Massively Parallel GPU Implementation of the Lattice-Boltzmann Method for the Simulation of Coupled Aero-Thermodynamic Systems

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ABSTRACT: The automotive industry is showing high demand for efficient design of cooling systems in electric vehicles. The development of complex aero-thermodynamic systems requires reliable, high-fidelity simulations of high Reynolds number flows. We implemented a numerical solver based on the double-distribution lattice-Boltzmann method (LBM). The main advantage of the LBM, compared to the Navier-Stokes-based solvers, is its computational efficiency and intrinsic parallelism, which allows for execution on massively parallel architectures (GPUs). We have validated our GPU implementation by simulating a natural convection flow and a heated cylinder in an enclosed cavity. Both cases show very good agreement with published literature. In the future, we aim to extend the usage of the LBM framework to industry-relevant cases like the simulation of various packaging concepts for electric vehicles.

KEY WORDS: heat · fluid, lattice-Boltzmann method, coupled aero-thermodynamic problems, heat exchange [D1]

1. Introduction

Natural convection phenomena are relevant for many industrial applications such as microelectronics cooling, heat exchangers, cooling of nuclear and chemical reactors, and air-conditioning of buildings and vehicles, to name a few. Various geometric configurations of a heated body embedded in a cooled enclosure have been investigated over the years[1,5]. Often, the numerical simulations are performed using conventional numerical methods based on the spatial and temporal discretization of the continuity, the Navier-Stokes and the energy equations. Such models highly depended on the quality of the mesh and its generation could be tedious and time-consuming for problems with complex geometries. An alternative approach which copes with the deficiencies mentioned above is the lattice-Boltzmann method (LBM). Inherited from its kinematic nature, the main advantages of the LBM are its intrinsic parallelism and the capability to simulate complex geometries with suitable accuracy[6]. Beyond that, the LBM has been adapted to simulate numerous complex problems such as turbulence[7,8], multiphase and multicomponent flows[9], porous media[10] and thermal flows[11].

The subject of the present study is to validate a massively parallel GPU (Graphics Processing Unit) implementation of the thermal LBM simulating a natural convection process, where a heated cylinder is placed within a square enclosure. The implemented model is based on the double-distribution LBM proposed by Guo et al.[12], coupling the fluid and temperature distribution functions using the Boussinesq approximation. The model is using the D3Q27 and the D3Q7 velocity sets for the flow field and for the temperature field, respectively. We have chosen the double-distribution LBM due to its superior properties such as locality, high numerical stability and relatively simple implementation of the boundary conditions in 3D compared to the multi-speed and hybrid methods. A similar study has been conducted by Lin et al.[13], however, they were using 2D lattice velocity sets and our implementation is targeting massively parallel multi-GPU systems instead of traditional CPU hardware. We show that the double-distribution LBM has a large potential when implemented for GPU architectures. The numerical results presented in this work are validated using the findings of Kim et al.[5], where a heated cylinder in a square enclosure is simulated by conventional numerical methods, namely a two-step time-split scheme for the flow field as well as an Adams-Bashforth scheme for the advection term and a Crank-Nicolson scheme for the diffusion term of the temperature field. For details please refer to Kim et al.[5] and the citations within.

The rest of the paper is organized as follows: first, we introduce the thermal LBM using the so-called Bhatnagar-Gross-Krook (BGK) collision operator[14]. In Section 3, we validate our implementation using a natural convection flow in a square cavity. In addition, we show the numerical results of a heated circular cylinder in a square enclosure and compare them with those of previous studies. Further discussions and conclusions are presented in Section 4.

