CIVA (Cubic Interpolation with Volume/Area Coordinates) and AMR (Adaptive Mesh Refinement) Method for Discrete Boltzmann Equation*

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In recent years, the Lattice Boltzmann Method (LBM) has been developed as an alternative numerical approach in Computational Fluid Dynamics (CFD). In particular, this method is promising for simulations of multiphase and multi component fluid flow involving complex interfacial dynamics. Unlike the conventional CFD methods based on NS equations, the LBM is based on the mesoscopic particle’s kinetic equation. This method has some advantages such as the simplicity of the algorithm (high efficiency on parallel processing), flexible reproduction of interfaces between phases. The conventional LBM, however, requires regular structured grids. But, for complex flow field, unstructured grids should be used. In this study, we describe a computational scheme based on two-dimensional unstructured grids using Cubic Interpolation with Volume/Area coordinates (CIVA) method and Adaptive Mesh Refinement method. As examples of tests of this scheme, single and two-phase flow simulations are presented.

Key Words: Computational Fluid Dynamics, Multi-Phase Flow, Lattice Boltzmann Method, Unstructured Grids, CIP, CIVA, Adaptive Mesh Refinement

1. Introduction

The Lattice Boltzmann Method (LBM)(1) has been developed as an alternative numerical approach in Computational Fluid Dynamics. But, the conventional LBM requires regular structured grids. To remove this constraint, during the past few years several workers have extended the LBM to use irregular lattices(2) – (5).

In this study, we describe a computational scheme based on two-dimensional unstructured grids using Cubic Interpolation with Volume/Area coordinates (CIVA) method(6), which has high accuracy for the analysis of the advection equation.

To apply the unstructured grids for the LBM, Discrete Boltzmann Equation is solved in Eulerian way. For the stability condition, the time step is severely restricted and consequently, more calculation time is required than the conventional LBM. In addition, it is desirable to refine the mesh at locations where the change of the physical quantity is intense for the accuracy. So, we apply the Adaptive Mesh Refinement method(7) for the improvement in calculation speed and the low memory consumption.

In addition, there are few studies about the LBM which apply the unstructured grids to analysis multi-phase flow(3). In this study, numerical analysis for two-phase flow using unstructured grids is carried out and evaluated its accuracy and validity.

2. Governing Equation

If a nine-velocity model is used, the Discrete Boltzmann Equation with an external force term is obtained.

$$\frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i = -\frac{1}{\lambda}(f_i - f_i^{eq}) + 3F \cdot (c_i - u_i)f_i^{eq}$$  \hspace{1cm} (1)

where $f_i$ is the single-particle distribution function, $c_i$ is the particle’s velocity, $\lambda$ is the relaxation time due to collision, $F$ is the external force, $i = 0, 1, \ldots, 8$. The discrete velocity $c_i$ is expressed as

$$c_i = \begin{cases} (0,0), & i = 0 \\ \cos(\theta_i,\sin \theta_i), & i = 1,3,5,7 \\ \sqrt{2} \cos(\theta_i,\sin \theta_i), & i = 2,4,6,8 \end{cases}$$  \hspace{1cm} (2)
The Boltzmann-Maxwellian equilibrium distribution $f_i^{eq}$ is expanded as a Taylor series,

$$f_i^{eq} = w_i n \left[ 1 + 3 (c_i \cdot u) + \frac{9}{2} (c_i \cdot u)^2 - \frac{3}{2} (u \cdot u) \right]$$  \hspace{1cm} (3)

with the weights $w_0 = 4/9$, $w_1 = w_3 = w_5 = 1/9$, and $w_2 = w_4 = w_6 = 1/36$. The macroscopic number density $n$ and velocity vector $u$ are related to the distribution function by

$$n = \sum_i f_i, \quad nu = \sum_i c_i f_i$$  \hspace{1cm} (4)

For the single-phase flow, pressure can be calculated from $p = c_i^2 n$ with the speed of sound $c_i = 1/\sqrt{3}$.

For the two-phase flow analysis, we used the model derived by Chen et al. \(^8\), \(^9\). In this model, the van der Waals's free energy is incorporated into the external force term, which is described as follows.

$$F = \left[ \frac{1}{3n} - \frac{3}{n(3n-2)} + \frac{3}{4T} \right] \nabla n + \kappa \nabla^2 \nabla n + g$$  \hspace{1cm} (5)

where $n$ is dimensionless number density, $T$ is dimensionless temperature (the system is assumed to be isothermal), $g$ is the gravitational acceleration, $\kappa$ is constant parameter determining the width of interface and strength of surface tension. Number density and temperature are normalized by critical density and temperature.

