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Moment Base Lattice Boltzmann Approach for Multiphysics Flow Problems

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Abstract: This paper describes a novel numerical approach for simulating multiphysics flow problems using several moments. Unsteady evolution of the moments are obtained by the lattice Boltzmann framework. Three dimensional incompressible isothermal flows can be described using lower ten moments. The Chapman-Enskog distribution functions for three dimensional lattice (for example, D3Q19) are temporary constructed from the moments. The time evolution of the moments can be obtained using the standard lattice Boltzmann method. As compared with the standard lattice Boltzmann method, the present method can save storage and improve numerical stability. Numerical experiments indicate that the advantage is more evident for multiphysics flow problems.

Keywords: Numerical Algorithms, Computational Fluid Dynamics, Lattice Boltzmann Method, Two-phase Flow, Thermal Lattice Boltzmann Model

1 Introduction

Nowadays the lattice Boltzmann method is widely used especially for simulating incompressible isothermal flows [1],[2]. Simpleness f the algorithm is one of the advantage of the lattice Boltzmann method. On the other hand, the method need more storage compared with the incompressible Navier-Stokes solver, especially for three dimensional multiphysics flow problems, such as thermal flows [3], [4] and two-phase flows [5], [6].

Even if we use the three dimensional D3Q19 model, the incompressible isothermal Navier-Stokes solution may be obtained using the lower ten moments instead of the nineteen lattice Boltzmann distribution functions. Unsteady evolution of those moments can be obtained using the simple algorithm of the standard lattice Boltzmann method. For thermal flows, additional four moments are only required of the nineteen thermal lattice distribution functions. In total only 14 moments of 38 distribution functions are required. Similar estimation can be made for two-phase flow problems Thus the moment base lattice Boltzmann method saves storage especially for multiphysics flow problems.

2 Lattice Boltzmann Method

In the Lattice Boltzmann method, unsteady evolution of the distribution function for incompressible isothermal flows are obtained simply as:

$$f_\alpha(t+\delta t, \mathbf{x}+\mathbf{e}_\alpha \delta t) = f_\alpha(t, \mathbf{x}) - \frac{1}{\tau}\left(f_\alpha(t, \mathbf{x}) - f_\alpha^{eq}(t, \mathbf{x})\right) \tag{1}$$

where $\mathbf{e}_\alpha$ are the discrete velocities, δt is the time step size, and τ is the relaxation time which is given with the kinematic viscosity ν as

$$\eta = 3\nu + \frac{1}{2} \tag{2}$$

The discrete velocities, for example, for two dimensional nine velocity (D2Q9) model are given by

$$\mathbf{e}_\alpha = \begin{cases} (0,0) & \alpha = 0, \\ (cos((\alpha-1)\pi/2), sin((\alpha-1)\pi/2)) & \alpha = 1,2,3,4 \\ \sqrt{2}\,(cos((2\alpha-9)\pi/4), sin((2\alpha-9)\pi/4)) & \alpha = 5,6,7,8 \end{cases} \tag{3}$$

and for three dimensional nineteen velocity (D3Q19) model are

$$\begin{gathered} \mathbf{e}_0 = (0,0,0) \\ \mathbf{e}_1 = (1,0,0),\ \mathbf{e}_2 = (-1,0,0),\ \mathbf{e}_3 = (0,1,0),\ \mathbf{e}_4 = (0,-1,0),\ \mathbf{e}_5 = (0,0,1),\ \mathbf{e}_6 = (0,0,-1) \\ \mathbf{e}_7 = (1,1,0),\ \mathbf{e}_8 = (1,-1,0),\ \mathbf{e}_9 = (-1,1,0),\ \mathbf{e}_{10}(-1,-1,0),\ \mathbf{e}_{11} = (0,1,1),\ \mathbf{e}_{12} = (0,1,-1) \\ \mathbf{e}_{13} = (0,-1,1),\ \mathbf{e}_{14} = (0,-1,-1),\ \mathbf{e}_{15} = (1,0,1),\ \mathbf{e}_{16}(-1,0,1),\ \mathbf{e}_{17} = (1,0,-1),\ \mathbf{e}_{18} = (-1,0,-1) \end{gathered} \tag{4}$$

