Comment on "Numerics of the lattice Boltzmann method: Effects of collision models on the lattice Boltzmann simulations"

I. V. Karlin,[1,2,*] S. Succi,[3,4,†] and S. S. Chikatamarla[2,‡]

[1]*Energy Technology Research Group, School of Engineering Sciences, University of Southampton, Southampton, GB-SO17 1BJ, United Kingdom*

[2]*Aerothermochemistry and Combustion Systems Lab, ETH Zurich, CH-8092 Zurich, Switzerland*

[3]*Istituto Applicazioni Calcolo CNR, Via dei Taurini 19, I-00185 Rome, Italy*

[4]*School of Soft Matter Research, Freiburg Institute for Advanced Studies, University of Freiburg, Albertstr. 19, D-79104 Freiburg, Germany*

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Critical comments on the entropic lattice Boltzmann equation (ELBE), by Li-Shi Luo, Wei Liao, Xingwang Chen, Yan Peng, and Wei Zhang in Ref. [1], are based on simulations, which make use of a model that, despite being referred to as the ELBE by the authors, is in fact equivalent to the standard lattice Bhatnagar-Gross-Krook equation for low Mach number simulations. In this Comment, a concise review of the ELBE is provided and illustrated by means of a three-dimensional turbulent flow simulation, which highlights the subgrid features of the ELBE.

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In a recent paper [1], authors Luo *et al.* claimed that the entropic lattice Boltzmann equation (ELBE) "does not improve the numerical stability of Lattice Bhatnagar-Gross-Krook (LBGK) model." They also stated that "the ELBE scheme . . . is unfit for carrying out numerical simulations in practice."

In this Comment, we point out that the above statements in Ref. [1] do not bear scientific relevance. The reason is simple: what Luo *et al.* have implemented in Ref. [1] is not the ELBE, but a model that is equivalent to the standard LBGK for low Mach number simulations.

Since the correct description of the ELBE was not presented in Ref. [1], let us remind that in the ELBE scheme, populations associated with the discrete velocities $\boldsymbol{v}_i$ evolve according to the following kinetic equation:

$$f_i(\boldsymbol{x}+\boldsymbol{v}_i,t+1)-f_i(\boldsymbol{x},t)=\alpha\beta\left(f_i^{\mathrm{eq}}-f_i\right). \tag{1}$$

In the above, f_i^{eq} is the local equilibrium, which minimizes the entropy function, $H(f)=\sum_i f_i\ln(f_i/W_i)$, where the weights W_i are lattice-specific constants. In Eq. (1), α is the maximal over-relaxation, which is operationally available as the positive root of the entropy condition

$$H(f+\alpha(f^{\mathrm{eq}}-f))=H(f). \tag{2}$$

This entropy estimate is the key, as it assures the discrete-time H theorem: For $\beta\in[0,1]$, the total entropy $\bar{H}(t)=\sum_{\boldsymbol{x}}H(f(\boldsymbol{x},t))$ is not increasing, $\bar{H}(t+1)\leqslant\bar{H}(t)$. Note that the validity of the H theorem requires not just the equilibrium to be evaluated through the minimization of H but also, and most importantly, the fulfillment of the entropy condition (2). For readers' convenience, we note a few implications of the entropy condition (2):

(i) Over-relaxation: Thanks to convexity of the entropy function, the solution to (2) always leads to over-relaxation, $\alpha>1$;

(ii) Duality: Let f be a population vector, and $f(\alpha)\equiv f+\alpha(f^{\mathrm{eq}}-f)$ its entropic mirror state, with the same value of the entropy, $H(f(\alpha))=H(f)$. If the entropy estimate is applied to $f(\alpha)$ instead of f, then the initial state is recovered in the form $f=f(\alpha)+\alpha'(f^{\mathrm{eq}}-f(\alpha))$, with another over-relaxation $\alpha'>1$, which satisfies a duality relation

$$\alpha'\alpha=\alpha'+\alpha. \tag{3}$$

Equation (3) implies that whenever $\alpha\lessgtr 2$, the opposite holds for the mirror state, $\alpha'\gtrless 2$.

Finally, whenever the simulation is resolved (populations stay close to the local equilibrium), the maximal over-relaxation parameter α becomes fixed automatically to the value $\alpha=2$ [and so is also the mirror value, $\alpha'=2$, according to (3)]. Then the ELBE [Eqs. (1), (2)] self-consistently becomes equivalent to the LBGK equation and recovers Navier-Stokes equations with the kinematic viscosity $\nu=c_{\mathrm{s}}^2(\frac{1}{2\beta}-\frac{1}{2})$, where c_{s} is speed of sound [an $O(1)$ lattice-dependent constant].

