

Reply to “Comment on ‘Numerics of the lattice Boltzmann method: Effects of collision models on the lattice Boltzmann simulations’”

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This Reply addresses two issues raised in the Comment [*Phys. Rev. E* **84**, 068701 (2011)] by Karlin, Succi, and Chikatamarla (KSC): (1) A lattice Boltzmann (LB) model, which is claimed to have an H theorem, is not qualified to be called an entropic lattice Boltzmann equation (ELBE); and (2) the real ELBE with a variable relaxation time performs exceedingly well, as exhibited by their simulations of decaying “Kida vortex” flow in a three-dimensional periodic cube free of no-slip boundary. The first issue is a semantic one. We note that it was Karlin, Succi, and others who “prove the H theorem for lattice Bhatnagar-Gross-Krook models,” which is the model we called ELBE in our original study to distinguish it from the *usual* lattice BGK model without the H theorem. Regardless of how this model is named, it does not affect the results and conclusions of our study in any way. Second, the focus of our original study is to quantify the errors of various LB models near no-slip boundaries. Hence, KSC’s example, which is free of no-slip boundaries, is not relevant to our study. The results in our original paper are valid and its conclusions remain unchallenged. On the other hand, KSC’s assertion that their real ELBE “provides a *reliable* subgrid simulation” of turbulence is not substantiated.

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In their Comment [1] on a recent work of ours [2], Karlin, Succi, and Chikatamarla (KSC) raise two issues. First, KSC state that the model we “have implemented as ELBE, [is] not the ELBE, but a model which is equivalent to the standard LBGK for low Mach number simulations.” Consequently KSC insist that “the conclusion of Ref. [2] (which is our original work) on ELBE is circular, hence devoid of scientific bearing” and our conclusions on the models we tested “do not bear scientific relevance.” And second, KSC assert that their real ELBE scheme works remarkably well, as backed up “by means of a three-dimensional turbulent flow simulation, which highlights the subgrid features of ELBE.” As I shall point out in this Reply, the first issue is semantic and the second point is unproven.

In our original work [2] we study the lattice Boltzmann equation (LBE) in two dimensions (2D) with various collision models in terms of their accuracy, stability, and computational efficiency [2]. The tested models include the lattice Bhatnagar-Gross-Krook (LBGK) model, the multiple-relaxation-time (MRT) model, the two-relaxation-time (TRT) model, and “the LBGK model,” which Karlin, Succi, and others proved to have an H theorem [3]; we called this model *ELBE with a constant relaxation time*. All the lattice Boltzmann (LB) models we have tested were clearly defined and described [2]. We chose the lid-driven cavity flow in 2D as a benchmark case for the following reasons. First, the flow can be solved with high precision by using spectral methods, thus an objective comparative study can be made to unequivocally expose and quantify the defects in the LB models. And second, it can be used to detect the defects of various LB models near no-slip boundaries. We found that the ELBE with a constant relaxation time performed the worst among the models tested, and does not improve the numerical stability of the LBGK model [3].

We note that none of the results in our study [2] has been challenged by KSC.

Let us directly address the first issue raised by KSC [1]. We separate the ELBE models into two types [4,5]. The first (type I) is to explicitly and analytically construct the equilibria which admit an H theorem (e.g., Ref. [3]), and the second (type II) is to construct a collision process which maximizes a given Lyapunov functional numerically (e.g., Ref. [6]). Karlin *et al.* [3] claimed that “for a suitable entropy function, we derive explicitly the hydrodynamic local equilibrium, prove the H theorem for lattice Bhatnagar-Gross-Krook models, and develop a systematic method to account for additional constraints.” This particular “LBGK” model [3] is what we classify as type-I ELBE [4,5]. The point is that we did not call this model “the ELBE” arbitrarily—it is so called because of its entropic property and the H theorem stated by Karlin *et al.* [3]. Although we were careful to qualify our conclusions [2], we note that in their Comment [1] KSC repeatedly misquote us by replacing “the ELBE” (which we clearly define in our work [2]) by “ELBE,” leaving a misimpression that our carefully qualified statements are more general than they are.

