A Lattice Boltzmann Method with Adaptive Mesh Refinement (AMR) for the simulation of gas-liquid flows

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1. Introduction

Two-phase flows with dynamic interfaces are ubiquitous in daily life as well as in many industrial applications. Gas bubbles and liquid droplets are typical forms of these two-phase flows. In chemical engineering, understanding the dynamics of these bubbles and droplets is crucial to the design and operation of the two-phase flow reactors, ranging from microfluidic devices to large systems such as bubble columns and three-phase fluidized beds. In recent years, advanced Computational Fluid Dynamics (CFD) simulation has been increasingly used to study the multiphase flow problems. In these CFD simulations, the interactions between different phases, including the various forces on the bubbles/droplets, need to be specified using closure models, which come from either experiment correlations, or more detailed numerical simulations. Direct numerical simulation (DNS) is capable of providing such closure relations, by detailed simulation of the motion of individual bubbles/droplets in which the motion of the gas-liquid interface is directly resolved. Several types of DNS methods have been developed, and they can be largely put into three categories: the front tracking method, the front-capturing method, and the diffused interface method. The front tracking method uses Lagrangian tracking particles to form a surface mesh that represents the interface, and these particles are convected by the local flow field in each time step to update the location of the interface. The front-capturing methods include the Volume of Fluid (VOF) and the level set method, in which the interface is represented by the contour of a scalar field, which can be the volume fraction of the gas phase in the computational cell (in VOF), or the distance to the interface (in level set method). The interfaces in both the front-tracking and front capturing methods are considered “physically sharp” with zero thickness, although they are numerically smoothed to avoid the abrupt discontinuity which causes numerical problems. In contrast, the interface in the diffused interface method is physically diffused. In other words, it has a finite thickness, and the density distribution inside the interface is determined by the thermodynamic laws.

Different from most fluid simulation methods that are rooted in the continuum Navier-Stokes equation, the Lattice Boltzmann method (LBM) focuses on the density distribution function of the “molecules” that comprise the fluid. This makes LBM a mesoscale method and can simulate more complicated problems. In addition, the algorithm in LBM is much simpler than that in traditional CFD methods, and parallel computation can be implemented with easy. When simulating interface between two fluid phases, 3 types of LBM techniques have been developed. Both the interaction potential model (Shan and Chen, 1993) and the free-energy model (Swift et al, 1996) employ the idea of diffused interface methods, while the LBM based on color function (Gunstensen and Rothman, 1991) is in fact similar to the their counterparts in sharp interface methods.

The LBM based on interaction potential model has the advantage of clear physical background and simple algorithm. In addition, the interface is formed naturally due to the attractive-repulsive interactions between the fluid "molecules", and therefore no interface tracking or capturing is required. In recent years, there have been several efforts that apply LBM to study the dynamics of bubbles. For example, Sankaranarayanan et al. (2002) used the interaction potential model to study the drag and virtual mass forces on bubbles.

Regardless of the numerical approach used, the central problem in the direct simulation of bubble flows is the accurate representation of the gas-liquid interface. As already mentioned, all numerical approaches use a numerically diffused interface, which spans typically to a thickness of 3~5 grid spacing. In order to have sufficient accuracy, the bubble size must be significantly larger than the interface thickness, and this sets a limitation for the maximum grid spacing, or the minimum grid points across the bubble diameter. For bubbles with small deformation, usually at least 16 grid points across the diameter are required to faithfully represent the bubble surface. This minimum grid number increases when the bubble undergoes larger deformation, for example, in higher Reynolds number flows. At the same time, the simulation domain needs to be significantly larger than the bubble size to avoid boundary effect in simulation, and the computation time and memory usage increase rapidly with the increasing mesh resolution and domain size. However, under the current computation capability, this resolution requirement often has to be compromised. As the result, most simulations to date consider only spherical or ellipsoidal bubble, while simulations for spherical cap and skirted bubbles that frequently appear in engineering applications are scarcely reported. Moreover, in numerical studies which explore the bubble interactions, the number of bubbles that can be put into the simulation domain is restricted due to the computation power. There is a demand for a simulation technique that can simultaneously keep sufficient mesh resolution near the bubble surface, while keeping the total computation cost under control.