The above is a direct implication of the built-in H theorem. Indeed, the resolved simulation, on the kinetic level, is characterized by the fact that all populations are asymptotically close to the local equilibrium. Then, the entropy function becomes well represented by its second-order approximation: At fixed locally conserved fields (density and momentum here), if $\delta f=f-f^{\mathrm{eq}}$, $|\delta f/f^{\mathrm{eq}}|\ll 1$, then $H(f)\approx H^{\mathrm{eq}}+(1/2)\sum_i\delta f_i^2/f_i^{\mathrm{eq}}$. The levels of the entropy are then asymptotically close to the levels of the above quadratic form. It is under such condition that the entropy estimate (2) results in $\alpha=2$. Note that the standard Chapman-Enskog approximation is valid under precisely the same condition of closeness to the local equilibrium, thereby the viscosity ν is the same for both ELBE and LBGK.

ELBE exploits the self-adaptive mechanism of stabilization by choosing automatically the over-relaxation α at each node, which guarantees the H theorem at all sites and all discrete

*karlin@lav.mavt.ethz.ch

†succi@iac.cnr.it

‡shyam_css@yahoo.com

time steps. When the grid is coarsened, over-relaxation α becomes smeared in an interval, $[\alpha_{\min},\alpha_{\max}]$, with $1 < \alpha_{\min} < 2$, and $\alpha_{\max} > 2$. The self-adapted over-relaxation set up by (2) results in two oppositely directed effects: If $\alpha < 2$, the relaxation parameter $\omega = \alpha\beta$ in (1) is less than the corresponding standard LBGK parameter $\omega_0 = 2\beta$ (set by the viscosity), and hence the ELBE relaxation will tend to smoothen any flow perturbation. On the other hand, if $\alpha > 2$, the flow perturbation is enhanced ($\omega > \omega_0$). In ELBE simulations, these two effects act simultaneously on various nodes, with the net effect combining stabilization (through smoothing, $\alpha < 2$) with the preservation of the resolution (through enhancement, $\alpha > 2$).

Instead of implementing the ELBE (1), which, by definition, requires the self-adjusted relaxation through the entropy estimate (2), calculations by Luo *et al.* make use of a constant relaxation time $\tau = \omega_0^{-1}$, that is

$$f_i(\boldsymbol{x} + \boldsymbol{v}_i, t+1) - f_i(\boldsymbol{x},t) = 2\beta\left(f_i^{\mathrm{eq}} - f_i\right). \tag{4}$$

The only remaining input from the ELBE in the above, is the local equilibrium f_i^{eq}, given by Eq. (14) in Ref. [1]. At this point, however, Eq. (4) is no longer ELBE, as it is in fact to all effects and purposes equivalent to the standard LBGK scheme (this is well understood, see, e.g., Refs. [2,3]). Indeed, the authors correctly state that "one difference between the ELBE and MRT-LBE is the $O(u^3)$ terms in the odd-order equilibrium moments," and "... the difference in the even-order equilibrium moments ... is of the terms of the order $O(u^4)$." This implies that the entropic equilibrium differs from its standard polynomial approximation only on the order of the overall errors of the lattice Boltzmann method for the low Mach number flows, and therefore Eq. (4) is equivalent to the standard LBGK method. The authors could have opted to replace the equilibrium by a polynomial approximation, to at least second order, thereby completing in full the identity between the standard LBGK and Eq. (4). The crucial point of ELBE is not the equilibrium by itself, but the entropy condition (2). The equilibrium can be used as an exact result of entropy minimization, whenever available, or as approximation thereof (see, e.g., Ref. [3] where standard polynomial approximations to equilibria were used in ELBE simulations). The discrete time H theorem cannot be proven for the fixed relaxation LBGK (4), with neither exact nor approximate equilibrium. More precisely, the H theorem is trivially valid on the uninteresting half of the linear stability interval, $0 < \beta \leqslant 1/2$, but for the most important case of low viscosity, $1/2 < \beta < 1$, that is, for the LBGK over-relaxation, one even cannot prove that populations stay non-negative after the collision (4).

