Validation of Three-Dimensional Grid Refinement for Efficient Resolution of Lattice Boltzmann Method

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The lattice Boltzmann method (LBM) is a method for modeling fluid dynamics which is based on discrete kinetic theory. It discretizes the continuous Boltzmann equation in velocity, spatial and temporal space and solves a transport equation for particle populations. To enable an efficient time-space discretization with discrete velocity sets, common LBM solvers employ uniform grids making them prohibitively expensive for the simulation of high Reynolds number flows. This paper describes the implementation of a vertex-centered grid refinement method with BGK operator in the Open-source Lattice Boltzmann code, OpenLB. The method is validated for flow around a 3D circular cylinder with Reynolds number varying from 100 to 300 and the 3D lid-driven cavity with Reynolds number equals 3200. The results are in good agreement with experimental measurements and the reference solutions with uniform grid spacing. The simulation with grid refinement allows for remarkable computational cost savings for a given accuracy.

I. Nomenclature

c_i	=	discrete particle velocity
c_p	=	pressure coefficient
c_s	=	non-dimensional speed of sound
δt	=	temporal derivative operator
δx	=	spatial derivative operator
Δt	=	discrete time step
Δx	=	discretization spacing
D	=	cylinder diameter
ϵ	=	order of magnitude of perturbation expansion terms
f_i	=	i component of the particle distribution function
$f_{i,c}, f_{i,f}$	=	i component of the particle distribution function on coarse and fine grid
f_i^{eq}, f_i^{neq}	=	i component of the equilibrium and non-equilibrium particle distribution function
f_i^*	=	i component of the post-collision particle distribution function
Kn	=	Knudsen number
λ	=	mean free path
L	=	characteristic length
Ma	=	Mach number
Ma_∞	=	free-stream Mach number
n	=	grid spacing ratio

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N	=	grid resolution per characteristic length
N_p	=	number of total points
N_t	=	number of total time steps
ν	=	kinematic viscosity
Ω	=	collision operator
p	=	pressure
p_0, p_∞	=	stagnation and free-stream pressure
Re	=	Reynolds number
σ	=	standard deviation
τ	=	relaxation time
τ_c, τ_f	=	relaxation time on coarse and fine grid
θ	=	angular coordinate in degree
U	=	velocity
U_x, U_y, U_z	=	x-, y- and z-component of velocity
U_{lb}	=	characteristic lattice velocity
W_x, W_y, W_z	=	x-, y- and z-component of vorticity
W_{mag}	=	magnitude of vorticity
x	=	spatial coordinate
t	=	time

II. Introduction

THE Lattice Boltzmann Method (LBM) is gaining popularity as a method for computational fluid dynamics. Developed from the lattice gas automata model, it discretizes the continuous Boltzmann equation in velocity, spatial and temporal space and solves a transport equation for particle populations, which represent the probability density functions of particles with a given microscopic velocity. The discretization in velocity space is chosen such that the continuum equations of fluid dynamics are recovered on the macroscopic scale. For computational efficiency, the particle transport is modelled as a collision and a streaming process over a discrete lattice mesh. The lattice, or grid, is inherently uniform. Although this uniform layout simplifies meshing, computation and communication, the computational resources needed grow considerably as the overall grid resolution increases for high Reynolds number simulations. As a result, grid refinement for LBM simulations at high Reynolds number flows is necessary.

In recent years multiple grid refinement models have been proposed. To understand these, it is first necessary to review the algorithm employed for particle propagation. The discrete Boltzmann equation for population, or particle distribution, f_i is given as:

$$f_i(x + c_i \Delta t, t + \Delta t) = f_i(x, t) - \frac{\Delta t}{\tau} (f_i(x, t) - f_i^{eq}(x, t)) , \quad (1)$$

where x is the spatial coordinate, c_i is the discrete particle velocity and Δt is the time step. The last term, referred to as the *BGK collision operator*, models the collision of particles as the gas is relaxing towards its equilibrium state f_i^{eq} by redistributing them among the different populations. The rate of this relaxation process is determined by the relaxation time τ . The discrete Boltzmann equation can therefore be modelled as two processes. First, the distribution function is locally collided during the *collision step*, and the post-collision distribution function, f_i^* is given as:

$$f_i^*(x, t) = f_i(x, t) - \frac{1}{\tau} (f_i(x, t) - f_i^{eq}(x, t)) . \quad (2)$$

