A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

Società Italiana di Fisica

sciences IOP Institute of Physics

An *H*-theorem for the lattice Boltzmann approach to hydrodynamics

To cite this article: A. J. Wagner 1998 *EPL* **44** 144

View the article online for updates and enhancements.

You may also like

- Three-dimensional modelling of the human carotid artery using the lattice Boltzmann method: I. Model and velocity analysis
J Boyd and J M Buick
- The finite-difference lattice Boltzmann method and its application in computational aero-acoustics
Michihisa Tsutahara
- Unsteady immiscible multiphase flow validation of a multiple-relaxation-time lattice Boltzmann method
S Leclaire, N Pellerin, M Reggio et al.

This content was downloaded from IP address 18.119.125.217 on 25/04/2024 at 22:30

EUROPHYSICS LETTERS 15 October 1998

Europhys. Lett., **44** (2), pp. 144-149 (1998)

An H-theorem for the lattice Boltzmann approach to hydrodynamics

A. J. WAGNER

Theoretical Physics, University of Oxford - 1 Keble Rd., Oxford OX1 3BN, Great Britain

(received 18 May 1998; accepted in final form 17 August 1998)

PACS. 05.20−y – Statistical mechanics.
PACS. 05.70Ln – Nonequilibrium thermodynamics, irreversible processes.
PACS. 47.11+j – Computational methods in fluid dynamics.

Abstract. – The lattice Boltzmann equation can be viewed as a discretization of the continuous Boltzmann equation. Because of this connection it has long been speculated that lattice Boltzmann algorithms might obey an H-theorem. In this letter we prove that usual nine-velocity models do not obey an H-theorem but models that do obey an H-theorem can be constructed. We consider the general conditions a lattice Boltzmann scheme must satisfy in order to obey an H-theorem and show why on a lattice, unlike the continuous case, dynamics that decrease an H-functional do not necessarily lead to a unique ground state.

Introduction. – The lattice Boltzmann approach is a method for the simulation of hydrodynamic flow that was originally developed as a model to directly simulate the statistical average densities of lattice gas models. However, deriving the collision term for the lattice Boltzmann model from a lattice gas collision term unnecessarily restricts the Boltzmann model. Early lattice Boltzmann methods also suffered from the exclusion principle (*i.e.*, there can be at most one particle at a given site), leading to an anomalous prefactor in the Navier-Stokes equation that breaks Galilean invariance [1]. This constraint was removed in the linearized lattice Boltzmann model first introduced by Higuera and co-workers [2], where it was observed that the collision operator can be linearized around a local equilibrium and need not correspond to the detailed choice of collision rules of the lattice gas automata, provided the operator conserves mass and momentum.

A further simplification was introduced by Qian, d'Humières and Lallemand [3], who proposed using the Bhatnagar-Gross-Krook (BGK) approximation [4] for the collision term in the lattice Boltzmann method. This approximation writes the collision operator as a function of the difference between the value of the distribution function and the equilibrium distribution function. For a recent review on the lattice Boltzmann method see [5].

Another interpretation of the lattice Boltzmann approach is as a discretized version of the continuum Boltzmann equation. The microscopic derivation of an H-theorem has been given by Boltzmann for the famous Boltzmann equation (see [6]). An H-theorem states that a functional can be defined which is a strictly decreasing function in time. For the continuous

© EDP Sciences

Boltzmann equation this is the famous H-functional:

$$H(t) = \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{v} f(\mathbf{x}, \mathbf{v}, t) \ln(f(\mathbf{x}, \mathbf{v}, t)). \tag{1}$$

Boltzmann was able to prove that for his equation $\frac{\mathrm{d}H(t)}{\mathrm{d}t} \leq 0$. This corresponds to the second law of thermodynamics, which states that the entropy is a monotonically increasing function in time. Isothermal situations are often considered for lattice Boltzmann simulations so the energy is not conserved. In this case an H-functional will no longer correspond to the entropy, but rather to the free energy, which has a monotonic time behaviour in thermodynamics.

In this letter we analyse the general conditions under which a BGK lattice Boltzmann model can obey an H-theorem. We show that lattice Boltzmann schemes do not automatically obey an H-theorem. It is possible, however, to define lattice Boltzmann schemes that do obey an H-theorem. For lattice gases Hénon proved an H-theorem if the collision rules obey semi-detailed balance [1]. This letter for the first time describes an H-theorem for lattice Boltzmann schemes.

