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A comparative study of lattice Boltzmann and front-tracking finite-difference methods for bubble simulations

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Abstract

This communication describes the results of bubble rise simulations using a lattice Boltzmann method and a front-tracking finite-difference method. The simulations, performed in a 2-D periodic box, consider two specific examples: a steadily rising bubble and a bubble rising in an oscillatory manner with accompanying shape change. We compare the shapes and rise velocities of the steadily rising and oscillating bubbles, the oscillation frequencies and amplitudes, and the bubble shapes at different phases of the oscillations. The simulations reveal that both numerical schemes afford qualitatively similar results, which are within a few percent quantitatively.

Keywords: Lattice Boltzmann method; Front-tracking finite-difference method; Bubble rise; Gas–liquid flow

1. Introduction

Over the past decade the lattice Boltzmann method (LBM) has evolved rapidly as a promising approach to solving certain classes of fluid flow problems. It has been shown in the literature (e.g. Chen and Doolen, 1998) that, in the low Mach number limit, the Navier–Stokes equation can be recovered from the LBM equations. Thus, LBM has been employed as an alternative to conventional computational fluid dynamics based on the Navier–Stokes equations (Chen and Doolen, 1998). As with every numerical scheme, the LBM has its limitations. For example, the fluid phase is treated as compressible in the LBM, so that flow of essentially incompressible liquids can

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be modeled only if the liquid is approximated as a modestly compressible fluid; this places limitations on the pressure drops which can be handled without creating unacceptably large changes in the liquid density. Because of such limitations, the LBM has been harshly criticized by some researchers, in spite of the fact that numerous benchmark calculations have been performed using LBM (e.g. Gustensen et al., 1991; Shan and Chen, 1993; Swift et al., 1995; Takada et al., 2000; Sankaranarayanan et al., 2002).

The first three authors of this communication have used LBM to study the rise behavior of a single gas bubble in periodic boxes of various dimensions (Sankaranarayanan et al., 2002) and extracted closures for two-fluid models. They have also performed many benchmark calculations to show that the computed results are consistent with literature correlations for rise velocity, bubble aspect ratio and wake shedding frequency. In spite of such validation, objections to LBM remain strong.

Tryggvason and coworkers have developed a front-tracking finite-difference method (FTFDM) to study bubbly suspensions and used this scheme to simulate a variety of bubble flow problems (Esmaeeli and Tryggvason, 1998, 1999; Tryggvason et al., 2001).

At various conferences, the researchers who object to LBM, have called for a head-to-head comparison of the LBM and FTFDM on some test problems to expose the similarities and differences. This is the goal of the present communication, where we describe the results of bubble rise in a two-dimensional periodic box generated using LBM and FTFDM. We present two examples. The first case is a steadily rising, but distorted, bubble. The second case involves a bubble rising in an oscillatory manner, whose shape is also changing in a periodic manner. Through a head-to-head comparison of the two methods for these two cases, we show that both methods yield essentially the same results.

1.1. The lattice Boltzmann method

The details of the LBM used in this communication has been described in an earlier work (Sankaranarayanan et al., 2002). The physical space (2-D in our examples) is first made dimensionless using an appropriate characteristic length and then represented by a square grid. The particles at each node are allowed to have one of nine possible (dimensionless) velocities, so chosen that after each dimensionless time step of unity, the particles reach one of eight neighboring sites or stay at the same node (corresponding to null velocity). The particle motion is driven by a combination of interparticle and external forces. In our examples, the gas bubble and the surrounding liquid medium are generated as coexisting phases of a two-component mixture in which the species interaction parameters are tailored to keep one component preferentially in the gas phase and the other in the liquid. The external force (gravity) is used to drive bubble rise. The evolution equation for single particle velocity distribution can be found in Sankaranarayanan et al. (2002). The mixture density, velocity and the temperature profiles are found from the moments of the distribution functions. We limit ourselves to an isothermal system.