This post-collision population is redistributed to the neighbor nodes during the *streaming step*:

$$f_i(x + c_i \Delta t, t + \Delta t) = f_i^*(x, t) . \quad (3)$$

The challenge of grid refinement methods is to establish a consistent link between the distribution functions, or populations, across an interface, connecting two grids with different grid sizes Δx and relaxation times τ . This involves *coupling* the populations at nodes where coarse and fine grid nodes coincide, and *interpolating* the unknown populations from the coarse grid to the fine grid at the other nodes.

Most grid refinement methods take advantage of the fact that the distribution function can be divided into two parts: the equilibrium part f_i^{eq} which is determined by the macroscopic fluid density and velocity, and the non-equilibrium

distribution function $f_i^{neq} = f_i - f_i^{eq}$ which represents local fluctuations from equilibrium state. The correct coupling of coarse populations, $f_{i,c}$, and fine populations, $f_{i,f}$, can be achieved by rescaling only the non-equilibrium part.

One of the first grid refinement methods was proposed by Filippova and Hänel [1]. They established a scaling relation between the fine and coarse grid populations based on the Chapman-Enskog analysis by approximating the first-order term of the Taylor-expansion of f_i over Knudsen number to f_i^{neq} . For constructing the unknown populations at fine nodes lying between coarse nodes, a second-order accurate interpolation approach was adopted. The refinement scheme was validated with a 2D benchmark problem of the steady and unsteady circular cylinder flow in a channel. The results were in good agreement with reference values and the CPU time was found to be comparable to that of incompressible finite-volume or finite-difference Navier-Stokes solvers. A more accurate spatial interpolation method using a symmetric, cubic spline fitting was proposed by Yu et al. [2]. This was combined with a three-point Lagrange interpolation for temporal scaling. The method was validated on 2D benchmark cases at Reynolds numbers $Re \leq 5000$ with a 5 block cascade domain (i.e. maximum spacing ratio is 32) and a 38 speed up was shown compared to a uniform grid solution. Dupuis et al. [3] improved stability by rescaling the post-streaming distribution function instead of the post-collision one. They achieved a similar performance to Filippova's method and demonstrated a significant speed up for a steady 2D Poiseuille flow. Lagrava et al. [4] introduced a non-weighted low-pass filter aiming at removing abundant information on the fine grid that was not resolved by the coarse grid, in order to avoid numerical instability at relative high Reynolds numbers. The filter was applied only on the non-equilibrium distribution functions to avoid an artificial increase of viscosity. They also demonstrated that a second order interpolation was not able to conserve the mass in the reconstruction process and a local cubic interpolation scheme was mandatory to meet the stability requirement of lattice Boltzmann method. This method was validated on two 2D benchmark cases: the flow past a circular cylinder at $Re = 100$ and the dipole-wall collision process. In the latter case, perturbations happened when Re reached 5000 when no filter technology was applied. They showed that introducing the filtering algorithm helped eliminate these perturbations.

A different grid layout, named the cell-centered, was used by Chen et al. [5] for a 2D grid refinement method. In this case, the missing populations are constructed in a volumetric way to strictly meet the conservation law and prevent a difference of the fluxes of mass and momentum at the refinement interface. Rohde et al. [6] extended Chen's model to 3D based on uniform redistribution method.

