Possibility and Impossibility of the Entropy Balance in Lattice Boltzmann Collisions

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We demonstrate that in the space of distributions operated on by lattice Boltzmann methods that there exists a vicinity of the equilibrium where collisions with entropy balance are possible and, at the same time, there exist an area of nonequilibrium distributions where such collisions are impossible. We calculate and graphically represent these areas for some simple entropic equilibria using single relaxation time models. Therefore it is shown that the definition of an entropic LBM is incomplete without a strategy to deal with certain highly nonequilibrium states. Such strategies should be explicitly stated as they may result in the production of additional entropy.

I. INTRODUCTION

Lattice Boltzmann schemes are a type of discrete algorithm which can be used to simulate fluid dynamics and more [2, 15]. Although such a method can be derived as a discretization of the fully continuous Boltzmann equation, some thermodynamics properties may be lost in this process. The Entropic lattice Boltzmann method (ELBM) was invented first in 1998 as a tool for the construction of single relaxation time lattice Boltzmann models which respects a H-theorem [10, 15]. 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 [2].

Nevertheless, controlling the proper entropy balance remained until recently a challenging problem for many lattice Boltzmann models [18]. Some discussions of modern ELBM implementations and results were published recently [11].

The distribution functions at the centre of lattice Boltzmann methods are often referred to and understood as particle densities. Of course for such an interpretation to be meaningful the distribution function should be strictly positive. Despite this some lattice Boltzmann implementations may, as a numerical scheme, tolerate negative population values. 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. A complete definition of an ELBM must include a strategy for what to do in such a situation. The choice of such a strategy should be explicitly given in any definition of an ELBM as it may have side-effects with modification of dissipation which should be understood separately from the influence of the proper entropy balance.

In this paper we study the regions in the spaces of distributions (populations) where collisions with entropy preservation are possible (near the equilibrium) and where they are impossible (sufficiently far from the equilibrium) and demonstrate that both such areas always exist apart some trivial degenerated cases.

II. SINGLE RELAXATION TIME LB SCHEMES

For fluids, LB systems can be derived as a discretization of the Boltzmann Equation

\[ \partial_t f + \mathbf{v} \cdot \partial_x f = Q(f) \]  

(1)

where \( f \equiv f(\mathbf{x}, \mathbf{v}, t) \) is a one particle distribution function over space, velocity space and time and \( Q(f) \) represents the interaction between particles, sometimes called a collision operation. A particular example of the interaction \( Q(f) \) is the Bhatnagar-Gross-Krook equation

\[ Q(f) = -\frac{1}{\tau}(f - f^{eq}). \]  

(2)

The BGK operation represents a relaxation towards the local equilibrium \( f^{eq} \) with rate \( 1/\tau \). The distribution \( f^{eq} \) is given by the Maxwell Boltzmann distribution,

\[ f^{eq} = \frac{\rho}{(2\pi T)^{D/2}} \exp\left(-\frac{\mathbf{v} - \mathbf{u})^2}{2T}\right). \]  

(3)

The macroscopic quantities are available as integrals over velocity space of the distribution function,

\[ \rho = \int f \, d\mathbf{v}, \quad \rho \mathbf{u} = \int \mathbf{v} f \, d\mathbf{v}, \quad \rho \mathbf{u}^2 + \rho T = \int \mathbf{v}^2 f \, d\mathbf{v}. \]

A discrete approximation to these integrals is the first ingredient to discretize this system. The scalar field of the population function (over space, vector space and time) becomes a sequence of vector fields (over space) in time \( f_i(\mathbf{x}, n_t \epsilon), n_t \in \mathbb{Z} \), where the elements of the vector each correspond with an element of the quadrature. Explicitly the macroscopic moments are given by,

\[ \rho = \sum_{i=1}^{n} f_i, \quad \rho \mathbf{u} = \sum_{i=1}^{n} \mathbf{v}_i f_i, \quad \rho \mathbf{u}^2 + \rho T = \sum_{i=1}^{n} \mathbf{v}_i^2 f_i. \]

The complete discrete scheme is given by

\[ f_i(\mathbf{x} + \epsilon \mathbf{v}_i, t + \epsilon) = f_i(\mathbf{x}, t) + \omega(f_i^{eq}(\mathbf{x}, t) - f_i(\mathbf{x}, t)) \]  

(4)

where \( \epsilon \) is the time step. For this system a discrete equilibrium must be used. The choice of the velocity...
set \{v_1, \ldots, 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 \(D\).

