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Optimal relaxation collisions for lattice Boltzmann methods

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ABSTRACT

The optimal relaxation time of about 0.8090 has been proposed to balance the efficiency, stability, and accuracy at a given lattice size of numerical simulations with lattice Boltzmann methods. The optimal lattice size for a desired Reynolds number can be refined by reducing the Mach number for incompressible flows. The functioned polylogarithm polynomials are defined and used to express the lattice Boltzmann equations at different time scales and to analyze the impact of relaxation times and lattice sizes on truncation errors. Smaller truncation errors can be achieved when relaxation times are greater than 0.5 and less than 1.0. The steady-state lid-driven cavity flow was chosen to validate the code of lattice Boltzmann procedures. The applications of the optimal relaxation parameters numerically balance the stability, efficiency, and accuracy through Hartmann flow. The optimal relaxation time can also be used to select the initial lattice size for the channel flow over a square cylinder with a given Mach number.

1. Introduction

The lattice Boltzmann method (LBM) has emerged as a promising alternative to the numerical scheme for high performance computational fluid dynamics (CFD) in the past twenty years. The numerical approaches based on the Boltzmann equation cover a wide range of the Knudsen number for practical applications. No effort for solving linear systems of equations is needed. The method is particularly competitive for fluid flow applications with complexities of geometries, boundaries, and interfacial dynamics [1]. The most commonly used collision operators are the single relaxation time (SRT) [2] and the multiple relaxation time (MRT) [3,4].

The LBMs can be applied to physical problems by means of nondimensionalization [5]. When both the physical system and the lattice system are equivalently scaled, three key dimensionless quantities: lattice size, relaxation time or collision frequency, and Mach number are yet to be determined for any CFD problems with a given Reynolds number. Different combinations of the key dimensionless quantities may numerically impact the stability, accuracy, and efficiency of the LBMs. The optimal relaxation time has been derived to balance the numerical properties. The optimal relaxation parameters are applicable for both the SRT and the MRT collision operators since no particular assumptions relative to collision operators have been made during their derivations.

The lattice Boltzmann method, which can be derived from the kinetic theory of gases, evolved from the lattice-gas automata. The primary variable is a one-particle probability distribution function $f(\mathbf{x}, \mathbf{e}, t)$. The macroscopic flow variables such as density, velocity, pressure, temperature, and stress can be expressed as the velocity moments of the one-particle probability distribution function.

The general transport equation reads

$$(\partial_t + \mathbf{e} \cdot \nabla_{\mathbf{x}} + \mathbf{a} \cdot \nabla_{\mathbf{e}}) f(\mathbf{x}, \mathbf{e}, t) = Q, \tag{1}$$

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where t is the time, $\mathbf{e}$ is the particle velocity, $\mathbf{x}$ is the special location, $\mathbf{a}$ is the acceleration due to an external force, and Q is a collision operator. To complete the Boltzmann equation from (1), the collision operator has to be specified. Four assumptions are made: (a) only binary collisions are taken into consideration, (b) the velocity of a molecule is not correlated to its space location, (c) the effect of the external force on the collision cross section is neglected, and (d) wall effects are ignored [6]. Under these assumptions, Boltzmann related the collision operator to the one-particle probability distribution function. One of the most commonly used collision operators is the linearized SRT or BGK collision operator [2]

$$Q = -\frac{1}{\tau}[f - f^{(\mathrm{eq})}], \tag{2}$$

where τ is a relaxation time.

With the Boltzmann H-theorem, the Maxwell–Boltzmann or equilibrium one-particle probability distribution function was given by

$$f^{(\mathrm{eq})} = \frac{\rho}{(2\pi RT)^{D/2}} \exp\left[-\frac{(\mathbf{e}-\mathbf{u})^2}{2RT}\right], \tag{3}$$

where D, R, T, ρ, and $\mathbf{u}$ are the dimensions of space, gas constant, temperature, density, and velocities, respectively.

