대한기계학회 2001년도 추계학술대회논문집 B pp. 468~474 KSME 01F223

Numerical Simulation of Shock Propatation by the Finite Difference Lattice Boltzmann Method

Ho-Keun Kang*, Michihisa Tsutahara**, Jeong-Hwan Kim*, Young-Ho Lee*

Key Words: finite difference lattice Boltzmann method(차분격자볼츠만법), the BGK model(BGK모델), compressible fluid(압축성 유체), shock wave(충격파), wave reflection(반사파)

Abstract

The shock process represents an abrupt change in fluid properties, in which finite variations in pressure, temperature, and density occur over a shock thickness which is comparable to the mean free path of the gas molecules involved. The fluid phenomenon is simulated by using finite difference lattice Boltzmann method (FDLBM). In this research, the new model is proposed using the lattice BGK compressible fluid model in FDLBM for the purpose of shortening in calculation time and stabilizing in simulation operation. The numerical results agree also with the theoretical predictions.

1. Introduction

In recent years, the lattice gas automata (LGA)[1,2] or the lattice Boltzmann method (LBM) [3] has received considerable attention as an alternative numerical scheme for simulating complex phenomena. The finite difference lattice Boltzmann method (FDLBM) [4] is one of the computational fluid mechanics which has been developed from the lattice Boltzmann method. In LBM, fluid is regarded as gathering of many particles repeating collision and translation (movement), and the motion of macroscopic fluid is expressed by calculation of these two motions of particles.

Although by using LBM & FDLBM until now, authors examine the flows such as the natural convection [5], the density-stratified flows and the unsteady shock wave [6], the thermo-hydrodynamic model is developed and has been verified.

However, LBM has many problems such as becoming unstable numerically to a heat flow problem or a high Reynolds number flow. The fluid phenomenon is also calculated by using the FDLBM, and the validity of this technique has been examined. But, the method is proven that there is a problem enormously taken the calculation time, when the application to flow of high Reynolds number and boundary fitted coordinate system is examined.

In this research, the new model is proposed using the lattice BGK compressible fluid model in FDLBM for the purpose of shortening in calculation time and stabilizing in simulation operation.

2. Foundation of FDLBM

The lattice BGK model in the finite difference lattice Boltzmann method which used until now in the collision term of fundamental equation has been expressed as

$$\frac{\partial f_i}{\partial t} + c_i \nabla f_i = -\frac{1}{\phi}(f_i - f^{i}_{(0)}) \qquad (1)$$

* Korea Maritime University
** Kobe University

Equation (1) has the Taylor expansion of lattice Boltzmann equation, and has a form equal to the approximate Boltzmann equation which adopts the first term.

The dynamics of the fluid can be described by the distribution function obeying the lattice BGK equation (1) and the macroscopic variables are given by the equilibrium distribution function.

Here, the fundamental physical variables are the density ρ, the momentum ρu_α and the internal energy e, and they are defined as

$$\rho = \sum_{\sigma, i} f_{\sigma i} = \sum_{\sigma, i} f_{\sigma i}^{(0)}, \tag{2}$$

$$\rho u_\alpha = \sum_{\sigma, i} f_{\sigma i} c_{\sigma i\alpha} = \sum_{\sigma, i} f_{\sigma i}^{(0)} c_{\sigma i\alpha}, \tag{3}$$

$$\rho e = \sum_{\sigma, i} \frac{1}{2} f_{\sigma i} c_{\sigma i\alpha}^2 - \frac{1}{2}\rho u^2$$

$$= \sum_{\sigma, i} \frac{1}{2} f_{\sigma i}^{(0)} c_{\sigma i\alpha}^2 - \frac{1}{2}\rho u^2. \tag{4}$$

In Eq.(1), the relation between coefficient of the kinematic viscosity ν deduced and the single relaxation coefficient ϕ, when the Navier-Stokes equation is induced, becomes $\phi \sim \nu$.

Here, when the finite difference calculation of Eq.(1) is used, if the time development is expressed by the Euler method, the equation is written as

$$f_i^{n+1} = f_i^n - \Delta t \cdot \left\{ c_{i\alpha} \frac{\partial f_i^n}{\partial r_\alpha} + \frac{1}{\phi}\left(f_i^n - f_i^{(0)} \right) \right\} \tag{5}$$

In Eq.(5), the coefficient which depends on the collision term is $\Delta t/\phi$, when we consider the collision term of right side.

As well as the relation of $1/\phi < 2.0$ which is stability condition of the collision term in LBM, the relation of $\Delta t/\phi < 2.0$ is established on this coefficient in FDLBM.