The equilibrium distribution function f_α^{eq} is written in the form

$$f_\alpha^{eq} = w_\alpha \rho \left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2\right] \tag{5}$$

Here the unit ratio of the lattice constant δx to the time step sizeδt is assumed for simplicity. The weighting factor w_α for D2Q9 model are given by

$$w_\alpha = \begin{cases} 4/9 & \alpha = 0 \\ 1/9 & \alpha = 1,2,3,4 \\ 1/36 & \alpha = 5,6,7,8 \end{cases} \tag{6}$$

and for D3Q19 model are

$$w_\alpha = \begin{cases} 1/3 & \alpha = 0, \\ 1/18 & \alpha = 1,2,...,6 \\ 1/36 & \alpha = 7,8,...,18 \end{cases} \tag{7}$$

The density ρ and the velocity $\mathbf{u}$ can be obtained by the moments

$$\rho = \sum_\alpha f_\alpha \tag{8}$$

and

$$\rho \mathbf{u} = \sum_\alpha \mathbf{e}_\alpha f_\alpha \tag{9}$$

3 Moment Base Lattice Boltzmann Method

The distribution function of D2Q9 model may be written in the following polynomial expression

$$f_\alpha = C^{(0)} + C_i^{(1)} e_{\alpha i} + C_{i,j}^{(2)} e_{\alpha i} e_{\alpha j} + C_i^{(3)} e_{\alpha i}^{\,2} e_{\alpha j} + C^{(4)} e_{\alpha i}^{\,2} e_{\alpha j}^{\,2} \tag{10}$$

Taking the lower 9 moments of bath side and obtaining the coefficients Cs, the distribution function can be written as

$$f_\alpha = f_\alpha^{eq} + w_\alpha \rho \left[S_{i,j}^{(2)} \left(e_{\alpha i} e_{\alpha j} - \frac{1}{3}\delta_{ij}\right) + S_i^{(3)} \left(e_{\alpha i}^{\,2} - \frac{1}{3}\delta i,j\right) e_{\alpha j} + S^{(4)} e_{\alpha i}^{\,2} e_{\alpha j}^{\,2}\right] \tag{11}$$

where the moments S are obtained by

$$\rho S_{i,j}^{(2)} = \frac{9}{2}\left(\sum_\alpha e_{\alpha i} e_{\alpha j} f_\alpha - \frac{1}{3}\rho\delta_{i,j} - \rho u_i u_j\right), \tag{12}$$

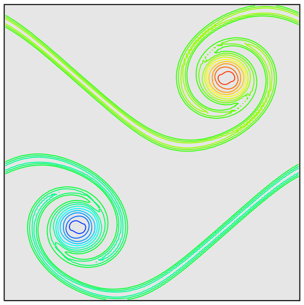

Figure 1: Vorticity contours obtained with MLBM on a 128×128 grid.

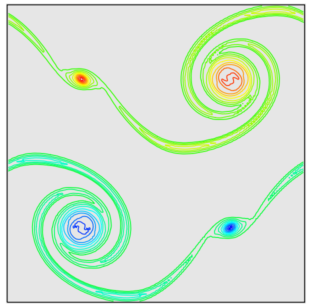

Figure 2: Vorticity contours obtained with LBM on a 128×128 grid.

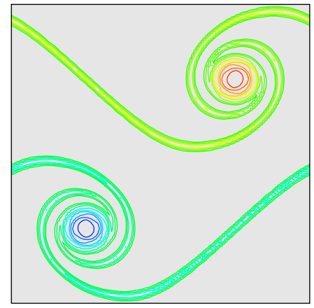

Figure 3: Vorticity contours obtained with PSM on a 128×128 grid.

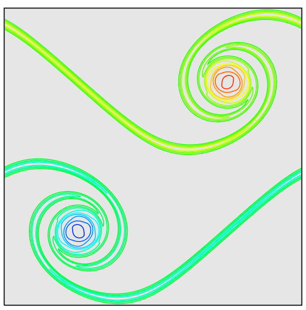

Figure 4: Vorticity contours obtained with MLBM on a 257×257 grid.