2. Lattice-Boltzmann Method

The LBM is based on the kinetic theory of gases and originates from the lattice-gas automata and the FHP models[15]. The lattice-gas models use only Boolean states, which requires non-equilibrium ensemble averaging to obtain the macroscopic variables. The idea behind the first LBM was to use the average values, called lattice populations, to perform the simulation. At first, the collision operator of the LBM mirrored the lattice-gas operator but nowadays, the most commonly used collision operator is the BGK operator[14]. The BGK collision operator relaxes the lattice populations towards a local equilibrium function, which allows for a significant simplification of Boltzmann’s original operator and recovers the mass, momentum and energy conservation equations.
Alexander et al.\(^{16}\) and Chen et al.\(^{17}\) are the pioneers in the development of the non-isothermal LBM. The thermal-lattice-Boltzmann models can be divided into three categories: multi-speed model\(^{16,17}\), hybrid model\(^{18,19}\) and double-distribution model\(^{11,12,20,21}\).

The multi-speed approach is a straightforward extension of the isothermal LBM. Within this approach, only one set of particle distribution functions is used to solve the thermo-hydrodynamic equations. To reconstruct the energy equation, higher-order kinetic moments of the density distribution function are required. Therefore, in the formulation of the multi-speed approach larger velocity sets are applied, which is the major reason for numerical instabilities and increased complexity in the implementation of boundary conditions. Due to the high-order velocity sets, the multi-speed approach becomes impractical for three-dimensional industrial applications. The model also limits the allowed temperature variations to a narrow range. The findings of Lallemand and Luo\(^{22}\) show that the extension to even larger velocity sets will not deliver a solution for the spurious mode coupling exhibited by the multi-speed model. They suggested solving the energy equation separately from the mass and momentum equations, however, this idea could be easily adopted in a different way by using the hybrid or the double-distribution thermal lattice-Boltzmann approach.

The hybrid model solves the velocity field using the lattice-Boltzmann equation and uses a conventional numerical method such as the finite difference method to reconstruct the temperature field\(^{18,19}\). This is a compromise solution and leads to difficulties in implementing effective parallelization strategies. In the hybrid approach, the viscous heat dissipation and compression work are often omitted.

The double-distribution approach, also known as multi-distribution approach, uses two separate distribution functions, one for the flow field and a second one for the temperature field. It has better numerical stability in comparison with the multi-speed approach. The viscous heat dissipation and compression work done by the pressure can be obtained by adding a viscous heat dissipation term to the thermal lattice-Boltzmann equation. However, since only the velocity field influences the heat equation, the method has one-way coupling and, in this formulation, is known as passive-scalar model. In the passive-scalar model, the temperature (concentration) is only advected by the flow field and has no influence on it. If the temperature distribution strongly affects the flow field, this phenomenon has to be modeled additionally, for example, by using the Boussinesq approximation. In the double-distribution model, usually an equation of state with constant temperature is recovered. This property characterizes the model as “decoupling”, which sets constraints on the temperature variations and limits the simulation problems to Boussinesq flows due to modeling errors. Li et al.\(^{23}\) suggest a “coupling” double-distribution LBM on standard lattices by modifying the equilibrium distribution function, such that they reconstruct the equation of state using the local temperature instead of the reference temperature.

In this study, however, we consider the “decoupling” double-distribution LBM using two separate population sets, one for the flow field and the second one for the thermal field. This approach preserves the locality of the LBM and allows for a straightforward and efficient parallelization on high-performance architectures. Using the Chapman-Enskog expansion, one can show that this method reconstructs the incompressible Navier-Stokes equations and the advection-diffusion equation\(^{24}\) given by

\[
\begin{align}
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} & = -\nabla p + \nabla \cdot \mathbf{σ} + \mathbf{F} \\
\frac{\partial T}{\partial t} & = \frac{1}{\rho C_p} \left( \nabla \cdot \mathbf{q} - \nabla T \right)
\end{align}
\]

where \( \mathbf{u} \) is the velocity, \( \mathbf{F} \) is the external force, \( p \) is the pressure, \( \rho \) is the density, \( C_p \) is the specific heat at constant pressure, \( \mathbf{σ} \) is the stress tensor and \( \mathbf{q} \) is the heat flux. The source terms \( \nabla \cdot \mathbf{q} \) and \( \nabla T \) describe the irreversible momentum transfer and heat flux, respectively.

