PHYSICAL REVIEW E **68**, 025103(R) (2003)

Galilean-invariant lattice-Boltzmann models with H theorem

Bruce M. Boghosian and Peter J. Love
Department of Mathematics, Bromfield-Pearson Hall, Tufts University, Medford, Massachusetts 02155, USA

Peter V. Coveney
Centre for Computational Science, Department of Chemistry, University College London, 20 Gordon Street, WC1H 0AJ London, United Kingdom

Iliya V. Karlin
Department of Materials, Institute of Polymers, ETH Zürich, ETH-Zentrum, Sonneggstrasse 3, ML J 19, CH-8092 Zürich, Switzerland

Sauro Succi
Istituto Applicazioni Del Calcolo, viale del Policlinico 137, 00161 Roma, Italy

Jeffrey Yepez
Air Force Research Laboratory, Hanscom Air Force Base, Massachusetts 01731-3010, USA

(Received 5 November 2002; published 26 August 2003)

We demonstrate that the requirement of Galilean invariance determines the choice of H function for a wide class of entropic lattice-Boltzmann models for the incompressible Navier-Stokes equations. The required H function has the form of the Burg entropy for $D=2$, and of a Tsallis entropy with $q=1-(2/D)$ for $D>2$, where D is the number of spatial dimensions. We use this observation to construct a fully explicit, unconditionally stable, Galilean-invariant, lattice-Boltzmann model for the incompressible Navier-Stokes equations, for which attainable Reynolds number is limited only by grid resolution.

DOI: 10.1103/PhysRevE.68.025103 PACS number(s): 47.11.+j

I. INTRODUCTION

Lattice-Boltzmann models of fluids [1,2] evolve a single-particle distribution function in discrete time steps on a regular spatial lattice, with a discrete velocity space comprising the lattice vectors themselves. The single-particle distribution corresponding to lattice vector $\mathbf{c}_i$ at lattice position $\mathbf{x}$ and time step t is denoted by $N_i(\mathbf{x},t)$. The simplest variety of lattice-Boltzmann models employ a Bhatnagar-Gross-Krook (BGK) operator [3], so that their evolution equation is

$$N_i(\mathbf{x}+\mathbf{c}_i,t+\Delta t)=N_i(\mathbf{x},t)+\frac{1}{\tau}[N_i^{\mathrm{eq}}(\mathbf{x},t)-N_i(\mathbf{x},t)],$$

for $i=1,\ldots,b$. Here b is the coordination number of the lattice, $N_i^{\mathrm{eq}}(\mathbf{x},t)$ is a specified equilibrium distribution function that depends only on the values of the conserved quantities at a site, and τ is a characteristic collisional relaxation time. Using the Chapman-Enskog analysis, it is possible to show that the mass and momentum moments of the distribution function will obey the Navier-Stokes equations for certain choices of equilibrium distribution [1].

The viscosity appearing in the Navier-Stokes equations obtained from these models is proportional to $\tau-\frac{1}{2}$. To lower this and thereby increase Reynolds number, practitioners often over-relax the collision operator by using values of τ in the range $(\frac{1}{2},1]$. For sufficiently small τ, however, the method loses numerical stability, and this consideration limits the lowest Reynolds numbers attainable.

In an effort to understand these instabilities, there has been much recent interest in *entropic lattice-Boltzmann models* [4–6]. These models are motivated by the fact that the loss of stability is due to the absence of an H theorem [6]. Numerical instabilities evolve in ways that would be precluded by the existence of a Lyapunov function. The idea behind entropic lattice-Boltzmann models is to specify an H function, rather than just the form of the equilibrium. Of course, the equilibrium distribution will be that which extremizes the H function. The evolution will be required never to decrease H, yielding a rigorous discrete-time H theorem; this is to be distinguished from other discrete models of fluid dynamics for which an H theorem may be demonstrated only in the limit of vanishing time step [7].

To ensure that collisions never decrease H, the collision time τ is made a function of the incoming state by solving for the smallest value τ_{min} which does not increase H. The value then used is $\tau=\tau_{\mathrm{min}}/\kappa$, where $0<\kappa<1$. It has been shown that the expression for the viscosity obtained by the Chapman-Enskog analysis will approach zero as κ approaches unity [4–6]. Thus, the entropic lattice-Boltzmann methodology allows for arbitrarily low viscosity together with a rigorous discrete-time H theorem, and thus absolute stability. The upper limit to the Reynolds numbers attainable by the model is therefore determined by loss of resolution of the smallest eddies, rather than by loss of stability [6,8,9].