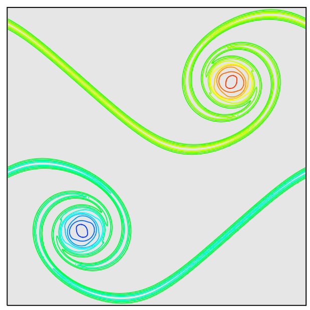

Figure 5: Vorticity contours obtained with LBM on a 257×257 grid.

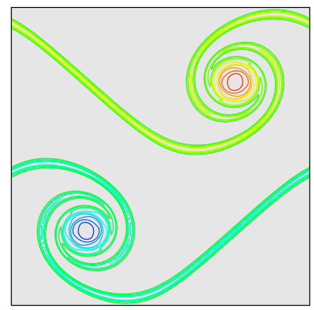

Figure 6: Vorticity contours obtained with PSM on a 257×257 grid.

$$\rho S_i^{(3)} = \frac{9}{2}\left(3\sum_\alpha {e_{\alpha}}_i^2 e_{\alpha j} f_\alpha - \rho u_j\right), \tag{13}$$

and

$$\rho S^{(4)} = \frac{9}{4}\left(9\sum_\alpha {e_{\alpha}}_i^2 {e_{\alpha}}_j^2 f_\alpha - \rho - 3\rho(u_i^2 + u_j^2) - \rho(S_{ii}^{(2)} + S_{jj}^{(2)})\right) \tag{14}$$

The kinetic theory indicates the solution of Navier-Stokes equations may be obtained using the distribution function constructed with proper number of lower moments. The solution of the incompressible isothermal flows may be obtained using the distribution function

$$f_\alpha = f_\alpha^{eq} + w_\alpha \rho \left(e_{\alpha i} e_{\alpha j} - \frac{1}{3}\delta_{i,j}\right) S_{i,j}^{(2)} \tag{15}$$

For the distribution function, Eq. (1) becomes the expression

$$f_\alpha(t+\delta t, \mathbf{x} + \mathbf{e}_\alpha \delta t) = f_\alpha^{eq}(t, \mathbf{x}) + (1 - \frac{1}{\tau}) w_\alpha \rho \left(e_{\alpha i} e_{\alpha j} - \frac{1}{3}\delta_{i,j}\right) S_{i,j}^{(2)}(t, \mathbf{x}) \tag{16}$$

Using the expression the solution of two dimensional incompressible isothermal flows can be obtained by the evolution of 6 moments (ρ, u_i, and $S_{i,j}^{(2)}$). Thus the number of unknown quantities, that is, memory can be reduced to $\frac{2}{3}$ compared to the original D2Q9 model. For D3Q19 model, since the solution can be obtained with similar 10 moments, the memory can be reduced to $\frac{10}{19}$.

Validation of the moment base lattice Boltzmann method is carried out for two dimensional doubly

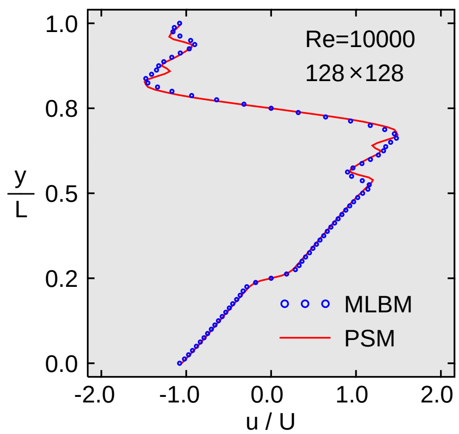

Figure 7: Comparison of x-component velocity between MLBM and PSM results on a 128×128 grid.

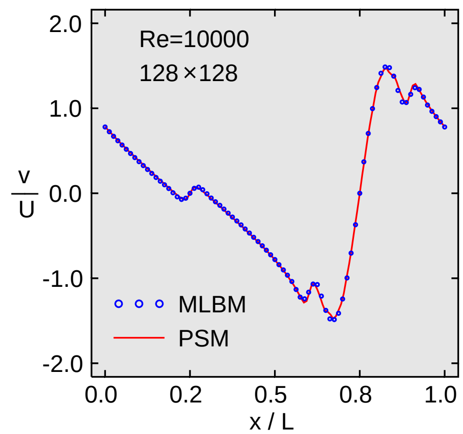

Figure 8: Comparison of y-component velocity between MLBM and PSM results on a 128×128 grid.