Adaptive Mesh Refinement (AMR) technique seems to be a natural candidate for such requirement in resolution and computation cost. Using AMR technique, the mesh resolution varies in the computation domain. Fine mesh resolution is used near the bubble surface to ensure the accuracy, while coarse mesh is applied in the bulk fluid faraway from the interface to reduce computation cost. The mesh resolution is updated dynamically during the simulation to reflect the motion of the interfaces. AMR techniques have been integrated into both traditional Navier-Stokes based methods as well as LBM. Hua et al (2008) combined the front-tracking method with AMR and successfully simulated wide range of bubble regimes, in particular the spherical cap and skirted bubbles. Tolke et al. (2006) employed AMR with LBM for bubble simulation. However, their LBM was based on the color function model for the interface, and therefore the interface is essentially captured as in the interface capturing methods, and lost the advantage of clear physical picture and natural interface in LBM. Several other LBM simulations related to the idea of AMR in single-phase flows also uses variable mesh resolution, and the mesh resolution is either dynamically updated or stationary during the simulation (Fares, 2006; Rhode, et al., 2006; Peng et al, 2006). In these

simulations, fine mesh was applied near the irregular solid boundary to greatly enhance the accuracy of the boundary condition. However, there is no straightforward extension of their single-phase algorithm to two-phase flow problems.

In this study, a new LBM approach with AMR capability is developed for the gas-liquid flows. The two-phase LBM is based on the interaction potential model developed by Shan and Chen (1993). The LBM-AMR algorithm will be introduced, followed by numerical examples of both single and two-phase flows.

2. LBM algorithm on uniform grid

The LBM algorithm is based on a special discretization of the Boltzmann equation in time, space, and velocity space. The main variable in LBM algorithm is the density distribution of the fluid "molecules", $f_i(\mathbf{x},t)$, which is the density distribution of fluid "molecules" with velocity $\mathbf{c}_i$ at location $\mathbf{x}$ and time *t*. The evolution of the distribution function obeys the LBM equation:

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{(eq)}(n,\mathbf{v})\right) \tag{1}$$

The left hand side of equation (1) is often called "streaming" or "propagation", and accounts for the migration of the fluid molecule from one grid point to the neighboring point. The right hand side is often named "collision", and models the relaxation process of the molecules towards to the local equilibrium distribution $f_i^{(eq)}$, which is the truncated Boltzmann distribution:

$$f_i^{(eq)}(n,\mathbf{v}) = \rho w_i\left[1+\frac{\mathbf{c}\cdot\mathbf{v}}{c_s^2}+\frac{(\mathbf{c}\cdot\mathbf{v})^2}{2c_s^4}-\frac{\mathbf{v}^2}{2c_s^4}\right] \tag{2}$$

The macroscopic variables such as density and momentum are related to the distribution function is such a way that

$$\rho(\mathbf{x},t) = \sum_i f_i(\mathbf{x},t), \quad \rho\mathbf{u}(\mathbf{x},t) = \sum_i \mathbf{c}_i f_i(\mathbf{x},t) \tag{3}$$

The pressure and kinematic viscosity are given as:

$$p = \rho c_s^2 \tag{4}$$

$$\nu = c_s^2\left(\tau - \frac{1}{2}\right)\frac{\Delta x^2}{\Delta t} \tag{5}$$

where τ is the relaxation factor in equation (1).

In practice, the variables in LBM are non-dimensionalized using Δx and Δt as the length and time scale. As the result, the non-dimensional mesh size and time step are both equal to 1.

3. Single phase LBM with AMR

When using different mesh resolution across the computation domain, it is crucial to understand which variables change with mesh size and which are independent of the grid.

In order to achieve the same lattice speed of sound $c_s = \sqrt{\frac{\Delta x}{3\Delta t}}$ across the entire domain, the time step needs to be proportional to the mesh size. Following the convention of LBM, the non-dimensional lattice speed of sound $\hat{c}_s = \frac{1}{\sqrt{3}}$ is used throughout the entire domain.