In FDLBM, ϕ is very small in the high Reynolds number on the relation between coefficient of kinematic viscosity and single relaxation coefficient $\phi \sim \nu$. Also, from the stability condition of the collision term, Δt must be taken small in order to satisfy the condition of the collision term. Therefore, the enormous calculation time is required to ensure appropriate calculation results.

3. Proposal of a New Model

Here, a new model is proposed in order to solve the problem described as the stated above.

To begin with, we consider that the finite difference lattice Boltzmann method regards as one scheme for deducing the Navier-Stokes equation. we also consider that the relation between coefficient of the kinematic viscosity ν and single relaxation coefficient ϕ is made to convert by disregarding the physical meaning of the fundamental equation, and adding some terms to the fundamental equation.

As the concrete method, the Taylor expansion is done to deduce the Navier-Stokes equation, when considering the derivation process of the viscosity term in LBM, then we deduce the viscosity terms by adoption in the secondary term.

From this fact, we note that the difference between LBM and the fundamental equation, which derivate the viscosity coefficient from the conventional FDLBM, is the existence of the term of the secondary order. Then, the term of the secondary order should be introduced into the equation of the conventional FDLBM.

Here, the term of the secondary derivative in the differential equation means the diffusion, and, in the point of the viscosity, it is regarded that the term of the secondary order is effective for the operation of the viscosity coefficient. Therefore, we can operate that the relation between the viscosity coefficient and the single relaxation coefficient converts by adding the term of the secondary order. Then, we intend to carry out the speed up, which is difficult in the conventional FDLBM model.

As a term of adding secondary order, the numerical calculation should be carried out by introducing the term $-ac_a \frac{\partial}{\partial r_a} \frac{f_i - f_i^{(0)}}{\phi}$.

In short, we transform the fundamental equation (1) as follows:

$$\frac{\partial f_i}{\partial t} + c_{ia}\frac{\partial f_i}{\partial r_a} - ac_{ia}\frac{\partial}{\partial r_a}\frac{f_i - f_i^{(0)}}{\phi} = -\frac{1}{\phi}(f_i - f_i^{(0)}) \tag{6}$$

Here, the added term is similar to $-ac_a \frac{\partial}{\partial r_a}\frac{f_i^{(1)}}{\phi}$, and it can be obtained when the governing equation of the flow is deduced by the Chapman-Enskog development.

Substituting Eqs.(2),(3) and (4) into Eq.(6), and taking terms up to the first order ε, we can obtain

$$\frac{\partial f_i^{(0)}}{\partial t_1} + c_{ia}\frac{\partial f_i^{(0)}}{\partial r_a} = -\frac{1}{\phi}f_i^{(1)} \tag{7}$$

Here, the added term is transformed with

$$a\tau c_a c_\beta \frac{\partial^2}{\partial r_a \partial r_\beta} f_i^{(0)} + a\tau c_a \frac{\partial^2}{\partial t_1 \partial r_a} f_i^{(0)} \tag{8}$$

When the Taylor expansion of LBM is done up to the second order, the equation is written as

$$\frac{\partial f_{\sigma i}}{\partial t} + c_{\sigma ia}\frac{\partial f_{\sigma i}}{\partial r_a} + \frac{1}{2}\tau c_{\sigma ia}c_{\sigma i\beta}\frac{\partial^2 f_{\sigma i}}{\partial r_a \partial r_\beta} + \tau c_{\sigma ia}\frac{\partial^2 f_{\sigma i}}{\partial t \partial r_a} + \frac{1}{2}\tau\frac{\partial^2 f_{\sigma i}}{\partial t^2} = -\frac{1}{\tau\phi}(f_{\sigma i} - f_{\sigma i}^{(0)}) \tag{9}$$

The form equal to that of the equation which removed the term of the second differential in the time, when it compared with the equation of LBM if the parameters are put with $\tau = 1.0$ and $a = 0.5$. By conducting such conversion, it is possible to convert the relationship between coefficient of the kinematic viscosity and the single relaxation coefficient from $\phi \sim \nu$ to $\phi - a \sim \nu$ in FDLBM.

By these procedure, the single relaxation coefficient ϕ becomes $\phi \rightarrow a$ in the flow of the high Reynolds number, and the proposed new model of FDLBM becomes possible to calculate by the fixed value of ϕ which is taken in the high Reynolds flow. Also, it becomes possible that calculation of Δt can easily or stably simulate up to large value, which $\Delta t/\phi < 2.0$ is a restriction on the collision term in the conventional FDLBM model.

