Maximum Entropy Principle for Lattice Kinetic Equations

Iliya V. Karlin* and Alexander N. Gorban
Computing Center RAS, Krasnoyarsk 660036 Russia
S. Succi and V. Boffi
Istituto Applicazioni Calcolo “M. Picone,” Via del Policlinico, 137, I-00161 Roma, Italy
(Received 17 September 1997; revised manuscript received 7 May 1998)

The entropy maximum approach to constructing equilibria in lattice kinetic equations is revisited. 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. [S0031-9007(98)06482-5]

PACS numbers: 05.20.Dd, 47.11.+j, 51.10.+y

Lattice-based simulations of hydrodynamic phenomena received much attention over the past decade [1]. One of the realizations, actively discussed at present, is the lattice Bhatnagar-Gross-Krook method (LBGK) [2]. In the LBGK method, populations of model fluid particles $N_i(r,t)$, residing on the link $i$ of the lattice site $r$ at the discrete time $t$, are updated according to the rule

$$N_i(r + c_i,t + 1) - N_i(r,t) = -\omega[N_i(r,t) - N_i^\text{eq}(r,t)],$$  

where $c_i$ is the $D$-dimensional vector of the $i$th link, and $i = 1, \ldots, b$. The right-hand side of Eq. (1) is the LBGK collision integral $\Delta$, the function $N_i^\text{eq}$ is the local equilibrium, and $\omega \geq 0$ is a dimensionless parameter. As the state of the lattice is updated long enough, the dynamics of $N_i$ becomes governed by macroscopic equations for a finite system of local averages. Depending on the geometry of the lattice, the averages of interest are $\rho(r,t) = \sum_i^b N_i(r,t)$, $\rho u(r,t) = \sum_i^b c_i N_i(r,t)$, and $2\rho E(r,t) = \sum_i^b c_i^2 N_i(r,t)$. Functions $\rho$, $u$, and $E$ are lattice analogs of the hydrodynamic quantities (local density, average velocity, and energy). If it is possible to cast the lattice macroscopic equations into the form of Navier-Stokes equations, then hydrodynamics is implemented in a fairly simple fully discrete kinetic picture (1).

The central issue of the LBGK method is the local equilibrium. Variational approach to the construction of $N_i^\text{eq}$ amounts to a maximization of a strictly concave function $S[N] = \sum_{i=1}^b F(N_i)$, subject to certain constraints. The minimal set of constraints consists of the hydrodynamic constraints which fix $\rho$ and $u$. Taking $F(x) = -x \ln x$, the formal solution is $N_i^\text{eq} = \exp(\alpha + b \cdot c_i)$. However, for lattices of interest, Lagrange multipliers $\alpha$ and $b$ cannot be explicitly expressed in terms of $\rho$ and $u$. This applies to all functions $S$, closely related to the Boltzmann entropy, and it has led to a perturbation technique through a low Mach number expansion (LMN) around the zero-flow equilibrium $N_i^\text{eq}(u = 0) = b^{-1}\rho$. At present, most of the definitions of $N_i^\text{eq}$ originate from the LMN expansions, and are motivated by a matching to the Navier-Stokes equations in the limit of small average velocities. These approaches, however, rarely address the entropy issue directly. This results in the lack of the $H$ theorem, which is, at least in part, responsible for instabilities at relatively low Mach numbers.

In this Letter we revisit the variational approach for the LBGK method. For the minimal set of hydrodynamic constraints, we construct a local equilibrium, specific to a finite system of velocities. This equilibrium has a simple analytic expression, and it is not based on the LMN expansions. We prove the $H$ theorem for the corresponding fully discrete LBGK model, and discuss an extension of the entropy maximum principle to take into account additional constraints.