3. Numerical Methods

To solve Eq. (1), solution procedure is split into “streaming step (left side of Eq. (1))” and “collision step (right side of Eq. (1))”. We apply the CIVA method\(^6\) for the streaming step. The governing equations for the spatial derivatives are solved as in the CIP method, so the Moving Least-Squares Method (MSLM)\(^10\) is applied to calculate the spatial derivatives of each value at the collision step.

**Streaming step:**

$$\frac{\partial \tilde{f}_i}{\partial t} + c_i \cdot \nabla f_i = 0, \quad \frac{\partial \tilde{f}_i}{\partial t} + c_i \cdot \nabla f_i = 0$$  \hspace{1cm} (6)

**Collision step:**

$$\frac{\partial f_i^{n+1}}{\partial t} = \tilde{\Omega}_i, \quad \Omega_i = -\frac{1}{J} (f_i - f_i^{eq}) + 3F \cdot (c_i \cdot u_i) f_i^{eq}$$

$$\frac{\partial f_i^{eq}}{\partial t} = \Omega_i^e, \quad \Omega_i^e = \nabla \left( \frac{\partial f_i^{n+1}}{\partial t} \right)$$  \hspace{1cm} (7)

In this procedure, viscosity of the fluid is evaluated by $\nu = (\lambda/\Delta t - 0.5)c_i^2 \Delta t(2)$.

3.1 CIVA method

For the streaming step, we apply the CIVA method\(^6\) which enables cubic interpolation with the local coordinate system, such as volume and area coordinates, by utilizing the concept of the CIP scheme.

The cubic function corresponding to the scalar quantity in a triangle is set in the following form using the area coordinates $(L_1, L_2, L_3)$.

$$f(L_1, L_2, L_3) = \sum_{i=1}^{3} \alpha_i L_i + \sum_{j=1, j \neq k}^{3} \beta_{jk} [L_j^2 L_k + c L_1 L_2 L_3]$$  \hspace{1cm} (8)

where,

$$\alpha_i = f_i$$

$$\beta_{jk} = f_j - f_k + (x_k - x_j) f_j^{eq} + (y_k - y_j) f_j^{eq}$$

$$c = 0.5$$

The derivatives can be calculated similarly by using following equations.

$$\frac{\partial f}{\partial x} = \frac{f_2 - f_1}{J} \frac{\partial f}{\partial L_1} + \frac{f_3 - f_1}{J} \frac{\partial f}{\partial L_2} + \frac{f_3 - f_2}{J} \frac{\partial f}{\partial L_3}$$

$$\frac{\partial f}{\partial y} = \frac{f_2 - f_1}{J} \frac{\partial f}{\partial L_1} + \frac{f_3 - f_1}{J} \frac{\partial f}{\partial L_2} + \frac{f_3 - f_2}{J} \frac{\partial f}{\partial L_3}$$

$$J = (x_2 - x_1)(y_3 - y_1) - (y_2 - y_1)(x_3 - x_1)$$

Usually a higher-order scheme results in oscillatory solutions. For the two-phase flow analysis, to prevent the overshoot and undershoot in the solution (particularly at interface), a filtering scheme\(^12\) is applied. Maximum and minimum limits in the evaluated triangle are calculated at each time step, and if the solution of a higher-order calculation is not included between them, second term of right side of Eq. (8) is omitted. Then, the scheme provides 1st order accuracy.

3.2 MSLM

For the collision step, the Moving Least-Squares Method (MLSM)\(^10\) is applied to calculate the spatial derivatives of each values. In the method, the value at a point is determined by minimizing following weighted residuals, using points in the neighborhood of the evaluation point.

$$J = \sum_{i=1}^{N} w(r_i) (f(x_i) - f_i)^2, \quad r_i = |x - x_i|$$  \hspace{1cm} (11)

where $N$ is number of points in the neighborhood of evaluation point, $x$ and $x_i$ are coordinates of evaluation point and points in the neighborhood respectively, $w(r_i)$ is the weight function, $f(x_i)$ is approximate function in the evaluation domain, $f_i$ is the value at each point. In this study, the following approximate function and weight function are used.

$$f(x) = a_0 + a_1 x + a_2 y,$$

$$w(r_i) = 1 - 6r_i/R^2 + 8r_i/R^3 - 3(r_i/R)^4 \quad (0 \leq r_i \leq R)$$

$$w(r_i) = 0 \quad (R < r)$$

$$R = \max(r_i) \times 1.5$$  \hspace{1cm} (12)

In order to obtain $a_0$, $a_1$ and $a_2$, we evaluate the partial differential of Eq. (11) by $a_0$, $a_1$ and $a_2$, which are equal to 0 at each evaluation point. To evaluate the third derivative of number density of Eq. (5), the above procedure is repeated.
3.3 AMR method

In order to use computer resources efficiently, it is necessary to use the Adaptive Mesh Refinement (AMR) method, which obtains higher resolutions by collecting many grids only in locations where the change of the physical quantity is intense.