In recent years, more grid refinement approaches for lattice Boltzmann methods emerged. Touil et al. [7] developed a grid refinement model of large eddy simulation (LES) solver for LBM based on D3Q19 model. Both direct numerical simulation (DNS) and LES were carried out on a turbulent plane-channel flow and validated against the reference data from a high-resolution pseudo-spectral simulation. When comparing with a Navier-Stokes LES solver based on finite-volume discretization, an improved accuracy in boundary layers was showed in LBM-LES model. Dorschner et al. [8] extended the vertex-centered grid refinement approach to entropic incompressible, thermal, and compressible 3D lattice Boltzmann models. Their approach was successfully validated on several turbulent benchmarks, including supersonic flow around NACA0012 airfoil with $Ma_\infty = 1.5$ and $Re = 10000$.

In summary, grid refinement method for two-dimensional LBM has been investigated and developed functionally, but the implementations and validations in 3D are rarely seen. This paper describes and validates a novel implementation of a vertex-centered 3D grid refinement method in the Open Source LBM solver OpenLB [9]. First, the grid refinement method will be explained and it will then be applied to two benchmark problems: flow around a circular cylinder and in a lid-driven cavity. While the former validates the method for transitional, unsteady and separated flows, the latter is useful for demonstrating convergence behavior and accuracy for complex wall bounded flows.

III. Grid Refinement Method

To illustrate a grid refinement interface, a coarse grid and a fine grid are shown in Fig. (1). The two grids overlap by one coarse grid spacing such that the boundary nodes of one grid coincide with interior fluid nodes of the other grid. This results in two interfaces, which are treated separately: a *fine coupling interface* at the boundary of the fine grid and a *coarse coupling interface* at the boundary of the coarse grid. The grid structure of a refinement interface is illustrated in the left figure in Fig. (1). Nodes belonging to the fine grid are denoted by crosses, while nodes of the coarse grid are denoted by circles. The nodes in blue color denote domain boundary nodes which require specific treatment during interpolation. To couple the two blocks, the post-collision functions will need to be constructed on the interface nodes and then be streamed back to the adjacent nodes in a normal fashion.

Fig. 1 General layout of a coarse and a fine grid. Coarse nodes are marked as $\circ$ and fine nodes are $\times$. Nodes marked in blue in the left figure are boundary nodes.

The post-collision population for both refinement levels are written in terms of the non-equilibrium distribution as:

$$\begin{aligned} f_{i,c}^*(x, t) &= \left(1 - \frac{1}{\tau_c}\right) f_{i,c}(x, t) + \frac{1}{\tau_c} f_{i,c}^{eq}(x, t) \\ &= f_{i,c}^{eq}(x, t) + \frac{\tau_c - 1}{\tau_c} f_{i,c}^{neq}(x, t), \end{aligned} \quad (4)$$

$$\begin{aligned} f_{i,f}^*(x, t) &= \left(1 - \frac{1}{\tau_f}\right) f_{i,f}(x, t) + \frac{1}{\tau_f} f_{i,f}^{eq}(x, t) \\ &= f_{i,f}^{eq}(x, t) + \frac{\tau_f - 1}{\tau_f} f_{i,f}^{neq}(x, t). \end{aligned} \quad (5)$$

At the interface, these two equations will need to be coupled by replacing the right-hand side with quantities from the other domain. Expressing the right-hand side in terms of equilibrium and non-equilibrium components simplifies this process because the $f_i^{eq}(x, t)$ is only determined by fluid density and velocity. In other words, at one physical position the equilibrium distribution function should be equal for both the coarse and fine grid node. The non-equilibrium part, on the other hand, needs to be scaled when transformed from one block to the other.

As illustrated in Fig. (1), there are two types of fine nodes at the interface, those sharing their location with a coarse node and those offset, lying mid-way between coarse nodes. This leads to three different interface treatments:

- 1) **Direct coupling from coarse to fine:** For fine nodes coincident with coarse nodes, the coarse populations are rescaled and directly assigned to the fine nodes.
- 2) **Interpolation from coarse to fine** For fine nodes located between coarse nodes, the new populations are interpolated from the surrounding coarse nodes and rescaled.
- 3) **Restricted coupling from fine to coarse** For coarse nodes coincident with fine nodes, the fine populations can, in theory, be rescaled and directly coupled to the corresponding coarse nodes. But to improve stability, a restriction process is used to take advantage of extra information on neighboring nodes.