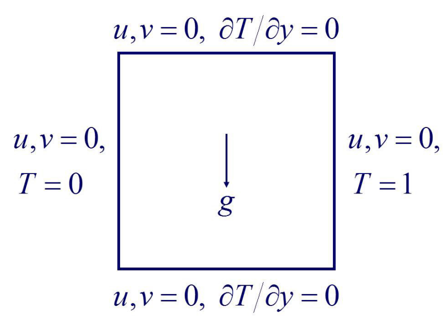

Figure 9: Numerical conditions of natural convection flow.

periodic shear layers. The computational domain is a square with unit length. The initial conditions are

$$u = \begin{cases} \tanh[\gamma(y-0.25)] & \text{for} y <= 0.5 \\ \\ \tanh[\gamma(0.75-y)] & \text{for} y >= 0.5 \end{cases} \tag{17}$$

and

$$v = \lambda \sin[2\pi(x+0.25)] \tag{18}$$

at γ of 80 and λ of 0.05. The Reynolds number is 10000. Figure 1 shows the vorticity contours obtained with the moment base lattice Boltzmann method (MLBM) at nondimensional time t of 1.0 on a 128×128 grid. For comparison, similar contours obtained with the normal lattice Boltzmann method (LBM) and a pseudo spectral method (PSM) are plotted in Fig. 2 and Fig. 3, respectively. The numerical results obtained with MLBM and PSM are in good agreement each other, while spurious vortices are observed in the result of LBM. The three numerical results obtained on a 257×257 grid are compared in Figs. 4 to 6. Since the LBM produces the reasonable result on the finer grid, three numerical results are well compared with one another. The x-component velocities along the line of $x = 0.75$ and the y-component velocities along the line of $y = 0.75$ are plotted in Fig. 7 and Fig. 8, respectively. The numerical results obtained with MLBM are compared with those of PSM. Although the results obtained on the coarse grid, good comparison is again observed.

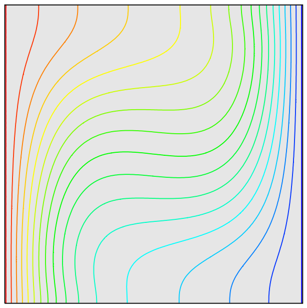

Figure 10: Temperature contours obtained with MTLBM at Ra of 10^4 on a 128×128 grid.

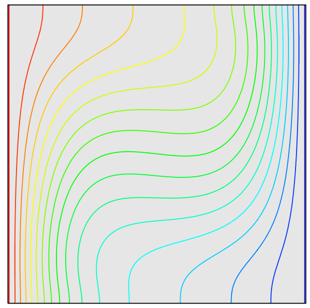

Figure 11: Temperature contours obtained with TLBM of Shi et al. at Ra of 10^4 on a 128×128 grid..

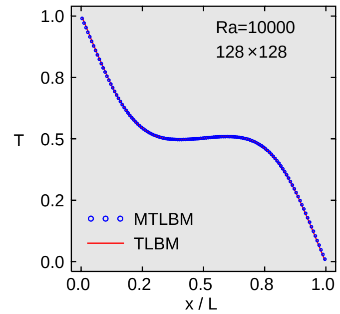

Figure 12: Comparison of temperature distribution at $y = 0.5$.

4 Moment Base Thermal Lattice Boltzmann Method

The moment base Lattice Boltzmann method is more effective for multiphysics problems, in which plural number of distribution function may be introduced. For thermal flow problems, Shi et al [4] propose a thermal lattice Boltzmann model using dual distribution functions, the density distribution function f_α and the temperature distribution function g_α. The unsteady evolution of the latter function g_α is obtained as

$$g_\alpha(t+\delta t, \mathbf{x}+\mathbf{e}_\alpha \delta t) = g_\alpha(t, \mathbf{x}) - \frac{1}{\eta}\left(g_\alpha(t,\mathbf{x}) - g_\alpha^{eq}(t,\mathbf{x})\right) \tag{19}$$

where η is the temperature relaxation time which is given with the thermal conductivity κ and specific heat c_v,

$$\eta = 3\frac{\kappa}{\rho c_v} + \frac{1}{2} \tag{20}$$

The equilibrium temperature distribution function g_α^{eq} is written in the form

$$g_\alpha^{eq} = w_\alpha \rho T \left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2\right] \tag{21}$$