The fact that the time step Δt varies with Δx has two consequences. Firstly, according to equation (5), to keep the fluid viscosity ν independent of grid size, the relaxation factor τ also need to change with Δx and must be calculated from equation (5). Secondly, the LBM algorithm performs more steps on fine mesh which requires smaller Δt than on the coarser mesh. Therefore, interpolation/average operations need to be performed at the coarse/fine resolution boundary at different moments in a complete time cycle.

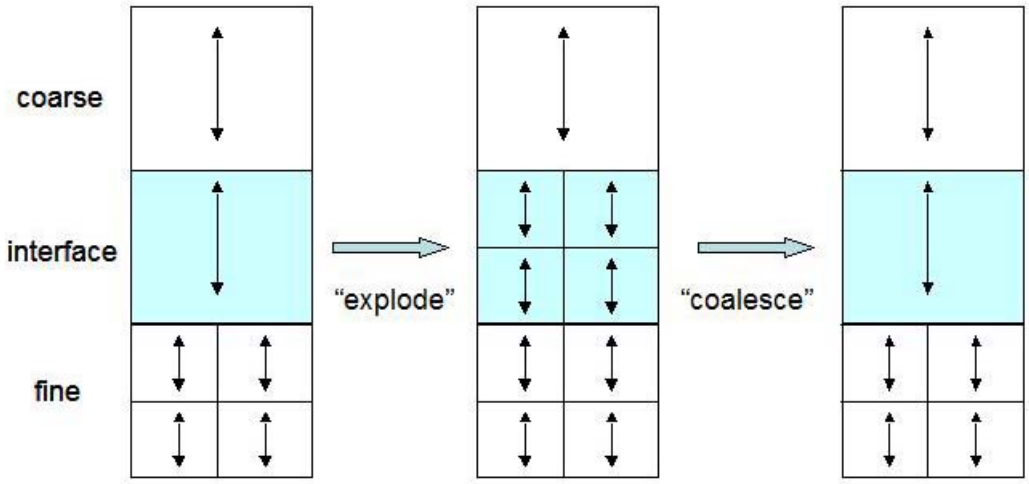


Figure 1. Schematic plot showing the "explode" and "coalesce" operation at refinement jump

The newly developed LBM-AMR approach is based on the multi-block structured grid. The entire computation domain is divided into a number of blocks that have identical grid structure but may have different grid resolutions. The blocks are categorized into different refinement levels, and grid sizes in each two consecutive levels differ by a factor of 2. At most one level difference in refinement levels is allowed at the boundary between two neighboring blocks. Inside each block, structured grid is used as in traditional LBM simulation. For the 2D computation in this study, the classical D2Q9 lattice is employed.

When a refinement level jump is presented between two neighboring blocks, special algorithm is devised to communicate information across block boundary. This process is shown schematically in figure 1. The coarse grid cell at the boundary between the coarse

and fine grid is named “interface” cell, as shown in the shaded zone in figure 1.It acts as the transition between two blocks, and operations “explode” and “coalesce” take place in these interface cells. These operations can be considered as specially designed interpolation and averaging operations.

The original “collide-propagate” algorithm is now complicated by the additional “explode” and “coalesce” operations. The flowchart of the computation procedure on two refinement levels is shown in figure 2. The computation on coarse level uses *dt* as its time step, while the fine grid has the time step of 0.5*dt*. Therefore, the “collide-propagate” operation happens twice on the fine level in each *dt*. The “explode” and “coalesce” steps each operate once during *dt*.