With this assessment, and fulfilling the usual low Mach number restrictions, the authors cannot make a "comparison of ELBE with LBGK," as the difference between (4) and the LBGK is of the overall order of errors of the LB method for low Mach number simulations. Instead, the authors continue as follows: "... it is unclear theoretically how the ELBE with a constant relaxation parameter τ can improve the numerical stability of the LBGK scheme, as it has been advocated [3,4]." However, neither in [3] nor in [4] (Refs. [4] and [5] here), is there any claim about constant relaxation parameter improving stability, and whenever stability of the ELBE was discussed in these papers, the entropy estimate (2) has always been provided (Eqs. (10) in [4] and (37) in [5]). In practice, the standard LBGK and Eq. (4) perform so similarly that Luo *et al.* state that "they are so similar to each other" that "only the results obtained by using ELBE are shown in Fig. 4" ([1], page 6). This twin behavior alone should have warned the authors, that the two allegedly different methods were basically the same.

Summarizing, for low Mach number simulations, ELBE with a constant relaxation time is equivalent to the standard LBGK model. The implementation of ELBE by Luo *et al.* missed its key component, the entropy estimate (2) (as stated in [1], "We did not test the ELBE with a variable relaxation time..."). Thus, what the authors achieve in the end is a circular result (i.e., a cross comparison of minor LBGK variants).

When the grid is coarsened, local instabilities due to lack of resolution typically lead to a collapse of LBGK. It is in this situation that ELBE proceeds with the adaptive relaxation. In this regard, we wish to point out that there has never been any mystery as to the fact that ELBE is a natural extension of LBGK into subgrid simulations with the distinctive trait that the stabilization mechanism is directly informed through the second principle (H theorem). This is well reflected by the specific way ELBE mends instabilities; most of the time during the simulation the relaxation parameter remains constant everywhere, so that indeed ELBE collapses to LBGK. It is only at the onset of a local instability, that ELBE deploys its built-in entropic stabilization capability. These stabilization events may be rare in time and very localized in space (so are incipient instabilities) but they make the whole difference. This local self-adaptive stabilization (no fine tuning of parameters) is what makes ELBE distinct from other LB methods.

As a practical illustration, we consider a three-dimensional turbulent flow in periodic domain, evolving from a symmetric initial condition (Kida vortex, see Refs. [3,6] for details). The flow is initialized by the velocity profile,

$$\begin{aligned} u_x(x,y,z,0) &= U_0 \sin x(\cos 3y \cos z - \cos y \cos 3z),\\ u_y(x,y,z,0) &= U_0 \sin y(\cos 3z \cos x - \cos z \cos 3x),\\ u_z(x,y,z,0) &= U_0 \sin z(\cos 3x \cos y - \cos x \cos 3y). \end{aligned} \tag{5}$$

The Reynolds number is defined as $\mathrm{Re} = U_0 N/\nu$, where N is the number of grid points in each direction, and $U_0 = 0.05$ was used in all simulations. For the standard D3Q15 lattice, equilibrium was used in the product form [7]; for the ELBE implementation, the entropy condition (2) was realized via bisection method, with the tolerance $\epsilon = 10^{-5}$ (a few simulations were run with a tolerance $\epsilon = 10^{-8}$ to confirm robustness). The LBGK simulation was produced through Eq. (4) (i.e., by switching off the ELBE root solver and setting $\alpha = 2$ instead). Two series of numerical experiments were performed to demonstrate ELBE as a method for subgrid simulation.

In the first set of simulations, we considered a low Reynolds number regime (although still turbulent), fixing $\mathrm{Re} = 4000$. Two grids of the size $N = 350$ and $N = 110$ were used. The former grid ($N = 350$) was used in Ref. [6] to compare the LBGK with spectral element direct numerical simulation (DNS); the latter ($N = 110$) is the coarsest grid at which LBGK simulation is numerically stable at $\mathrm{Re} = 4000$. First, in Fig. 1, snapshots of the velocity field are reported for