The following will explain these treatments in detail.

A. Direct Coupling from coarse to fine

As discussed previously, for fine nodes coincident with coarse nodes, no interpolation is necessary. However, the terms on the right-hand side of Eq. (5) must be rescaled to the new grid spacing. This requires scaling of both the relaxation time and the population.

1. Interpolation from coarse to fine

The rescaling of relaxation time τ is quite straightforward as τ is only determined by physical viscosity ν and discretization spacing Δx . At each level of grids τ is thus a constant. The relation given by Chapman-Enskog analysis is:

$$\nu_f = c_s^2(\tau_f - \frac{1}{2}) \frac{\Delta x_f^2}{\Delta t_f} = \nu_c = c_s^2(\tau_c - \frac{1}{2}) \frac{\Delta x_c^2}{\Delta t_c}, \quad (6)$$

where $c_s = 1/\sqrt{3}$ is a constant in the basic isothermal LBM that represents the speed of sound and the subscript f represents quantities of the fine grids and the subscript c represents those of the coarse grids. Meanwhile, there are two scaling relation of Δt and Δx : the convective and diffusive scaling. The diffusive scaling requires the temporal scale to be proportional to the square of the spatial scale ($\Delta t \sim \Delta x^2$) in order to reduce the compressibility error terms ($O(Ma^2)$) when simulating incompressible flows. In the convective scaling (also known as the acoustic scaling) the temporal scale is proportional to the spatial scale ($\Delta t \sim \Delta x$) which makes it more computationally efficient compared to the diffusive scaling. In this research, where low-speed flows dominate, the convective scaling is usually adopted for computational efficiency. Consequently, the relaxation time relationship of these two blocks is controlled by grid spacing ratio $n = \Delta x_c/\Delta x_f$ and is

$$\begin{aligned} \tau_f &= \frac{1}{2} + \frac{\Delta x_c}{\Delta x_f}(\tau_c - \frac{1}{2}) \\ &= \frac{1}{2} + n(\tau_c - \frac{1}{2}). \end{aligned} \quad (7)$$

Similarly, the relaxation time of the coarse block is

$$\tau_c = \frac{1}{2} + \frac{1}{n}(\tau_f - \frac{1}{2}). \quad (8)$$

2. Restricted coupling from fine to coarse

Once the relaxation parameter of one grid can be transferred to the other, the remaining parameter to be rescaled is the distribution function $f_i(x, t)$. As mentioned previously, the equilibrium part of the distribution function is identical between different grids, so it is sufficient to scale the non-equilibrium part. From Dupuis [3], the relation of non-equilibrium distribution function on coarse and fine grid can be derived as:

$$\begin{aligned} f_{i,c}^{neq} &= \frac{\tau_c}{\tau_f} \frac{\Delta t_c}{\Delta t_f} f_{i,f}^{neq} \\ &= \frac{n\tau_c}{\tau_f} f_{i,f}^{neq}. \end{aligned} \quad (9)$$

Finally, the direct coupling relation can be summarized as

$$f_{i,f}^{new}(x, t) = f_{i,c}^{eq}(\rho(x, t), u(x, t)) + \frac{\tau_f}{n\tau_c} f_{i,c}^{neq}(x, t) \quad c \rightarrow f, \quad (10)$$

$$f_{i,c}^{new}(x, t) = f_{i,f}^{eq}(\rho(x, t), u(x, t)) + \frac{n\tau_c}{\tau_f} f_{i,f}^{neq}(x, t) \quad f \rightarrow c. \quad (11)$$

B. Interpolation from Coarse to Fine

Populations on fine nodes located between coarse nodes cannot be directly mapped from coarse nodes but need to be re-constructed based on the local physical state. A fourth-order accurate interpolation method is adopted and at least 4×4 neighboring coarse grid is needed for each fine cell. This is illustrated in Fig. 2a, where the red cross marks the interpolation location. Since the nodes are uniformly spaced, the weight coefficients used for the interpolation are fixed. If all surrounding 4×4 nodes are available, the weights are symmetric. The weight function on each coarse node is simply the product of 1D weight functions of each direction. When a node is located close to a boundary, the weights become asymmetric as shown in Fig. 2b and 2c. For fine nodes in line with the coarse grid, i.e. whose x or y -location is equal to that of a coarse node, the bicubic interpolation is simplified to a 1D cubic interpolation because the weight function in the other dimension are always 1 locally and 0 elsewhere. The 1D interpolation is illustrated in Fig. 3a, for a fine node in a row of coarse nodes.

