Three-Dimensional Micro-Droplet Collision Simulation using the Lattice Boltzmann Method

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Abstract The modelling of binary droplet collisions has important applications in many engineering problems, including spray coating and fuel injection. The Lattice Boltzmann method (LBM) is a well established technique for modelling multiphase fluids, and does so without the difficulties of explicit interface tracking found in other CFD methods. However, simulating droplet collisions under realistic conditions remains a complex problem. Challenges include reproducing the different collision outcomes observed experimentally (Qian and Law, 1997), and maintaining a stable simulation at sufficiently high Reynolds and Weber numbers, and with a high density ratio between the liquid and gas phases. Although previous studies have achieved these goals individually, they have not been successfully combined to simulate droplet collisions with realistic physical parameters.

A number of different methods for extending the LBM for multiphase flow exist, with the Shan-Chen interparticle potential method (Shan and Chen, 1993) being the basic model used here. Many extensions to improve the original Shan-Chen method have been proposed, to improve achievable Reynolds number and density ratio. Using combinations of these, both coalescence and separation of two-dimensional droplets were successfully simulated at density ratios of order 1000, and high Weber numbers (Lycett-Brown et al., 2011).

In this study, the developed methodologies in Lycett-Brown et al. (2011) are extended to simulate three dimensional micro-droplet collisions by making use of the LBM's excellent scalability on massively parallel computers. These high-resolution simulations are also compared with low-resolution three-dimensional simulations using a multiple-relaxation-time LBM approach (Monaco and Luo, 2008).

Keywords: Lattice Boltzmann Method, Multiphase Flow, Binary Droplet Collision

1. Introduction

The Lattice Boltzmann Method (LBM) is a rapidly developing approach to computational fluid dynamics (CFD). It offers a computationally efficient alternative to conventional numerical methods, with advantages in simulating micro flows, complex geometries, and multiphase fluids (Succi, 2001). As the LBM solves mesoscopic kinetic equations, it is particularly suited to incorporating the interfaces between different phases. The discrete kinetic equations solved are designed in such that they reproduce the Navier-Stokes equation in the hydrodynamic limit.

A number of different approaches to simulating multiphase fluids with the LBM have been suggested. The Shan-Chen interparticle potential model (Shan and Chen, 1993) is the basis of the method used here. While this method is only computationally stable when the density ratio between the gas and liquid phase is small, a number of different solutions to this problem have been proposed. Here the grid refinement method (Sbragaglia et al., 2007) is used to allow a density ratio of 1000 to be stably simulated.

The study of binary droplet collisions presents a significant challenge for LBM, and other CFD methods. LBM is at an advantage as it does not have to track the complex merging, and in some cases splitting, of the droplet interfaces. However to date

simulations have either achieved high density ratios at low Reynolds number, or vice versa (Inamuro et al., 2004, Monaco, 2009).

A useful property of the LBM is its suitability to large scale parallel computing. To take full advantage of high end multi-core computers CFD codes must scale well as the number of processors are increased, up to the order of tens of thousands on the largest machines currently available. Here a multiphase LBM code is used on thousands of processors, allowing a large grid size to be used. With this, droplet collisions at high Reynolds numbers and high density ratios can be simulated.

The paper is organised as follows: The LBM is briefly described in Section 2, with the multiphase component of the model discussed in Section 3. Section 4 gives details and scaling results for the parallelization of the multiphase and grid refinement LBM codes. This is then applied to the case of a binary droplet collision at a high density ratio and Reynolds number in Section 5. Section 6 concludes the paper.

2. The Lattice Boltzmann Method

The LBM is a discretisation of the Boltzmann transport equation, which describes the evolution of the density function, *f*, of a gas of point like particles