4. The Calculation Speedup

In this section, we consider whether the calculation speedup becomes possible by converting the relationship between the viscosity coefficient ν and the single relaxation coefficient ϕ by adding the term in Eq.(6).

To begin with, there are large difference between the proposed FDLBM model and the conventional FDLBM model, when the high Reynolds number is considered. In the difference, when it is made to be Re $\rightarrow \infty$, the relaxation time is $\phi \rightarrow 0.0$ in the conventional FDLBM, whereas that of proposed model is $\phi \rightarrow a$.

From this fact, in order to satisfy $\Delta t/\phi < 2.0$ which is a condition of the coefficient depending on the collision term, though the calculation stability could not

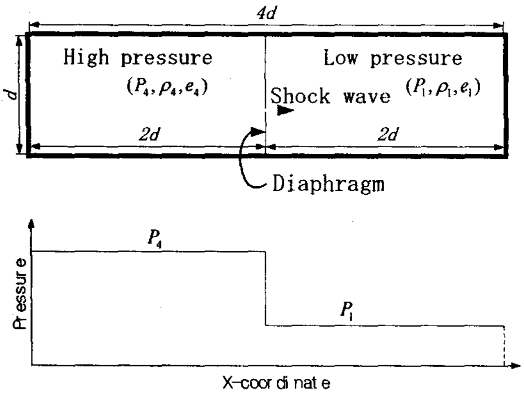


Fig.1 Simulated flow field in a shock tube (2D21V)

operate if $\Delta t \rightarrow 0$ is not given in the conventional FDLBM, the time becomes $\Delta t \rightarrow 2.0 \cdot a$ in the proposed FDLBM.

Therefore, we can easily promote the calculation stability in Δt to some extent size.

5. Numerical Results

To examine characteristics of shock wave and reflection wave and verify the proposed FDLBM, we use both the conventional model and the proposed model.
The shock propagation process represents an abrupt change in fluid properties. Shocks also

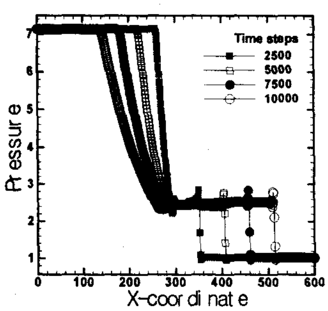
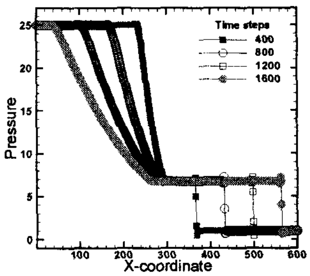
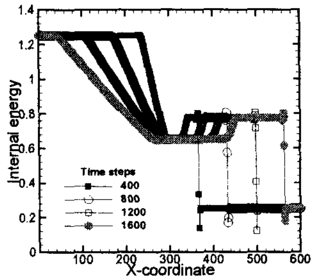


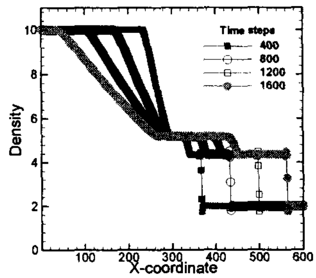
Fig.2 Flow field in a shock tube simulated with 2D21V model by the conventional FDLBM



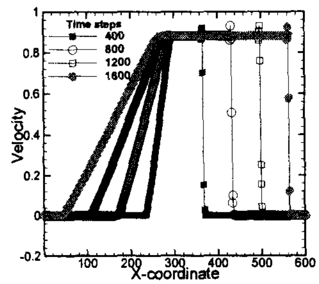
(a) Pressure



(b) Internal energy



(c) Density



(d) Velocity

Fig.3 Flow field in a shock tube simulated with 2D21V model by the proposed FDLBM

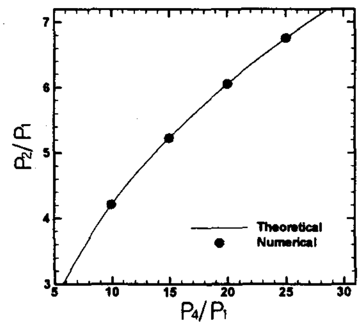


Fig.4 Results of the pressure of the front and rear of shock wave(by the proposed FDLBM)

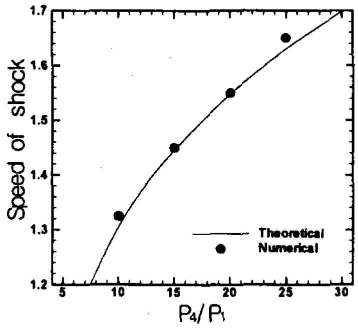


Fig.5 Results of the speed of shock (by the proposed FDLBM)

occur in the flow of a compressible medium through ducts or nozzles and thus may have a decisive effect on these flows. An understanding of the shock process and its ramifications is essential to a study of compressible flow.

