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Allowed and forbidden regimes of entropy balance in lattice Boltzmann collisions

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We study the possibility of modifying collisions in the lattice Boltzmann method to keep the proper entropy balance. We demonstrate that in the space of distributions operated on by lattice Boltzmann methods which respect a Boltzmann type H theorem, there exists a vicinity of the equilibrium where collisions with entropy balance are possible and, at the same time, there exists a region of nonequilibrium distributions where such collisions are impossible. In particular, for a strictly concave and uniformly bounded entropy function with positive equilibria, we show that proper entropy balance is always possible sufficiently close to the local equilibrium and it is impossible sufficiently far from it, where additional dissipation has to appear. We also present some nonclassical entropies that do not share this concern. The cases where the distribution enters the region far from equilibrium typically occur in flows with low viscosity and/or high Mach number flows and in simulations on coarse grids.

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The problem of proper entropy balance is crucial in many areas of computational physics. For classical computational methods, including various versions of finite difference and finite element methods, many efforts were applied to create methods that guarantee proper values of entropy production [1,2]. This problem persists because any new family of methods requires an analysis of entropy balance and significant efforts may be necessary to provide proper entropy production.

Lattice Boltzmann schemes are a type of discrete algorithm which can be used to simulate fluid dynamics and more [3,4]. The problem of entropy balance in lattice Boltzmann methods (LBMs) attracted much attention during the past decades [5–9] and still remains unsolvable, and even a solvability of this problem for many versions of LBM is now not completely clear. In this Rapid Communication we demonstrate that near a positive equilibrium which respects a strictly convex and uniformly bounded H function there always exists a vicinity where it is possible to introduce LBM collisions with proper entropy balance. At the same time, we prove that there always exist areas of nonequilibrium distributions where LBM collisions with the proper entropy balance are impossible. The distribution function may regularly enter these regions in low viscosity or high Mach number fluids and in simulations on coarse grids. In these regions we cannot redefine the collisions for proper entropy balance and always have to introduce additional dissipation. We calculate and graphically represent these areas for some simple models of entropic collisions. We provide the analysis in the frame of the entropic lattice Boltzmann method (ELBM). It was invented in 1998 as a tool for the construction of single relaxation time lattice Boltzman models which respects an H theorem [5,6,10]. For this purpose, instead of the mirror image with a local equilibrium as the reflection center, the entropic involution was proposed, which preserves the entropy value. Later, it was called the *Karlin-Succi involution* [11]. An ELBM usually involves an evaluation of a Boltzmann type entropy function, which does not exist for negative populations, hence such an ELBM cannot ever tolerate a negative population value. Due to this there are population values for which an entropic involution cannot be performed.

We discuss enhanced entropic collisions and demonstrate that they provide the proper balance of entropy under wider conditions because they do not require existence of the entropic involution and use the entropic contraction instead. We demonstrate also that two one-parametric distinguished families of nonclassical entropies with singularity at the boundary of positivity allow us to perform entropic collisions without restrictions.

LBGK, ELBGK and enhanced entropic collisions. The lattice Boltzmann discrete algorithm consists of two alternating steps, advection and collision, which are applied to n single particle distribution functions $f_i \equiv f_i(\mathbf{x},t)(i = 1 \dots n)$, each of which corresponds with a discrete velocity vector $\mathbf{v}_i$ $(i = 1 \dots m)$. The values f_i are also sometimes known as *populations* or *densities*. The advection operation is simply free flight for the discrete time step ϵ in the direction of the corresponding velocity vector. The collision operation is instantaneous and can be different for each distribution function but depends on every distribution function. Collisions do not change the macroscopic variables (moments). The standard hydrodynamic moments are given by

$$\rho = \sum_i f_i, \quad \rho\mathbf{u} = \sum_i \mathbf{v}_i f_i, \quad \rho\mathbf{u}^2 + \rho T = \sum_i \mathbf{v}_i^2 f_i.$$

