Without loss of generality, the cavity inclined at 15° is considered to study the effect of non-aligned boundaries. In addition, different grid sizes (from $N^2 = 50^2$ to 400^2) are tested to clarify its effect on the ML problems.

Fig. 3 shows the history of the overall ML for both aligned and inclined cavity using different grid resolutions. As can be observed, the mass leakage accumulates with time in all the cases. For the simulations with non-aligned boundaries, the mass leakage is so significant that all the simulations crash in the early stage. In contrast, for the cases with aligned boundaries, the mass leakage decreases significantly with refining grid spacing, from about -80% using $N^2 = 50^2$ to about 3% using $N^2 = 400^2$ at $U_{ref} t / L = 250$. However, even with relatively low increasing rate, the accumulated ML still leads to computation crash finally, e.g. this occurs at around $U_{ref} t / L = 400$ in the case with $N^2 = 200^2$. The observed dependence of ML on grid spacing and boundary orientation is consistent with the theoretical analysis of ML reported in Ref.³¹ for general LB methods.

FIG. 3. Time histories of mass leakage at $Ra = 10^7$ for aligned and inclined cavity (lines with square markers). The x markers indicate crashed computation.

FIG. 4. Time history of $\overline{Nu}$ (a) and temperature profile at $x/L = 0.5$ and $U_{ref}t/L = 250$ (b). In (b), result from Ref.³⁵ (lines with markers) is included for comparison.

To clarify the influence of the observed ML on the solutions, time histories of the averaged Nusselt number along the aligned wall in the right side and the temperature profiles at $x/L = 0.5$ and $U_{ref}t/L = 250$ are plotted in Fig. 4(a) and (b), respectively. As we can see, for all the tested grid resolutions, $\overline{Nu}$ (see Fig. 4(a)) firstly increases with time during the thermal convection establishment, but it then decreases gradually after $U_{ref}t/L = 250$ to the end of the simulations. Similar to the ML displayed in Fig. 3, the decreasing rate of $\overline{Nu}$ as well as the discrepancy of the temperature profiles (see Fig. 4(b)) reduces with increasing N . Although these behaviours are usually deemed as a pure grid spacing converging process (e.g. in Ref.³⁵), the problem is actually beyond that because of two reasons. First, the monotonic decreasing trend of $\overline{Nu}$ is non-physical

since the simulations are supposed to reach a steady state featuring a constant $\overline{Nu}$. Second, due to the accumulating mass leakage, the reasonable result obtained using very fine grid (e.g. $N = 400$) can not be maintained with more time steps simulated. Therefore, it can be concluded that, for the considered thermal simulation, ML is a critical challenge that refining grids could relieve it. In addition, as shown in Fig. 4(b), the grid spacing depended discrepancy of the temperature profiles is more obvious in the result reported in Ref.³⁵ using an improved density-based LB method, indicating that the ML challenge might be also critical in other LB frameworks.

B. Effectiveness of the mass correction scheme

To cure the mass leakage problem observed in the last subsection, we implemented a local mass correction (MC) method in the solver based on the theoretical analysis proposed in §III. Effectiveness of the MC method is assessed here. First, similar to the ML analysis in §V A, the cases with aligned boundaries considering different grid resolutions ($50 \leq N \leq 400$) are analyzed. Second, the heated cavity inclined at different angles from 0° to 45° is simulated to assess the robustness of the mass corrected LB method. Still, the most representative $Ra = 10^7$ is considered.

Before detailed physical analysis, it is pointed out that mass leakage measured by Eq. (15) in all the considered simulations is exactly zero, indicating that the theoretical mass leakage analysis for Farag's pressure-based LB method is accurate and reliable.

Fig. 5(a) and 5(b) display the time history of $\overline{Nu}$ and the temperature profiles at $x/L = 0.5$, respectively, for the cases with aligned boundaries. As shown in Fig. 5(b), all the results with N from 50 to 400 converge well to the reference data from Ref.¹¹, exhibiting substantially improvement compared to those without mass correction shown in Fig. 4(a). Consistently, all the temperature profiles shown in Fig. 5(b) achieve excellent agreement with the reference data, which is significantly improved from those without mass correction shown in Fig. 4(b). Clearly, the mass correction not only improves the reliability of the simulations, but also allows using coarse grid resolution to achieve good results thus significantly improve the computational efficiency. Besides, the observed improvement using mass correction also confirms that the problems observed in §V A is mainly caused by mass leakage.