In (3), the advection-diffusion equation for temperature is depicted, where \( \mathbf{T} \) defines the fluid temperature in Kelvin (K). This equation is often called heat equation and the \( q_a \) term is the heat flux, which is proportional to the local temperature gradient. The Fourier’s law describes this relation as

\[
q_a = -k \nabla T
\]

with \( k \) representing the thermal diffusivity.

The source terms \( F_a \) and \( S \) in equations (2) and (3), respectively, represent external forces. In the performed simulations, we neglect the heat source term \( S \) in the heat equation because viscous dissipation and compression work do not have a significant effect on the investigated physical phenomena.

We use a BGK LBM for the flow and for the temperature fields with a small modification in the formulation of the BGK collision operator for the fluid field compared to its standard version. According to Geier et al.\(^{25}\), this modification is beneficial for the stability of the method. The coupling procedure is modeled using the Boussinesq approximation. The whole approach is integrated into the commercial GPU-based Computational Fluid Dynamics (CFD) solver ultraFluidX, developed by Fluidyna GmbH. The LBM is explicit in time, inherently transient and requires only nearest-neighbor information for the computation. That allows the method to leverage the computational power of the massively parallel architectures of GPUs, additionally, the usage of CUDA-aware MPI allows for simulating relevant industrial application problems on multiple GPUs with highly reduced turnaround times compared to traditional approaches\(^{26}\).

2.1. Lattice-Boltzmann Method for the Flow Field

The lattice-Boltzmann equation describes the probability of a particle \( f_i \) moving with velocity \( v_i \) to the neighboring cells \( x + v_i \) in time \( t + 1 \). The probability density function evolves in time according to the Boltzmann equation

\[
f_i(x + v_i, t + 1) = f_i(x, t) + \Omega(f_i)
\]
where $\Omega(f_i)$ is a collision operator chosen in such a way that all the conserved quantities are not changed during the collision process. The BGK collision operator is defined as

$$\Omega(f_i) = -\frac{1}{\tau_f} (f_i - f_i^0),$$

where $\tau_f$ is the relaxation time and $f_i^0$ is a local equilibrium distribution function for the flow field.

Using the first set of populations $f_i(x, t)$, we ensure mass (1) and momentum (2) conservation. In this case, the local density $\rho$ and the momentum density $\rho u_a$ have to be recovered using the zero and first velocity moments

$$\rho = \sum_i f_i = \sum_i f_i^0,$$

$$\rho u_a = \sum_i v_{ia} f_i = \sum_i v_{ia} f_i^0.$$

In the LBM, the local conservation of mass and momentum is ensured since the equilibrium distribution functions also ensure since the equilibrium distribution functions also

The local equilibrium function $f_i^0$ should satisfy the following higher-order velocity moments

$$\rho \delta_{a\beta} = \sum_i v_{ia} v_{\beta i} f_i^0 = \rho \delta_{a\beta} + \rho u_a u_{\beta},$$

$$
\Omega(\rho \delta_{a\beta}^0) = \sum_i v_{ia} v_{\beta i} \delta_{a\beta} f_i^0
= \rho \delta_{a\beta} (u_\alpha \delta_{\alpha \beta} + u_\beta \delta_{a\alpha} + u_\gamma \delta_{a\beta})
+ \rho u_a u_{\beta} u_{a},
$$

where $\tau_g$ is the relaxation time for the temperature populations. The local fluid temperature can be computed from the temperature distribution function

$$T = \sum_i g_i = \sum_i g_i^0.$$ (17)