The temperature T is obtained by the moment

$$\rho T = \sum_\alpha g_\alpha \tag{22}$$

In our moment base thermal lattice Boltzmann method, the temperature distribution function is expressed as

$$g_\alpha = g_\alpha^{eq} + w_\alpha \rho e_{\alpha i} T_i^{(1)} \tag{23}$$

where the moments $T_i^{(1)}$ are obtained by

$$\rho T_i^{(1)} = 3\sum_\alpha e_{\alpha i} g_\alpha - \rho T u_i \tag{24}$$

The evolution of the temperature is obtained from

$$g_\alpha(t+\delta t, \mathbf{x}+\mathbf{e}_\alpha \delta t) = g_\alpha^{eq}(t,\mathbf{x}) + (1-\frac{1}{\eta}) w_\alpha \rho \; e_{\alpha i} T_i^{(1)}(t,\mathbf{x}) \tag{25}$$

Using the expression the solution of two dimensional thermal flows can be obtained by the evolution of 9 moments (ρ, u_i, $S_{i,j}^{(2)}$, T, and $T_i^{(1)}$). Thus the number of unknown quantities, that is, memory can be

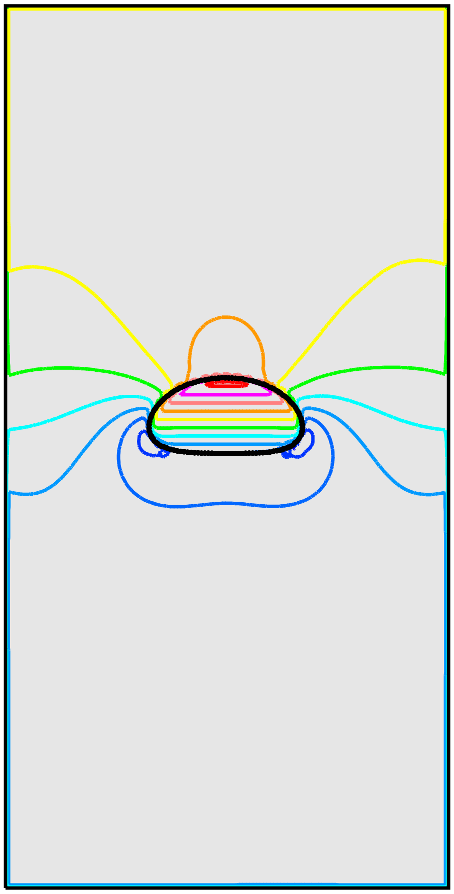

Figure 13: Relative pressure contours obtained with the present method at $Mo = 10^{-2}$, $Bo = 10$, $\frac{\rho_l}{\rho_g} = 1000$, and $\frac{\mu_l}{\mu_g} = 100$.

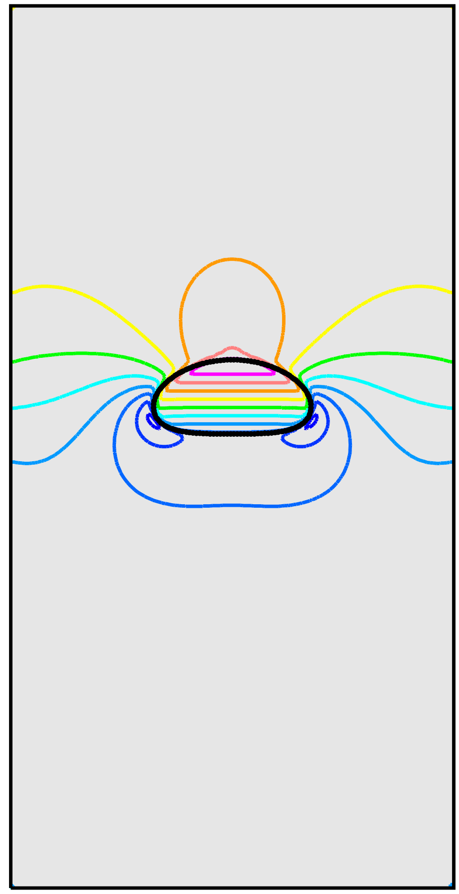

Figure 14: Relative pressure contours obtained with the NS solver at $Mo = 10^{-2}$, $Bo = 10$, $\frac{\rho_l}{\rho_g} = 1000$, and $\frac{\mu_l}{\mu_g} = 100$.

reduced to $\frac{1}{2}$ compared to the original D2Q9 model. For D3Q19 model, since the solution can be obtained with similar 14 moments, the memory can be reduced to $\frac{7}{19}$.