1.2. Front-tracking/finite difference method

The front-tracking/finite difference method uses a single set of equations for both the liquid and gas phase. Interfacial tension is therefore introduced as a delta-function concentrated at the surface of the bubble. The fluids are incompressible and immiscible, and the density and viscosity of each fluid is constant. We use a fixed, regular, staggered grid and discretize the Navier–Stokes equations using a conservative, second-order centered difference scheme for the spatial variables and an explicit second-order time integration method. The pressure equation is solved by multigrid iteration. In addition to the fixed grid used to solve the conservation equations, the front is resolved by discrete computational points that are moved by interpolating their velocities from the grid. These points are connected by lines to form a front that is used to keep the density and viscosity stratification sharp and to calculate the interfacial tension. For a detailed description of the method and various validation tests, see Unverdi and Tryggvason (1992), Esmaeeli and Tryggvason (1998), and Tryggvason et al. (2001).

1.3. Results

We performed simulations in 2-D at three different resolutions (64×64, 128×128 and 256×256 grids) using both the LBM and FTFDM for two distinct cases: (1) a steadily rising bubble; and (2) a bubble undergoing shape oscillation and rising in an oscillatory fashion. The simulations took place with doubly periodic boundary conditions, and a gas fraction of 0.0881. In order to ensure that the momentum of the gas–liquid mixture did not change in time, we imposed a pressure gradient which equaled the weight of the mixture (see e.g. Sankaranarayanan et al., 2002; Esmaeeli and Tryggvason, 1998, 1999).

We present the results in terms of the following dimensionless groups: Reynolds number ($Re = Vd/v$), Eötvös number ($Eo = g\Delta\rho d^2/\sigma$), Morton number ($Mo = g\rho_\ell^2\Delta\rho v^4/\sigma^3$), a dimensionless period of oscillation Tv/d^2 and a dimensionless amplitude of oscillation (A/d). In these, ρ_ℓ is the density of the continuous (liquid) phase; g is the acceleration due to gravity; v is the kinematic viscosity of the liquid; σ is the interfacial tension; $\Delta\rho$ is the density difference between liquid and gas phases; V is the magnitude of the slip velocity; d is the (area equivalent) diameter of the bubble; T is the period of oscillation; and A is the amplitude of oscillation. In our simulations, Eo and Mo are input parameters, whereas Re and bubble shape are outputs. In both numerical schemes, we first created a circular bubble in the absence of gravity and then turned on gravity to achieve the desired Eo and Mo. Both numerical schemes yielded steadily rising bubbles (henceforth, case 1) for $Eo = 2.1337$ and $Mo = 1.6425 \times 10^{-4}$, and bubbles rising in an oscillatory manner (henceforth, case 2) for $Eo = 8.5348$ and $Mo = 6.57 \times 10^{-4}$. These results are described below.

In Fig. 1 we show the shapes of a steadily rising bubble obtained with the two numerical schemes for case 1. Both methods give shapes which are in close agreement with each other, and the Reynolds numbers are within 2%. The rise velocities of the bubbles were determined by tracking the centroids as functions of time.

Fig. 2 shows the trajectory of the centroid of the oscillatory bubble, as computed by the LBM (panel a) and FTFDM (panel b). The dimensionless amplitude (A/d) is 0.50 for LBM and 0.46 for FTFDM. The dimensionless periods of oscillation (Tv/d^2) for the two methods are 0.20 and 0.21, respectively. The Reynolds numbers, based on average vertical velocity over a period of the fully developed oscillation cycle, are within 6%. In both numerical approaches, when the gravity was turned on, the bubbles began to rise vertically, deformed quickly and assumed nearly identical shapes. This can be seen in Fig. 3a and b, which compare shapes at early times in the bubble rise