We consider a class of lattices which satisfy usual symmetry requirements $\sum_{i=1}^b c_i x_i = 0$, and $\sum_{i=1}^b c_i x_i c_j = \xi^2 \delta_{ij}$, where $\alpha, \beta = 1, \ldots, D$ label components of vectors. Maximization of a concave function $S$, subject to the constraints of fixed $\rho$ and $u$, yields $N_i^\text{eq} = G(\alpha + b \cdot c_i)$. First, disregarding the variational origin of the function $G$, we ask for a dependence such that the constraints, $\sum_{i=1}^b G(\alpha + b \cdot c_i) = \rho$ and $\sum_{i=1}^b c_i G(\alpha + b \cdot c_i) = \rho u$, have an explicit solution in terms of $\rho$ and $u$. This occurs in the simplest nontrivial case $G(\cdots) = (\cdots)^2$.

The corresponding quadratic hydrodynamic equilibrium (QHE) has the form

$$N_i^\text{eq} = (\rho/b)[R + c_i^{-2}u \cdot c_i + (4c_i^2 R)^{-1}(u \cdot c_i)^2].$$  

(2a)

Here $c_i^2 = b^{-1}\xi^2$ is the sound speed squared, and $R$ is a function of the Mach number squared, $M^2 = u^2/c_s^2$,

$$R = (1/2)(1 + \sqrt{1 - M^2}).$$  

(2b)

The QHE equilibrium (2) is a positive real-valued function inside the domain $M \leq 1$. For $M > 1$, there are no real-valued solutions to the constraints for the quadratic dependence $G$. We denote $\Omega = \{N_i \mid N_i \geq 0, \rho^2[N] < c_i^2\}$ the set of admissible non-negative populations which can be mapped onto the equilibrium (2). The result of this mapping is $N_i^\text{eq}[N] = N_i^\text{eq}[\rho(N), u(N)]$, which we will further denote simply as $N_i^\text{eq}$. 

© 1998 The American Physical Society
As the next step, we find that the equilibrium (2) maximizes the concave function $S$,
\[ S = -\sum_{i=1}^{b} N_i \sqrt{N_i}, \]
subject to the constraints of fixed density and average velocity. Function $S$ has a formal relation to the well known Tsallis entropy with $q = 3/2$ [3]. Now we can take advantage of the variational origin of the equilibrium (2) to prove the $H$ theorem.

First, we consider the global $H$ theorem. The local entropy production $\sigma(\mathbf{r}, t)$ in the admissible state $N_i$ reads
\[ \sigma = \sum_{i=1}^{b} \frac{\partial S}{\partial N_i} \Delta[N] = \frac{3}{2} \omega \sum_{i=1}^{b} \sqrt{N_i} (N_i - N_i^{eq}). \tag{4a} \]

From the variational problem it follows that
\[ \sum_{i=1}^{b} \sqrt{N_i^{eq}} (N_i - N_i^{eq}) = 0. \]
Thus, Eq. (4a) may be rewritten as
\[ \sigma = \frac{3}{2} \omega \sum_{i=1}^{b} (\sqrt{N_i} - \sqrt{N_i^{eq}}) (N_i - N_i^{eq}) \geq 0, \tag{4b} \]
where we have taken into account that $(\sqrt{X} - \sqrt{Y}) (X - Y) \geq 0$ for $X, Y \geq 0$. The local $H$ theorem (4b) immediately results in the global $H$ theorem for the discrete velocity continuous space-time counterpart of the LBGK equation (1), $\partial_t N_i + c_i \cdot \nabla N_i = -\omega [N_i - N_i^{eq}]$, and has the usual form $d\mathcal{S}/dt = \mathcal{P}$, where the overbar denotes integration over a volume $V$, and where suitable conditions at the boundary $\partial V$ (making surface integrals equal zero) are assumed.