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\boldsymbol{\nabla}_{\mathbf{x}} f + \mathbf{a}\cdot\boldsymbol{\nabla}_{\mathbf{p}} f = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}}, \qquad (1)$$

where $\mathbf{a}$ is an external force. As is common in many LBM methods the right hand side is approximated here by the Bhatnagar-Gross-Krook (BGK) collision term. Discretisation of this equation, details of which can be found in many papers, including He and Luo (1997), leads to the Lattice BGK method. The method involves the streaming of distribution functions between fixed nodes along lattice velocities $\mathbf{v}_\alpha$, and then relaxing these distributions to their local equilibrium, $f_\alpha^{\text{eq}}(\mathbf{x}, t)$, at each lattice node

$$f_\alpha(\mathbf{x}+\mathbf{v}_\alpha, t+1) = \left(1-\frac{1}{\tau}\right) f_\alpha(\mathbf{x}, t) + \frac{1}{\tau} f_\alpha^{(eq)}(\mathbf{x}, t), \qquad (2)$$

where τ is the relaxation time, and the forcing term has been left out, this will be discussed in the following section. In computation the left and right hand sides are separated into a streaming and calculation step respectively. Macroscopic quantities are recovered from moments of the distribution function

$$\rho = \sum_\alpha f_\alpha, \qquad (3)$$

$$\rho\mathbf{u} = \sum_\alpha \mathbf{v}_\alpha f_\alpha. \qquad (4)$$

These are used to calculate the equilibrium distribution functions at each node. The 3-dimensional lattice used in this work has 27 velocities, (0, 0, 0), (±1, 0, 0), (0, ±1, 0), (0, 0, ±1), (±1, ±1, 0), (±1, 0, ±1), (0, ±1, ±1) and (±1, ±1, ±1), and is labelled the D3Q27 lattice. Its equilibrium distribution function, to second order in velocity, is given by

$$f_\alpha^{(eq)} = w_\alpha \rho \left\{ 1 + \frac{(\mathbf{v}_\alpha\cdot\mathbf{u})}{c_s^2} + \frac{(\mathbf{v}_\alpha\cdot\mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2} \right\} \qquad (5)$$

where w_α is a weighting function, and c_s is the speed of sound. This equilibrium is designed in such a way as to reproduce the Navier-Stokes equation in the macroscopic limit, with $c_s^2 = 1/3$.

3. Multiphase LBM

3.1 The Shan-Chen Model

The Shan-Chen multiphase method (Shan and Chen, 1993) introduces an interparticle potential to induce phase separation. This potential is given by

$$V(\mathbf{x}, \mathbf{x}+\mathbf{v}_\alpha) = G\psi(\mathbf{x})\psi(\mathbf{x}+\mathbf{v}_\alpha), \qquad (6)$$

where G controls the strength of the interaction, and ψ is an effective number density. This potential produces a change of momentum at each site

$$\frac{dP}{dt}(\mathbf{x}) = -G\,\psi(\mathbf{x})\sum_{\alpha}\psi(\mathbf{x}+\mathbf{v}_{\alpha})\mathbf{v}_{\alpha}. \qquad (7)$$

The equilibrium distribution function, Eq. (5), is then calculated using a modified velocity, $\mathbf{u}'$, given by

$$\rho\mathbf{u}' = \rho\mathbf{u} + \tau\frac{dP}{dt}. \qquad (8)$$

Using this form of the interaction force, the resulting equation of state of the system is now

$$P = \rho c_s^2 + G\frac{c_s^2}{2}\psi(\mathbf{x})^2, \qquad (9)$$

where the second term on the right hand side alters the ideal gas equation of state as a result of the interaction force. For phase separation to occur a suitable $\psi(\rho)$ must be chosen, and G must be negative and below a certain critical value. Here we use

$$\psi(\rho) = \sqrt{\rho_0}\left(1 - \mathrm{e}^{-\frac{\rho}{\rho_0}}\right) \qquad (10)$$

where ρ_0 is a reference density. This choice is similar to that originally proposed by Shan and Chen (1993), it is a monotonically increasing function of density and therefore provides the correct form for the pressure to induce phase separation. It also has the advantage that it becomes constant at high density and therefore prevents high density areas collapsing.

This model is only stable for density ratios between the gas and liquid phases of $\mathcal{O}(10)$. The grid refinement method of Sbragaglia et al. (2007) allows this to be greatly increased.