As to KSC’s real ELBE, no one has been able to prove that it solves the Navier-Stokes equations. Furthermore, KSC’s ELBE is computationally inefficient. By “using a combination of the Newton-Raphson method and the bisection method,” KSC’s ELBE with nine velocities in 2D “is an order of magnitude slower compared to the BGK method” [7]. If only the bisection method is used [1], then the required number of iterations with a given tolerance $1 > \epsilon > 0$ in estimating α is $n \geq |\ln \epsilon / \ln 2|$, e.g., $n > 16$ for $\epsilon \leq 10^{-5}$. Thus, KSC’s ELBE requires at least a tenfold computational overhead. Such a severe computational overhead for the sole purpose of numerical stability is not justifiable, especially for a scheme which cannot be proved to solve the Navier-Stokes equations. There exists no evidence to show that KSC’s ELBE “becomes

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efficient for the simulations at high rather than at low Reynolds numbers” [1]. If the numerical stability is the sole objective as is for KSC’s ELBE, a simple limiter can serve the purpose much more effectively and efficiently (cf., e.g., Refs. [8,9]). For the above reasons, the only comment about the ELBE with a variable relaxation time in our study [2] is the following statement: “We do not test the ELBE with a variable relaxation time, which is supposed to guarantee numerical stability, because it is computationally inefficient and unphysical with a viscosity depending on space and time; a stable but inaccurate, unphysical, and inefficient scheme is simply not a viable one.” Clearly, all the conclusions in our study [2] are qualified only for “the ELBE” with a constant relaxation time, as we explicitly and repeatedly stated in our study [2].

We now address the second issue raised by KSC in their Comment [1]—the efficacy of their ELBE. KSC provide an example of the decaying “Kida vortex” flow in a three-dimensional cube free of no-slip boundary to demonstrate that their ELBE is more stable than the LBGK scheme. Not only is it unnecessary, because we explicitly acknowledge this fact, but it is also not relevant to our study [2], which emphasizes quantifying the errors of various LB models *especially near no-slip boundaries*. Thus the technical content of KSC’s Comment [1] is not relevant to our original work [2]. To settle this controversy definitely, KSC could compare their *existing* results of the cavity flow obtained by using their ELBE [7,10–12] with readily available accurate solutions. It should also be noted that the results depend critically on the accuracy of the numerical root-finding in KSC’s ELBE, and thus on implementation details that were not reported by KSC. For example, Packwood [13,14] was unable to reproduce the shock tube behavior reported by Ansumali and Karlin [15].

KSC’s Comment [1] raises several issues which deserve critical scrutiny. First, KSC state that their ELBE scheme is “a *natural* extension of LBGK into subgrid simulations” for turbulence. However, this point has not been substantiated. The result of the decaying “Kida vortex” flow shown in the Comment [1] does not constitute a demonstration of the ELBE’s capability of subgrid turbulence modeling—the results in KSC’s Comment only illustrate that their ELBE is more dissipative than the LBGK model in small scales (larger k). However, the dissipation in KSC’s ELBE is solely based on the consideration of *numerical stability* and has nothing to do with the underlying physical process or turbulence.

Second, KSC maintain that their “ELBM provides [an] entropy function H for the LBM which restores thermodynamic consistency and ensures its compliance with [the] second law of thermodynamics.” However, KSC’s ELBE

model does *not* respect the first law of thermodynamics, i.e., energy conservation, hence it is more appropriate to be called *athermal* (as opposed to isothermal). The “temperature” is not conserved by collisions in KSC’s ELBE model, but instead is reset to a prescribed constant value after every collision. It is thus not a dynamical variable in the usual sense of thermodynamics. Furthermore, KSC’s “entropy” [1] is in fact a Lyapunov function which is a *numerical stabilizer* without any thermodynamic significance. Consequently it is somewhat confusing to invoke the second law of thermodynamics and thermodynamic consistency while the H function in KSC’s ELBE has no physical significance at all.

Third, KSC assert that “most of the time during the simulation the relaxation parameter remains constant everywhere, so that indeed ELBE collapses to LBGK. . . . These stabilization events may be rare in time and very localized in space. . . .” We would like to point out that the stabilization events are certainly not rare in general and definitely not so for the cavity flow—it contradicts the authors’ own results (cf. Fig. 4 in Ref. [10], Fig. 1 in Ref. [11], and Figs. 4 and 5 in Ref. [12]).

Fourth, KSC insist that “the ELBE” we implemented in our work [2] “is in fact equivalent to the *standard* lattice Bhatnagar-Gross-Krook equation for low Mach number simulations.” This is simply not factual. It is well known that these models are different in terms of errors in the bulk flow and especially near a no-slip boundary, which are the subjects clearly *quantified* in our study [2]. More specifically, the discrete entropy-minimizing equilibria [1,3,7] do not have the correct second- and third-order moments to reproduce the Navier-Stokes equations.

Fifth, KSC state that the “entropy condition” always leads to $\alpha > 1$, hence to the overrelaxation of their ELBE scheme. This is incorrect—their ELBE scheme is overrelaxed if and only if $\alpha\beta > 1$ (cf. Eq. (1) in KSC’s Comment [1]).

Sixth, KSC’s statement “that LBGK is a *fast* and *efficient* DNS method for low-Mach number isothermal simulations” defies mounting evidence to the contrary [2,16–20].

In conclusion, KSC’s Comment offers no evidence to invalidate the results in our original work [2], and thus the conclusions in our original work remain unchallenged.

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