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An improved entropic lattice Boltzmann model for parallel computation

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ABSTRACT

In this paper, we suggest two kinds of approximation methods based on Taylor series expansion which can solve the non-linear equation in entropic lattice Boltzmann model without using any iteration methods such as Newton–Raphson method. The advantage of our methods is to be able to avoid the load imbalance in parallel computation which occurs due to the differences of iteration number on each calculation grid. In this study, ELBM simulations using our methods were compared with those using Newton–Raphson method for the channel flow past a square cylinder in $Re = 1000$ and the validity of the results and computational effort were investigated. As a result, it was found that the solutions obtained by our methods are qualitatively and quantitatively reasonable and CPU time is shorter than those obtained by Newton–Raphson method.

1. Introduction

Lattice Boltzmann Method (LBM) has been developed as the method which can solve macro-scale fluid dynamics through meso-scale approach by calculating translation and collision of particle. The algorithm appropriates for the parallel computing using multi-core CPU and GPU computing because, for example, for well-known LBGK model, only the information of on-site and the nearest neighbor grid points are required to get the solutions. But it was known that in well-known LBGK model a solution becomes unstable in high Reynolds number (Re) region due to the disruptive non-linear instability. In order to overcome such shortcoming, entropic lattice Boltzmann model (ELBM) was developed by Karlin et al. [1–3], and expanded by several researchers recently [4–7]. ELBM can get stable solution by satisfying the second principle of the thermodynamic by imposing the monotonicity and the minimality of the H-function. However, in the algorithm of ELBM, non-linear equation must be solved to calculate the relaxation adjusting parameter which adjusts the relaxation time locally in such a way that monotonisity of H function is guaranteed. The non-linear equation solver using the iteration method, such as Newton–Raphson (N.R.) method, causes the increase of computational effort for parallel computing due to the load imbalance which is occurred by the difference of iteration number on each grid point. In order to avoid such problem, the direct method which can solve the non-linear equation is required. But there are a few previous studies [8] about the direct solution method for the relaxation adjusting parameter. In the present study, we considered two kinds of approximation methods based on Taylor series expansion for getting the solution of the non-linear equation and the methods were applied to a channel flow past a square cylinder in $Re = 1000$ and the validity of the result and computational effort were investigated. The detail comparison for accuracy, stability and efficiency between ELBM with N.R. method and LBGK model has already investigated in our previous study [9] and it was found that the ELBM enhances the stability and decreases the computational effort compared with LBGK model. So, in this paper, we mainly focuses on the comparison of the results of our approximation methods with those of ELBM with N.R method with respect to the accuracy, computational effort and stability.

2. Numerical methods

2.1. Outline of entropic lattice Boltzmann model

In the present work, we treat two-dimensional nine-speed (D2Q9) ELBM [9]. ELBM is different mainly on two points from standard LBGK model.

First point, the equilibrium distribution function is derived not from the expansion of Maxwell–Boltzmann distribution but from the minimization of H function under the conserving of mass and momentum. The discrete H function is given as follow

$$H(\boldsymbol{f}) = \sum_{i=0}^{q-1} f_i \ln(f_i/w_i), \tag{1}$$

where f_i is the distribution function in i direction, and q is the number of direction of speed, in the present model $q = 9$. By calculating

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the minimization problem of Eq. (1), the local velocity equilibrium distribution function in i direction f_i^{eq} is obtained as follow

$$f_i^{eq} = w_i\rho\prod_{j=1}^{d}\left[\left(2-\sqrt{1+3u_j^2}\right)\left\{\left(2u_j+\sqrt{1+3u_j^2}\right)/(1-u_j)\right\}^{c_{ij}}\right], \tag{2}$$

where ρ is the fluid density, d is the number of spatial dimension, u_j is the component of macroscopic velocity in j direction.