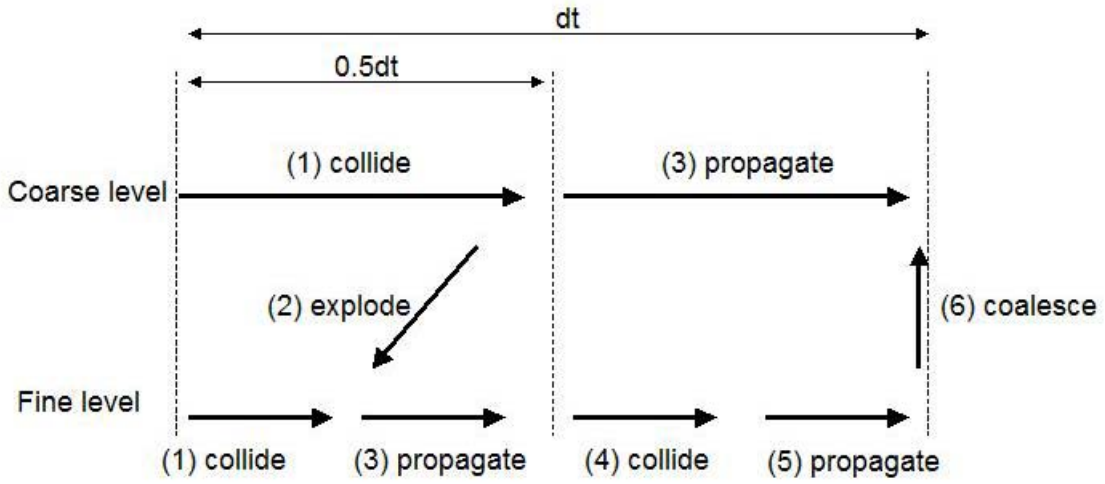
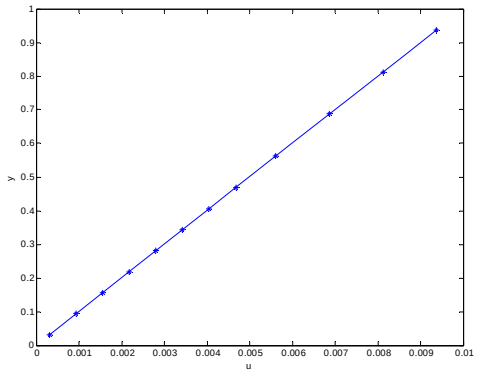


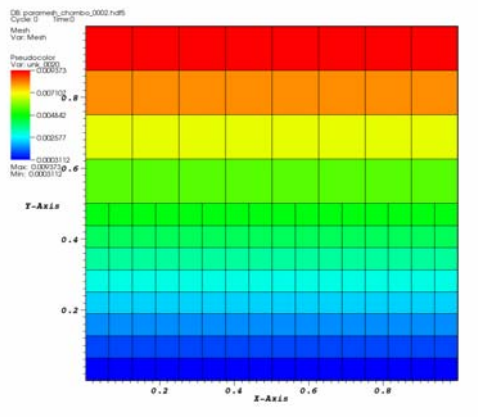
Figure 2. Flowchart of the computation steps for two refinement levels

The simulation code used in this study is developed using the open-source software package Paramesh. Paramesh provides the utilities for mesh generation and management, as well as the framework for parallel computation. The LBM algorithm has been integrated with Paramesh to realize the LBM-AMR technique.

Simulation results for flows between parallel plates driven by either shear or pressure are shown in figure 3. The dots and curves in (a) and (c) presents the simulated velocity profile and the analytical solutions obtained by solving the Navier-Stokes equation, respectively. Figure 3(b) shows the velocity contour and the computation grid used for Couette flow simulation, while 3(d) shows the velocity vectors and the grid for Poisueillie flow. The numerical results matches the analytical results and this proves the accuracy of the LBM-AMR algorithm for single phase flows.



(a)



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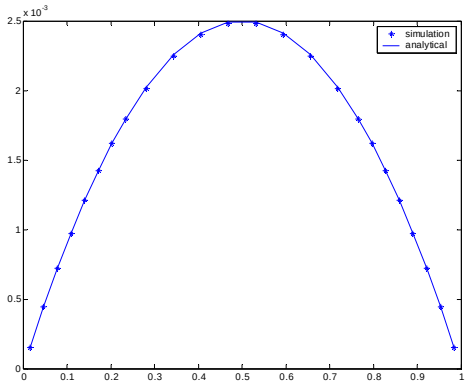
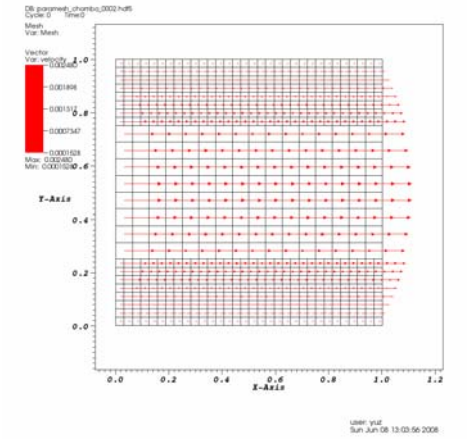