In the next section we will introduce a general BGK lattice Boltzmann scheme. We then examine which general properties we can deduce for a lattice Boltzmann scheme that obeys an H-theorem. This will lead to a consistency condition for the equilibrium distribution. We then show that any lattice Boltzmann scheme with an equilibrium distribution that obeys the consistency condition will also obey an H-theorem, and we can construct the H-functional. Lastly we show that usual equilibrium distributions do not obey the consistency condition and construct one example that does obey it.

The BGK lattice Boltzmann scheme. – For a single-component fluid the BGK lattice Boltzmann evolution equation is

$$f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left(f_i^0(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right) , \tag{2}$$

where $\mathbf{x}$ is a discrete vector to a lattice site and the $\mathbf{v}_i$'s are velocity vectors. These are chosen in a way such that $\mathbf{v}_i \Delta t = \mathbf{e}_i$ is a lattice vector of the underlying lattice. Formally, the evolution can be decomposed into two steps: the streaming step and the collision step. The collision step collides the densities according to

$$f_i^{\mathrm{c}}(\mathbf{x}, t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left(f_i^0(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right) \tag{3}$$

and the streaming step moves the density on the lattice according to

$$f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i^{\mathrm{c}}(\mathbf{x}, t). \tag{4}$$

Combining eqs. (3) and (4) recovers the full evolution equation (2). Many lattice Boltzmann applications are isothermal and do not conserve energy so the H-functional corresponds to the free energy instead of the entropy. The case of an isothermal model and a model that conserves energy can thus be treated equivalently for our purpose. We will point out the differences where they arise.

The local density $n(\mathbf{x}, t)$, the local net velocity $\mathbf{u}(\mathbf{x}, t)$ and, for a thermal model, the local kinetic energy $\epsilon(\mathbf{x}, t)$ are given by

$$n = \sum_{i=0}^{N} f_i, \quad n\mathbf{u} = \sum_{i=0}^{N} f_i \mathbf{v}_i \text{ and } n\epsilon = \sum_{i=0}^{N} f_i |\mathbf{v}_i|^2, \tag{5}$$

where the sum is over the N velocity vectors, $\mathbf{v}_i$, of the model. In order for this approach to simulate the continuity, the Navier-Stokes and, for a thermal model, the heat equation, the equilibrium distribution, f_i^0, has to respect the conservation of mass, momentum and energy. To reproduce the right form of the transport coefficients it has to respect additional constraints, namely higher-order velocity moments of the f_i have to correspond to the equivalent moments of the continuum Boltzmann distribution (although this is often relaxed for practical applications, *e.g.* by restricting the method to incompressible flow).

The H-theorem. – Let us now consider whether or not the scheme described can obey an H-theorem. If we have a functional that always decreases in time, then the H-functional must be locally minimal if the distribution function is the equilibrium distribution.

To derive the general form of this H-functional, we will show that the streaming step cannot change the value of the H-functional. Let us consider the collisionless limit ($\tau \to \infty$) where we have only streaming. In a periodic system it follows that the time evolution also has to be periodic for $L!$ steps if L is the number of lattice sites. Thus, if this system obeys the H-theorem, the streaming step cannot change the H-functional.

A different way of seeing that the H-functional has to be invariant under the streaming step is to consider a system for which the H-functional has the value H_1 and then to perform a streaming step to a new system for which the H-functional has the value H_2. If the evolution obeys an H-theorem, it follows that $H_1 \geq H_2$. We then invert all the velocities. It seems reasonable to assume that this operation should not change the value of the H-functional. If we now perform a streaming step on the new system, we arrive at the original system with inverted velocities, and we can conclude $H_2 \geq H_1$ and, therefore, $H_1 = H_2$.

From the invariance of the H-functional under the streaming step we can conclude that there can be no cross-terms between the densities in the H-functional. It can therefore be written as a sum of functions of the f_i separately:

$$H[\{f_i\}](t) = \sum_{l=1}^{L} \sum_{i=0}^{N} h_i[f_i(\mathbf{x}_l, t)], \tag{6}$$

where L is the number of lattice points and l is an index that numbers all points of the lattice.