3.2 Grid Refinement

One major drawback of the original Shan-Chen multiphase method is the inability to independently vary density ratio and surface tension. To improve stability at higher density ratios it would be useful to be able to spread the interface over a larger number of points, however as the interface width is related to surface tension this is not possible. To resolve this Sbragaglia et al. (2007) generalised Eq. (7) to include both nearest and next-nearest neighbours

$$\boldsymbol{F} = -\psi(\mathbf{x})\sum_{\alpha} w(|\mathbf{v}_{\alpha}|^2)\times \left[G_1\psi(\mathbf{x}+\mathbf{v}_{\alpha}) + G_2\psi(\mathbf{x}+2\mathbf{v}_{\alpha})\right]\mathbf{v}_{\alpha}. \qquad (11)$$

The pressure tensor is now

$$P_{ij} = \left(\rho c_s^2 + \frac{A_1 c_s^2}{2}\psi^2 + \frac{A_2 c_s^4}{4}|\nabla\psi|^2 + \frac{A_2 c_s^4}{2}\psi\nabla\psi\right)\delta_{ij} - \frac{A_2 c_s^4}{2}\partial_i\psi\partial_j\psi + O(\partial^4), \qquad (12)$$

where

$$A_1 = G_1 + 2G_2, \qquad A_2 = G_1 + 8G_2. \qquad (13)$$

The surface tension is now given by

$$\sigma = -\frac{A_2 c_s^2}{2}\int_{-\infty}^{\infty}\left|\partial_y\psi\right|^2 dy. \qquad (14)$$

As there are now two tuneable parameters in the system, G_1 and G_2, the equation of state, and therefore the density ratio, and the surface tension can be controlled separately. With ψ in the form given by Eq. (10), it can be shown (Sbragaglia et al., 2007) that rescaling coordinates using $x' = \rho_0 x$, allows the interface width to be changed by varying ρ_0, keeping density ratio and surface tension constant, as long as A_2 is varied according to

$$A_2 = \frac{A_2'}{\rho_0^2}. \qquad (15)$$

Using this method density ratios of $\mathcal{O}(1000)$ can be simulated.

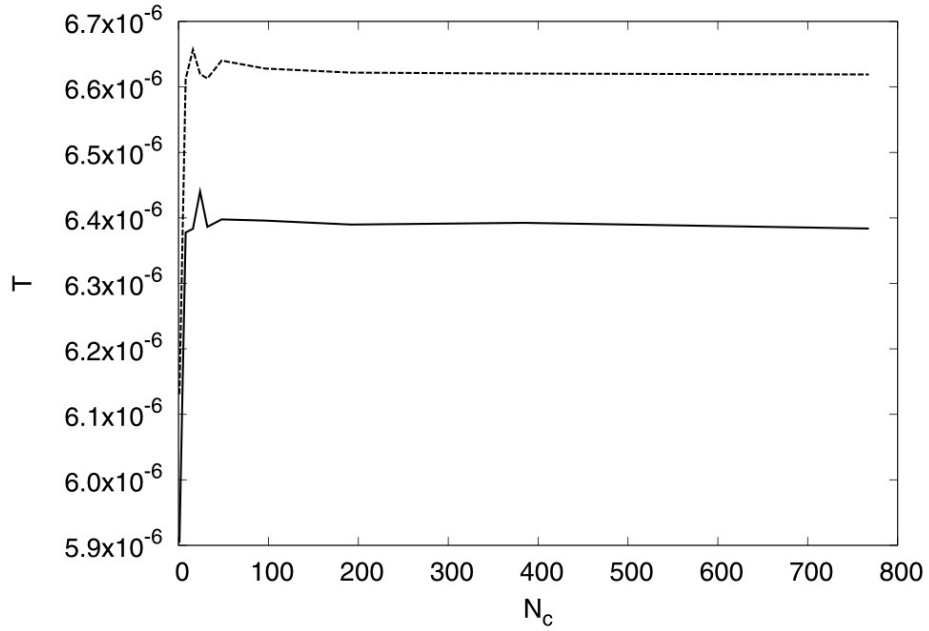

Fig. 1. Time per iteration per grid point on a grid size of 96^3 per core, for the Shan-Chen multiphase LBM (solid line), and grid refinement method (dashed line).