Fig. 6 shows the temperature contours at $U_{ref}t/L = 250$ for inclination angle increasing from 0° (aligned boundaries) to 45° with an increment of 15° . As can be seen, the solutions are almost independent of the inclined angles. The most observable discrepancy is near the bottom wall of 45°

FIG. 5. Time history of $\overline{Nu}$ (a) and temperature profile at $x/L = 0.5$ and $U_{ref}t/L = 250$ (b) for $Ra = 10^7$.

inclined cavity. Similar conclusion can be also drawn from the corresponding $\overline{Nu}$ listed in Table I. The observed discrepancy is supposed to be associated with the fact observed in Ref.³¹ that boundary nodes along 45° inclined boundaries tend to produce the most significant mass leakage, which might introduce unfavorable coupling with the heat flux in the considered configuration.

FIG. 6. Temperature contour of $Ra=10^7$ and grid resolution $N^2 = 400^2$ at inclined angle 0° (solid line), 15° (dashed line), 30° (dash dotted line) and 45° (dash dot dot line)

TABLE I. Average Nusselt number at different angles of inclination α compared with reference Vierendeels, Merci, and Dick¹¹

α	0°	15°	30°	45°	Ref
$\overline{Nu}$	16.24	16.22	16.13	15.40	16.24
Error (%)	0.0	-0.12	-0.67	-5.17	—

C. Performance over $10^3 \leq Ra \leq 10^7$

The performance of Farag's pressure-based method using mass correction in heat-dominated flow over $10^3 \leq Ra \leq 10^7$ is assessed now. The value of Ra is changed by altering L with the other parameters (e.g. T_1, T_2) unchanged. The cavities are inclined at 15° to include the influence of non-aligned boundaries. Grid convergence is performed for all the considered Ra with good results represented by Fig. 4(a) and (b) at $Ra = 10^7$. To facilitate consistent comparison with previous studies, results for $Ra = 10^3, 10^4, 10^5, 10^6, 10^7$ are presented with $N^2 = 100^2, 100^2, 200^2, 200^2, 400^2$, respectively.

Table II display $\overline{Nu}$ of the considered simulations. As can be seen, the heat flux increases significantly with Ra from $\overline{Nu} = 1.11$ at $Ra = 10^3$ to $\overline{Nu} = 16.22$ at $Ra = 10^7$, indicating a physically increasing thermal convection. The increasingly dominating thermal convection is corroborated by the increasing Mach number shown in Fig. 7 where the maximum Ma increases from 7.5×10^{-5} at $Ra = 10^3$ to 2×10^{-4} at $Ra = 10^7$ (the reference sound speed corresponding to $T_0 = 600K$ is unchanged). Meanwhile, for the considered $10^3 \leq Ra \leq 10^7$, the present results achieve good agreement (relative difference within 1%) with the data reported in Ref.¹¹, and considerably outperform those reported by Feng *et al.* applying an improved density-based LB method using very fine grids ($N = 800$) in an aligned cavity. In addition, profiles of temperature and velocity along different lines are shown in Fig. 8(a)-(c). As can be observed, the above observed increasing trend of $\overline{Nu}$ is consistent with the increasing temperature gradient near the wall shown in Fig. 8(b). Meanwhile, the present results agree well with the reference data reported in Ref.¹¹, indicating that the heat-dominated flows are well reproduced by the solver.

TABLE II. $\overline{Nu}$ at inclined angle 15° in the range of $10^3 \leq Ra \leq 10^7$. Data reported by Feng *et al.* in Ref.³⁵ is included for comparison, and those in Ref.¹¹ is used as the reference.

Ra	Present	Feng <i>et al.</i> ³⁵	Ref. ¹¹	Error (%) Present VS Feng <i>et al.</i> ³⁵
10^3	1.11	—	1.11	0.0 vs —
10^4	2.20	2.28	2.22	0.9 vs 2.70
10^5	4.45	4.55	4.48	0.67 vs 1.56
10^6	8.72	8.82	8.69	0.35 vs 1.50
10^7	16.22	16.26	16.24	-0.12 vs 0.12

FIG. 7. Profiles of Mach number (normalized by speed of sound at $T_0 = 600K$) at $x/L = 0.5$ with the cavity inclined at 15° .