In the fully discrete case, to which we turn now, the $H$ theorem is different. First, we consider a pure relaxation due to the space-independent version of the LBGK equation (1): $N_i(t + 1) = (1 - \omega)N_i(t) + \omega N_i^{eq}$. Average velocity $\mathbf{u}$ is a constant, and if the initial population was admissible, and if $0 \leq \omega \leq 1$, then $N_i(t) \in \Omega$ for all $t \geq 0$. The entropy at time step $t + 1$ is
\[ S(t + 1) = -\sum_{i=1}^{b} [(1 - \omega)N_i(t) + \omega N_i^{eq}]/3/2. \tag{5} \]
Applying the well known inequality $f([1 - \omega]x + \omega y) \geq (1 - \omega)f(x) + \omega f(y)$ to the concave function on the right-hand side of Eq. (5), we derive an estimate for the entropy variation,
\[ S(t + 1) - S(t) \geq \omega[S^{eq} - S(t)]. \tag{6} \]
From the variational origin of $N_i^{eq}$ it follows that $S^{eq} \geq S(t)$. Thus, the right-hand side of Eq. (6) is non-negative. On the other hand, applying inequality $f(\omega) \leq f(0) + f'(0)\omega$ to the concave function on the right-hand side of Eq. (5), we derive an estimate from above,
\[ S(t + 1) - S(t) \leq \sigma(t), \tag{7} \]
where $\sigma(t)$ is the entropy production (4b) at time step $t$. Inequalities (6) and (7) prove the $H$ theorem in the space-independent case for $\omega \in [0, 1]$ if the initial population is admissible, then the entropy increases monotonically in the course of relaxation to the equilibrium (6), and since there are no dissipation mechanisms except for LBGK collisions, the increase of entropy per each time step cannot exceed the amount of entropy produced at this step (7).

Let us discuss qualitatively the case $\omega > 1$. Formally, substituting into the right-hand side of Eq. (5) the function $N_i = N_i^{eq} + \epsilon \Delta N_i$, where $\epsilon \ll 1$ and $\sum_{i=1}^{b} \Delta N_i/N_i^{eq} = 0$, and keeping the lowest order terms (which are of the order $\epsilon^2$), we derive
\[ S_q(t + 1) - S_q(t) = \frac{2 - \omega}{2} \sigma_q(t). \tag{8} \]
Here the subscript indicates quadratic approximation to the entropy and entropy production, $S_q = S^{eq} - (3/8)Q$ and $\sigma_q = (3/4)Q$, while $Q = \sum_{i=1}^{b} \Delta N_i^{2}/\sqrt{N_i^{eq}}$ is a non-negatively definite quadratic form. Equation (8) implies that close to equilibrium variation of the entropy per time step is equal to a non-negative fraction of the entropy production, if $\omega$ belongs to the well known LBGK linear stability interval, $0 \leq \omega \leq 2$. However, a justification is required because functions $N_i(\omega) = (1 - \omega)N_i + \omega N_i^{eq}$ become negative for large enough $\omega > 1$, and then Eq. (5) is not valid. A qualitative argument is as follows: If $|\mathbf{u}| < c_v$, equilibrium (2) is positive, and therefore it has a nonempty positive neighborhood $U$. Thus, $N_i^{eq}$ has a nonempty neighborhood $U_\Omega$ in the admissible domain ($U_\Omega = U \cap P$, where $P$ is the hyperplane of populations with fixed $\mathbf{u}$). This neighborhood $U_\Omega$ can be taken small enough to make $S_q$ a valid approximation, and each of the two states $N_i^{eq} = N_i^{eq} + \epsilon \Delta N_i$ belongs to $U_\Omega$. Then the segment $L$ joining $N_1^+$ and $N_1^-$ also belongs to $U_\Omega$, and it consists of two parts, $L_+$ (between $N_1^+$ and $N_1^{eq}$). Let us take one of the population $N_1^{eq}$ (say, $N_1^{eq}$ for the initial condition, and consider $S_q$ at the subsequent time as a function of $\omega$. This function $S_q(\omega)$ increases as $\omega$ varies from 0 to 1. As $\omega$ exceeds 1, function $S_q(\omega)$ starts decreasing but its value remains higher than in the initial state $N_1^+$, until $\omega$ reaches the value 2. Then $S_q(2) = S_q(0)$, and the update has arrived into $N_1^-$. If $\omega \in [0, 1]$, populations $N_i(t)$ are confined to the segment $L_+$, and they tend to $N_i^{eq}$. If $\omega \in [1, 2]$, populations $N_i(t)$ are confined to the segment $L_-$. They also tend to $N_i^{eq}$ but in a different way, jumping (“overrelaxing”) each time from $L_-$ to $L_+$. This qualitative consideration highlights the entropic origin of the linear stability interval, and indicates the importance of pairs of states with equal entropy. A more quantitative analysis, in particular, corrections to the size of stability interval due to the difference between $S$ and $S_q$, requires an estimate of the neighborhoods $U$ and $U_\Omega$, and it is left for a future work.