To numerically solve for f given in (1)–(3), the velocity space $\mathbf{e}$ is simplified by a finite set of velocity vectors $\mathbf{e}_i$, which is chosen for isotropy. For the *D2Q9* model, the discrete velocity vectors can be practically expressed as $\mathbf{e}_0 = (0, 0)$, $\mathbf{e}_1 = -\mathbf{e}_3 = (c, 0)$, $\mathbf{e}_2 = -\mathbf{e}_4 = (0, c)$, $\mathbf{e}_5 = -\mathbf{e}_7 = (c, c)$, and $\mathbf{e}_6 = -\mathbf{e}_8 = (-c, c)$. The lattice speed $c = \delta x/\delta t$ is the ratio of a lattice spacing δx to a time step δt. The low Mach number expansion of (3) at a constant temperature is given by [7]

$$f_i^{(\mathrm{eq})} = \rho w_i \left[1 + \frac{3}{c^2}(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2c^4}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2c^2}(\mathbf{u} \cdot \mathbf{u})\right], \tag{4}$$

where the weighting factors w_i are specifically given by $w_0 = 4/9$, $w_1 = w_2 = w_3 = w_4 = 1/9$, and $w_5 = w_6 = w_7 = w_8 = 1/36$. The leading moments of the truncated equilibrium distribution function (4) for incompressible flows can be evaluated as

$$\rho = \sum_{i=0}^{8} f_i = \sum_{i=0}^{8} f_i^{(\mathrm{eq})}, \tag{5}$$

$$\rho u_\alpha = \sum_{i=1}^{8} e_{i\alpha} f_i = \sum_{i=1}^{8} e_{i\alpha} f_i^{(\mathrm{eq})}, \tag{6}$$

$$\frac{1}{3}c^2\rho\delta_{\alpha\beta} + \rho u_\alpha u_\beta = \sum_{i=1}^{8} e_{i\alpha} e_{i\beta} f_i^{(\mathrm{eq})}, \tag{7}$$

$$\frac{1}{3}c^2\rho(\delta_{\alpha\beta}u_\gamma + \delta_{\beta\gamma}u_\alpha + \delta_{\gamma\alpha}u_\beta) = \sum_{i=1}^{8} e_{i\alpha} e_{i\beta} e_{i\gamma} f_i^{(\mathrm{eq})}, \tag{8}$$

where $e_{i\alpha}$ is the projection of $\mathbf{e}_i$ on α-axis.

In (6) through (8), the summation is taken from 1 to 8 because of a rest particle devised for better computational stability. For ideal gases, the equation of state relates density ρ to pressure p with the following equation

$$p = \rho RT = \frac{1}{3}\rho c^2. \tag{9}$$

Eqs. (1) and (2), by introducing the collision frequency $\omega = 1/\tau$, can be discretized in space $\mathbf{x}$ and time t with the lattice spacing of $\delta\mathbf{x} = \mathbf{e}_i\delta t$ as

$$f_i(\mathbf{x} + \mathbf{e}_i\delta t, t + \delta t) - f_i(\mathbf{x}, t) = -\omega[f_i(\mathbf{x}, t) - f_i^{(\mathrm{eq})}(\mathbf{x}, t)]. \tag{10}$$

This is the lattice Boltzmann equation with the BGK simplification. The lattice BGK model can be solved in two steps: first by collision and then by streaming. Therefore, the relaxation of local collision and advection of particle distribution functions evolve from one lattice to another by

$$\widetilde{f}_i(\mathbf{x}, t + \delta t) = (1 - \omega) f_i(\mathbf{x}, t) + \omega f_i^{(\mathrm{eq})}(\mathbf{x}, t), \tag{11}$$

$$f_i(\mathbf{x} + \mathbf{e}_i\delta t, t + \delta t) = \widetilde{f}_i(\mathbf{x}, t + \delta t), \tag{12}$$