In this study, the Bisection algorithm(7) is used for the refinement of the elements. A triangle element is divided into two by dividing the longest edge at the midpoint (Fig. 1). The refinement criterion, based on vorticity (for single-phase flow) or number density (for two-phase flow),

\[
\phi_{\text{vorticity}} = \sqrt{\left(\frac{\partial \omega}{\partial x}\right)^2 + \left(\frac{\partial \omega}{\partial y}\right)^2}, \quad \omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}
\]

\[
\phi_{\text{density}} = \sqrt{\left(\frac{\partial n}{\partial x}\right)^2 + \left(\frac{\partial n}{\partial y}\right)^2},
\]

is calculated at each node, and if it is greater than the threshold value for the refinement, all triangle elements surrounding the node is refined. If it is smaller than the threshold value for the coarsening, the node is to be removed. The refinement is limited by specifying the minimum edge length.

3.4 Boundary condition

Boundary condition for non-slip wall must be provided if \(c \cdot n < 0\) where \(n\) is a unit vector outward normal to the local boundary surface. Only at streaming step, we apply the bounce-back rule of the nonequilibrium distribution proposed by Lee et al.(2)

\[
(f^n + 1 - f^n) - (f^{\alpha + 1} - f^{\alpha}) = 0
\]

where \(\alpha\) is \(\beta\)'s opposite direction. The physical Dirichlet and Neumann conditions (density and velocity) are imposed through the macroscopic value in \(f^{eq}\).

4. Numerical Analysis

4.1 Lid-driven cavity flow

Numerical simulation of lid-driven cavity flow is a well-known benchmark problem. To capture flow phenomena near numerical singularities at the top corners, it is desirable to refine the mesh near those points. Usually, lid-driven cavity flow is treated as steady-state problem, but in this study, in order to evaluate the scheme, is treated as transient problem.

The simulations are carried out for \(Re = 400\) and 1 000. The Reynolds number, \(Re\) is defined as \(Re = UL/\nu\), where \(U\) is the uniform velocity of the top plate, \(L\) is the length of the top plate. Here, \(U = 0.1, L = 1.0, \Delta t = 1.0e^{-3}\), and initial number density \(n = 1.0\). The equilibrium distribution function is used to specify initial conditions. For \(Re = 400\), AMR is not applied and the computational grid consists of uniform right angled triangle elements with some fixed sizes (edge length is 1/50, 1/100 and 1/200, respectively). For \(Re = 1 000\), initial grid consists of uniform right angled triangle elements (edge length is 1/25). The AMR is carried out once to 10 time steps, using threshold value for the refinement and coarsening as 2, and the minimum edge length is 1/200.

We compare the results of \(Re = 400\) calculated on each computational grids. Figure 2 shows the comparison of the profiles of the horizontal velocity component in the vertical symmetry plane at steady state. We can see that the accuracy of a value is increasing as computational grid becomes fine. Particular, results on 1/200 grid shows good agreement with the previous results(11), which are also displayed for comparison.

The AMR method is applied for calculation of \(Re = 1 000\). Figures 3 and 5 (c) show contour plots of pressure and vorticity at time \(t = 200\), respectively. The flow structure is good agreement with previous results(11). Comparison of the profiles of the horizontal and vertical velocity component in the vertical and horizontal symmetry plane is shown in Fig. 4. The results are good agreement with the previous results(11). Figure 5 shows the time evolu-
Profiles of normalized velocity component $u$ and $v$ through the geometric center of the cavity at $t = 200$ (●: Ghia et al.\(^{(11)}\), line: Present result) ($Re = 1000$)

Time evolutions of computational grids and vorticity contours ($Re = 1000$)

Time evolution of density distribution (maximum is black and minimum is white)

Fig. 4 Profiles of normalized velocity component $u$ and $v$ through the geometric center of the cavity at $t = 200$ (●: Ghia et al.\(^{(11)}\), line: Present result) ($Re = 1000$)

Fig. 5 Time evolutions of computational grids and vorticity contours ($Re = 1000$)

Fig. 6 Time evolution of density distribution (maximum is black and minimum is white)

Numerical analysis of phase separation is demonstrated to evaluate the validity of the two-phase model. The initial condition is uniform distributions of the averaged dimensionless number density $n = 1.0$. Random noises of magnitude 0.1 have been added to represent the nuclei in the density field. The system is quenched from the critical point to the state of dimensionless temperature $T = 0.9$.