The goal now is to extend the above consideration to the space-dependent case. We address here the case $\omega \in [0, 1]$. There are three operations involved in the LBGK equation (1): propagation which acts as a shift,
If the function $TN_i(r, t)$ is admissible, then the right-hand side of Eq. (9) is positive, and the total entropy $\overline{S}(t + 1)$ may be written as

$$\overline{S}(t + 1) = -\sum_r \sum_{i=1}^b \left[ (1 - \omega)TN_i(r, t) + \omega ETN_i(r, t) \right]^{3/2},$$

where summation in $r$ goes over all lattice sites. Under suitable boundary conditions (periodic, for instance), we can write $N_i(r, t)$ in place of $TN_i(r, t)$ in the latter expression. (Specification of boundary conditions plays the same role as in the proof of the global $H$ theorem in the continuous space-time case.) In this case, the above results for the space-independent $H$ theorem are immediately extended onto the space-dependent case by summing over all lattice sites in Eqs. (6) and (7).

Now we come to the most delicate point of analysis: Do populations stay admissible after the propagation step? Since propagation does not violate positivity, we have to check that the average velocity of the population $TN_i$ is below the boundary value $c_s$. If this is the case, then $TN_i$ can be mapped into local equilibrium, and the LBGK update (9) exists. Since there is no mechanism in the system which would keep the average velocity below $c_s$, the answer to this question depends on the choice of initial conditions. Here we present some explicit results.

For simplicity, we consider the incompressible case $\rho = 1$. First, we need to specify populations in $\Omega$, for which moments after propagation can be explicitly evaluated. We consider convex linear combinations of equilibrium populations (2),

$$N_i(r) = \sum_{j=1}^m a_j(r)N_i^{eq}(u_j),$$

where $N_i^{eq}(u_j)$ are equilibrium (2) with fixed vectors $u_j$ of admissible length, and where non-negative functions $a_j(r)$ satisfy $\sum_{j=1}^m a_j(r) = 1$ for all sites $r$. Functions (10) constitute a subset $\Omega^l \subset \Omega$. In particular, $\Omega^l$ contains local equilibrium populations. Propagation transforms populations (10) into $TN_i(r) = \sum_{j=1}^m a_j(r - c_s)N_i^{eq}(u_j)$. Moments of the population $TN_i(r)$, and, in particular, the average velocity, are explicitly computable. [With space Fourier transform of functions $a_j$, it amounts to finding the moments generating function, $G(k, u) = \sum_{i=1}^b \exp(-ik \cdot c_i)N_i^{eq}(u)$, which can be done explicitly for any lattice.]

We present here the result for the simplest case of the one-dimensional lattice with spacing $c$, and with three velocities, $c_s = \pm c$, and $c_0 = 0$. In this case, $c_s^2 = (2/3)c^2$. Exact expression for the average velocity after propagation, $Tu(r)$, reads

$$Tu(r) = \sum_{j=1}^m a_j^+(r)u_j - \frac{c(c^2 - c_s^2)}{6c_s^2} \sum_{j=1}^m Y(u_j)a_j^-(r).$$