As for the velocity field, the equilibrium distribution function $g_i^0$ is given by the second-order Maxwell-Boltzmann distribution

$$g_i^0 = w_i T \left( 1 + \frac{v_i \cdot u}{c_s^2} + \frac{(v_i \cdot u)^2}{2c_s^2} - \frac{u \cdot u}{2c_s^2} \right).$$ (18)

One could also use the first-order equilibrium distribution function, but this leads to velocity-dependent diffusivity$^{24,31}$. The discrete velocities $v_i$ and the respective weights $w_i$ define the lattice velocity set. In the following, we use 27 discrete velocities in three dimensions (D3Q27) for the flow field which is shown in Fig. 1. The weights of the D3Q27 velocity set are

$$w_i = \begin{cases}
\frac{8}{27}, & i = 0 \\
\frac{2}{27}, & i = 1.6 \\
\frac{1}{54}, & i = 7.18 \\
\frac{1}{216}, & i = 19.26.
\end{cases}$$ (14)

Based on the findings of White and Chomel$^{27}$, the D3Q19 lattice model brakes the rotational invariance, a problem which could not be resolved by increasing the grid resolution$^{27}$. Though, it has been shown that by using the D3Q27 model we can achieve the anticipated axis-symmetrical results. In the last years, this hypothesis was tested and confirmed by independent research groups$^{28,30}$. However, one should not neglect the fact that the D3Q27 model comes with the price of approximately 35% more computational cost.

2.2. Lattice-Boltzmann Method for the Temperature Field

To recover the advection-diffusion equation (3), a second set of populations $g_i(x, t)$ is solved. The lattice-Boltzmann equation for the temperature evolution reads

$$g_i(x + v_i t + 1) = g_i(x, t) + \Omega(g_i)$$ (15)

which resembles the lattice-Boltzmann formulation of the velocity evolution given in equation (7). The term $\Omega(g_i)$ is the BGK collision operator for the temperature field given as

$$\Omega(g_i) = \frac{1}{\tau_g} (g_i - g_i^0).$$ (16)

2.3. Coupling Strategy

In the Boussinesq approximation, the density variations are ignored as long as they are not triggering buoyancy forces. In this vein, the buoyancy force density $F_b$ reads

$$T = \sum_i g_i = \sum_i g_i^0,$$ (20)

with $\gamma$ being the gravity acceleration and $T_0$ being the reference temperature given by $T_0 = (T_{\text{hot}} - T_{\text{cold}})/2$. The buoyancy
forcing term is added to the right-hand side of the flow field evolution equation (7) using the exact difference method proposed by Kupershtoh\(^{(2)}\).

The Boussinesq approximation introduces a modeling error which can be undesirably large if the problem experiences significant density variations caused by the temperature differences. Gray and Giorgini\(^{(13)}\) as well as Bückle and Perić\(^{(14)}\) investigated the theoretical and numerical range of the validity of the Boussinesq approximation. They found that the modeling errors are negligible (in the order of 1%) when the temperature variations are smaller than 10 K (for air), but they become significant beyond 30 K.

Therefore, physical phenomena such as natural convection, ventilation, air conditioning or central heating that deal with small temperature and velocity variations can be simulated without considerable modeling errors using the Boussinesq approximation. Relevant Boussinesq flow applications in the automotive industry are, for example, the simulation of the battery packaging for electric vehicles, heat transfer between small elements, air-conditioning and ventilation of the vehicle interior\(^{(35)}\).