VI. CONCLUSIONS

In this paper, we extend the recently developed Farag's pressure-based LB method implemented in the commercial software ProLB, which has exhibited outstanding capability for supersonic flow, to heat-dominated flow at low Ma with large temperature difference considering both aligned and inclined boundaries. As demonstrated in ProLB, Farag's pressure-based LB method prefers an efficient hybrid strategy that solves the energy equation in a conventional FD manner, and directly includes the conventionally solved temperature in the zeroth order moment of the distribution functions to restore the energy equation. To address the thermal-coupled mass conservation challenge, we theoretically quantify the mass leakage (ML) at the boundary nodes within Farag's LB framework, and implemented a local mass correction in the solver based on that.

(a) Temperature profiles at $x/L = 0.5$

(b) Temperature profiles at $y/L = 0.5$

(c) Velocity profiles

FIG. 8. Profiles of temperature ((a)-(b)) and velocity (c) inclined cavity for different Rayleigh number, markers represent reference data¹¹.

The canonical natural thermal convection in a square cavity heated by a large temperature difference $\Delta T/T_{ref} = 1.2$ is considered to assess the performance of the mass corrected pressure-based LB method with the Rayleigh number ranging from 10^3 to 10^7 and the cavity inclined at different angles. The numerical results show that the mass leakage is a serious challenge leading to simulation crashes. Although the problem could be significantly relieved by applying aligned boundaries with very fine grid resolutions, the reliability of simulations is still supposed to be ruined when more time step is simulated. Fortunately, the proposed theoretical ML identification is accurate, based on which the applied local mass correction is able to remove it cleanly. Together

with the mass correction, the high-speed featured Farag’s LB method implemented in ProLB performs well over the considered $10^3 \leq Ra \leq 10^7$ for both aligned and inclined boundaries.

The presented capability extension of Farag’s pressure-based LB method is limited to low Ma regime. However, it clearly illustrates the way to apply the method for thermal problems with complex geometry involved. Moreover, it also enables the solver to deal with practical problems where both low and high Ma thermal physics emerges, e.g. a cooling fan might has low Ma area near the fix hub but high Ma area around the blade tips. That probably will be our next research topic.

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Appendix A: The discrete velocity model D3Q19

The discrete velocities (c_i) as well as the corresponding weight factors (ω_i) of the applied D3Q19 model are detailed in Table. III:

TABLE III. Discrete velocities and corresponding weights of D3Q19. The sub-index α in $c_{i\alpha}$ refers to the coordinates x , y , and z .

	D3Q19	
$c_{i\alpha}$ ω_i	(0,0,0)	1/3
	($\pm 1,0,0$)	1/18
	($\pm 1,\pm 1,0$)	1/36

Noticeably, to reduce the defect of rotation invariant using D3Q19, a set of Hermite basis with improved orthogonality is adopted in the recursive regularization of the distribution functions. The

improved Hermite basis is formulated as

$$\mathcal{H}_{i,(\alpha\beta\gamma)\subset(x,y,z)}^{(3)} = \begin{pmatrix} \text{cyc}(H_{i,xy}^{(3)} + H_{i,yz}^{(3)}) \\ \text{cyc}(H_{i,xz}^{(3)} + H_{i,xy}^{(3)}) \\ \text{cyc}(H_{i,yz}^{(3)} + H_{i,xz}^{(3)}) \\ H_{i,xy}^{(3)} - H_{i,yz}^{(3)} \\ H_{i,xz}^{(3)} - H_{i,xy}^{(3)} \\ H_{i,yz}^{(3)} - H_{i,xz}^{(3)} \end{pmatrix} \quad (\text{A1})$$

where $(\alpha\beta\gamma) \subset (x,y,z)$, and $H_{i,\alpha\beta\gamma}$ is the original 3rd order Hermite basis tensor

$$H_{i,\alpha\beta\gamma}^{(3)} = c_{i,\alpha}c_{i,\beta}c_{i,\gamma} - c_s^2[c_i\delta]_{\alpha\beta\gamma} \quad (\text{A2})$$

Appendix B: Governing equations and the hybrid solving process

By combining Farag's pressure-based LB method and finite-difference method, the commercial software ProLB solves the full compressible Navier-Stokes equations, i.e.,

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\alpha}{\partial x_\alpha} = 0 \quad (\text{B1a})$$

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta} \left[\mu \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3} \frac{\partial u_\gamma}{\partial x_\gamma} \delta_{\alpha\beta} \right) \right] + F_\alpha \quad (\text{B1b})$$

$$\frac{\partial s}{\partial t} + \mathbf{u} \frac{\partial s}{\partial x_\alpha} = \frac{1}{\rho T} \left[\mu \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3} \frac{\partial u_\gamma}{\partial x_\gamma} \delta_{\alpha\beta} \right) \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial}{\partial x_\alpha} \left(\lambda \frac{\partial T}{\partial x_\alpha} \right) \right] \quad (\text{B1c})$$

where F_α is the external force, e.g., the gravity used in this study, and s is the entropy.