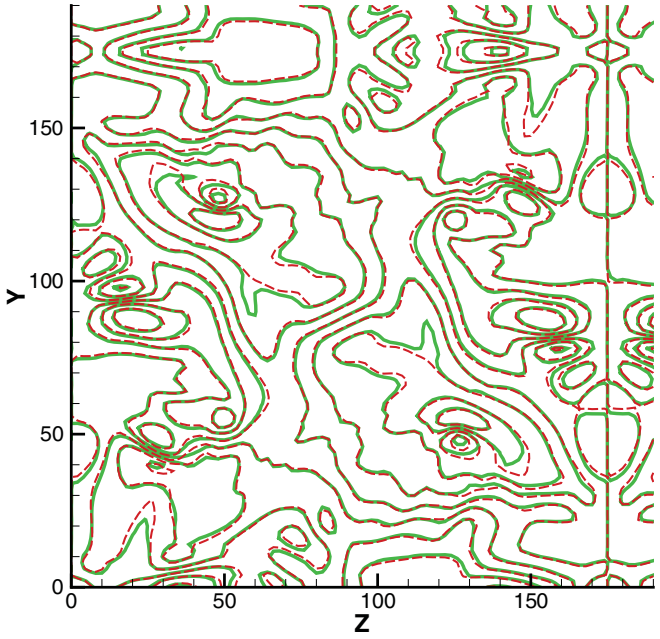

FIG. 1. (Color online) Isocontours of the z component of the velocity on a slice through the simulation domain at $x = 20$, at $\mathrm{Re} = 4000$. Grid size 350^3. One quarter of the slice is shown due to flow symmetry. Solid line: ELBE; Dashed: LBGK.

both the LBGK and ELBE on the fine grid ($N = 350$). Results are in agreement within even the finest flow structures, thus demonstrating that ELBE has the correct limit of DNS when simulation is sufficiently resolved. Second, in Fig. 2, the energy spectrum for both ELBE and LBGK simulations on the coarse grid ($N = 110$) are compared with the DNS [6]. ELBE compares well with the resolved simulation for

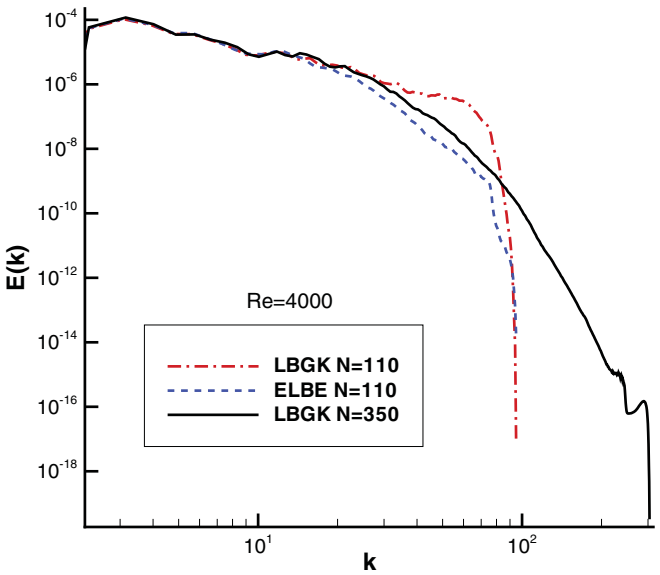

FIG. 2. (Color online) Energy spectrum at $\mathrm{Re} = 4000$. Solid line: Resolved DNS [6] (LBGK, grid 350^3); Dashed: ELBE, grid 110^3; Dot-dashed: LBGK, grid 110^3. Accumulation of energy at the short-wave end of the spectrum for LBGK is a precursor of numerical instability, which terminates the LBGK simulation on the grid 100^3.

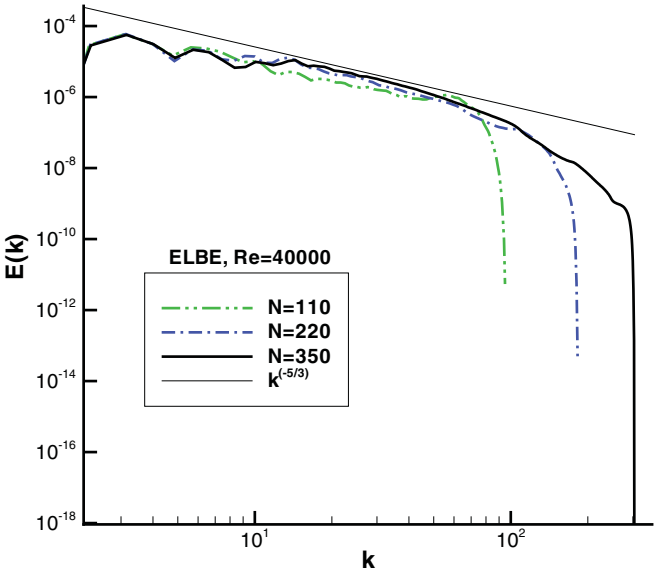

FIG. 3. (Color online) Energy spectrum at $\mathrm{Re} = 40\,000$. ELBE simulations on grids 110^3 (double dot-dashed), 220^3 (dot-dashed) and 350^3 (solid line). Line with the slope $-5/3$: Kolmogorov's scaling.