In a recent review of the subject, Succi, Karlin, and Chen [10] have pointed out that entropic lattice-Boltzmann models have three important desiderata: Galilean invariance, nonnegativity of the distribution function, and ease of determining the local equilibrium distribution at each site and at each time step.

In this paper, we shall construct entropic lattice-Boltzmann models for the incompressible Navier-Stokes equations which are Galilean invariant to second order in the Mach number expansion of the distribution function (quasiperfect in the terminology of Ref. [10]). We shall show that the requirement of Galilean invariance makes the choice of H function unique. We shall show that the required function has the form of the Burg entropy [11] in two dimensions, and the Tsallis entropy in higher dimensions. While the analogous problem for the compressible Navier-Stokes equations is difficult and remains outstanding, the purpose of this paper is to point out that the incompressible case is nontrivial and interesting in its own right.

Finally, a point of clarification: Throughout this paper, when we describe the lattice-Boltzmann model as "incompressible," we really mean that it is faithful to the Navier-Stokes equations only in the asymptotic limit of incompressibility. This means that the Mach number must scale with the Knudsen number, and the fluctuation of density about its mean must scale with the Knudsen number squared. Indeed, this is the same sense in which any quasicompressible fluid model may be said to simulate incompressible fluid equations. In this asymptotic limit the pressure is determined by an elliptic equation, and the equation of state becomes irrelevant.

II. EQUILIBRIUM DISTRIBUTION

We consider a Bravais lattice of coordination number b in D dimensions. We denote the lattice vectors by $\mathbf{c}_i$, where $i=1,\ldots,b$, and their magnitudes by $c=|\mathbf{c}_i|$. The restriction to a single-speed model on a Bravais lattice is done solely for the sake of simplicity in presentation. A future publication will generalize the results of this paper to multispeed lattice-Boltzmann models [12].

We demand that the lattice symmetry group be sufficiently large that the only fourth-rank tensors that are invariant under its group action are isotropic. The mass and momentum densities are given by

$$\rho=\sum_{i=1}^{b} mN_i \tag{1}$$

and

$$\rho\mathbf{u}=\sum_{i=1}^{b} m\mathbf{c}_i N_i, \tag{2}$$

where m is the particle mass and $\mathbf{u}$ is the hydrodynamic velocity D vector. These $D+1$ quantities must be conserved in collisions.

If we regard N_i, for $i=1,\ldots,b$, as coordinates in a b-dimensional space, the conservation laws (1) and (2) restrict the collision outcomes to a $[b-(D+1)]$-dimensional subspace. Since the conserved quantities are linear functions of N_i's, the non-negativity requirement

$$N_i \geqslant 0 \tag{3}$$

is satisfied within a compact polytope whose faces are given by the b equations, $N_i=0$ for $i=1,\ldots,b$. In order to ensure that H is altered only by collisions and not by propagation, we assume that the H function is of trace form

$$H=\sum_{i=1}^{b} h(N_i),$$

where $h'(x)\geqslant 0$ for $x>0$. If $\lim_{x\to 0}h'(x)=\infty$, then the normal derivative of H goes to negative infinity on the polytope boundary, enforcing the non-negativity constraint [Eq. (3)]. The purpose of this paper is to demonstrate that the requirement of Galilean invariance uniquely determines the choice of function $h(x)$.

In passing, we note that our choice of the form of H differs from that of Karlin, Ferrante, and Öttinger [5], which is of the form $H=\Sigma_i^b N_i \ln(N_i/W_i)$, where W_i are speed-dependent weights (equal to the global equilibrium at zero flow). That is, prior work has allowed weighted contributions to H and found solutions for which h has the form of a (relative) Boltzmann entropy, while the present work assumes uniform contributions to H and finds solutions for which h is not a Boltzmann entropy. Both approaches are capable of yielding Galilean-invariant hydrodynamics. A more general form for H which will subsume both approaches as special cases remains an interesting theoretical challenge.

The equilibrium distribution function may be found by extremizing H with respect to N_i, subject to the constraints [Eqs. (1) and (2)]

$$0=\frac{\partial}{\partial N_i}\left(H-\frac{\mu}{m}\rho-\frac{\boldsymbol{\beta}}{m}\cdot\rho\mathbf{u}\right),$$

where μ/m and $\boldsymbol{\beta}/m$ are Lagrange multipliers. We quickly find

$$0=h'(N_i)-\mu-\boldsymbol{\beta}\cdot\mathbf{c}_i,$$

and so

$$N_i^{\mathrm{eq}}=\phi(\mu+\boldsymbol{\beta}\cdot\mathbf{c}_i), \tag{4}$$

where the function ϕ is the inverse function of h'. The constants μ and $\boldsymbol{\beta}$ are determined by Eqs. (1) and (2). It is usually difficult to find an exact analytic expression for them in terms of the conserved quantities ρ and $\rho\mathbf{u}$, though some equilibria are known for which this is possible [8,9]. Alternatively, one may solve for them numerically or perform a Taylor expansion in Mach number. We adopt the latter approach below.

