Rayleigh-Bénard convection via Lattice Boltzmann method: code validation and grid resolution effects

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Abstract. Thermal plumes, formed at the wall of turbulent natural convection cells, play an important role in the re-suspension and dispersion process of inertial particles. For this reason, a good resolution of the region close to the wall is necessary to correctly describe the plumes and, consequently, the particle dynamics. In this work, a Lattice Boltzmann Method (LBM) coupled with Lagrangian particle tracking is used to understand the effects of the filtering action exerted by the grid resolution on particle trajectories. A validation of the numerical method against the work of Kunnen (2009) and Schumacher (2009) is presented and, in this framework, mean and RMS statistics on fluid temperature are considered and analyzed in detail.

1. Introduction
The dispersion of inertial particles in turbulent convection has direct relevance for many industrial and environmental applications, where the fluid heat transfer can be modified by the presence and deposition of particles at the walls (e.g. nuclear power plants, petrochemical multiphase reactors, cooling systems for electronic devices, pollutant dispersion in the atmospheric boundary layer, aerosol deposition, etc.). Over the past years, turbulent convection has been the subject of extensive studies (see e.g. [1, 5, 7]), which attempted to determine the main flow features and the relation between the different parameters which characterize the fluid velocity and temperature fields, but only few of them focused on Lagrangian statistics. A Lagrangian tracking of tracer particles has been employed in [8] to study the properties of the mixing zone, the zone close to the wall dominated by rising and falling thermal plumes. The behaviour of heavy particles in stably stratified turbulence has been studied in [11] focusing on the relation between preferential concentration and flow stratification.

The focus of the present work is to evaluate the effects of the grid resolution on the flow characteristics and on particle behaviour in a turbulent Rayleigh-Bénard cell. To this aim a Lattice Boltzmann Method (LBM) coupled with a Lagrangian particle tracking has been chosen to solve for the fluid and particle velocity and temperature fields. Unlike the conventional numerical schemes based on discretization of macroscopic continuum equations, LBM is based on simplified kinetic models that incorporate the essential physics of mesoscopic scales, so that
the macroscopic averaged properties obey the desired macroscopic equations (see e.g. the review articles [2, 4]). For what concerns single-phase turbulent flows, the LBM can be considered as an alternative numerical method with low algorithm complexity and good parallelization capabilities. However, if a local grid refinement is not considered, the LBM is restricted to a discretization onto a regular grid which might be not enough to capture correctly the physics in the close vicinity of the wall where the velocity and temperature boundary layers are formed. As in the present work the code is based on a uniform grid and, of course, we expect the LBM to perform as other discretization schemes, we need to understand which grid spacing is accurate enough for the purposes of this study. For this reason, the code has been validated against other two numerical works by [5] and [8] at different Rayleigh numbers. A good agreement between the LBM and the other methodologies has been found, confirming that the method provides an accurate description of the fluid momentum and temperature fields and, therefore, suitable for an analysis of particle resuspension dynamics in the domain. In Section 3, some preliminary results on tracer particles tracked in the same physical system described with three different domain discretizations, are also presented. Results showed that the grid resolution has a strong impact on particle behaviour exhibiting a lower dispersion if a coarser grid is used.

2. Methodology

The Lattice Boltzmann method is a well established tool described in detail in many previous publications (see e.g. [10] and [2]), so here only the main features characterizing this technique are reported. The simplest lattice Boltzmann equation, under the BGK approximation, can be written as follows:

\[ f_i(x + \Delta x, t + \Delta t) - f_i(x, t) = -\frac{\Delta t}{\tau} [f_i(x, t) - f_{eq}^i(x, t)] + F_i \Delta t \]  