III. ELBM

In the continuous case the Maxwellian distribution maximizes entropy, as measured by the Boltzmann \(H\) function, and therefore also has zero entropy production. In the context of lattice Boltzmann methods a discrete form of the \(H\)-theorem has been suggested as a way to introduce thermodynamic control to the system [3,10].

A variation on the LBGK is the ELBGK [1]. In this family of methods, the equilibria are 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 [9]. A slightly different notation is used for the discrete Boltzmann algorithm,

\[ f_i(x + cv_i, t + \epsilon) = f_i(x, t) + \alpha\beta(f_i^{eq}(x, t) - f_i(x, t)). \quad (5) \]

The single parameter \(\omega\) is replaced by a composite parameter \(\alpha\beta\). In this case \(\beta\) controls the viscosity and \(\alpha\) is varied to ensure a constant entropy condition according to the discrete \(H\)-theorem. With knowledge of the entropy function \(S\), \(\alpha\) is found as the non-trivial root of the equation

\[ S(f) = S(f + \alpha(f^* - f)). \quad (6) \]

The trivial root \(\alpha = 0\) returns the entropy value of the original populations. ELBGK then finds the non-trivial \(\alpha\) such that \(D\) holds. This version of the BGK collision one calls entropic BGK (or EBGK) collision. A solution of \(D\) must be found at every time step and lattice site. The EBGK collision obviously respects the Second Law (if \(\beta \leq 1\), and simple analysis of entropy dissipation gives the proper evaluation of viscosity.

In general the entropy function is based upon the lattice. For example, in the case of the simple one dimensional lattice with velocities \(v = (-c, 0, c)\) and corresponding populations \(f = (f_-, f_0, f_+)\) an explicit Boltzmann style entropy function is known [9]:

\[ S(f) = -f_\cdot \log(f_-) - f_0 \log(f_0/4) - f_+ \log(f_+). \quad (7) \]

IV. REGIONS OF EXISTENCE AND NON-EXISTENCE OF ENTROPIC INVOLUTION

Let us study the entropic involution in the distribution simplex \(\Sigma\) given by \(\sum f_i = const > 0\), \(f_i \geq 0\).

Let us prove that under very natural assumptions about some properties of the entropy that the simplex of distributions can be split into two subsets \(A\) and \(B\): in the set \(A\) the entropic involution exists, and for distributions from the set \(B\) equation \(D\) has no non-trivial solutions. Both sets \(A\) and \(B\) have non-empty interior (apart of a trivial symmetric degenerated case).

Let the entropy \(S\) be a strictly concave continuous function in the distribution simplex \(\Sigma\). 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, \(\Sigma_+\), where \(\sum f_i = const\), \(f_i > 0\) 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.

Macroscopic variables are linear functions of \(\mathbf{f}\). The sets with given values of the macroscopic variables in the simplex \(\Sigma\) are polyhedra, intersections of \(\Sigma\) with linear manifolds with the given values of moments. We assume that in any such a polyhedron the entropy achieves its (conditionally) global maximum at an internal point. This assumption holds for the Boltzmann relative entropy because of the logarithmic singularity of the “chemical potentials” \(\mu_i = (\ln(W_i))\) on the border of positivity. These maximizers are equilibria. If \(\mathbf{f}\) is sufficiently close to a positive equilibrium then, due to the implicit function theorem, the nontrivial solution to equation \(D\) exists and it gives \(\alpha = 2 + o(\mathbf{f} - \mathbf{f}^*)\). The value \(\alpha = 2\) corresponds to the mirror image, the small term \(o(\mathbf{f} - \mathbf{f}^*)\) 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 possible, let us consider one 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 \(\mathbf{f}^*\). Let us draw a straight line \(l\) through points \(\mathbf{f}^*\) and \(\mathbf{f}^+\). The intersection \(l \cap \Sigma\) is an interval and \(S\) achieves its global minimum on this interval at the point \(\mathbf{f}^*\). 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 exists for \(\mathbf{f}^*\) and some vicinity around it.