Fig. 2 Interpolation on 2D center (a), edge (b) and corner (c) node

Fig. 3 Interpolation on 1D center (a) and edge (b) node

C. Restricted Coupling from Fine to Coarse

When coupling from a fine node to its corresponding coarse node, the macroscopic physical properties, i.e. the fluid density and velocity, can be directly mapped. The coupling of the non-equilibrium distribution function f_i^{neq} is slightly different. From a physical meaning view, f_i^{neq} represents the difference between current state to its equilibrium state and is dependent of local shear stress. Therefore, to obtain an accurate coupling of f_i^{neq} from fine grid to coarse, not only the coincident fine node but also the neighboring fine nodes should be taken into consideration. If no filtering method is used, a drop in accuracy and stability may occur due to the variance in stress field. The mean value of these fine nodes is used instead to calculate the new f_i^{neq} and this filtering procedure is called the restriction process. One simple restriction method proposed by Lagrava [4] is to take the average of all f_i^{neq} of surrounding fine nodes over each lattice direction as

$$f_{i,c}^{neq}(x, t) = \frac{1}{q} \sum_{i=0}^{q-1} f_{i,f}^{neq}(x + c_i \Delta x_f, t). \quad (12)$$

D. Specific Treatment on Periodic Boundaries

Special attention should be paid to the periodic boundary condition when applied to a refinement interface. In OpenLB periodic boundary conditions are implemented using ghost nodes, as shown in Fig. (4a), the fluid boundary node marked in red is mapped to the periodic ghost node on the other side for communication. But with refinement grid, the different grid sizes will result in a $0.5\Delta X$ dislocation on periodic boundaries. This dislocation will produce a discontinuity near the interface and a gap in cross-sectional area. By re-organizing the grid structures as illustrated in Fig. (4b), one more fluid layer is added to fine grid to enforce same mapping locations of periodic ghost nodes and fluid

Fig. 4 Problematic (a) and corrected (b) grid layout for periodic boundary

Fig. 5 Collision and streaming in overlapped region

nodes. Homologous fluid node are now mapped to one physical position and the mass flow is correctly captured with an equal cross-sectional area of both grids.

E. Overall Collision And Streaming Process

The overall collision and streaming process in the overlapped region, where the fine and coarse couplings take place, is illustrated in Fig. (5). A whole computation step with time interval dt contains one collision and streaming process in coarse grid and two in fine grid. The time step length is proportional to grid spacing in order to maintain a constant grid velocity. Normal collision and streaming take place on both grids firstly, resulting in mismatched populations on interface nodes. These populations are re-calculated from neighboring fluid nodes of the other grid. Note that the collision-and-streaming and coupling on fine nodes occurred twice in a coarse time step, so the mid-state of coarse nodes are used in the first fine coupling step.

IV. Results

The simulations and results of two benchmark cases will be discussed in this section to validate the implementation of 3D grid refinement approach. The flow around a circular cylinder is firstly studied paying attention to the turbulent transition in the vortex shedding wake. The pressure coefficient and velocity profiles in near wake are examined against experimental and numerical results [10–12]. The lid-driven cavity case involves a moving wall boundary and a complex flow with multiple interacting vortical structures with varying bulk flow velocities ranging from almost stagnant to possibly high speed ones.