where \( f_i(x, t) = f_i(x, v = c_i, t), i = 1, ..., n \) is the probability of finding a particle at lattice site \( x \) at time \( t \), moving along the lattice direction defined by the discrete speed \( c_i \) during a time step \( \Delta t \). The left-hand side of the equation represents the so-called streaming term, which corresponds to the evolution in time of the probability function \( f \). The RHS describes the collision via a simple relaxation towards local equilibrium \( f_{eq}^i \) (a local Maxwellian distribution expanded to second order in the fluid speed) in a time lapse \( \tau \). This relaxation time fixes the fluid kinematic viscosity as \( \nu = c_s^2(\tau - 1/2) \), where \( c_s \) is the speed of sound of the lattice fluid, \( (c_s^2 = 1/3 \) in the present work). Finally, \( F_i \) represents the effects of external forces. The set of discrete speeds must be chosen such that rotational symmetry is fulfilled to the required level of accuracy. The fluid density \( \rho = \sum_i f_i \), and speed \( u = \sum_i f_i c_i / \rho \) can be shown to evolve according to the (quasi-incompressible) Navier-Stokes equations of fluid dynamics. In this paper, we will refer to the nineteen speed D3Q19 model shown in Figure 1a. The temperature population \( g_i \) is evolved on the lattice according to the same formulation of the Boltzmann equation used for the fluid momentum. The temperature is modeled as a scalar \( T = \sum_i g_i \), and it provides an external forcing via a buoyancy term, which is taken into account by introducing a suitable shift of the velocity and temperature fields entering the local equilibrium distributions.

The reference geometry, shown schematically in Figure 1b, is a Cartesian slab bounded by two horizontal walls having dimensions equal to the size of the computational grid employed for the calculations. Since in the present work a Lattice Boltzmann approach with a grid resolution equispaced in all directions has been chosen, it becomes useful to validate the code against other numerical works to check its capability in correctly capturing the flow field properties in the vicinity of the wall. The two works chosen as reference for this benchmark are: the finite-difference code by [5] and the pseudo-spectral code by [8]. The former has been selected for its relatively low Rayleigh number, the use of grid refinement close to the wall according to a log-normal distribution of the grid nodes and for the more realistic choice of no-slip boundary
Figure 1. (a) Scheme of the D3Q19 model for the velocities in the LBM, (b) Sketch of the computational domain.

Table 1. The code has been validated against the numerical works by Kunnen et al. (2009) and Schumacher (2009) and for each test case two grid resolutions under the same physical parameters have been tested with the Lattice Boltzmann Method. The parameters used for the two benchmarks are here summarized.

| Grid                     | Grid type | b.c. vel/T       | $\Delta T$ | Ra        | Pr        |
|--------------------------|-----------|------------------|-------------|-----------|-----------|
| Kunnen et al. (2009)     | 128x128x64| Refined No-slip   | $/T_{fixed}$| 1         | $2.5 \cdot 10^6$| 1        |
| LBM                      | 128x128x64| 256x256x128      | Regular No-slip | $/T_{fixed}$| 1         | $2.5 \cdot 10^6$| 1        |
| Schumacher (2009)        | 2048x2048x512| Regular Stress-free | $/T_{fixed}$| 2$\pi$    | $1.2 \cdot 10^8$| 0.7      |
| LBM                      | 1024x1024x256| 512x512x128      | Regular Stress-free | $/T_{fixed}$| 2$\pi$    | $1.2 \cdot 10^8$| 0.7      |

conditions. The latter because it employs a pseudo-spectral code, considered to be one of the most accurate Navier-Stokes solvers, on a regular grid at relatively high Rayleigh number using stress-free boundary conditions. To mimic the two numerical works as close as possible, the system properties, the grid resolution and the boundary conditions have been modified accordingly in the LBM. In Table 1 the parameters used in the validation tests are summarized. Periodic boundary conditions are imposed on both the velocity and the temperature field in the directions parallel to the walls. The no-slip and the stress-free conditions are implemented using a standard bounce back method which assures a second-order accuracy with the wall situated between two grid nodes. The temperature field is decomposed into a linear profile $T_{\text{lin}}$ and fluctuations $T'$ about the profile which are evolved in time. Since the total temperature is prescribed to be constant at the bottom ($Z = 0$) and top wall ($Z = 1$) the condition $T' = 0$ follows there, so a mid-grid bounce back method is employed also for the temperature field.

The Rayleigh number is defined as $Ra = (\alpha g \Delta T H^3) / \nu \kappa$ where $g$ is the gravitational acceleration, $\alpha$ the coefficient of thermal expansion, $\Delta T$ the temperature difference between the two walls, $\kappa$ the thermal diffusivity and $\nu$ is the fluid kinematic viscosity. The Prandtl number is defined as the ratio of the kinematic viscosity to the thermal diffusivity of the fluid as $Pr = \nu / \kappa$.

As by definition in LBM the grid resolution corresponds to the size of the computational domain,
to maintain the same $Ra$ and $Pr$ number for different grid sizes i.e. for different values of $H$, the values of $\alpha g$, $\nu$ and $\kappa$ have been varied.