III. GALILEAN INVARIANCE

We seek to Taylor expand the equilibrium distribution in Mach number because (i) we can do so analytically, (ii) only the first two terms of that expansion determine the form of the incompressible Navier-Stokes equations, and (iii) that expansion is a useful initial guess for any numerical solution. From general symmetry arguments, it is clear that $\boldsymbol{\beta}$ will be proportional to the hydrodynamic velocity $\mathbf{u}$, so that we may begin our Mach number expansion by expanding Eq. (4) for small $\boldsymbol{\beta}$. We get

$$N_i^{\mathrm{eq}}=\phi(\mu)+\phi'(\mu)\boldsymbol{\beta}\cdot\mathbf{c}_i+\frac{1}{2}\phi''(\mu)\boldsymbol{\beta}\boldsymbol{\beta}:\mathbf{c}_i\mathbf{c}_i+\cdots.$$

Inserting this into Eqs. (1) and (2), and using general properties of the Bravais lattice, we find

$$\rho=mb\phi(\mu)+\frac{mbc^2}{2D}\phi''(\mu)\beta^2+\cdots$$

and

$$\rho\mathbf{u}=\frac{mbc^2}{D}\phi'(\mu)\boldsymbol{\beta}+\cdots,$$

where the ellipses denote third or higher order terms in Mach number. Inverting this perturbatively we find that, to second order in Mach number, the Lagrange multipliers are given by

$$\mu=x-\frac{D}{2c^2}\frac{\left(\frac{\rho}{mb}\right)^2\phi''(x)}{[\phi'(x)]^2}u^2+\cdots,$$

where $x\equiv h'(\rho/mb)$, and by

$$\boldsymbol{\beta}=\frac{D}{c^2}\frac{\frac{\rho}{mb}}{\phi'(x)}\mathbf{u}+\cdots.$$

Inserting these into Eq. (4), we obtain the equilibrium distribution

$$N_i^{\mathrm{eq}}=\frac{\rho}{mb}\left[1+\frac{D}{c^2}\mathbf{c}_i\cdot\mathbf{u}+\frac{D^2}{2c^4}\frac{\phi(x)\phi''(x)}{[\phi'(x)]^2}\times\left(\mathbf{c}_i\mathbf{c}_i-\frac{c^2}{D}\mathbf{1}\right):\mathbf{u}\mathbf{u}+\cdots\right]. \tag{5}$$

Now, for lattice-Boltzmann models on a Bravais lattice, it is well known that a Chapman-Enskog analysis based on the equilibrium distribution

$$N_i^{\mathrm{eq}}=\frac{\rho}{mb}\left[1+\frac{D}{c^2}\mathbf{c}_i\cdot\mathbf{u}+\frac{D(D+2)}{2c^4}g\left(\mathbf{c}_i\mathbf{c}_i-\frac{c^2}{D}\mathbf{1}\right):\mathbf{u}\mathbf{u}+\cdots\right] \tag{6}$$

will give rise to the incompressible Navier-Stokes equations

$$\boldsymbol{\nabla}\cdot\mathbf{u}=0$$

and

$$\frac{\partial\mathbf{u}}{\partial t}+g\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u}=-\frac{1}{\rho}\boldsymbol{\nabla}P+\nu\nabla^2\mathbf{u}.$$

Comparing Eqs. (5) and (6), we identify

$$g=\left(\frac{D}{D+2}\right)\frac{\phi(x)\phi''(x)}{[\phi'(x)]^2}.$$

If the factor g is not unity, Galilean invariance will be broken. Thus we demand $g=1$, and this yields the second-order nonlinear differential equation

$$\phi(x)\phi''(x)=\left(1+\frac{2}{D}\right)[\phi'(x)]^2.$$

The general solution to this equation is of the form

$$\phi(x)=C^{D/2}(x-aC)^{\gamma},$$

where C and a are arbitrary constants, and γ is to be determined. We quickly find that γ must be either 0 or $-D/2$. Since a constant ϕ would not yield a well defined h', we see that we must have $\phi(x)=C^{D/2}(x-aC)^{-D/2}$, whence $h'(x)=C(a+x^{-2/D})$, and this integrates to give