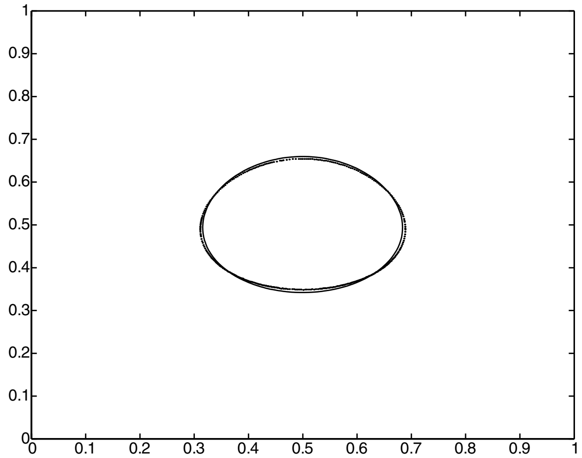

Fig. 1. Shape of a rising 2-D bubble. 128×128 nodes. $Mo = 1.6425 \times 10^{-4}$; $Eo = 2.1337$. Bubble area fraction = 0.0881. (—) LBM, $Re = Vd/\nu = 10.79$; (- - -) front-tracking finite difference, $Re = 10.97$. In both cases, the bubbles rise vertically upwards.

simulations. The oscillatory rise (and the concomitant shape oscillation) evolved more slowly and their growth times depended on the numerical round-off and truncation errors inherent in the two schemes. Hence it is not meaningful to compare the temporal evolution of the structures by comparing shapes at identical times. It is, however, easy to compare the details of the fully developed oscillatory state, which is presented in Fig. 4a and b. In these figures, we begin from a state where the centroid of the bubble is close to the extremum on the right side (see where the dotted line begins at the bottom of each of these figures) and show the shapes of the bubbles at various times after that. The grid spacing in the Y-axis in these figures represent one-half box height. It is clear that the bubble shapes at various phases of the oscillation cycle are very similar for both methods.

We tested the effect of resolution on bubble rise velocity by repeating the LBM and FTFDM simulations for 64×64 and 256×256 grids, and the results are summarized in Tables 1 and 2. The rise velocities for case 1 obtained with the 256×256 simulations are within 0.3% of each other, and the shapes are essentially indistinguishable (not shown). Thus, there is no question that both methods are converging towards the same solution in this case.

It is clear from this table that the estimates for the rise velocities are only weakly dependent on spatial resolution for the case of steadily rising bubbles (case 1), while this dependence is more pronounced for the case where the bubble shape is changing with time (case 2). This is not surprising, since the oscillatory motion is accompanied by wake shedding which requires simulations at higher resolution. The differences seen between the LBM and the FTFDM results are comparable to those observed with different grid resolutions in LBM. It does appear that the LBM results converge towards the FTFDM results as the grid resolution is increased. However, it is disappointing that, in both schemes, a grid-size independent average rise velocity is not achieved even with 256×256 grids. Linear extrapolation of the computed Re at various grid sizes to zero grid size led to an estimate of 15.84 for both methods. Such an extrapolation is not rigorous, but it