(c)



(d)

Figure 3. Simulation results using LBM-AMR for Couette and Poiseuille flow. (a) Velocity profile for Couette flow. (b) Velocity contour and grid for Couette flow. (c) Velocity profile for Poiseuille flow. (d) Velocity vector and grid for Poiseuille flow.

4. Multiphase LBM with AMR

The multiphase LBM-AMR simulations in this study are based on the interaction potential model developed by Shan and Chen (1993). In reality, the attractive and repulsive interactions between the fluid molecules give rise to the non-ideal Equation of State (EOS) of the fluid, and the gas and liquid phases become separated according to the thermodynamics. Interaction potential based LBM simulations mimic the physics of phase separation by introducing a force term to account for the interactions between fluid molecules. The interaction force is written as:

$$\mathbf{F} = -G\psi \sum_i T_i \psi(\mathbf{x} + \mathbf{c}_i)\mathbf{c}_i \approx -G\psi\nabla\psi \qquad (6)$$

Where $\psi(\rho)$ is the interaction potential and G is the interaction strength constant. The Equation of State of the fluid changes accordingly:

$$p = \rho c_s^2 + \frac{1}{2} c_s^2 G \psi^2(\rho) \tag{7}$$

In order for the interaction potential model to be integrated with AMR technique, again it is important to understand how different variables in the model change with grid resolution. As demonstrated in the single phase LBM-AMR, the relaxation factor τ has different values in regions with different mesh sizes. One problem with the original formulation of the interaction potential model is that the equilibrium for the two stable phases varies when τ changes. This problem is less important in LBM with uniform mesh size. However, for LBM on different mesh size, it causes the fluid to have different equilibrium point in different parts of the computation domain and no consistent phase properties can be achieve throughout the entire domain. In this work, the cause of the problem has been identified to be the way in which the interaction force is incorporated into LBM. While the approach proposed by Shan and Chen (1993) introduces an error on the order of O($\boldsymbol{F}^2$), other approaches, although more complicated, can eliminate this error and achieve identical equilibrium point for different τ.

Besides the effect of the force term, the equilibrium properties are also related to the structure of the interface between phases. This is a direct result of the diffused interface nature of the interaction potential LBM model. Once the formulation of the interaction force is specified, the density profile of the interface can be derived from the mechanical equilibrium condition, and properties such as equilibrium densities, interface thickness, and surface tension can be obtained analytically. The analytical approach to find these properties has been recently reported by Shan (2008). The approach has been tested extensively with different parameters in the current study, and the simulations prove the validity of the analysis by Shan.