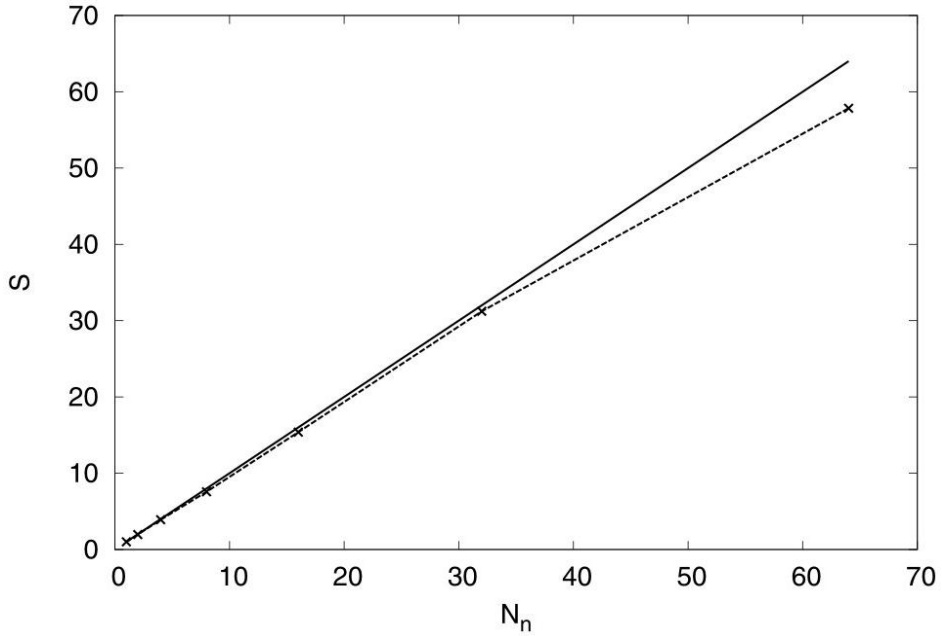

Fig. 2. Speedup for Shan-Chen multiphase LBM (dashed line) and linear speedup (solid line). Grid size 192^3. N_n is number of nodes, with 12 cores per node.

4. Parallel LBM

On a single processor in 3-dimensions the largest grid size it is possible to use is of $\mathcal{O}(100^3)$. As the LBM only requires information from its nearest neighbours at each time step it is naturally well suited to parallelisation for use on many core machines. The domain is divided up evenly between the available cores, and at each time step the outer nodes of each domain require information from their neighbouring domains. In the single phase case this is only required once per time step, when the particle distribution functions are streamed along lattice nodes. In the multiphase case a second series of

communications is required for the calculation of $\boldsymbol{F}$. The original Shan-Chen method only requires nearest neighbours for this, however the grid refinement method also requires next nearest neighbours, and therefore more information must be passed between cores. The algorithm iterates over the following subroutines:

- Calculate the RHS of Eq. (2)
- Communicate boundary site propagation
- Propagate internal sites
- Calculate $\rho, \mathbf{u}$ and ψ at each site
- Communicate ψ
- Calculate $\boldsymbol{F}$ and $\mathbf{u}'$
- Calculate $f^{(eq)}$, Eq. (5)

where the first communication is the same in all cases, single and multiphase. The second communication requires moving twice as much data when using grid refinement as for the basic Shan-Chen method. This algorithm was tested on HECToR, a Cray XE6 System. Each XE6 computer node contains two AMD 2.1 GHz 12-core processors, up to 32 of which are used here, giving 768 cores in total. Scaling tests were conducted on the codes, with results given in Figs. 1 and 2. For weak scaling the problem size used was 96^3 per core. The multiphase LBM shows excellent scaling for both Shan-Chen and grid refinement cases, in both cases the communications require an overhead of less than 10%, and importantly as the number of cores is increased this is not seen to change. Therefore as the number of cores is increased with problem size, the time taken remains constant. In the strong scaling case, the Shan-Chen method shows good scaling, until problem size per node becomes smaller than would practically be of use.