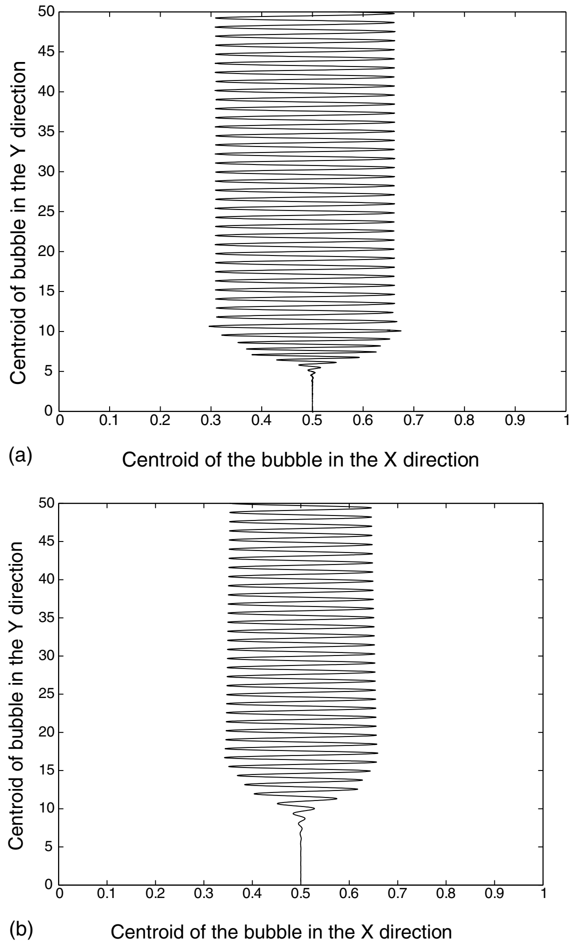

Fig. 2. Trajectory of the centroid of a 2-D bubble rising in an oscillatory manner. 128 × 128 nodes. $Mo = 6.57 \times 10^{-4}$; $Eo = 8.5348$. Bubble area fraction = 0.0881. (a) LBM, $Re = 16.88$, amplitude of the oscillation, $A/d = 0.50$, period of oscillation, $T\nu/d^2 = 0.20$; (b) Front-tracking finite difference, $Re = 17.35$, amplitude of the oscillation, $A/d = 0.46$, period of oscillation, $T\nu/d^2 = 0.21$.

suggests that the inaccuracy in either scheme may be about 3–4% even at the highest resolution employed in this comparative study.

2. Summary

In this communication we have compared the LBM and a FTFDM for 2-D simulations of bubble rise in a periodic box. The examples presented illustrate that both methods yield qualitatively similar results. The quantitative agreement between the methods is better for the case of a steadily rising bubble and it deteriorates (to ~6% for the example presented) when the bubble shape oscillates intensely with time. The bubble shape oscillations are very similar. The LBM has

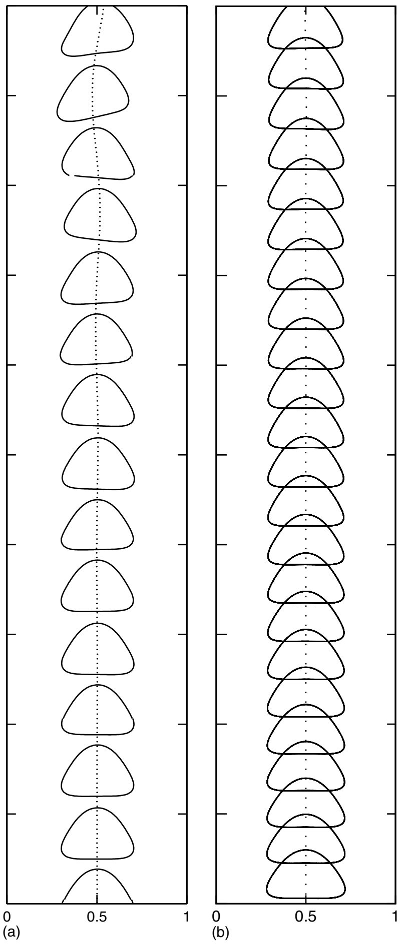

Fig. 3. Snapshots of bubble shapes at various times during the early stages of the development of the oscillatory flow. Conditions are as in Fig. 2. (a) LBM; (b) FTFDM. The y-coordinates are arbitrary and the distance between grid points in the y-axis is one-half of a box height.

been criticized by some researchers as being flawed and unreliable. The simulation of an oscillating bubble presented here is a fairly complex problem and the fact that LBM is able to capture rather closely the results of the FTFDM shows that when applied properly LBM can yield meaningful results.

Every numerical scheme has its limitations and LBM is no exception. In the lattice Boltzmann scheme used in our study, the liquid is treated as a slightly compressible fluid, and is indeed far more compressible than any typical liquid. Consequently, this scheme is not appropriate for flows with large pressure drops, where the changes in liquid density (in the LBM simulations) can become large and unphysical. In the periodic-domain simulations presented here, such large pressure drops do not arise. Also, the LBM scheme is equivalent to the Navier–Stokes equation only in the low Mach number limit. Therefore, if the intent is to employ LBM as an alternative to conventional CFD of the Navier–Stokes equations, one must ensure that the Mach number in the