The equilibrium distribution, f_i^0, is the distribution that minimizes the H-functional under the constraint that its moments have the same values for the conserved quantities of the distribution before the collision. We can eliminate this constraint by introducing Lagrange multipliers into the the H-functional:

$$H[\{f_i\}] = \sum_{i=0}^{N} h_i(f_i) - a\left(\sum_{i=0}^{N} f_i - n\right) - \mathbf{b}\left(\sum_{i=0}^{N} f_i \mathbf{v}_i - n\mathbf{u}\right) - c\left(\sum_{i=0}^{N} f_i |\mathbf{v}_i|^2 - n\epsilon\right). \tag{7}$$

The variation of the H-functional has to vanish for the equilibrium distribution. We therefore obtain for the variation

$$\delta H[\{f_i\}] = \sum_{i=0}^{N} \delta f_i \left(h_i{}'(f_i) - a - \mathbf{b}\mathbf{v}_i - c\mathbf{v}_i^2\right). \tag{8}$$

Because the δf_i are independent, the terms for all i have to vanish independently at equilibrium. This gives us the consistency condition for the local equilibrium distribution

$$f_i^0 = h_i{}'^{-1}(a + \mathbf{b}\mathbf{v}_i + c\mathbf{v}_i^2). \tag{9}$$

This yields a unique definition for f^0 if the h_i' are strictly monotonic, *i.e.*, if the h_i are convex. The Lagrangian multipliers are determined by the conservation constraints

$$n = \sum_{i=0}^{N} f_i^0, \quad n\mathbf{u} = \sum_{i=0}^{N} f_i^0 \mathbf{v}_i \quad \text{and, for a thermal model, } n\epsilon = \sum_{i=0}^{N} f_i^0 |\mathbf{v}_i|^2. \tag{10}$$

For an isothermal model we use $c = 0$ in eq. (7).

Local H-theorem. – We can now show that for the collision step (3) with an equilibrium function that obeys the consistency condition (9), the value of the H-functional decreases. Because we are only concerned with the collision term we drop the $\mathbf{x}$-dependence. We then get for the time development of the local H-functional H^ℓ

$$H^\ell[\{f_i\}](t + \Delta t) - H^\ell[\{f_i\}](t) \leq 0, \qquad \forall \Delta t < \tau. \tag{11}$$

The constraint $\Delta t < \tau$ excludes over-relaxation, which is often used to simulate high Reynolds number flow because the viscosity for lattice Boltzmann schemes has a factor $\tau - (\Delta t)/2$. The condition $\tau = (\Delta t)/2$ corresponds to a vanishing viscosity, and one can prove that in this limit no H-theorem can exist. The case of $(\Delta t)/2 < \tau < \Delta t$ is an interesting problem that still warrants closer investigation.

We now provide the proof for the H-theorem. It is technically difficult to prove it for discrete time steps. As a mathematical simplification we introduce a continuation of the definition of the densities for continuous time in the collision step (3). The continuation is chosen so that the densities obey the conservation constraints at all times. For these continuous time densities we can then prove an infinitesimal H-theorem over which we integrate to obtain the exact H-theorem for discrete time.

Proof:
We define for real $s \in [0, \Delta t]$

$$f_i(t + s) = f_i(t) + \frac{s}{\tau}\left(f_i^0 - f_i(t)\right). \tag{12}$$

Observe that $f_i^0 = f_i^0(n, \mathbf{u}, \epsilon)$ is the equilibrium distribution for all $f_i(s)$ since the conserved quantities are the same for all $f_i(s)$.

Now we can prove the local H-theorem using the definition of H from (7):

$$\begin{aligned}
&H[\{f_i\}](t + \Delta t) - H[\{f_i\}](t) \\
&\quad = \int_0^{\Delta t} \mathrm{d}s \sum_{i=0}^{N} \partial_{f_i}\big(h_i(f_i(t+s)) - a f_i(t+s) - \mathbf{b} f_i(t+s)\mathbf{v}_i - c f_i(t+s)\mathbf{v}_i^2 \\
&\qquad + \frac{1}{N}(an + \mathbf{b}n\mathbf{u} + cn\epsilon)\big)\partial_s f_i(t+s) \\
&\quad \overset{(12)}{=} \int_0^{\Delta t} \mathrm{d}s \sum_{i=0}^{N} \left(h_i{}'(f_i(t+s)) - a - \mathbf{b}\mathbf{v}_i - c\mathbf{v}_i^2\right) \times \frac{1}{\tau}\left(f_i^0 - f_i(t)\right) \\
&\quad \overset{(9)}{=} \int_0^{\Delta t} \mathrm{d}s \sum_{i=0}^{N} \left(h_i{}'(f_i(t+s)) - h_i{}'(f_i^0)\right) \times \frac{\alpha(s)}{\tau}(f_i^0 - f_i(t+s)) \\
&\quad \leq 0
\end{aligned} \tag{13}$$