Fig. 6 Simulation domain of 3D cylinder containing three levels of refinement around cylinder and two levels of refinement around outlet

A. Validation on Vortex Shedding Flow around a Circular Cylinder

The simulation domain and layout of refinement levels are illustrated in Fig. (6). The domain size is $25D \times 8D \times 8D$ with the cylinder diameter D to be 0.1. The cylinder is placed slight off-center to trigger the onset of shedding phenomenon. A constant velocity inlet and a pressure outlet are preset. The same magnitude velocity U is prescribed on the side boundaries to approximate a free-stream environment and the domain is initialized with uniform U . Periodic condition is assumed in spanwise direction to approximate an infinitely long cylinder. The periodic condition with refinement grid requires a different grid structure as stated in previous chapter. The simulation is conducted at $Re=100$, 200 and 300 by varying the relaxation parameter of the BGK operator. An example of simulation parameters on different levels of grids at $Re = 300$ is shown in Table. (1). The lattice velocity U_{lb} is fixed to 0.02 at all levels of grids in order to maintain same propagation speed of populations. Three levels of refinement around the cylinder and two around the outlet are applied with the coarsest resolution $N=100$. The number of total active cells in the refined case is reduced to 29 million compared with the 819 million active cells of the finest uniform grid with resolution $N = 800$.

Table 1 Simulation parameters of cylinder at $Re=300$

N	U_{lb}	τ	Re	Ma	Δx	Δt
100	0.02	0.502	300	0.035	0.01	$2e^{-4}$
200	0.02	0.504	300	0.035	0.005	$1e^{-4}$
400	0.02	0.508	300	0.035	0.0025	$5e^{-5}$
800	0.02	0.516	300	0.035	0.00125	$2.5e^{-5}$

Apart from the 2D primary instability, which leads the wake to transition from 2D steady to 2D periodic, two further three-dimensional instabilities are involved when Re keeps increasing. It has been shown the onset of corresponding three-dimensionality in the wake cannot be captured in 2D experiments and numerical simulations [13]. The first 3D wake transition occurs from the spanwise-periodic deformation of primary vortices at Re around 180 and is marked as mode A by Williamson [14]. The other mode B instability near $Re=230$ possesses a smaller spanwise wavelength and fine-scale wave pattern, indicating a different vorticity structure from mode A.

The transient velocity contour on the midspan section are shown in Fig. (7). The upper plot is the contour of velocity magnitude at each Reynolds number, showing an overall development of the vortex street. The vortex pairs are still regular at $Re=200$ but exhibits chaotic dislocation when Re reaches 300. This disorder can be explained with the contour of velocity components in each direction. The y-component, which is in the tangential direction, undergoes little changes in magnitude and wave pattern. In contrast, the magnitude of spanwise z-component rises from $O(10^{-9})$ at $Re=100$ to

Fig. 7 Contour of velocity magnitude, y- and z-component at Re=100, 200 and 300 with refined grid in LBM

Fig. 8 Pressure coefficients around cylinder at Re=100

$O(10^{-5})$ at Re=200 and $O(10^{-1})$ at Re=300. This relatively small component makes no contribution in the wave pattern when Re is low. While Re reaches to 300, the transverse velocity has grown to about same magnitude as the other two and results in a transition in cylinder wake. It can therefore be deduced that this transition is dominated by spanwise deformation of vortex structures. This development in the third direction that cannot be revealed by two-dimensional approaches shows the wake transition is three-dimensional inherently. From the velocity contours it can also be observed that the continuity of velocity field is preserved across the refinement interfaces.

Further validation on the time-averaged pressure coefficient C_p given by Eq. (13) around cylinder and velocity profiles in the near wake are shown in Fig. (8) and Fig. (9). The pressure coefficient at Re=100 with refined grid is in good agreement with reported values [10, 11]. At $Re = 300$ the time-averaged U_x and U_y are plotted at two streamwise locations $x/D = 1$ and $x/D = 2$ behind the cylinder. Note that the deflection in the wake is accurately captured compared to reference [12]. The external flow exhibits a bit higher U_x due to the imposed velocity in the boundaries.