The simplest single relaxation time LBM is the *lattice Bhatnagar-Gross-Krook model (LBGK)*,

$$f_i(\mathbf{x} + \epsilon\mathbf{v}_i, t + \epsilon) = f_i(\mathbf{x},t) + \omega\big(f_i^{\mathrm{eq}}(\mathbf{x},t) - f_i(\mathbf{x},t)\big), \quad (1)$$

where ϵ is the time step and the relaxation coefficient $\omega = 2\epsilon/(2\tau + \epsilon)$, τ is the continuous BGK relaxation time, and at first order in ϵ, the viscosity $\nu = c_s^2\tau$, where c_s is the speed of sound. $\omega \in [1,2)$, $\omega = 1$ $(\tau = \epsilon/2)$ corresponds to equilibrating at each time step and $\omega = 2$ corresponds to a reflection and the zero viscosity limit. The choice of the velocity set $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ and the discrete equilibrium distribution f_i^{eq} should provide the best approximation of the transport equations for the moments by the discrete scheme (1). A variation on the LBGK is the *entropic LBGK (ELBGK)* [12]. In this family of methods, the equilibria are

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defined as the conditional entropy maximizers under given values of macroscopic variables (*entropic equilibria*). The entropies have been constructed in a lattice dependent fashion in Ref. [13]. Some conditions for nonexistence of the entropic representation for given equilibria were found, and this class [8,9] includes standard polynomial equilibria. As well it was shown Ref. [9] that other types of equilibria only satisfy a H theorem under some additional constraints on the Mach number. Nevertheless, if the entropy is given, then, in some range of the constraints, the corresponding entropic equilibria exist. For the entropic lattice Boltzmann algorithm,

$$f_i(\mathbf{x}+\epsilon\mathbf{v}_i,t+\epsilon) = f_i(\mathbf{x},t) + \alpha\beta\big(f_i^{\mathrm{eq}}(\mathbf{x},t) - f_i(\mathbf{x},t)\big). \quad (2)$$

The single parameter ω is replaced by a composite parameter $\alpha\beta$. With knowledge of the entropy function S, α is found as the nontrivial root of the equation

$$S(\mathbf{f}) = S(\mathbf{f} + \alpha(\mathbf{f}^{\mathrm{eq}} - \mathbf{f})). \quad (3)$$

The trivial root $\alpha = 0$ returns the entropy value of the original populations. ELBGK then finds the nontrivial α such that (3) holds and the limit of the collision operation is zero entropy production, and $\beta = \omega/2$ controls how much entropy is produced. A solution of (3) must be found at every time step and lattice site. The ELBGK collision obviously respects the second law (if $\beta \leqslant 1$), and a simple analysis of entropy production gives the proper evaluation of viscosity.

We also introduce a different form of the ELBGK collision operation, which we call *enhanced entropic collisions (EECs)*. We directly search for the distribution function $\mathbf{f}' = \mathbf{f} + \alpha(\mathbf{f}^{\mathrm{eq}} - \mathbf{f})$ ($\alpha \geqslant 1$) which satisfies the equation ($1 \leqslant \omega < 2$)

$$S(\mathbf{f}') - S(\mathbf{f}^{\mathrm{eq}}) = \sqrt{\omega - 1}(S(\mathbf{f}) - S(\mathbf{f}^{\mathrm{eq}})). \quad (4)$$

The parameter ω directly controls the amount of entropy to be added into the system, and the coefficient $\sqrt{\omega - 1}$ is used due to the essentially quadratic nature of the entropy function S near the equilibrium $\mathbf{f}^{\mathrm{eq}}$. Hence, where the entropic involution exists, solutions of (4) and (3) coincide to the second order in $\mathbf{f} - \mathbf{f}^{\mathrm{eq}}$. If ω is close to 2, then EEC approaches ELBGK collisions. If $\mathbf{f}$ is close to $\mathbf{f}^{\mathrm{eq}}$, then both EEC and ELBGK coincide with the simple LBGK in the main order. If ω is close to 1, then EEC coincides with LBGK. This is not true for ELBGK because the nontrivial solution to (3) may not exist. Its existence does not depend on ω but only on the populations. Attempting to solve (3) assumes that the entropic reflection exists, which is a strong requirement of existence of collisions with *preservation of entropy*, whereas we just need a proper entropy balance.

It has been shown [14] that, inside the region where the entropy balance exists, the ELBGK produces a nonlinear viscosity correction proportional to the strain rate tensor. This type of correction must necessarily occur when the relaxation parameter depends on the nonequilibrium part of the distribution and has led to ELBM being characterized as a subgrid method [14,15].