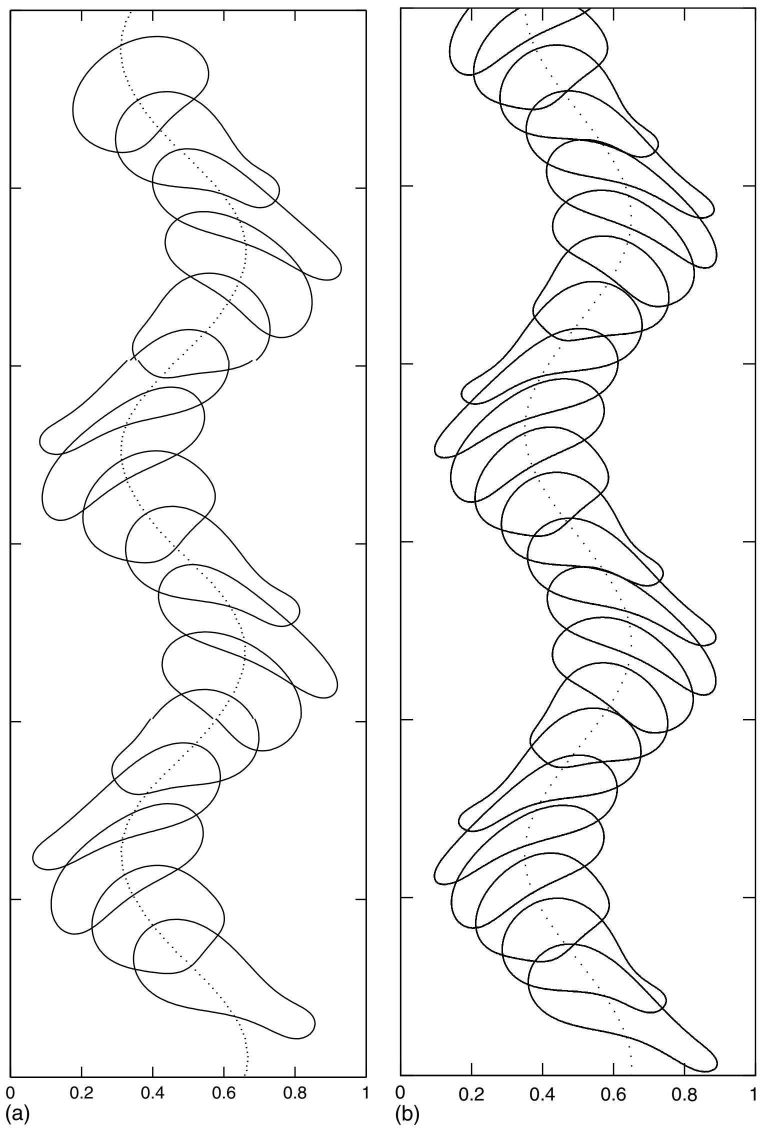

Fig. 4. Snapshots of bubble shapes in a fully developed oscillatory flow. Conditions are as in Fig. 2. (a) LBM; (b) FTFDM. The y-coordinates are arbitrary and the distance between grid points in the y-axis is one-half of a box height.

LBM simulations is indeed small. As the compressibility of the liquid in our LBM simulations is appreciably larger than the true compressibility, the Mach number in the LBM simulations is much larger than the true Mach number of the flow. In the LBM simulations shown in this paper, the Mach number is kept below 0.1 at all times and all locations. The comparisons presented in this paper indicate that, as long as such simple restrictions are recognized, LBM can indeed serve as an alternative to finite-difference or finite-element simulations of the Navier–Stokes equations. The LBM may be more convenient to program for a class of problems (when compared to the

Table 1
LBM simulation results

Resolution	Case 1	Case 2		
	Re	*Re*	A/d	$T\nu/d^2$
64×64	11.02	17.60	0.35	0.19
128×128	10.79	16.88	0.50	0.20
256×256	10.98	16.20	0.45	0.21

Table 2
FTFDM simulation results

Resolution	Case 1	Case 2		
	Re	*Re*	A/d	$T\nu/d^2$
64×64	10.99	18.23	0.43	0.22
128×128	10.97	17.35	0.46	0.21
256×256	10.95	16.28	0.47	0.22

conventional CFD), but at the same time there is no basis for arguing that it is a superior method. It is simply a possible alternate scheme.

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