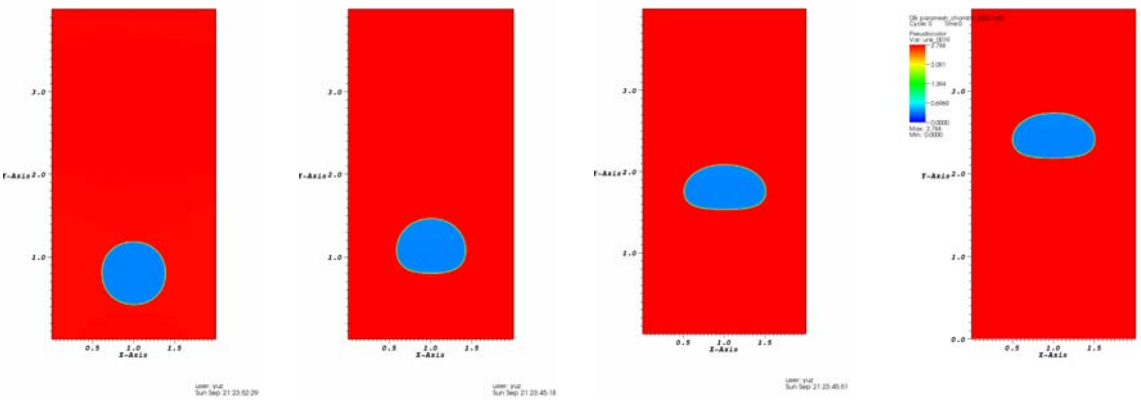


Figure 4. Ellipsoidal bubble. Eo=4.1, Mo=3.3*10^{-4}.
From left to right, time step=0, 1500, 3500, 5500.

It is well known that the surface tension in the interaction model comes from the higher order term in the interaction force. More detailed analysis shows that the value of the surface tension in the original interaction model is proportional to the grid size dx. To compensate for the difference due to grid size effect, an additional higher order term must be included in the interaction force to achieve consistent surface tension throughout the domain. The new interaction force has the form

$$\mathbf{F} = -G\psi\nabla\psi + k\psi\nabla\nabla^2\psi \tag{8}$$

where the second term is the correction to the grid size effect.