The solving process is illustrated in Fig. 9. Clearly, the LB process in the left-hand side solves the mass and momentum equations (the first two in Eq. (B1)), while the FD process in the right-hand side solves the energy equation. The two processes are deeply coupled: the LB process relies on the thermal variable $\theta = T/T_0$ solved by the FD process to include thermal and compressible effects, and, in turn, the FD process uses ρ and $\mathbf{u}$ solved by the LB process to complete the heat convection. The FD process will be detailed in the followed Appendix C.

FIG. 9. Sketch of the hybrid strategy adopted in ProLB

397 Appendix C: Numerical schemes for the energy equation

398 The energy equation in Eq. (B1) is solved using a FD method taking the entropy as the di-
 399 rect thermal variable. The temporal derivative and convective term in the left-hand side are
 400 discretized using the first-order explicit Euler scheme and the second-order Monotonic Upwind
 401 Scheme for Conservation Laws (MUSCL-Hancock)³⁷, respectively. The viscous heat dissipation
 402 and Fourier heat transfer terms on right-hand side are discretized using second order central dif-
 403 ference schemes.

404 1. Discretization of terms on the left-hand side

405 The terms on the left-hand side of Eq. (B1c) are discretized as

$$406 \quad \frac{s_i^{n+1} - s_i^n}{\Delta t} + \frac{F(s_{i+\frac{1}{2}}^n) - F(s_{i-\frac{1}{2}}^n)}{\Delta x} \quad (C1)$$

407 where n , i and $i \pm \frac{1}{2}$ represent respectively the time step, cell identity and boundary of the i^{th} cell.

408 The convective flux $F(s_{i+\frac{1}{2}}^n)$ and $F(s_{i-\frac{1}{2}}^n)$ are computed through the following three steps:

1. Data reconstruction. The inter-cell values at the left and right sides of the i^{th} cell is firstly evaluated by extrapolation, i.e.,

$$s_{i,L} = s_i - \frac{1}{2}\Delta_i \quad (C2a)$$

$$s_{i,R} = s_i + \frac{1}{2}\Delta_i \quad (C2b)$$

409 where the Δ_i is a high order approximation of the slop at the center of i^{th} cell which is
 410 calculated by

$$411 \quad \Delta_i = \frac{1}{2} \left[(1 + \Phi)(s_i - s_{i-1}) + (1 - \Phi)(s_{i+1} - s_i) \right] \quad (C3)$$

412 with $\Phi = \frac{1}{3} \left[\frac{2\Delta t u_i}{\Delta x} - \text{sign}(u_i) \right]$ proposed by Toro³⁷.

2. Data evolution. The boundary values of the cell is further evolved by a semi-time step $\frac{\Delta t}{2}$, i.e.,

$$\bar{s}_{i,L} = s_{i,L} + \frac{2\Delta t u_i}{\Delta x} (s_{i,L} - s_{i,R}) \quad (C4a)$$

$$\bar{s}_{i,R} = s_{i,R} + \frac{2\Delta t u_i}{\Delta x} (s_{i,L} - s_{i,R}) \quad (C4b)$$

3. Piece-wise construction of convective flux. The convective flux $F(s_{i+\frac{1}{2}})$ and $F(s_{i-\frac{1}{2}}^n)$ are then evaluated by

$$F(s_{i+\frac{1}{2}}) = \begin{cases} u_i \bar{s}_{i,R} & \text{if } u_i \geq 0 \\ u_i \bar{s}_{i+1,L} & \text{if } u_i \leq 0 \end{cases} \quad (\text{C5a})$$

$$F(s_{i-\frac{1}{2}}) = \begin{cases} u_i \bar{s}_{i-1,R} & \text{if } u_i \geq 0 \\ u_i \bar{s}_{i,L} & \text{if } u_i \leq 0 \end{cases} \quad (\text{C5b})$$