Second point, the relaxation time of ELBM is locally adjusted in such a way that the monotonicity of the H-function is satisfied through the relaxation adjusting parameter α. The parameter α is determined by solving following non-linear equation:

$$H(\boldsymbol{f}) = H(\boldsymbol{f}+\alpha\Delta), \tag{3}$$

where Δ represents the local non-equilibrium value of distribution function, $\boldsymbol{f}^{eq}-\boldsymbol{f}$. Once the parameter α is given by solving Eq. (3), the distribution function at new time step can be obtained by following time developed lattice BGK equation:

$$f_i(\mathbf{x}+c_i, t+1) = f_i(\mathbf{x},t) + \alpha\{f_i^{eq}(\mathbf{x},t) - f_i(\mathbf{x},t)\}/(2\tau_0), \tag{4}$$

where τ_0 is the relaxation time in LBGK model. As shown in Eq. (4), the relaxation time in ELBM τ is given by $\tau = 2\tau_0/\alpha$, therefore in the case of $\alpha = 2$, ELBM is equivalent to LBGK model. From the distribution function, the macroscopic variables can be calculated by using following relationship:

$$\rho = \sum_{i=0}^{q-1} f_i, \rho\mathbf{u} = \sum_{i=0}^{q-1} c_i f_i \tag{5}$$

2.2. Approximation method for solving the relaxation adjusting parameter α

In this section, we represent two methods to approximately solve the relaxation adjusting parameter α in Eq. (3). For convenience, we call those two methods, 'Method 1' and 'Method 2', respectively, below. First of all, let us define α in Eq. (3) as the sum of the values α^* and α' as follows:

$$\alpha = \alpha^* + \alpha', \tag{6}$$

where α^* is the α at one calculation time step before and α' is the difference between α and α^*. Substituting Eq. (6) into Eq. (3), right-hand side of Eq. (3) is written as follows:

$$H\{\boldsymbol{f}+(\alpha^*+\alpha')\Delta\} = H(\boldsymbol{f}+\alpha^*\Delta+\alpha'\Delta) = H(\boldsymbol{f}^*+\alpha'\Delta), \tag{7}$$

where $\boldsymbol{f}^* = \boldsymbol{f}+\alpha^*\Delta$. Assuming $\alpha'\Delta \ll 1$, the right hand side of Eq. (7) can be expanded by Taylor series expansion as follows:

$$H(\boldsymbol{f}^*+\alpha'\Delta) = H(\boldsymbol{f}^*) + H(\boldsymbol{f}^*)'(\alpha'\Delta) + H(\boldsymbol{f}^*)''(\alpha'\Delta)^2/2 + H(\boldsymbol{f}^*)'''(\alpha'\Delta)^3/6 + \cdots, \tag{8}$$

where subscription $'$ represents the partial differential with respect to $\boldsymbol{f}^*$.In Method 1, the terms order $O\{(\alpha'\Delta)^2\}$or smaller on the right hand side of (8) are neglected and then substituting the result into Eq. (3), Eq. (3) becomes

$$H(\boldsymbol{f}) = H(\boldsymbol{f}^*) + H(\boldsymbol{f}^*)'(\alpha'\Delta). \tag{9}$$

The second term of right hand side in Eq. (9) is deformed by using Eq. (1) as:

$$H(\boldsymbol{f}^*)'(\alpha'\Delta) = \partial H(\boldsymbol{f}^*)/\partial\boldsymbol{f}^*(\alpha'\Delta) = \alpha'\sum_{i=0}^{q-1}[\{1+\ln(f_i^*/w_i)\}\Delta_i] = \alpha'\sum_{i=0}^{q-1}\{\ln(f_i^*/w_i)\}\Delta_i. \tag{10}$$

Then substituting the Eq. (10) into Eq. (9) and solving the equation with respect to α', α' can be obtained as:

$$\alpha' = \{H(\boldsymbol{f}) - H(\boldsymbol{f}^*)\}\Big/\sum_{i=0}^{q-1}\{\ln(f_i^*/w_i)\}\Delta_i. \tag{11}$$

Then by the definition of Eq. (6), we can get approximate solution of α for Method 1 as below

$$\alpha = \alpha^* + \{H(\boldsymbol{f}) - H(\boldsymbol{f}^*)\}\Big/\sum_{i=0}^{q-1}\{\ln(f_i^*/w_i)\}\Delta_i. \tag{12}$$

Eq. (12) is equivalent to that of N.R. method in which only one iteration is carried out.