2.4. GPU Implementation and Performance Aspects

We have designed the data structures and algorithms such that our framework can achieve unprecedented performance for thermal LBM methods. In principle, any well-designed GPU-based LBM code for solving the flow field can serve as a basis for the thermal LBM approach as described in this work, however, the way how the thermal part is added is crucial to minimize the impact on simulation performance. The most important part is to perform the collision of the two velocity sets and the coupling in a single GPU kernel to guarantee a minimum amount of global memory accesses. For example, \(u\) and \(T\) are both needed for the thermal collision as well as the addition of the buoyancy force via the exact difference method, and \(u\) is also needed for the fluid collision. Therefore, it is optimal to first load the fluid distributions into the local memory to compute \(u\) and perform the fluid collision, then to load the thermal distributions to compute \(T\) and perform the thermal collision using \(u\) and \(T\), and then to use these known values of \(u\) and \(T\) to add the buoyancy force to the fluid distributions before writing all the variables back to global memory. In a similar manner, the interpolated boundary conditions for both velocity sets that are mentioned in the following sections can reuse some information like the wall distance of the directions 1 to 6, if both the fluid and the thermal boundary condition are applied together per direction of the respective distributions in the same GPU kernel.

Following the concepts of reusing data as outlined above as much as possible, solving the additional temperature field only has a minor influence on the overall simulation performance. Our current implementation achieves approx. 2,200 million node updates per second (MNUPS) on a set of four NVIDIA Tesla V100 GPUs on a DGX Station using single precision. CPU-based LBM frameworks such as wallerBerla reach a performance of up to approx. 5 MNUPS per core for non-uniform grids and about 2-2.5x more for uniform grids using double precision and a single D3Q19 velocity set only for the flow field\(^{(36)}\). Therefore, if we assume that the performance gain of using single precision would roughly be compensated by the need for 15 additional velocity distributions (8 more for the flow field and 7 for the temperature field) and the coupling between the fields, the resulting approx. 10 MNUPS per core would require using more than 50 CPU cores to achieve the performance of our framework on a single V100 GPU.

Thus, ultraFluidX has the potential to execute simulations for large industrial applications on single GPU servers such as the NVIDIA DGX Systems with 4, 8 or 16 V100s (DGX Station, DGX-1 and DGX-2), where large CPU clusters with hundreds of cores would be necessary to achieve similar performance. Ren et al.\(^{(37)}\) recently also presented a GPU implementation of the double-distribution LBM with passive scalar transport, but they do not comment on their overall achieved performance and we use full coupling between the fields with the Boussinesq approximation instead.

3. Results and Discussion

To verify our parallel implementation of the thermal LBM, we present two general validation scenarios. First, we show the results for a natural convection problem. As a second validation case, we simulate a heated cylinder in an enclosed cavity with varying position of the center of the cylinder.

3.1. Natural Convection in a Square Cavity

benchmark solution for the natural convection problem was proposed by De Vahl Davis\(^{(38)}\), Fig. 2 shows a schematic representation of the respective configuration, where the horizontal walls are held at constant temperature (\(T_{\text{hot}}\) and \(T_{\text{cold}}\), respectively) and the rest of the walls are adiabatic. A mesh resolution of \(160 \times 160 \times 8\) was employed for the validation. The simulations are performed in 3D, however, since the problem has a 2D solution, we assume periodicity and use a domain with only a small extent in \(z\)-direction. To ensure that our 3D implementation is valid, we have performed additional tests with arbitrary chosen periodicity direction and the obtained results have been identical (not depicted here). All the results shown in the current study represent a slice in the \(z\)-normal plane for the velocity and for the temperature fields.

The constant temperature boundary condition is implemented using the scheme proposed by Li et al.\(^{(39)}\) for interpolated thermal boundary conditions. The bounce-back scheme is used for the adiabatic walls. No-slip fluid boundary conditions are imposed on all the boundaries and they are also implemented using the bounce-back scheme. In the \(z\)-direction of the domain, periodicity boundary conditions are imposed for the two population sets.