Here $a_j^+ = (1/2)[a_j(r + c) + a_j(r - c)]$ are symmetric and asymmetric parts of the functions $a_j$, and function $Y(u)$ depends on the average velocity through Mach number squared: $Y = M^2R^{-1}(M^2)$, while $R$ is defined by Eq. (2b). The part of Eq. (11) which contains $a_j^+$ keeps $u$ below $c_s$, and it causes no problems (this part is “space averaging”). The second part which contains $a_j^-$ can drive the population out of the admissible domain (this part “re-solves” average velocity at neighboring sites). The rate of this process is controlled by values of Mach numbers, and “smoothness” of functions $a_j(r)$. Various estimates can be derived from Eq. (11). The simplest (and rather crude) one is as follows: Let $|u_j(r)| < c_s(1 - \eta)$, where $1 > \eta > 0$. Taking the absolute value of the right-hand side in Eq. (11), and replacing $Y$ by its maximal value 2 at $M = 1$, we derive the following: For $1 > \eta > \sqrt{3/6}\sqrt{2} \approx 0.2$, population stays admissible after propagation step, independently of spatial behavior of functions $a_j(r)$.

Thus, we have demonstrated that there exists a subset $\Omega^l \subset \Omega^l$ which remains inside the admissible domain $\Omega$ after the first time step. Better estimates become available if we take into account functions $a_j$ which vary in space smoothly (in some appropriate sense) because for $a_j = \text{const}$ the asymmetric terms in (11) vanish. Analysis of further time steps is more complicated (though possible for at least $\omega$ close to 1), and will be addressed in a separate paper.

Macroscopic equations for the LBGK model (1) with $N_i^{eq}(2)$ can be established in a usual way [1]. For example, in the case of two-dimensional hexagonal lattice (the FHP lattice, Ref. [1]), the macroscopic equations on the Euler (inviscid) level have the form

$$\partial_t \rho + \partial_a (\rho u_a) = 0, \quad \partial_t (\rho u_a) + \partial_{\beta} P_{a\beta}^{eq} = 0.$$

Here $P_{a\beta}^{eq} = \sum_{i=1}^b c_i\rho \delta_{a\beta} N_i^{eq}$ is the pressure tensor in the equilibrium (2),

$$P_{a\beta}^{eq} = \rho c_s^2 \delta_{a\beta} + (4R)^{-1}\rho(u_a u_\beta - (1/2)u^2 \delta_{a\beta}).$$

(12)

Deviations from the real-fluid case ($P_{a\beta}^{eq} = c_s^2 \rho \delta_{a\beta} + \rho u_a u_\beta$) are twofold. First, the well-known feature of the FHP lattice is present ($P_{a\alpha}^{eq} = 2c_s^2 \rho$ for any equilibrium on the FHP lattice). Second, the nonexistence of $N^{eq}(2)$ at $M > 1$, as implemented by the factor $R$ (2b), causes the velocity-dependent density $\rho = (4R)^{-1}\rho$ in the advection term.

Deviations from hydrodynamic equations are not surprising since only the minimal set of constraints, $\rho$ and $u$ was used to construct the equilibrium. As is well known, this problem can be fixed by invoking further constraints
on the equilibrium population, and thus forcing higher moments to have an appropriate form [4]. We will discuss briefly an extension of our approach to account for additional constraints. Specifically, we seek maximum of the function $S(3)$, subject to an extended set of constraints: $\rho, u$, and $\sum_i c_i^2 N_i = 2\rho E$. In the general case, this problem is not solvable explicitly. However, since the QHE is explicit, we can utilize this to account the additional (energy) constraint approximately.

The full problem is equivalent to the sequence of two subproblems. First, we find a maximum of the function $S$, subject to the hydrodynamic constraints, and disregarding the energy constraint. The solution is the QHE $N^0_i(\rho, u)$. Now the full problem is equivalent to the maximization of the function $S(N_0^0 + \Delta N)$, subject to the constraints $\sum_i c_i^2 \Delta N_i = 2\rho \Delta E$. Here $\Delta N_i$ is the unknown deviation from the QHE $N_0^0$ due to the energy constraint. The solution is controlled by one parameter, $\Delta E = E - E_0(u^2)$, where $E_0$ is the value of the energy in the QHE $N_0^0$. For small $\Delta E$, the problem is well approximated if we confine only the quadratic in $\Delta N_i$ terms in the expansion of the function $S$ around $N_0^0$. Thus, we finally come to the problem of finding a maximum of a quadratic form, subject to the linear constraints. The solution has the form $N^eq = N^0_i(\rho, u) + \Delta N_i(\rho, u, \Delta E)$, and is always explicitly found from the corresponding linear algebraic problem. This method was used earlier to derive Grad-like approximations for the Boltzmann equation [5].