if h' is non-decreasing or, equivalently, if h is convex. We have $\alpha(s) = (1 - s/\tau)^{-1}$, which is always positive because $s < \Delta t < \tau$.

Global H-theorem. – The total entropy $H[\{f_i\}](t)$ defined in (6) is non-increasing at every lattice site in the collision step and is unchanged in the streaming step. We therefore have the global H-theorem

$$H[\{f_i(\mathbf{x})\}](t+\Delta t) - H[\{f_i(\mathbf{x})\}(t)] \leq 0 \qquad \forall \tau > \Delta t. \tag{14}$$

The global equilibrium distribution. – In statistical mechanics the H-theorem is used to prove the existence of a unique equilibrium state of the system. It will turn out that for lattice systems this is not necessarily the case. Demanding the existence of a well-defined ground state gives us a constraint for the structure of the lattice. This is equivalent to the constraint that there are no spuriously conserved quantities.

Since we have a global H-theorem and the H-functional is bounded, we know that the scheme has to converge to some minimal value of the H-functional. We will now examine what information about the final state we can extract from our H-theorem.

Since the H-functional does not change in the final state, we know that it also cannot change locally in the collisions. Therefore the local distributions must be equilibrium distributions $f_i(t) = f_i^0$. We can conclude that for large t the system converges to a state that has local equilibrium distributions everywhere. Furthermore, the streaming step has to transform one state of local equilibrium into another (or the same) state of local equilibrium.

Whether these conditions force the global equilibrium to be homogeneous depends on the lattice and the set of velocity vectors $\{\mathbf{v}_i\}$. This question is related to the problem of spurious invariants (see, for instance, [7] and references therein). Spurious invariants are conserved quantities that do not correspond to any physical quantities. In a four-velocity model on a square lattice, for instance, the total momentum of all even and odd lattice sites is separately conserved. If the global equilibrium is constrained to be homogeneous, then there cannot be any spurious invariant. If, however, inhomogeneous final states are possible, then these states can be characterized by at least one spuriously conserved quantity.

Why conventional lattice Boltzmann schemes cannot have an H-theorem. – We show that assuming an H-theorem leads to a structure of the equilibrium distribution that is different from the usual structure of the equilibrium distribution. The usual BGK lattice Boltzmann schemes have a polynomial equilibrium distribution. For an isothermal model it takes the form [3, 8-10]

$$f_i^0 = A_\sigma n + B_\sigma n u_\alpha v_{i\alpha} + C_\sigma n u_\alpha u_\alpha + D_\sigma n u_\alpha u_\beta v_{i\alpha} v_{i\beta}, \tag{15}$$

where $A_\sigma, B_\sigma, C_\sigma$, and D_σ are constants and σ is an index distinguishing velocities with different magnitudes. If this equilibrium distribution is to be derived from an H-functional of the form given in eq. (6), then the $h'^{-1}(x)$ have to be quadratic polynomials. We obtain

$$\begin{aligned} f_i^0 &= {h_i}'^{-1}(a + b_\alpha v_{i\alpha}) \\ &= \alpha_\sigma + \beta_\sigma(a + b_\alpha v_{i\alpha}) + \gamma_\sigma(a + b_\alpha v_{i\alpha})^2 \\ &= (\alpha_\sigma + \beta_\sigma a + \gamma_\sigma a^2) + (\beta_\sigma + 2\gamma_\sigma a) b_\alpha v_{i\alpha} + \gamma_\sigma b_\alpha b_\beta v_{i\alpha} v_{i\beta}\,, \end{aligned} \tag{16}$$