2. Discretization of terms on the right-hand side

The Fourier part $\frac{\partial}{\partial x_\alpha} \left(\lambda \frac{\partial T}{\partial x_\alpha} \right)$ and the viscous heat dissipation $(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3} \frac{\partial u_\gamma}{\partial x_\gamma} \delta_{\alpha\beta}) \frac{\partial u_\alpha}{\partial x_\beta}$ are discretized here. Since λ in the Fourier part varies with T , the term is decomposed into two parts: $\frac{\partial \lambda}{\partial x_\alpha} \frac{\partial T}{\partial x_\alpha}$ and $\lambda \frac{\partial^2 T}{\partial x_\alpha^2}$. Apparently, the first-order spatial derivatives of u , λ and T as well as the second-order spatial derivatives of T are required to be discretized. In ProLB, all of them are discretized using second-order accurate center difference schemes, i.e.,

$$\frac{\partial \phi}{\partial x_\alpha} = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x_\alpha} \quad (\text{C6a})$$

$$\frac{\partial^2 T}{\partial x_\alpha^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x_\alpha^2} \quad (\text{C6b})$$

where $\phi = u$, λ and T , and $\alpha \in [x, y, z]$.

Appendix D: A cut-cell immersed boundary treatment

A cut-cell immersed based recursive regularized boundary treatment is adopted in ProLB to reconstruct the LB distribution functions and the temperature. In the method, the macroscopic variables (e.g., p , u and T) are reconstructed through interpolation, based on which $\rho = p/(RT)$ and the equilibrium parts of the distribution functions are directly calculated using Eq. (2). Meanwhile, the off-equilibrium parts are reconstructed from the spatial derivatives of macroscopic variables according to the recursive regularization analysis³⁸ with the required spatial derivatives are calculated using the finite difference method (centered or not) using values of the previous time step. As an introduction of the immersed boundary method, the following is focused on the details of the reconstruction of the macroscopic variables.

The interpolation of macroscopic variables is illustrated in Fig. 10. As shown in Fig. 10, two reference points (i.e., Ref₁ and Ref₂ one and two grid spacing away from the boundary node,

respectively) in the fluid domain along the local normal direction of the wall are introduced to assist the interpolation. With the variables at the reference points interpolated from the surrounding fluid nodes, values at the concerned boundary node are interpolated from the reference points according to specific boundary conditions.

FIG. 10. Sketch of interpolation-based immersed boundary method. The black square and blue circles represent a boundary node and its neighbor nodes, respectively.

Firstly, the macroscopic variables at the reference points are computed through an inverse distance weighting (IDW) method, i.e.,

$$\phi_{x_{ref}} = \sum_{i=1}^N \frac{d(x_i, x_{ref})^{-p}}{\sum_{i=1}^N d(x_i, x_{ref})^{-p}} \phi_{x_i} \quad (D1)$$

where ϕ represents the required macroscopic variables (e.g., ρ , u and T), $d(x_i, x_{ref})$ the distance of the i^{th} neighbor point to the reference point, and the coefficient $P = 2$ is preferred here^{39,40}.

Then, the macroscopic variables at the concerned boundary node is interpolated from those at the reference points to implement different kinds of boundary condition. In this paper, two kinds of boundary condition, the Dirichlet and Neumann boundary conditions, are implemented. For Dirichlet boundary conditions, e.g., the velocity of static walls and T at isothermal walls, the projection point (see Ref_w in Fig. 10) of the concerned boundary node at the wall is included in the interpolation stencil. The interpolation can be formulated as

$$\phi_{BN} = \frac{2\Delta x^2}{(\Delta_w + \Delta x)(\Delta_w + 2\Delta x)} \phi_w + \frac{2\Delta_w}{\Delta_w + \Delta x} \phi_1 - \frac{\Delta_w}{\Delta_w + 2\Delta x} \phi_2 \quad (D2a)$$

where ϕ_{BN} is the required variables at the boundary node, ϕ_w is those at the projection point, ϕ_1 and ϕ_2 are those at Ref₁ and Ref₂, respectively, and δ_w and δ_x represent the wall distance of boundary node and the local grid spacing, respectively. For the Neumann boundary condition, such as $\frac{\partial p}{\partial n} = 0$ and the adiabatic wall ($\frac{\partial T}{\partial n} = 0$), the second order Lagrangian interpolation is used to reconstruct the required variables as

$$\phi_{BN} = \frac{4(\Delta x + \Delta_w)\phi_1 - (\Delta x + 2\Delta_w)\phi_2}{2\Delta_w + 3\Delta x} \quad (\text{D3a})$$

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