In order to validate the moment base thermal lattice Boltzmann method (MTLBM), numerical simulation of the natural convection flow in a two dimensional square cavity is carried out. Flow conditions are illustrated in Fig. 9. Figure 10 shows the temperature contours obtained with MLBM at Rayleigh number Ra of 10000 on a 128×128 grid. For comparison, numerical results obtained with the original thermal lattice Boltzmann model (TLBM) of Shi et al. are plotted in Fig. 11. The temperature distribution along $y = 0.5$ is compared in Fig. 12. Results of MTLBM agree well with those of TLBM.

5 Multiphase Moment Base Lattice Boltzmann Method

For multiphase flow problems, dual distribution functions, the pressure distribution function f_α instead of the density and the distribution function h_α for a level set function ϕ [7] are introduced as

$$f_\alpha = f_\alpha^{eq} + w_\alpha \rho(\phi) \left(e_{\alpha i} e_{\alpha j} - \frac{1}{3} \delta_{i,j} \right) S_{i,j}^{(2)} \tag{26}$$

and

$$h_\alpha = h_\alpha^{eq} + w_\alpha e_{\alpha i} H_i^{(1)} \tag{27}$$

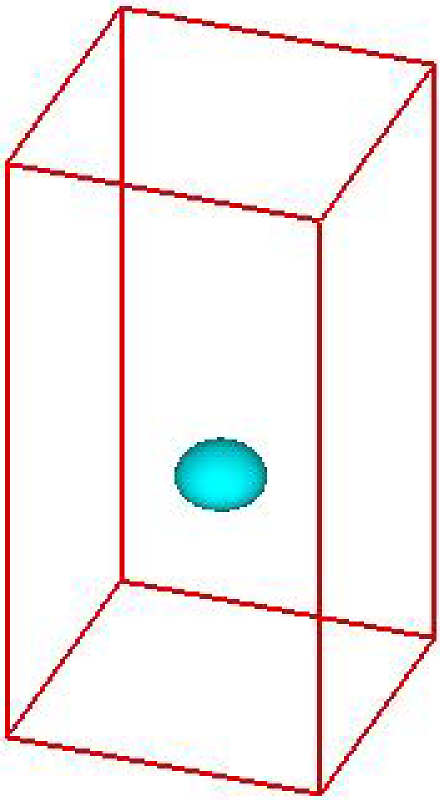

Figure 15: Rising bubble shape obtained at $\sqrt{d}\ t/\sqrt{g} = 4$ with the present method at $Mo = 10^{-2}$, $Bo = 10$, $\frac{\rho_l}{\rho_g} = 100$, and $\frac{\mu_l}{\mu_g} = 10$.

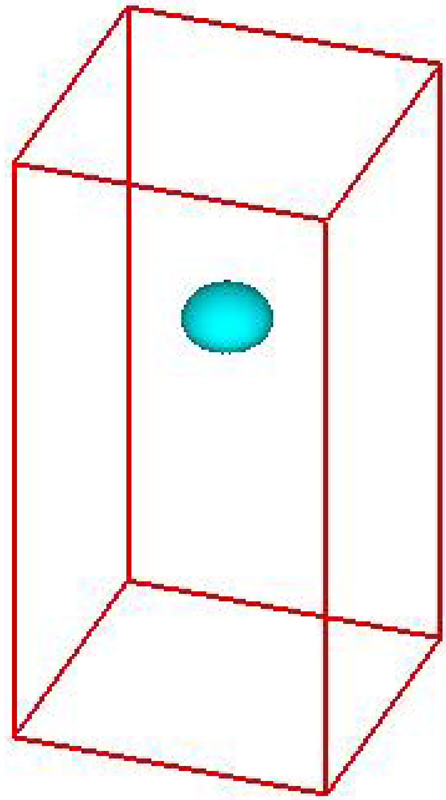

Figure 16: Rising bubble shape obtained at $\sqrt{d}\ t/\sqrt{g} = 8$ with the present method at $Mo = 10^{-2}$, $Bo = 10$, $\frac{\rho_l}{\rho_g} = 100$, and $\frac{\mu_l}{\mu_g} = 10$.