The main idea in the entropic collisions is the direct control of local entropy production. Recently, this idea was developed in various directions [16], such as entropic limiters [17] or the entropy viscosity method [18] where a nonlinear viscosity based on the local amount of entropy production is added to the numerical discretization.

Regions of existence and nonexistence of entropic collisions. Let us study the entropic involution in the distribution simplex Σ given by $\sum f_i = \mathrm{const} > 0$, $f_i \geqslant 0$. Let us prove that under very natural assumptions about some properties of the entropy the simplex of distributions can be split into two subsets A and B: In set A the entropic involution exists, and for distributions from set B, Eq. (3) has no nontrivial solutions. Both sets A and B have nonempty interiors (apart from a trivial symmetric degenerated case).

Let the entropy S be a strictly concave continuous function in the distribution simplex Σ. We assume also that S is twice differentiable, the Hessian of S, $\partial^2 S/\partial f_i \partial f_j$, is negative definite in the interior of the simplex, Σ_+, where $\sum f_i = \mathrm{const}$, $f_i > 0$, and the global maximizer of S, the equilibrium, belongs to the interior of the simplex. For example, the relative Boltzmann entropy, $S = -\sum f_i[\ln(f_i/W_i) - 1]$, $W_i > 0$, satisfies these conditions, because $f \ln f \to 0$ when $f \to 0$ and $\partial^2 S/\partial f_i \partial f_j = -\delta_{ij}/f_i$, whereas the relative *Burg entropy* $S = \sum W_i[\ln(f_i/W_i)]$ does not satisfy these conditions because it does not exist on the border of the simplex (where some $f_i \to 0$).

The sets of distributions $\mathbf{f}$ with given values of the macroscopic variables in the simplex Σ are polyhedra, and intersections of Σ with linear manifolds with the given values of moments. We assume that in any such polyhedron the entropy achieves its (conditionally) global maximum at an internal point (equilibrium). This assumption holds for the Boltzmann relative entropy because of the logarithmic singularity of the "chemical potentials" $\mu_i = \ln(f_i/W_i)$ on the border of positivity. If $\mathbf{f}$ is sufficiently close to a positive equilibrium, then, due to the implicit function theorem, the nontrivial solution to Eq. (3) exists and it gives $\alpha = 2 + o(\mathbf{f} - \mathbf{f}^{\mathrm{eq}})$. The value $\alpha = 2$ corresponds to the mirror image, and the small term $o(\mathbf{f} - \mathbf{f}^{\mathrm{eq}})$ gives the corrections to the value $\alpha = 2$. Therefore, in some vicinity of the equilibrium the entropic involution exists.

To prove the existence of the area where entropic involution is impossible, let us consider a polyhedron with given values of the macroscopic variables and a positive equilibrium. The local minima of the entropy in this polyhedron are situated at the vertices. At least one of them is a global minimum. Let this vertex be $\mathbf{f}^{\mathrm{v}}$. Let us draw a straight line l through points $\mathbf{f}^{\mathrm{v}}$ and $\mathbf{f}^{\mathrm{eq}}$. The intersection $l \cap \Sigma$ is an interval and S achieves its global minimum on this interval at the point $\mathbf{f}^{\mathrm{v}}$. If the dimension of the polyhedron is more than one, then the opposite end of this interval is not even a local minimum of S in the polyhedron and the entropic involution does not exist for $\mathbf{f}^{\mathrm{v}}$ and some vicinity around it. A special degeneration is possible when the polyhedra are one dimensional (1D), i.e., intervals, and the values of the entropy at both ends of each interval coincide. For example, for two-dimensional distributions, f_+, f_-, the entropy $S = -f_+ \ln f_+ - f_- \ln f_-$ and the macroscopic variable $\rho = f_+ + f_-$. Apart from such symmetric one-dimensional cases there exists an area near the maximally nonequilibrium vertex $\mathbf{f}^{\mathrm{v}}$ where the entropic involution cannot be defined. Such an area may also exist near some other vertices.