To understand the impact of the grid resolution on particle dynamics, a Lagrangian approach has been used to track a swarm of $1.6 \times 10^5$ tracer particles dispersed in the domain at $Ra = 5 \times 10^6$. No-slip boundary condition and constant temperature have been imposed on the velocity and temperature fields respectively. Three grid resolutions have been employed in this particular test case: $256 \times 256 \times 128$, $128 \times 128 \times 64$ and $64 \times 64 \times 32$. Particles are initially released at random positions on a plane placed at the same physical location from the bottom wall in all the grids considered. Specifically, the position $H_0$ of the plane in the lower resolution case is $0.5$ lattice unit from the bottom wall (which sits $0.5$ grid points below the first lattice node) and it is then multiplied by 2 and 4 to obtain the starting height in the other two grids. This particular configuration has been chosen to capture the effects of the plumes on particle resuspension at the early stages of the simulation, when hot plumes start to form at the bottom plate and particles are still non-homogeneously distributed in the domain. As particles have zero inertia, their equation of motion reduces to the simple kinematic relationship $dx/dt = u$, where $u$ is the fluid velocity at the particle position and their temperature is equal to the fluid one calculated at the particle position. An explicit Adams-Bashforth scheme is used for the time integration of the equation of particle motion and a linear interpolation scheme is used to obtain both the fluid velocity and temperature at the point of the particle.

3. Results

3.1. Benchmark tests of the LBM code

In this section, results of the benchmark tests between the Lattice Boltzmann code and the works of [5] and [8] are presented.

In Figure 2a the mean temperature profile obtained with the Lattice Boltzmann method (symbols) is compared with the results obtained by [5] (black curve). All the curves are nicely overlapping on top of each other, thus suggesting that mean quantities are not really sensitive to both the numerical scheme and the employed grid resolution. It is possible to notice that the LBM, despite the regular grid, is capable to correctly capture the thermal boundary layer thickness $\delta_T$ in its geometrical extrapolation (see the inset of Figure 2a) if compared to the finite-difference code result. A value of about 0.045 in non-dimensional units is found. This value is consistent with the position of the peak in the temperature RMS profile visible in Figure 2b. However, some discrepancies in the RMS profile are still present in the bulk of the cell. This can be mainly due to two effects: (i) the different simulation time which is slightly longer in the finite difference case with respect to the present work, as it was checked by calculating the time-averaged statistics using different time windows and (ii) the different grid resolution used in the bulk region of the flow which is higher in the LBM with respect to the work of [5], thus providing a better description of this flow region. Since we are mostly interested in the dynamics of the boundary layer, this discrepancy can be considered negligible for the purposes of this study.

To quantify the total (conductive and convective) turbulent heat transport inside the domain, the volume and time averaged Nusselt number, normalized by the conductive heat flux obtained in absence of convection, has been calculated as:

$$Nu(z, t) = \frac{(u_z T)_{A,t} - \kappa \partial_z \langle T \rangle_{A,t}}{\kappa \Delta T / H}$$

$$Nu = \frac{1}{H(t - t_0)} \int_0^H \int_0^t Nu(z, t) dz dt = 1 + \frac{H}{\kappa \Delta T} \langle u_z T \rangle_{V,t}$$

In [5] (see also [6]) a value of 11.08 for the total Nusselt number was found. In the present case a Nusselt number of $11.07 \pm 1.03$ and $11.16 \pm 1.15$ has been obtained for the low and high resolution
Figure 2. Benchmark between the LBM code using two grid resolutions (symbols) and the work by [5] (solid black line). (a) Mean temperature profile varying with the cell height with, in the inset, geometrical extrapolation of the thermal boundary layer thickness and (b) RMS of the temperature varying with the cell height with zoom in of the region where sharp temperature gradients are present.

case respectively. This result confirms the good agreement between the two codes and, as the introduced error between both approaches is around or less than 1%, the non-sensitivity of the results to the grid resolution. Using these values for the Nusselt number the boundary layer thickness can be calculated as:

\[ \delta_T = \frac{H}{2Nu} \]  

A value of 0.045 ± 0.005 has been found for both resolution, thus confirming the previous result obtained with the geometrical extrapolation.