The evolution of the distribution function is obtained by

$$f_\alpha(t+\delta t, \mathbf{x}+\mathbf{e}_\alpha \delta t) = f_\alpha^{eq}(t,\mathbf{x}) - (1-\frac{1}{\tau^*})w_\alpha \rho(\phi^*)\left(e_{\alpha i}e_{\alpha j} - \frac{1}{3}\delta_{i,j}\right)S_{i,j}^{(2)}(t,\mathbf{x}) + F_\alpha \tag{28}$$

and

$$h_\alpha(t+\delta t, \mathbf{x}+\mathbf{e}_\alpha \delta t) = h_\alpha^{eq}(t,\mathbf{x}) + (1-\frac{1}{\zeta})w_\alpha e_{\alpha i} H_i^{(1)}(t,\mathbf{x}) \tag{29}$$

where F_α is forcing terms and ζ is the relaxation time. The level set function ϕ and the moments $H_i^{(1)}$ are obtained by

$$\phi = \sum_\alpha h_\alpha \tag{30}$$

and

$$H_i^{(1)} = 3\sum_\alpha e_{\alpha i} h_\alpha - \phi u_i \tag{31}$$

The equilibrium pressure distribution function f_α^{eq} and the equilibrium level set distribution function h_α^{eq} are given by

$$f_\alpha^{eq} = w_\alpha \left\{ p + \rho(\phi^*) \left[3(\mathbf{e}_\alpha \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2 \right] \right\} \tag{32}$$

and

$$h_\alpha^{eq} = (\phi + \delta\phi) \left\{ \Phi_\alpha + w_\alpha \left[3(\mathbf{e}_\alpha \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2 \right] \right\} \tag{33}$$

where the weighting factor Φ_α are given by

$$\Phi_\alpha = \begin{cases} 1 & \alpha = 0, \\ 0 & \alpha \neq 1 \end{cases} \tag{34}$$

In order to reinitialize the level set function, $\delta\phi$ is included in Eq. (29), which is obtained by

$$\delta\phi = \omega \; sgn(\phi)(1 - |\nabla\phi|) \tag{35}$$

where sgn is the sign function and ω is an adjusting constant.

The density $\rho(\phi^*)$ is evaluated at $\mathbf{x} + \mathbf{e}_\alpha \delta t$ by

$$\rho = \begin{cases} \rho_1 & \text{if} \quad \phi > \epsilon \\ \rho_2 & \text{if} \quad \phi < -\epsilon \\ \bar{\rho} + \Delta\rho \cos(\pi\phi/\epsilon) & \text{otherwise} \end{cases} \tag{36}$$

where $\bar{\rho} = (\rho_1 + \rho_2)/2$ and $\Delta\rho = (\rho_1 - \rho_2)/2$. Similarly τ^* is evaluated with the density $\rho(\mathbf{x} + \mathbf{e}_\alpha \delta t)$ and the viscosity $\mu(\mathbf{x})$ which is given by

$$\mu = \begin{cases} \mu_1 & \text{if} \quad \phi > \epsilon \\ \mu_2 & \text{if} \quad \phi < -\epsilon \\ \bar{\mu} + \Delta\mu \cos(\pi\phi/\epsilon) & \text{otherwise} \end{cases} \tag{37}$$

where $\bar{\mu} = (\nu_1 + \mu_2)/2$ and $\Delta\mu = (\mu_1 - \mu_2)/2$.