The entropic involution is always possible for two families of entropies [20]: the *convex combinations of the Boltzmann and the Burg relative entropies* $S = -\sum[\alpha f_i \ln(f_i/W_i) - (1-\alpha)W_i \ln(W_i/f_i)]$ $(0 \leqslant \alpha < 1)$. The same is true for the relative entropy of the form $S = -\beta^{-1}\sum W_i((W_i/f_i)^{\beta} - 1)$ $(\beta > 0)$ that tends to the Burg entropy when $\beta \to 0$. This *negative branch of the relative Tsallis entropy* is less known then the usual positive branch [19]. These two families of entropies are defined by the following conditions [20]: (i) They increase in Markov processes, (ii) they have the form of the sum over states (the *trace from condition*), (iii) there exist a monotonic transformation that makes these entropies additive with respect to joining of independent subsystems, and (iv) they tend to $-\infty$ at the border of positivity.

We now demonstrate the population function values where the involution cannot be performed for some simple examples. We use the standard 1D lattice with velocities $\mathbf{v} = (-c,0,c)$ and corresponding populations $\mathbf{f} = (f_-, f_0, f_+)$. The explicit Boltzmann style entropy function is [13]

$$S(\mathbf{f}) = -f_- \log(f_-) - f_0 \log(f_0/4) - f_+ \log(f_+). \quad (5)$$

We begin with an LBM with only one conserved moment in collision, namely, density. The equilibrium is $f_-^{\rm eq} = \frac{\rho}{6}$, $f_0^{\rm eq} = \frac{2\rho}{3}$, $f_+^{\rm eq} = \frac{\rho}{6}$. In Fig. 1(a), the simplex Σ of positive populations with a fixed density $\rho = 1$ is the triangle given by the intersection of three half planes, $f^+ \geqslant 0, f^- \geqslant 0$, and $1 - f^+ - f^- \geqslant 0$. Within that region we plot several entropy level contours $S(\mathbf{f}) = c$ and the unique equilibrium point. The region is divided into the parts where the entropic involution is possible (around the equilibrium) and where it is impossible. Additionally the extended possibility boundary given by using the EEC for $\omega = 1.2$ is given.

A more common use of lattice Boltzmann involves a second fixed moment, momentum. The entropic equilibria used by the ELBGK are available explicitly as the maximum of the entropy function (5),

$$f_{\mp}^{\rm eq} = \frac{\rho}{6}(\mp 3u - 1 + 2\sqrt{1+3u^2}), \quad f_0^{\rm eq} = \frac{2\rho}{3}(2 - \sqrt{1+3u^2}).$$

These equilibria form a curve in the simplex $\rho =$ const. In Fig. 1(b) all relaxation occurs parallel to the lines of constant u. The region where entropic involution is possible is again given. Again the extended possibility boundary given by using the EEC for $\omega = 1.2$ is given.

We calculate these borders with the accuracy 10^{-3} guaranteed. The possibility boundaries in Fig. 1 are the images of the simplex boundary under the entropic involution (3) or the transformation (4) for all the boundary points $\mathbf{f}$ where they exist. In this method we draw a straight line l through a boundary point $\mathbf{f}$ and the equilibrium and find the intersection $l \cap \Sigma$ which consists of all points on l with non-negative coordinates. One end of this interval is $\mathbf{f}$, and another end is also a boundary point, $\mathbf{f}^b$. The entropic involution for $\mathbf{f}$ exists if and only if $S(\mathbf{f}^b) \leqslant S(\mathbf{f})$. The solution of (4) exists if and only if $S(\mathbf{f}^{\rm eq}) - S(\mathbf{f}^b) \geqslant \sqrt{\omega - 1}[S(\mathbf{f}^{\rm eq}) - S(\mathbf{f})]$. After we check this inequality, we can solve the equations and find the images. We choose these examples because an LBM with three discrete velocities is simple to visualize. The analysis is equally valid for larger velocity sets in higher dimensions, and in such cases the dimension of the simplex Σ will increase. The shape and size of the region A within that simplex, where entropy balance is possible, will be dependent on the particular choice of the conserved macroscopic moments and the equilibrium. Without making more assumptions about the equilibrium it is not possible to more precisely define the regions A, B than to say that they both exist.