A special degeneration is possible when the polyhedra are one-dimensional, 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 non-equilibrium vertex \(\mathbf{f}^*\) where the entropic involution cannot be defined. Such an area may also exist near some other vertices, where local entropy minima are reached.

For the Burg entropy, the entropic involution is always
possible because it tends to $-\infty$ at the border of positivity. The same is true for the relative entropy of the form $S = -\beta^{-1} \sum W_i ((W_i / f_i)^\beta - 1)$ that tends to the Burg entropy when $\beta \to 0$. This negative branch of the relative Tsallis entropy is less known. The standard Tsallis entropy is finite at the border of positivity, hence, collisions with entropy preservation are not always possible for it.

We now demonstrate the population function values where the involution cannot be performed for some simple examples. We use the standard 1-D lattice described in Section [III] with the discrete equilibrium given in Eq (7). We begin with an LBM with only one conserved moment in collision, namely density. The equilibrium is $f^- = \frac{\rho}{6}$, $f_0 = \frac{2\rho}{3}$, $f^+ = \frac{\rho}{6}$.

In Fig. 1, the simplex $\Sigma$ of positive populations with a fixed density $\rho = 1$ is the triangle given by the intersection of three half-planes, $f^+ > 0$, $f^- > 0$, and $1 - f^+ - f^- > 0$. Within that region we plot several entropy level contours $S(f) = c$ 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.

A more common use of lattice Boltzmann involves a
second fixed moment, momentum. The entropic equilib-ria used by the ELBGK are available explicitly as the maximum of the entropy function [7].

\[ f_u = \frac{\rho}{6}(3u - 1 + 2\sqrt{1 + 3u^2}), \quad f_0 = \frac{2\rho}{3}(2 - \sqrt{1 + 3u^2}). \]

In this case the dimension of the equilibrium is one greater. In Fig. 2 all relaxation occurs parallel to the lines of constant \( u \). The region where entropic involution is possible is again given.

In each experiment the region is discretized into many individual points. For each point a value for \( \alpha \) is possible is again given.

\( \alpha \) begins with a guess of \( \alpha = 1 \) and then add increments of \( 10^{-3} \) until a solution of Eq. (6) occurs, or the edge of the positivity domain is reached. This method would be in-appropriate to use in a usual ELBM, due to the very large computational cost, but it is very robust and hence useful for this experiment with many highy non-equilibrium distributions. Another approach (with the same result) implies calculation of the entropic involution for all the distributions. Another approach (with the same result) implies calculation of the entropic involution for all the boundary points where it exists. In this method we draw a straight line \( l \) through a boundary point \( f \) 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 \( f \), another end is also a boundary point, \( f' \). The entropic involution for \( f \) exits if and only if \( S(f') \leq S(f) \). After we check this inequality, we can solve Eq. (6). The images of these involutions form the border that separates sets \( A \) and \( B \) (see Figs).

V. CONCLUSION

The entropic involution is not always possible to perform. We have demonstrated that apart some special one-dimensional spaces of distributions with additional symmetry there exist domains where collisions with the preservation of entropy are not possible. We illustrated this statement by some simple and well known 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 non-equilibrium distributions there exists no non-trivial root of equation (6). A collision which preserves entropy does not exist for this area. Therefore, for the regimes close to equilibrium (the vicinities \( A \) of equilibria, Figs 1,2), ELBM schemes guaranty the precise balance of the entropy and for more nonequilibrium regimes, when at some sites the distribution belongs to sets \( B \), ELBM schemes work as limiters [5], with additional dissipation. It is necessary for any complete definition of an ELBM algorithm to prescribe what to do when the involution is not possible. A reasonable choice would be to over-relax the maximum amount possible while maintaining positive population values. Such a technique is independently in use as a stabilizer for lattice Boltzmann schemes, sometimes called the ‘positivity limiter’ [4, 5, 12, 13, 16]. An effect of this operation is a local increase in viscosity/entropy production. Hence, if an ELBM were to apply such a scheme it would necessarily break the proper entropy balance. In this sense, ELBM belongs to a large family of add-ons that regularise LBM by the management of the additional dissipation [6].

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