The natural convection phenomenon is characterized by the Rayleigh number that describes the transition from conductive to convective transport,

\[
Ra = \frac{ag\Delta T L^3}{\nu k}
\]

(21)
in which $\alpha$ is the thermal expansion coefficient, $\Delta T = T_{hot} - T_{cold}$ is the temperature difference, $L$ the length of the domain, $\nu$ the kinematic viscosity and $\kappa$ the thermal diffusivity. We validate our implementation by calculating the averaged Nusselt number

$$Nu = \frac{1}{L} \int_0^L \frac{1}{\Delta T} \frac{\partial \theta}{\partial y} \, dy,$$

with the local Nusselt number

$$Nu_l = \frac{q_x L}{\lambda \Delta T},$$

where $q_x$ is the heat flux in x-direction and $\lambda$ is the heat conductivity. The obtained results are shown in Table 1. They are in very good agreement with the De Vahl Davis$^{(3)}$ benchmark solution.

| Table 1 | Comparison of the averaged Nusselt number ($\bar{Nu}$) of the present study with the De Vahl Davis$^{(3)}$ benchmark solution. |
|---------|---------------------------------------------------------------|
| $Ra$    | $\bar{Nu}$ at the hot wall | Ref.$^{(3)}$ | Error (%) |
| $10^3$  | 1.1174 | 1.118 | 0.05 |
| $10^4$  | 2.2482 | 2.243 | -0.23 |
| $10^5$  | 4.5291 | 4.519 | -0.22 |
| $10^6$  | 8.8127 | 8.800 | -0.14 |

3.2. Heated Cylinder in an Enclosed Cavity

For this part of the study, we consider an enclosure around a heated cylinder, as depicted in Fig. 3. The walls of the enclosure are kept at constant cold temperature $T_{cold}$, while the cylinder walls are heated at temperature $T_{hot}$. For the flow field, no-slip boundary conditions are imposed on all the walls. We again use the interpolated thermal boundary conditions for the thermal field and a bounce-back scheme for the flow field. The problem is uniformly discretized with 500 $\times$ 500 $\times$ 8 cells and all the cells within the solid circular cylinder have been deleted before simulation. Like for the natural convection problem, all the simulations are performed in 3D, although the flow around an enclosed heated cylinder has a 2D solution. Thus, we again assume periodicity in the $z$-direction and only show a slice in the $z$-normal plane.

We compare our findings with the work of Kim et al.$^{(5)}$, where the authors use the Navier-Stokes approach to show how the position of the cylinder influences the flow field and the temperature distribution. The simulations are performed with varying Rayleigh number from $10^3$ to $10^5$ and with a Prandtl number ($Pr = \nu/\alpha$) fixed at 0.71 for air. Since the flow at $Ra = 10^3$ is very much dominated by conduction and we are mainly interested in coupled aero-thermodynamic problems, we neglected this case for the current study. Kim et al.$^{(5)}$ simulated such low Rayleigh numbers and showed that the flow and temperature field results are very similar to the results at $Ra = 10^4$. Instead, we perform simulations at $Ra = 10^5$, which to our best knowledge were not fully investigated in previous studies. The ratio between the length of the square domain $L$ and the radius of the cylinder ($r = R/L$) is taken as $r = 0.2$. Three different values for the position of the center of the cylinder delta are tested: $0.2L$, $0.0L$ and $-0.2L$. To the best of the authors knowledge, no comparison results are found for the scenarios at $Ra = 10^7$ with $\delta = 0.2L$ and $\delta = -0.2L$.

3.2.1. Flow and temperature fields at $\delta = 0.0L$

In Fig. 4, the center of the cylinder is in the middle of the square enclosure ($\delta = 0.0L$). The steady state of the present scenario has a symmetric solution about the $y$-axis through the center of the circular cylinder ($x = 0$). This two-folded symmetry was also shown by Kim et al.$^{(5)}$ and Moukalled and Acharya$^{(6)}$. Characteristic for the flow of the investigated heated cylinder in an enclosed cavity is that the hot thinner fluid rises along the heated surface of the cylinder. Once the fluid reaches the cold surface of the enclosure, the fluid cools down becoming denser and moves downwards following the surface of the cold walls. This behavior is observed regardless of the position of the
According to the data obtained at $Ra = 10^4$ and $Ra = 10^5$, a good agreement has been found for the flow field and the thermal distribution with Kim et al.\(^5\). At $Ra = 10^7$, the convection is significant, and the fluid recirculation becomes stronger. Due to flow separation, a vortex is formed at the bottom of the domain that was also reported in Ref.\(^{40}\). Kim et al.\(^5\) observed a separation of the flow and a tiny vortex formation even at $Ra = 10^6$, which is not visible in our findings. We anticipate that the main two reasons for the deviation in our results are the grid generation and resolution. In their work, Kim et al.\(^5\) used a stretched grid with finer resolution near the surfaces, while we applied a uniform grid with lower resolution. This could possibly be resolved either by uniformly increasing the number of grid points or by multi-resolution mesh refinement near the hot and cold surfaces.