5. Droplet Collisions

The difficulty in reproducing experimental results for binary droplet collisions comes from matching the following dimensionless parameters in the real system in a stable simulation. The first of these, the density ratio between the gas and liquid components is of $\mathcal{O}(1000)$. The second is Reynolds number, defined for the case of two droplets of equal radius, *R*, colliding as

$$Re = \frac{2RU}{\nu_l}, \tag{16}$$

where U is the relative velocity of the droplets, and ν_l is the kinematic viscosity of the liquid, given by

$$\nu_l = c_s^2\left(\tau - \frac{1}{2}\right), \tag{17}$$

experimentally Reynolds number is typically of $\mathcal{O}(1000)$. The third is Weber number, defined as

$$We = \frac{2R\rho U^2}{\sigma}, \tag{18}$$

which experimentally takes values up to $\mathcal{O}(100)$.

Of the three parameters for increasing Reynolds number, the velocity is limited by the low Mach number expansion in the equilibrium to $\mathbf{u} < 0.1$. For high density ratio multiphase systems it is found that simulations are unstable for any τ slightly less than 1, which limits low viscosities. This leaves only the radius which can only be increased by increasing the size of the system. For the Weber number the surface tension is limited by the need to maintain a wide enough interface to give a stable simulation, and again the radius remains the only free parameter.

Previous studies have approached this problem in various ways, including using multiphase methods other than the Shan-Chen interparticle potential method, and using techniques for increasing the lower bounds on viscosity. These include Inamuro et al. (2004) using the projection method applied to the free energy model (Swift et al., 1995). Results for a head on droplet collision at a Reynolds number of 2000 and a Weber number of 80 where produced, but at a density ratio of only 50. Monaco (2009) used the Shan-Chen method, but with a different equation of state, which allows high density ratios to be reached (Yuan and Schaefer, 2006), and a multi-

relaxation time method (D'Humieres et al, 2002) to allow slightly lower viscosities. At a density ratio of 1000 this allowed simulations of head on droplet collision at *Re* = 15, and *We* = 0.2.

On a 640×640×480 grid a binary droplet collision with droplets of radius 165 impacting at $U = 0.16$, was simulated, the result shown in Fig. 2. 10,000 time steps took around an hour to compute using 3072 cores on HECToR with an unoptimised code. For this $\tau = 1$, $\rho_0 = 1$, $G_1 = 0$ and $G_2 = -5.3$, giving $\rho_r = 940$. The simulation was at *Re* = 320 and *We* = 9.6, significantly higher than previously simulated at this density ratio.

6. Conclusion

Using the inherent parallelism of the LBM algorithm very large grid sizes can easily be used on many core machines. Even in the multiphase case, and when using the grid refinement method, it is shown that the LBM codes scale extremely well. Here, a large grid resolution allowed a 3-dimensional simulation of a head-on binary droplet collision to be carried out at a higher Reynolds number than had previously been achieved.

Acknowledgments

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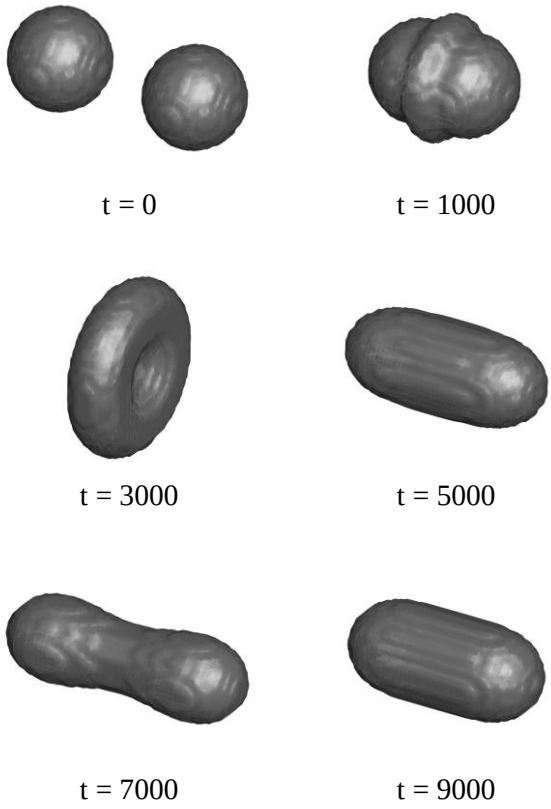

Fig. 2. Head-on binary droplet collision on a 640×640×480 grid, with density ratio = 1000, *Re* = 320 and *We* = 0.2.

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