$$c_p = (p - p_\infty)/(p_0 - p_\infty) \quad (13)$$

The detailed spanwise vortex structure is further illustrated in Fig. (10) by contouring the vorticity magnitude and its streamwise component. The isovorticity surface plot in the left shows pure 2D vortex structures at Re=100. The spanwise wave pattern can be revealed in streamwise vorticity component contour on the right-hand side. Although showing an elementary shape in isosurface contours of W_x , the strength of this instability is too small to impact the primary vortex structures. The onset of mode A instability around Re=200 is due to the development and stretch of

Fig. 9 Velocity profiles in the cylinder wake of $Re=300$ at $x/D = 1$ and $x/D = 2$

Fig. 10 Isosurface contours of vorticity magnitude and its x-component at $Re=100, 200$ and 300

primary vortex pairs. The influence of mode A instability on vortex street structure is still not obvious but W_x already

Fig. 11 Domain geometry and refinement layout of 3D lid-driven cavity

shows a periodic spanwise wave pattern with wavelength of around 3-4 cylinder diameters. Mode B instability, on the other hand, has a remarkable impact on the primary vortex structure as shown in isovorticity contours at $Re=300$. The strength of W_x and W_y reaches to the same magnitude as W_z . The secondary vortex structure becomes complicated and the wavelength of spanwise wave pattern is now only around 1 diameter. Another interesting phenomenon is the out-of-phase vortices from one braid to the next one in mode A instability. This separation of streamwise vortex pattern indicates independent originations. The vortices in mode B, in contrast, are in-phase and in a continuous arrangement. These streamwise vortices are developed from upstream in a successive manner. Overall, the observation in Williamson's experiments of two instability modes and wave patterns can be accurately reproduced in this study.

B. Validation on Lid-Driven Flow in a Cavity

Another well-known benchmark for 3D incompressible flow with moving boundary is the lid-driven cavity. The geometry of the simulation domain is depicted in Fig. (11). The cubic cavity is surrounded by 5 no-slip walls and 1 top moving boundary with uniform $U_x = 1$ velocity. The accuracy and stability of the numerical simulation may be affected due to the discontinuity in the velocity at edges of rigid wall and the top moving boundary [15]. Higher resolution is needed to limit the affected region and improve stability. Simulation of two refinement layouts are performed to compare with the result of uniform resolution. The first case involves an all-bounded refinement along all the boundaries and a further refinement grid is employed near the top boundary to help resolve flows around singularities. The Reynolds number is fixed to 3200 and the lattice velocity is fixed to 0.02 for incompressible condition. A comparison of computational resources for uniform and refined grids are summarized in Table. (2). All simulations are carried out on parallel clusters with 48 processors. The number of total active cells of 1 level refinement simulation is around 4.7 million, which is considerably less than 8.1 million lattice points in the uniform case with same finest resolution.

Table 2 Computational costs that scaled with “Uniform $N = 100$ ” case, of which $\Delta t = 2e^{-4}$, total active cells are 1 million, total convergence time is 3.7 hours

	physical Δt	total active cells	total convergence time
Uniform $N = 100$	1	1	1
Uniform $N = 200$	0.5	8.1	6.9
Refinement 1	1	4.7	3.9
Refinement 2	1	10.9	6.9

The convergence of the simulation is assessed via examination of continuously updated statistics, that is, mean and standard deviation σ in Eq. (14), computed in a selected set of points. The plane $y = 0.5$ is then selected for convergence monitoring in this case. Recording of these statistics commences after the initial unphysical transient stemming from

Fig. 12 Measured standard deviation of flow velocity versus computation steps after convergence

initialization using constant values has passed. This is assumed to be the case after energy residuals fall below 10^{-5} . As illustrated in Fig. (12), the standard deviations of both U_x and U_z are plotted against computation steps. Both curves start from infinite small values and reach to a constant region after sharp increases. The increase of σ is as expected because the error terms are accumulated from an initial state. Flow statistics can be therefore considered as converged.