where the coefficients α_σ, β_σ and γ_σ are constants that cannot depend on n or $\mathbf{u}$. The Lagrange multipliers a and b_α are determined by the conservation laws. In order for the coefficients in (16) to be linear in n, we require $\alpha_\sigma = \beta_\sigma = 0$. Evaluation shows that the resulting coefficients are not quadratic in u_α for any choice of γ_σ. In particular, we get

$$a^2 = n \frac{\gamma_1 + 2\gamma_2 + \sqrt{(\gamma_1 + 2\gamma_2)(-2u^2\gamma_0 + (1-8u^2)\gamma_1 + 2(1-4u^2)\gamma_2)}}{2(\gamma_1 + 2\gamma_2)(\gamma_0 + 4(\gamma_1 + \gamma_2))}\,, \tag{17}$$

which has a more complicated u-dependence for all γ_σ than eq. (15). All lattice Boltzmann schemes of which we are aware have a polynomial u-dependence and therefore cannot obey an H-theorem.

A lattice Boltzmann scheme with an H-theorem. – If we use the classical choice for the H-functional

$$H(\{f_i\}) = \sum_l \sum_i f_i \ln(f_i) \tag{18}$$

for a thermal model, *i.e.*, a model with mass, momentum and energy conservation, we get for the equilibrium equation a Maxwell-Boltzmann distribution

$$f_i^0 = N \exp\left[(\mathbf{v}_i - \mathbf{U})^2/T\right] , \tag{19}$$

where N, $\mathbf{U}$ and T are the Lagrange multipliers. This scheme simulates the continuity, Navier-Stokes and heat equations to an approximation that depends on the choice of lattice (because the higher-order moments needed for the Chapman-Enskog expansion do not necessarily coincide for the discrete and continuum case). Unfortunately, the Lagrange multipliers cannot be expressed analytically in terms of the conserved quantities, but have to be found by numerically solving the non-linear equation. For a regime where the Navier-Stokes and heat equations are recovered, the Lagrange multipliers are well approximated by $\mathbf{U} \sim \mathbf{u}$ and $T \sim \theta = 1/d(\epsilon - n\mathbf{u}^2)$, where d is the number of spatial dimensions.

The advantage of this scheme is that it is numerically stable for $\tau > \Delta t$. This is ensured by the H-theorem because numerical instabilities lead to inhomogeneities that would increase the H-functional.

Conclusions. – We have shown how lattice Boltzmann models can be constructed to obey an H-theorem and that the usual choice of the equilibrium distribution is incompatible with an H-theorem. For traditional schemes no H-functional can exist.

It will be interesting to investigate further examples and applications of lattice Boltzmann methods which obey an H-theorem. One apparent advantage of these schemes is the numerical stability that results from the constraint which minimizes the H-functional. We believe that constructing lattice Boltzmann schemes with H-functionals will help to improve the stability lattice Boltzmann schemes.

***

It is a pleasure to thank D. D'HUMIÈRES and C. MARSH for several helpful discussions.

REFERENCES

[1] FRISCH U., D'HUMIÈRES D., HASSLACHER B., LALLEMAND P., POMEAU Y. and RIVET J. P., *Complex Systems*, **1** (1987) 649.
[2] HIGUERA F. J. and JIMÉNEZ J., *Europhys. Lett.*, **9** (1989) 663.
[3] QIAN Y. H., D'HUMIÈRES D. and LALLEMAND P., *Europhys. Lett.*, **17** (1992) 479.
[4] BHATNAGAR P., GROSS E. P. and KROOK M. K., *Phys. Rev.*, **94** (1954) 511.
[5] CHEN S. and DOOLEN G. D., *Annu. Rev. Fluid Mech.*, **30** (1998) 329.
[6] HUANG K., *Statistical Mechanics*, second edition (John Wiley & Sons, New York-Chichester-Brisbane-Toronto-Singapore) 1987.
[7] BENZI R., SUCCI S. and VERGASSOLA M., *Phys. Rep.*, **222** (1992) 145.
[8] FLEKKØY E. G., *Phys. Rev. E*, **47** (1993) 4247.
[9] SWIFT M. R., OSBORN W. R. and YEOMANS J. M., *Phys. Rev. Lett.*, **75** (1995) 830.
[10] ORLANDINI E., SWIFT M. R. and YEOMANS J. M., *Europhys. Lett.*, **32** (1995) 463.