Conclusion. It is not always possible to perform an entropic involution. We have demonstrated that, apart from some special one-dimensional spaces of distributions with additional

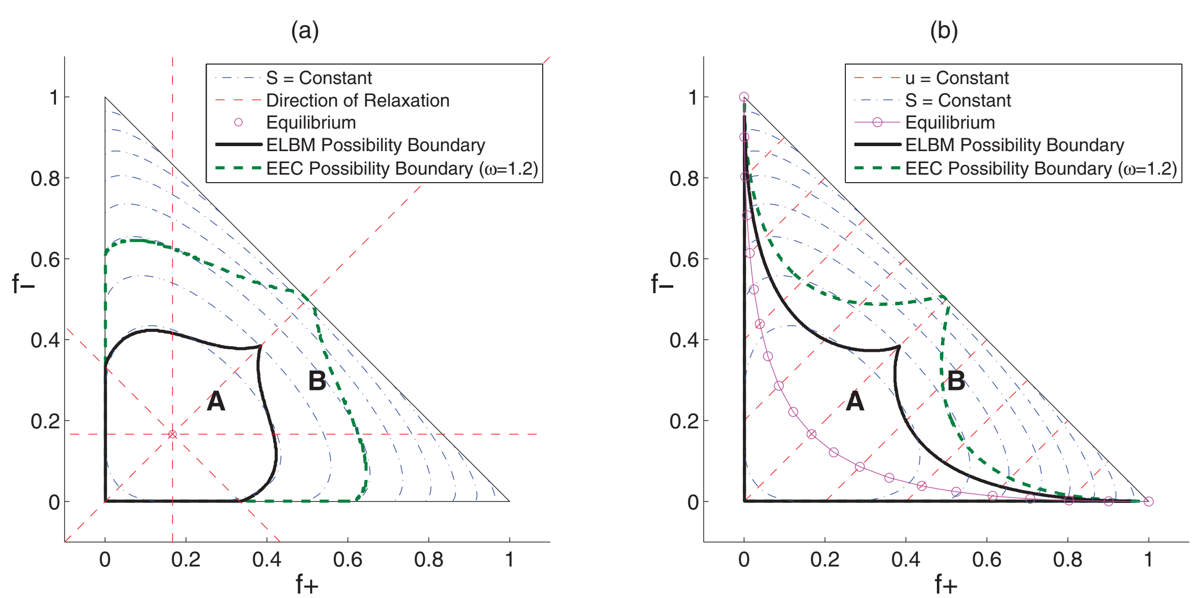

FIG. 1. (Color online) The simplex Σ is given by the triangle. (a) Populations relax through the equilibrium given by the single point. (b) Populations relax through the their corresponding equilibrium point along the line $u =$ const. In both cases the boundary of the possibility of involution is given. The regions A (the entropic involution is possible) and B (it is impossible) divided by this boundary are presented. The boundary of the possibility region for the EEC with $\omega = 1.2$ is plotted.

symmetry, there exist domains with collisions where the preservation of entropy is not possible if the entropy is finite at the border of positivity. We illustrated this statement by some simple examples of ELBGK systems for which we directly calculated the areas where entropic collisions exist and where they do not exist. Such phenomena should be observable in all ELBM schemes with the classical entropies: There exists a vicinity of the equilibrium where the entropic involution is possible, but for some areas of nonequilibrium distributions there exists no nontrivial root of Eq. (3). A collision which preserves entropy does not exist for this area. Therefore, for the regimes close to equilibrium (the vicinities A of equilibria, Fig. 1), ELBM schemes guarantee the precise balance of the entropy. For more nonequilibrium regimes, when at some sites the distribution belongs to sets B, ELBM schemes work as *limiters* with additional dissipation. For any complete definition of ELBM it is necessary to prescribe what to do when the involution is not possible in the sets B. A reasonable choice would be to over-relax the maximum amount possible while maintaining positive population values. Such a technique is in use as a stabilizer for lattice Boltzmann schemes (the "positivity limiter" [17,21–24]), and this is an example of a class of limiters applied to stabilize LB methods [16,17]. An effect of this operation is a local increase in viscosity and in entropy production. The use of the EEC allows the proper entropy production in a wider domain of populations without the entropic reflection necessarily existing. Our formal analysis is valid for all types of (linear) conservation constraints including both thermal and athermal LBM.

Our work addresses a long-lasting discussion, whether the proper entropy balance is always possible in an LBM which respects a H theorem. The answer for any values of the macroscopic variables is as follows: It is always possible if the distribution belongs to some vicinity of the local equilibrium and, at the same time, additional dissipation always appears for sufficiently nonequilibrium distributions. In addition, we stress that (i) the convex combinations of the Boltzmann and the Burg relative entropies and (ii) negative branch of the relative Tsallis entropy allow us to perform entropic collisions without restrictions.

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