In Figure 3a a comparison between the mean temperature profile varying with the cell height obtained with the LBM (symbols) and the pseudo-spectral code by [8] (black line) is reported. An overall good agreement among the curves is found. However, discrepancies are present in the close vicinity of the wall for the lower resolution case, as visible in the inset, where a small portion of the domain is considered for visualization. The black line indicates the value of the boundary layer thickness as in [8], whereas the colour dotted lines refer to the geometrical interpretation of \( \delta_T \) obtained with the LB method. The lower grid resolution overestimates the value of \( \delta_T \) and it is obviously not enough to correctly capture the dynamics in the boundary layer at this high Rayleigh number. In Figure 3b the temperature RMS varying with the cell height is presented. As expected, the lower grid resolution is overestimating the boundary layer thickness, but deviations are found in the bulk of the cell with both grid resolutions\(^1\) of our LBM simulations. If we compare the value of the volume and time averaged Nusselt number a good agreement is found, also in this case. The obtained values of 57.0 ± 1.7 on the 1024 × 1024 × 256 grid and of 55.3 ± 4.3 on the lower grid resolution compare well with the 56.4 ± 0.6 of [8]. The error in the Nusselt number, estimated by calculating the time averaged RMS of Nusselt number, is higher in the LBM case with respect to the pseudo-spectral code. This can be due to the different grid resolution employed in the two works which was limited in the LBM case by the computational resources available.

\(^1\) As only a portion of the available computational resources was dedicated to the validation of the methodology, the low resolution case, being less expensive from a computational viewpoint, was run for a period longer than the higher resolution case. This allowed to obtaining slightly better results in the bulk of the cell with respect to the high resolution case.
3.2. Lagrangian insights

In this section some preliminary results on tracer particles dynamics are presented. The reader should refer to Section 2 for details on particle tracking methodology and simulation parameters used in the following discussion.

The Lagrangian trajectories of tracer particles has put into evidence the direct impact that the computational grid has on the trajectory of the particles dispersed in the flow. In Figure 4a, the mean square displacement of particle position varying in time using three grid resolutions is shown. The mean square displacement has been calculated as the square of the difference between the particle initial position at time $t = 0$ and the particle position at time $t$ as:

$$\langle \sigma(t)^2 \rangle = \frac{1}{N_p} \sum_{i=0}^{N_p} (x_i(t) - x_i(t = t_0))^2$$  \hspace{1cm} (5)

The statistics have been normalized in the vertical direction by the particle initial position $H_0$ and by the large circulation time scale on the horizontal axis. A coarser grid seems to under-predict single particle dispersion causing, with its implicit filtering action, particles to be confined in a smaller region of the domain. The reason for this can be found in the close relationship between the small-scale thermal plumes developing at the wall and particle dynamics. The sheetlike plumes close to the wall are responsible, in their morphological evolution, for the formation of mushroom-like plumes in a region confined to few $\delta_T$ [9, 7]. These three dimensional plumes are accountable, depending on their temperature, for the upward or downward particle transport. Changing the grid resolution modifies the statistical presence, the shape and the properties (velocity, temperature etc.) of sheetlike plumes and consequently affects the overall dispersion of particles in the cell. In Figure 4b an instantaneous snapshot of particles coloured with their temperature is shown. It is possible to notice that cold regions of fluid (green) are surrounded by warm (red) regions that correspond to the sheetlike structures. As we are focusing on the initial transient period when the convection starts to develop inside the domain, tracer particles are pushed at the edges of the sheetlike plumes, and bursts of particles are starting to rise due to the formation of mushroom-like type of structures, thus confirming the importance of these plumes in particle suspension.
4. Conclusions

A Lattice Boltzmann approach, coupled with Lagrangian particle tracking of passive tracers, is used in this work to understand the effects of the grid resolution on particle behaviour in a Rayleigh-Bénard cell. Results of a code validation against two other numerical works by [5] and [8] have been discussed. Good agreement in the mean temperature profile has been found in both cases. In the comparison with Kunnen and co-authors a good agreement, in the vicinity of the wall, is found also in RMS profiles for all grid resolutions considered, suggesting that at this low Rayleigh number the LBM results are independent from the grid resolution. Discrepancies are found in the bulk of the flow due to differences in both the simulation time lengths and the local grid resolutions. In the comparison with the work of [8] discrepancies are found in the temperature RMS profiles especially for the lower grid resolution which is not enough to correctly capture the thermal boundary layer thickness. Preliminary results on tracer particles suggest that particle motion is strongly influenced by the grid resolution as it impacts on the description of the small scales of the flow which are more effective in particle re-suspension and dispersion. Indeed, particles released in a flow obtained with the most refined grid are traveling longer distances with respect to those in the other two resolutions.

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