We will illustrate this approach with an example of the one-dimensional lattice with $2m + 1$ velocities $c_i = i\epsilon$, where $i = -m, \ldots, 0, \ldots, m$. For the QHE, we find

$$N^0_i = \rho \left( \frac{R_m}{2m + 1} + \frac{iu}{2r_m} + \frac{(2m + 1)i^2 u^2}{16r_m^2 R_m c^2} \right),$$

where $R_m$ is given by Eq. (2b) with sound speed squared $c_{sm}^2 = (2r_m c^2)/(2m + 1)$, where $r_m = \sum_{j=1}^m i^2$. The improved equilibrium, subject to the energy constraint, has the form

$$N^eq_i = N^0_i + \rho \left( 1 + \frac{(2m + 1)i u}{4r_m R_m c} \right) (\mu + \nu i + \varphi i^2),$$

where $\mu$, $\nu$, and $\varphi$ are found from a linear algebraic system,

$$\mu + \frac{u}{2R_m c} \nu + \frac{2r_m}{2m + 1} \varphi = 0,$$

$$(2m + 1)u \frac{R_m}{4r_m R_m c} \mu + \nu + \frac{(2m + 1)l_m u}{4r_m^2 R_m c} \varphi = 0,$$

$$r_m l_m \mu + (2m + 1)u \frac{R_m}{4r_m R_m c} \nu + \varphi = \frac{\Delta E}{l_m c^2}.$$  

Here $l_m = \sum_{j=1}^m i^4$. The approximation is valid for $|\Delta E| \ll l_m c^2$. Recall that $\Delta E$ is the deviation of the energy parameter from its value $E_0(u^2) [6]$ in the QHE $N^0$ (13). For $\Delta E \neq 0$, Eq. (15) has a solution, if this system is not degenerated. However, the system (15) becomes degenerated for the following value $u_m^*$:

$$u_m^* = \frac{4i^{1/2} R_m^3/2}{r_m^2 + (2m + 1)l_m c^2}.$$  

For each $m$, the average velocity $u_m^*$ belongs to the domain of existence of the QHE ($u_m^* < c_{sm}$). The solution to the system (15) is easily found explicitly, and we do not represent the final result here. Instead, we will discuss what happens at the critical average velocity $u_m^*$.

Since the density scales out, the equilibration on the lattice has the form $N^eq_i = \rho n_i(u, E)$. For $|u| < c_{sm}$, the family of normalized local equilibria $n_i(u, E)$ is two-parametric if only $|u| \neq u_m^*$. For small $\Delta E$, this family is constructed above. If, however, $|u| = u_m^*$, this two-parameter family becomes only one-parametric. In other words, for $|u| = u_m^*$, the energy parameter cannot be chosen independently of the average velocity, and only the value $E^* = E_0((u_m^*)^2)$ is coexistent with the rest of the constraints.

In this Letter, we have constructed a class of nonperturbative lattice equilibria (2) using the maximum entropy principle, introduced a method for taking into account additional constraints, and given proofs of $H$ theorems for LBKG models.

I. V. K. acknowledges the support of the CNR and the SD RAS; also the support of the RFBR (Grant No. 95-02-03836-a) is acknowledged (A. N. G. and I. V. K.).

*Author to whom correspondence should be addressed. Present address: IAC/CNR, V. del Policlinico, 137, 00161 Roma, Italy.


[6] Explicitly, $2E_0 = \rho c_{sm}^2 + \tilde{\rho}(u^2) u^2$, where $\tilde{\rho} = \rho(8r_m^2 R_m)^{-1}[2m + 1/l_m - 2r_m^2]$. 

9