Whereas, in Method 2, the terms order $O\{(\alpha'\Delta)^3\}$ or smaller on the right hand side of Eq. (8) are neglected and then substituting the result into Eq. (3), Eq. (3) becomes as:

$$H(\boldsymbol{f}) = H(\boldsymbol{f}^*) + H(\boldsymbol{f}^*)'(\alpha'\Delta) + H(\boldsymbol{f}^*)''(\alpha'\Delta)^2/2, \tag{13}$$

where $H(\boldsymbol{f}^*)''$ is the second order partial deferential with respect to $\boldsymbol{f}^*$, and $H(\boldsymbol{f}^*)''(\alpha'\Delta)^2$ in the right hand side of Eq. (13) can be deformed by using Eq. (1) as follows:

$$H(\boldsymbol{f}^*)''(\alpha'\Delta)^2 = \{\partial H^2(\boldsymbol{f}^*)/\partial\boldsymbol{f}^{*2}\}(\alpha'\Delta)^2 = \alpha'\sum_{i=0}^{q-1}\{(1/f_i^*)\Delta_i^2\}, \tag{14}$$

Eq. (13) can rewrite to the quadratic equation with respect to α'

$$\alpha'^2 H(f^*)''\Delta^2/2 + \alpha' H(\boldsymbol{f}^*)'\Delta + H(\boldsymbol{f}^*) - H(\boldsymbol{f}) = 0, \tag{15}$$

by using the quadratic formula, α' can be obtained as

$$\alpha' = \{-C_2 + (C_2^2 - 4C_1C_3)^{1/2}\}/(2C_1), \tag{16}$$

where the constant coefficients C_1, C_2 and C_3 in (16) are defined as follows, respectively:

$$C_1 = H(\boldsymbol{f}^*)''\Delta^2/2, C_2 = H(\boldsymbol{f}^*)'\Delta, C_3 = H(\boldsymbol{f}^*) - H(\boldsymbol{f}). \tag{17}$$

Finally, we can get the following approximate solution for Method 2

$$\alpha = \alpha^* + \{-C_2 + (C_2^2 - 4C_1C_3)^{1/2}\}/(2C_1). \tag{18}$$

2.3. Calculation condition

Fig. 1 shows the computed geometry in the present calculation. A square cylinder which has the size of D is symmetrically placed in the 2-dimensional channel with respected to the channel centerline and the x-position is $12.5D$ from the channel inlet. The channel has the dimension of $8D$ wide and $50D$ long. As boundary condition, parabolic velocity profile with the maximum velocity at the channel center, U_{max} (= 0.058) which corresponds to Mach number of 0.1, is imposed at the inlet boundary, half way bounce-back conditions are given on the channel walls and the cylinder surface, and at outlet boundary, the distribution functions are extrapolated from the upstream side of the boundary. We use

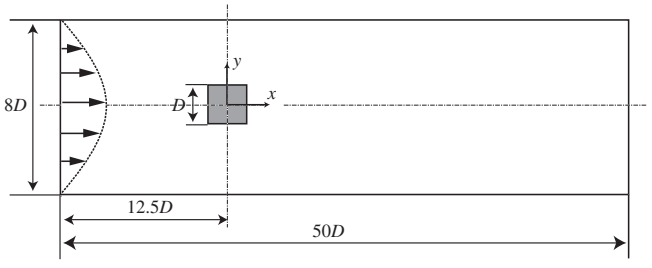

Fig. 1. Definition of the computed geometry.