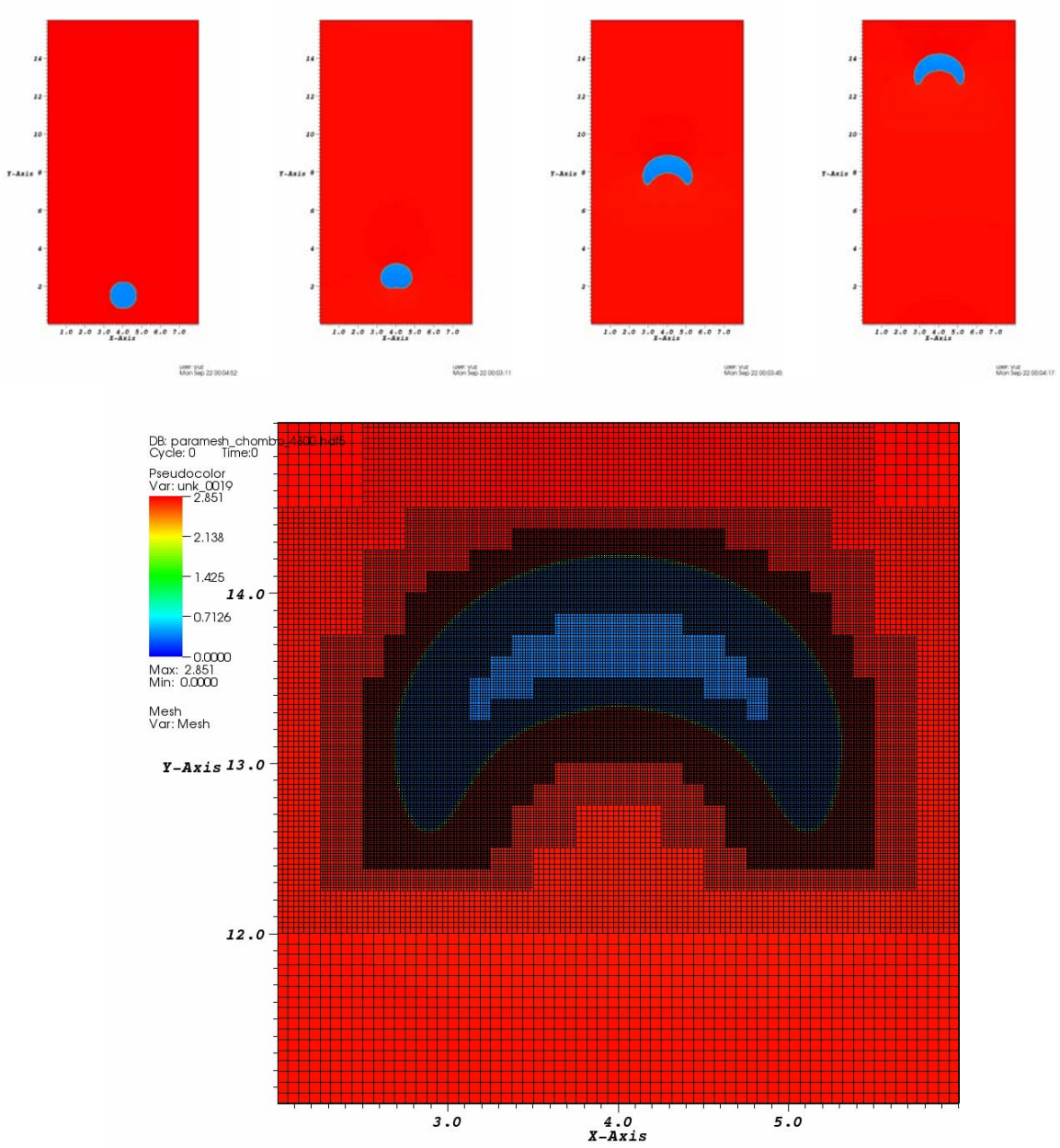


Figure 5. Ellipsoidal cap bubble. Eo=62, Mo=135.
Top: from left to right, time step =0, 200, 1000, 1800
Bottom: mesh near bubble, t=3800

The multiphase LBM-AMR technique is applied to simulate single gas bubble rising in liquid. Two typical cases are presented for the ellipsoidal bubble and the ellipsoidal cap bubble. 4 levels of grids are used for the ellipsoidal bubble, while 9 levels are used for the ellipsoidal cap bubble. The time sequences of the bubble rising are shown in figures 4 and 5. The bubble shapes compare well with the experimental results obtained by Bhaga

and Weber (1980). An enlarged view of the hierarchical mesh near the bubble is included in figure 5. It can be concluded that the current LBM-AMR approach is able to simulate bubbles with moderate to large deformations.

5. Conclusion

In this work, the principle for LBM-AMR technique is discussed. The dependency of different variables on the grid size is analyzed. The newly developed method is applied to first study the single phase flows, and then multiphase flows in which a gas bubble rises in liquid is also presented. The results show that the LBM-AMR is an accurate and efficient method for direct simulation of both single phase and gas-liquid flows.

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References:

Bhaga, D. and Weber, M. E., 1981, Bubbles in viscous liquids: shapes, wakes, and velocities. Journal of Fluid Mechanics, 105, 61-85

Fares, E., 2006, Unsteady flow simulation of the Ahmed reference body using a lattice Boltzmann approach. Computer and Fluids, 35, 940-950.

Gunstensen , AK, Rothman D., 1991. Lattice Boltzmann model of immiscible fluids. Physical Review A. 43(8) 4320-7

Hua, JS. Stene, JF. Lin P., 2008. Numerical simulation of 3D bubbles rising in viscous liquid using a front tracking method. Journal of Computational Physics, 227: 3358-3382

Peng, Y. et al. 2006. Application of multi-block approach in the immersed boundary-lattice Boltzmann method for viscous fluid flows. Journal of Computational Physics, 218, 460-478.

Rohde, et al. 2006. A generic mass-conservative local grid refinement technique for lattice Boltzmann scheme. International journal for numerical methods in fluids. 51: 439-468.

Sankaranarayanan, K., Shan, X., Kevrekidis, I. G., and Sundaresan, S., 2002, Analysis of drag and virtual mass forces in bubbly suspensions using an implicit formulation of the lattice Boltzmann method, Journal of Fluid Mechanics, 452, 61-96

Shan, XW. and Chen, H.D., 1993, “Lattice Boltzmann model for simulating flows with multiple phase and components”, Physical Review E 47 1815-1819

Shan, XW. 2008. Pressure tensor calculation in a class of non-ideal gas lattice Boltzmann models. Physical Review E, 77: 066702.

Swift, M. R., Orlandini, E., Osborn, W. R., and Yeomans J. M., 1996, Lattice Boltzmann simulations of liquid-gas and binary fluid systems, Physical Review E, 54(5) 5041-5052

Tolke, J., Freudiger, S., and Krafczyk, M., 2006, An adaptive scheme using hierarchical grids for lattice Boltzmann multiphase flow simulations. Computer and Fluids, 35, 820-830.