The forcing terms F_α may be given as

$$F_\alpha = 3(\mathbf{e} - \mathbf{u}) \cdot \left[\sigma \nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|} \right) \delta(\phi) \nabla\phi + \mathbf{G} \right] w_\alpha \left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2 \right] \tag{38}$$

where σ is the surface tension, G is the gravitational force, and $\delta(\phi)$ is the modified delta function defined by

$$\delta(\phi) = \begin{cases} 1 & \text{if} \quad |\phi| < \epsilon \\ 0 & \text{otherwise} \end{cases} \tag{39}$$

The multiphase moment base lattice Boltzmann method is applied to the simulation of a rising bubble in a liquid at rest. At first several two dimensional test cases are calculated. Figure 13 shows the contours of the relative pressure to the hydrostatic pressure obtained with the present method at the Morton number Mo of 10^{-2}, the Bond number Bo of 10, the density ratio $\frac{\rho_l}{\rho_g}$ of 1000, and the viscosity ratio $\frac{\mu_l}{\mu_g}$ of 100 on a 128×256 grid over $4d \times 8d$ computational domain, where d is the initial diameter of the bubble. At the high density ratio case, a limit function of the pressure at the interface is introduced in order to stabilize the present method. For comparison, reference solution, which is obtained using a fractional step method for the incompressible Navier-Stokes equations with the level set function, is plotted in Fig. 14. The interface thickness parameter ϵ is set at $2\delta x$ for both methods. Good comparison is observed.

Figures 15 and 16 show the three dimensional shape of rising bubble obtained with the present method at the Morton number Mo of 10^{-2}, the Bond number Bo of 10, the density ratio $\frac{\rho_l}{\rho_g}$ of 100, and the viscosity ratio $\frac{\mu_l}{\mu_g}$ of 10 on a $128 \times 128 \times 256$ grid over $4d \times 4d \times 8d$ computational domain.

Finally area or volume conservation for the bubbles are examined. Figures 17 and 18 show bubble area and volume as a function of nondimensional time ($\sqrt{g}\, t/\sqrt{d}$) obtained with the present method for the two dimensional case and three dimensional case, respectively. Adjusting the relaxation time ζ, the conservation of the present method properly good.

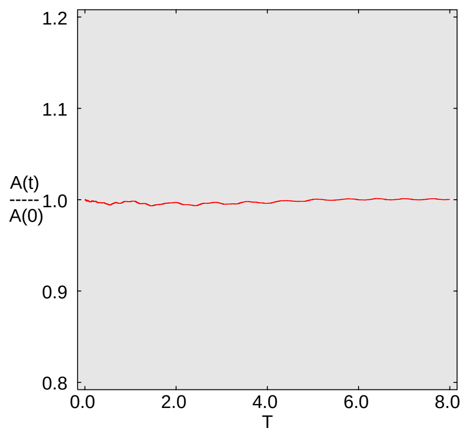

Figure 17: Bubble area as a function of nondimensional time ($\sqrt{g}\ t/\sqrt{d}$) obtained at $Mo = 10^{-2}$, $Bo = 10$, $\frac{\rho_l}{\rho_g} = 1000$, and $\frac{\mu_l}{\mu_g} = 100$.

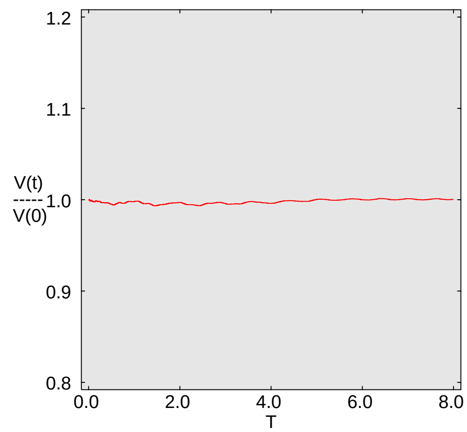

Figure 18: Bubble volume as a function of nondimensional time ($\sqrt{g}\ t/\sqrt{d}$) obtained at $Mo = 10^{-2}$, $Bo = 10$, $\frac{\rho_l}{\rho_g} = 100$, and $\frac{\mu_l}{\mu_g} = 10$.

6 Conclusion

Novel numerical approach for simulating multiphysics flow problems using minimum number of necessary moments. Unsteady evolution of the moments are obtained by the lattice Boltzmann framework. The validation of the method carried out unsteady shear flow, natural convection flow, and a rising bubble flow. Numerical experiments indicate that the moment base lattice Boltzmann Method can improve numerical stability and save storage as compared with the standard lattice Boltzmann method. The advantage is more evident for mulltiphysics flow problems.

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