$$\sigma = \frac{1}{N_p} \sum_{p=1}^{N_p} \sqrt{\frac{1}{N_t - 1} \sum_{t=1}^{N_t} (U_{p,t} - \bar{U}_{p,t})^2} \quad (14)$$

The time-averaged velocity contours of U_x and U_z are illustrated in Fig. (13). The refinement interfaces are marked by red lines and the positive and negative values of velocity are denoted by solid line and dotted line. The primary vortex and three secondary vortices are captured and the location of impingement points of flow jets and boundary walls are recorded correctly in comparison to results of a large eddy simulation [16]. The position of impingement points showed increased accuracy after adding refined grid as compared with reference value (0.717, 0) and (0, 0.197). Another remarkable difference is the smoothness and shape of velocity contours, which is largely influenced by top edge singularities. The refinement layer around the top boundary “blocked” the corner fluctuations from streaming into the bulk flow. In addition, the secondary vortices on the bottom left and bottom right are not accurately captured in U_z contour of $N=100$ and U_x contour of 1 level refinement case. The structure of these small vortices is disturbed by background instabilities and deformed to an asymmetric shape. In comparison, when the top refinement is employed, these vortices are well resolved.

To investigate the flow continuity across the refinement interface, the transient streamline contours of each case are illustrated in Fig. (14). The streamline directions are not affected when passing through refinement interfaces. And no blockage nor distortion to the velocity field is detected, indicating a continuous flow feature across the interface.

The time-averaged velocity profile of U_x along z -axis at $x = 0.5$ and U_z along x -axis at $z = 0.5$ on the plane of symmetry ($y = 0.5$) is shown in Fig. (15). Results of two refinement cases are compared with two uniform simulation with resolution 100 and 200 and experiments by Prasad et al. [17]. The deployment of first refinement grid around wall boundaries retains a similar accuracy level in boundary layer as $N = 200$ uniform grid. The grid of coarse resolution has better performance in the bulk flow region than fine grid. It is known [18], that the performance of the BGK operator is sensitive to τ . Figure. (16) shows how this sensitivity is grid dependent, which is consistent with the fact that the physical viscosity is a function of grid size and relaxation parameter (see Eq. (6)). The implication is that reproducing a given physical viscosity in a given mesh implies tailoring the relaxation parameter. Since the analysis of the performance of BGK operators is out of the scope of this work, a value for which the coarse mesh gives good results far from the walls has been chosen, and used throughout. Overall, from the comparison between refined grids and uniform grids it can be observed that with grid refinement good accuracy is obtained both in near-boundary region and bulk flow area.

Fig. 13 Time-averaged contours of velocity of N=100 uniform, 1 level refinement and 2 levels refinement cases on the plane of symmetry ($y=0.5$)

Fig. 14 Instantaneous streamline contours of N=100 uniform, 1 level refinement and 2 levels refinement case on the plane of symmetry ($y=0.5$)

V. Conclusion

A 3D grid refinement method is implemented in open-source code OpenLB and validated against two benchmarks: vortex shedding of a circular cylinder at $Re = 100 \sim 300$ and lid-driven flow in a cubic cavity at $Re = 3200$. The three-dimensionality in cylinder's wake transition is reproduced and two instability modes with different spanwise patterns are captured. The continuity across refinement interface is shown and a good capability of grid refinement method and periodic boundary is validated in cylinder case. The refinement around the outlet boundary also helps smooth out the instabilities caused by the vortices leaving out of the domain. The simulation of lid-driven flow in cavity, in which the moving wall boundary is problematic, indicates that the refinement helps stabilize complex boundary condition and reduce the effect of the artificial discontinuity. An important conclusion is that refining boundaries is

Fig. 15 Time-averaged U_x along z -axis at $x = 0.5$ and U_z along x -axis at $z = 0.5$ on $(y = 0.5)$ plane

Fig. 16 Time-averaged U_x and U_z profiles of uniform grid with resolution $N = 200$ of different lattice velocity

a good practice. In both cases, quality of the results is quantitatively improved without requiring the computational resources of a uniformly spaced finer mesh.

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