almost the entire range of scales available. Note that ELBE slightly underpredicts the energy at smaller scales, as it is expected for a viable subgrid simulation. On the contrary, the LBGK significantly overpredicts the energy at the same scales; accumulation of the energy toward the end of the spectrum is not sustainable for LBGK, and is the reason for its collapse if the grid is further reduced (e.g., at $N = 100$).

It is important to realize that the range of Reynolds numbers for performing simulations dramatically increases with ELBE. In order to demonstrate this, in the second simulation, the Reynolds number was increased by order of magnitude, $\mathrm{Re} = 40\,000$, and a series of grids was used to probe the subgrid capability of ELBE. Results are presented in Fig. 3. It is clearly visible that: (i) The larger (nonuniversal) scales are well matched even on a coarse grid ($N = 110$) and (ii) The inertial regime becomes well captured starting with the reasonably coarse grid ($N = 220$). Thus, already with $N \gtrsim 220$, ELBE provides a reliable subgrid simulation.

Note that ELBE remains stable for much coarser grids and/or extreme Reynolds numbers. However, at such extreme regimes, the flow physics becomes corrupted, and therefore the grid resolution has to be kept reasonable. It is also important to stress that ELBE becomes efficient for the simulations at high rather than at low Reynolds numbers. In the present example, the LBGK would require a grid of the order of $N \sim 1000$ for $\mathrm{Re} \sim 40\,000$. It should be mentioned that for a given grid size, ELBE is typically 3–6 times slower than LBGK [depending on optimization of solution to Eq. (2)]. Since the computational time and memory scale as the fourth and the third power of N, respectively, a conservative estimate for $\mathrm{Re} \sim 40\,000$ makes ELBE ($N \sim 300$) no less than 10 times faster than LBGK ($N \sim 1000$), with about a factor 30 savings in memory.

Summarizing, the above simulations demonstrate a reliable subgrid capability of ELBE for a range of high Reynolds numbers. In fact, ELBE just features the same trend of

improvement, as LBGK, under grid refinement but at much higher Reynolds numbers.

In conclusion, we summarize the entropic lattice Boltzmann method (ELBM). Entropy considerations were first invoked in Ref. [8] in order to explain why conventional LB models are reliable only in well-resolved simulations. And ever since ELBM was proposed, a decade ago in Refs. [2,9], it has grown into a consolidated framework that explains LBM and its relation to the Boltzmann and Navier-Stokes equations. ELBM can be understood on three different levels: (i) ELBM provides entropy function H for the LBM, which restores thermodynamic consistency and ensures its compliance with second law of thermodynamics. The advantages of defining LBM through an entropy function are multiple. It gives us the relation of LBM to the Boltzmann equation and provides us with a systematic description of higher order lattices [10]. (ii) The equilibrium in the entropic LB is given as the minimizer of entropy function under fixed local conservations. As already mentioned, this implies the standard LBGK, once the equilibrium is expanded to second order. Exact solution for equilibria were found [11], a subsequent development of this approach has led to a product and Maxwell forms for equilibria [7]. Product-form equilibria offer an efficient way to perform LB simulations on higher-order lattices [6]. Applications of ELBM equilibria include LB models with energy conservation, multicomponent mixtures, and microflows. Extension of the ELBM equilibrium delivered a thermodynamically consistent LB model with tunable bulk viscosity [12]. (iii) Subgrid simulations: It must be understood that LBGK is a fast and efficient DNS method for low Mach number isothermal simulations [6]. However, the reduction in grid resolution leads to a breakdown of LBGK simulation. This is largely (and inappropriately) interpreted as a problem with LBM simulations. In that respect, ELBE [Eqs. (1), (2)] provides a means for subgrid simulations by bringing the entropy nonadhering nodes back to entropy-compliant conditions.

All of the above demonstrates that ELBM is a diverse and consolidated framework for constructing LB models and performing simulations, of which the subgrid ELBE is one important facet. It comes unwarranted that Luo *et al.* [1] categorically negate ELBM, without studying even a single aspect of it.

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