3.2.2. Flow and temperature fields at $\delta = 0.2L$

As shown by Kim et al.\(^5\), the evolution of the flow can be investigated as a function of $\delta$. The flow and thermal fields are strongly dependent on the distance between the heated cylinder and the cold enclosure walls. When the cylinder is moved upwards closer to the top wall as depicted in Fig. 5, the flow structures at $Ra = 10^4$ get merged into one large vortex structure. For low Rayleigh numbers the flow recirculation vortex is located below the heated cylinder and rises upwards towards the top wall when the Rayleigh number is increased. Larger temperature gradients and strong convective flow are observed between the hot inner cylinder and the top wall of the domain. Due to the smaller distance between the cylinder surface and the top wall, the isotherms are dense and only small distortion of the isotherms exists. In contrast, the isotherms in the bottom part of the cavity are coarse.

Our findings at $\delta = 0.2L$ for low Rayleigh numbers ($Ra = 10^4$ and $Ra = 10^5$) are consistent with the work of Kim et al.\(^5\). However, for high Rayleigh numbers, the authors show small tertiary vortices formed at $Ra = 10^6$, which cannot be seen in the current study. We assume that the observed deviations are mainly...
due to the different strategies applied in mesh generation and resolution as mentioned in Section 3.2.1.

3.2.3. Flow and temperature fields at δ = −0.2L

If we move the heated cylinder downwards as shown in Fig.6, the space between the cylinder and the bottom wall becomes smaller. The larger temperature gradients close to the top boundary give rise to a longer and a sharper plume formation. In Fig. 6, the streamlines and isotherms at \( Ra = 10^5 \)–\( 10^6 \) resemble the results obtained using the Navier-Stokes approach in Ref.\(^\text{19}\). At a higher Rayleigh number (\( Ra = 10^7 \)), which was not investigated by Kim et al.\(^\text{19}\), the flow and temperature fields get even more distorted because of the significant convection effects. In the flow field, two separate vortices appear, one is located in the upper region of the enclosed cavity and a second one is located at approximately the same height as the center of the heated cylinder. The temperature field shows strong temperature gradients and distorted plume structures.

4. Summary and Outlook

In this paper, we validated our implementation of the thermal LBM by simulating natural convection in a square cavity and a heated cylinder in a cooled square enclosure. The double-distribution LBM was implemented for massively parallel GPU architectures and all the performed simulations were executed in 3D with assumed periodicity in \( z \)-direction. For the heated cylinder, we analyzed the effect of different Rayleigh numbers from \( 10^4 \)–\( 10^7 \) and the influence of the position of its center. The results were depicted using streamline and isotherm plots. The behavior of the flow and thermal fields agrees well with previously published results, which verifies the correctness of our parallel implementation for thermal phenomena. To resolve the finer flow structures even better, higher resolution or multiresolution mesh refinement are necessary and will therefore be subject of future work.

To expand the applicable scope of our 3D thermal lattice-Boltzmann implementation, we intend to investigate more complex geometries with industry-relevant application, such as the indoor air flow simulation conducted by van Treeck et al.\(^\text{20}\) and convective heat transfer over a wall-mounted cube.

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