Comment on “Maximum Entropy Principle for Lattice Kinetic Equations”

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In a recent Letter [1], Kurlin et al. proposed a class of athermal lattice Bhatnagar-Gross-Krook (LBGK) models which purportedly admit an $H$ theorem when the LBGK equation is under-relaxed and the equilibrium $f_i^{(eq)}$ is positive. Since then a considerable number of papers on “entropic lattice Boltzmann equation” (ELBE) has been published (cf. [2–4]). In this comment we would like to point out that the positivity condition $f_i^{(eq)} > 0$ does not ensure an $H$ theorem. We can prove that there exists no $H$ theorem in some positivity domain of $f_i^{(eq)}$, and that the validity domain of the $H$ theorem is strictly smaller than the positivity domain [5, 6].

For a lattice Boltzmann equation (LBE) with $N$ distinctive discrete velocities in $d$-dimensions (denoted as $DdQN$), the discrete velocity set $\{c_i|i=1,2,\ldots,N\}$ is assumed to have the following symmetry property: $\sum_i c_i c_i = N c_0^2 d_{i,\beta}$, where $c_0 > 0$ is a constant and $c_{i,\alpha}$ is a Cartesian component of $c_i$. We shall assume that $\{c_i\}$ is symmetric, i.e., $\{c_i\} = -\{c_i\}$. The strictly convex function $h_i(x) = \frac{2}{3} x^{3/2}$ for $x > 0$, together with the (athermal) conservation constraints $\sum_i f_i^{(eq)} = \rho$ and $\sum_i c_i f_i^{(eq)} = \rho u_i$, is used to obtain $f_i^{(eq)}$ by solving [1]

$$h_i'(f_i^{(eq)}) = \sqrt{f_i^{(eq)}} = a + b \cdot c_i,$$

(1)

where $a$ and $b$ are the Lagrange multipliers, and $\rho$ and $u$ are the flow density and velocity, respectively. Equation (1) yields the following solution for $f_i^{(eq)}$:

$$f_i^{(eq)}(\rho, u) = \frac{1}{N \rho} \left\{ R + \frac{c_i \cdot u}{c_i^2} + \frac{(c_i \cdot u)^2}{4 c_i^2 R} \right\},$$

(2)

where $R = (1 + \sqrt{1 - M^2})/2$ and $M := u/c_s$.

For $M \leq 1$, $R$, hence the model, is well defined. The following inequality is claimed to hold for the model:

$$\sum_k N \sum_{i=1}^N h_i(f_i(x_k, t_{n+1})) \leq \sum_k N \sum_{i=1}^N h_i(f_i(x_k, t_n))$$

(3)

for all $t_n \in \delta_1 \mathbb{N} := \delta_1 \{0, 1, 2, \ldots\}$, leading to the claim of existence of an $H$ theorem [1].

From Eq. (1), we see clearly that $a + b \cdot c_i \geq 0 \ \forall \ i$, which is equivalent to the following inequality [5, 6]:

$$M \leq \min_{i: |c_i| \geq e_i} \frac{2 c_i |c_i|}{c_i^2 + |c_i|^2} = M_{\text{max}},$$

(4)

Because there always exists at least one $c_i$ such that $|c_i| > c_s$, therefore $M_{\text{max}} < 1$. Consequently the above upper bound on $M$ is strictly lower than the positivity criterion $M \leq 1$. Thus, the validity domain of the $H$ theorem seems strictly smaller the positivity domain.

To complete our argument, we show that a convex function other than $h_i$, which leads to an $H$ theorem, does not exist, if there exist $c_i \neq c_j$ such that $c_i \cdot c_j = 0$ and $|c_i| \geq 2 c_s$. This can be done by choosing two macroscopic states $S_1 := (\rho_1, u_1) \neq S_2 := (\rho_2, u_2)$ such that

$$f_i^{(eq)}(S_1) \neq f_i^{(eq)}(S_2), \quad f_k^{(eq)}(S_1) = f_k^{(eq)}(S_2),$$

(5)

where $k \in \{i, j\}$, and $c_i := -c_j$. The above conditions contradict the strictly convexity of $h_i$ stated by Eq. (1) (cf. Theorem 2.2 in [6]). In particular, for the D3Q15 model with $c_i^2 = 2/3$, by choosing $c_i = (1,1,1)$ and $c_j = (0,0,0)\, S_1 = (\rho_0,0), \rho_0 \neq 0$, and $S_2 = ((1-\theta)^{-1} \rho_0, \theta c_i), \theta := 4 c_i^2/(4 c_s^2 + |c_i|^2) = 8/17, \quad M = \theta |c_i|/c_s \in (M_{\text{max}}, 1), \quad M_{\text{max}} = 6\sqrt{3}/11$, we can easily show that conditions of (5) are satisfied and thus $H$ theorem does not exist. This proof can be applied to models more general than the LBGK models [5, 6].

There are additional problems in the ELBE which should be noted. First, in order to maintain the $H$ theorem, the relaxation time (the viscosity) in the ELBE is not a constant, therefore the time evolution of such an ELBE is unphysical. Second, $f_i^{(eq)}$ of Eq. (2) has error terms of $O(u^4)$ and beyond which are absent in the polynomial equilibria. And third, the maximum velocity allowed in the ELBE is usually much smaller than that in other models [4]. These conditions and the under-relaxation restriction would make the ELBE inefficient and ineffective for flow simulations.

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