Here, the AMR is not applied and the computational grid consists of uniform right angled triangle elements with fixed sizes (edge length is 1/100). Computational domain’s size is $1 \times 1$ and the periodic boundary condition is applied for all boundaries. $\kappa = 1.0e^{-4}$ and $\Delta t = 1.0e^{-3}$.

Snapshots of phase separation at different time are shown in Fig. 6. From the figures, we can see the processes of phase separation and coalescence of droplets. At the final equilibrium, a large liquid droplet is formed among the gaseous phase. Theoretically, the dimensionless number densities of two bulk coexisting phase corresponding to the dimensionless temperature $T = 0.9$ are about 1.657 (liquid phase) and 0.426 (gas phase) respectively. In this simulation, finally, the maximum and minimum number density values are 1.662 and 0.428 respectively.

**4.3 Interfacial density profile**

The interface profiles calculated on some computational grids are compared with the theoretical results\(^{(9)}\) based on the original theory of van der Waals. The computational grid, not to apply the AMR, consists of uniform right angled triangle elements with some fixed sizes (edge length is 1/50, 1/100 and 1/200, respectively). On the other hand, the initial element’s edge length is 1/25 for the grid to apply the AMR. The AMR is carried out once to 10 time steps, using threshold value for the refine-
Analysis model is shown in Fig. 7. The initial density distribution is set up that the dimensionless number density at the area named “Low density” in Fig. 7 is 0.4 and other area is 1.6. The length of the system is 1.0×0.16 and the periodic boundary condition is applied at all boundaries. \( \kappa = 2.5 \times 10^{-5}, \Delta t = 1.0 \times 10^{-3} \), and the dimensionless temperature \( T = 0.9 \).

Figure 8 shows the computational grid at \( t = 200 \). We can see that the adequate refinement of mesh at the interface and the coarsening of mesh at other area. At boundary elements, in order to apply periodic boundary condition smoothly, we divided the element intentionally.

Figure 9 shows the \( t = 200 \)’s interfacial density profiles obtained from the each calculation at the area named “evaluated region” in Fig. 7. We can see that the accuracy of a value is increasing as computational grid becomes fine. Particular, results on the AMR grid and the fixed 1/200 grid show good agreement with the theoretical result. Nevertheless there are 3 310 grid points in the AMR grid and 6 633 points in the fixed 1/200 grid, those density profiles are overlapped in the graph. In addition, it is cleared that adequately refined mesh (edge length is 1/200) is required at the interface in this condition (\( T = 0.9 \)).

4.4 Droplet collision

Finally, numerical analysis of binary droplet collision is demonstrated to evaluate the validity of the numerical methods applied in this study. Two liquid droplets with the same radius are placed among the gaseous phase, and they collide with the opposite direction’s velocity.

Initial grid consists of uniform right angled triangle elements (edge length is 0.08). The initial density distribution is set up that the dimensionless number density of
droplets is 1.6 and other area is 0.4. The length of the system is \(2.0 \times 2.0\) and the periodic boundary condition is applied at all boundaries. \(\kappa = 5.0e^{-5}\), \(\Delta t = 1.0e^{-3}\), \(\nu = 1.5e^{-3}\), and the dimensionless temperature \(T = 0.9\). Radius of each droplet is 0.3. After adequate relaxation, the horizontal velocity 0.15 and \(-0.15\) is imposed on each droplet. The AMR is carried out once to 10 time steps, using threshold value for the refinement and coarsening as 10, and the minimum edge length is 1/200.

Figure 10 shows the time evolutions of droplet’s shape and computational grids. After droplets collide, they form a disk-like droplet. Then, the droplet oscillates and circular form is formed by work of surface tension and viscous force. We can see that the adequate refinement of mesh at the interface and the coarsening of mesh at other area at each time.

5. Conclusions

From the results of this study, it is indicated that the applicability of the computational scheme for the Discrete Boltzmann Equation, based on CIVA and AMR. Single and two-phase flow simulations are presented on the unstructured grids with adequate refinement of the elements (at the two-phase’s interface and so on).

In this study, for two-phase flow analysis, we investigate only the state of dimensionless temperature \(T = 0.9\). We are presently trying simulation at the state of lower temperature, which causes higher density ratio.

References