To begin with, we examine a shock tube flow. The shock tube is a device in which normal shock waves are generated by the rupture of a diaphragm separating a high-pressure gas from one at low pressure. After rupture of the diaphragm, the system eventually approaches thermodynamic equilibrium, with the final state in the close-end tube determined from the first law of thermodynamics. With no external heat transfer, the total internal energy of the gases at the final state is equal to the sum of the internal energy of the gases initially present on either side of the diaphragm.

However, of primary interest is not the final equilibrium state of the gases, but the transient shock phenomena occurring immediately after rupture of the diaphragm. Upon rupture of the diaphragm, a normal shock wave moves into the low-pressure side, with a series of expansion waves propagating into the high-pressure gas.

The conceptual scheme of shock tube is shown in Fig.1. The pressure distribution is also illustrated.

The speed of shock c_s is defined as

$$c_s = M_s a_{s1} \tag{10}$$

where M_s is the shock Mach number and a_s is explained later.

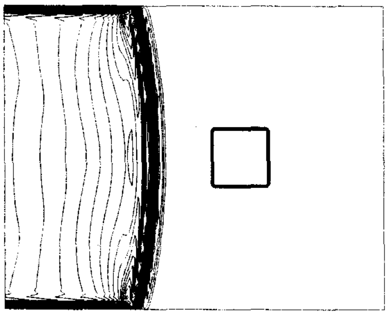
The fundamental equation of shock tube can be written as

$$\frac{P_4}{P_1} = \frac{P_2}{P_1}\left[1 - \frac{(\gamma_4 - 1)(a_{s1}/a_{s4})(P_2/P_1)}{\sqrt{2\gamma_1}\sqrt{2\gamma_1 + (\gamma_1 + 1)(P_2/P_1 - 1)}}\right]^{-2\gamma_4/(\gamma_4 - 1)} \tag{11}$$

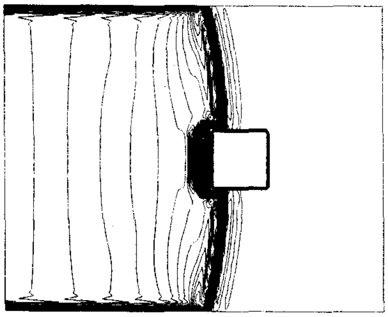
where a_{s1}, a_{s4} are the front sound velocity and the rear sound velocity of shock wave, respectively.

As the initial parameters, we set the initial pressure ratio of P_4/P_1 at 7.0, the time $\Delta t = 0.01$ and the temperature in both chambers at $e_1 = e_4 = 0.85$, and then, the shock Mach number becomes $M_s = 1.645$. The pressure distribution is shown in Fig.2 and the pressure ratio over 7.0 is not completed by using the conventional FDLBM.

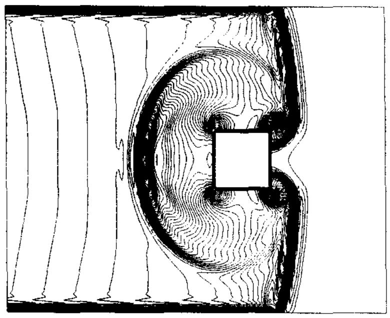
With the proposed FDLBM, we put the



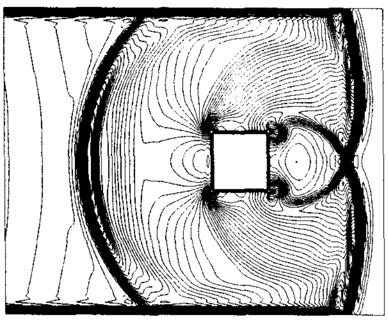
(a) 1800 time steps



(b) 2000 time steps

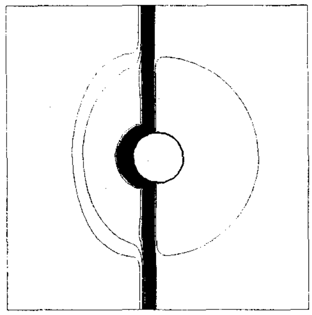


(c) 2200 time steps

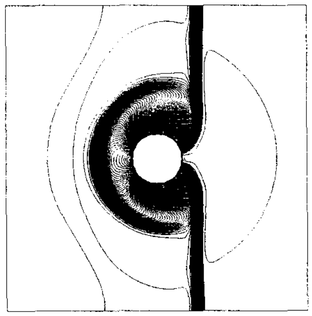


(d) 2400 time steps

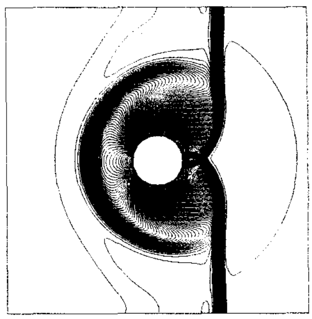
Fig.6 Unsteady shock wave passing through the rectangular column. The shock Mach number $M_s = 2.215$, initial pressure ratio $P_4/P_1 = 25.0$



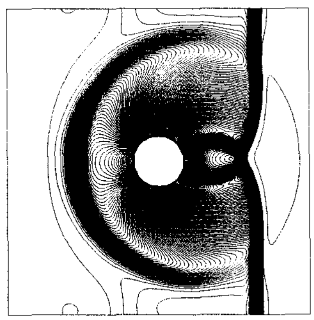
(a) 1000 time steps



(b) 1350 time steps



(c) 1500 time steps



(d) 1760 time steps

Fig.7 Unsteady shock wave passing through the circular cylinder. The shock Mach number $M_s = 2.043$, initial pressure ratio $P_4/P_1 = 15.0$

initial pressure ratio of P_4/P_1 at 25.0, the time $\Delta t = 0.1$ as initial condition, and the shock Mach number $M_s = 2.215$, and the flow field is shown in Figs.3(a) ~ (d). Here, we know that the proposed model is stably completed even in the pressure ratio over 3 times from the conventional model in the calculation. Also, from Fig.2 and Fig.3, we are certain that it is possible to shorten the calculation time over 10 times further than that of the conventional model, when we simulate by using the proposed new model.

In Fig.3(a), the shock wave are resolved by 5 lattices, and there is not the vibration which often observed in the wave surface back.

Figure 4 shows the relation between the initial pressure ratio and the pressure of the front and rear of shock wave. In this case, we obtain that an error is within 0.02% and the results agree with the theoretical predictions.

Figure 5 shows that an error between the theoretical shock speed and that measured from numerical result is within 1.24%, and the both agree with each other.

In Figs.6(a) ~ (d), the unsteady shock wave passing through the rectangular column which put in the low-pressure gas chamber is shown as time step go on. The initial pressure ratio $P_4/P_1 = 25.0$, the time $\Delta t = 0.1$ and the shock Mach number $M_s = 2.215$ are set, as an initial condition. Shock wave and reflected wave have also been well expressed.

In Figs.7(a) ~ (d), the unsteady shock wave passing through the circular cylinder is shown. The radius is made to be the 25 lattice nodes. As an initial condition, the initial pressure ratio $P_4/P_1 = 15.0$, the time $\Delta t = 0.1$ and the shock Mach number $M_s = 2.043$ are set. The numerical results are well expressed the unsteady shock wave and the reflected wave as time step go on.

6. Conclusions

By solving the lattice BGK compressible fluid model using the difference, we showed that the calculation of flow field (strong shock wave) where exists large pressure ratio is possible.

The new model is also proposed in the finite difference lattice Boltzmann method for the purpose of the stabilization of calculation and the shortening the calculation time.

With the shock tube, we examined the theoretical and the numerical results. In this calculation, we obtained the numerical results which agree with the theoretical predictions.

Finally, we expressed well the shock wave and reflected wave through some examples.

Reference

(1) McNamara, G., and Zanetti, G., Use of the Boltzmann Equation to Simulate Lattice-Gas Automata, Phys. Rev. Lett., 61, (1988), pp. 2332-2335.

(2) Rothman, D. and Zaleski, S., Lattice-Gas Cellular Automata, Cambridge UP 1997.

(3) Chen, Y., Ohashi, H., and Akiyama, M., Thermal Lattice Bhatnagar-Gross-Krook Model without Nonlinear Deviations in Macrodynamic Equation, Phys. Rev. E, 50, (1994), pp. 2776-2783.

(4) Cao, N., Chen, S., Jin, S. and Martinez, D., Phys. Rev. E, 55, (1997), pp.21.

(5) 蔦原道久, 高田尙樹, 片岡武, 格子氣體法 ・格子ボルツマン法, コロナ社, (1999).

(6) 姜鎬根, 蔦原道久, 差分格子ボルツマン法における壓縮性流れの數値シミュレーション, 日本流體力學講演會論文集, (2001).