$$h(x)=\begin{cases} h_0+C[ax+\ln x] & \text{if } D=2\\ h_0+C\left[ax+\left(\frac{x^{1-2/D}-1}{1-2/D}\right)\right] & \text{if } D\neq 2,\end{cases} \tag{7}$$

where h_0 is constant. In fact, the only effect of nonzero h_0 is to introduce an additive constant to H, and the only effect of nonunity C is to scale H by a constant factor. In other words, $h(x)$ is uniquely specified only to within additive and multiplicative constants. With this understanding, we may say that the requirement of Galilean invariance has uniquely specified the choice of H. We also note that $\lim_{x\to 0}h'(x)=\infty$, so the non-negativity constraint will be enforced by the dynamics.

Finally, we write the global Lyapunov function $\mathcal{H}\equiv\Sigma_{\mathbf{x}}H$ by summing $h(N_i(\mathbf{x},t))$ over the lattice. Since the total mass is conserved we have complete freedom to choose a, and so to within additive and multiplicative constants $\mathcal{H}$ may be written

$$\mathcal{H}(t)\propto\begin{cases} \sum_{\mathbf{x}}\sum_i \ln[N_i(\mathbf{x},t)] & \text{for } D=2\\ \sum_{\mathbf{x}}\sum_i \frac{[N_i(\mathbf{x},t)]^{1-2/D}-N_i(\mathbf{x},t)}{2/D} & \text{for } D\neq 2,\end{cases}$$

for appropriate choices of a and C. This has the form of a Burg entropy [11] for $D=2$, and a subadditive Tsallis entropy [13] with parameter

$$q=1-\frac{2}{D}$$

for $D\neq 2$. We note that $D\leqslant 2$ corresponds to $q\leqslant 0$, and $D>2$ corresponds to $0<q<1$. It is interesting that it is only in the infinite-dimensional limit, $D\to\infty$, where the set of velocities becomes infinite, that $q\to 1$ and we recover the Boltzmann-Gibbs entropy [14]. We might also expect the limit of large b at constant D to yield the Boltzmann-Gibbs entropy, but that demonstration will require the multispeed generalization of the present analysis; that work, which will also provide the details of the Chapman-Enskog analysis, is in progress [12]. The numerical implementation of the model described herein is likely to require some careful algorithmic optimization, and is likewise left to future publication.

The appearance of the Burg and Tsallis entropies in this context is fascinating. In a footnote of their recent review, Succi, Karlin, and Chen [10] noted that the entropy that gave rise to the above-mentioned solvable model for a compressible fluid was related to the Tsallis entropy with $q=3/2$, so there may be more than one connection with Tsallis thermostatistics [13] lurking here. There are precious few situations in which the origins of Tsallis thermostatistics can be traced analytically to an underlying microscopic dynamical model, as we have done here.

IV. CONCLUSIONS

We have presented Galilean-invariant, entropic lattice-Boltzmann models for the incompressible Navier-Stokes equations. We expect that these models will be useful for the simulation of two- and three-dimensional turbulence. As noted by Succi, Karlin, and Chen [10], the problem of finding perfect models for lattice models of the *compressible* Navier-Stokes equations is much more difficult and may well be impossible. We found it interesting that the simpler problem, for incompressible fluids, is itself very nontrivial. In particular, the appearance of the Burg and Tsallis entropies for the H function is surprising. These entropies have heretofore been associated with long-range interactions, long-time memory, or a fractal space-time structure. This work indicates that they may also be relevant to models with discretized space-time and finite domain connectivity, and this surely warrants future study.

ACKNOWLEDGMENTS

B.M.B. was supported in part by the U.S. Air Force Office of Scientific Research under Grant No. F49620-01-1-0385, and in part by MesoSoft Corporation. He performed a portion of this work while at the Center for Computational Science, Department of Chemistry, Queen Mary, University of London under RealityGrid Contract No. GR/R67699. P.L. was supported by the DARPA QuIST program under AFOSR Grant No. F49620-01-1-0566.

[1] S. Succi, *The Lattice Boltzmann Equation-For Fluid Dynamics and Beyond* (Oxford University Press, 2001).
[2] R. Benzi, S. Succi, and M. Vergassola, Phys. Rep. **222**, 145 (1992).
[3] Y.H. Qian, D. d'Humieres, and P. Lallemand, Europhys. Lett. **17**, 479 (1992).
[4] I.V. Karlin, A.N. Gorban, S. Succi, and V. Boffi, Phys. Rev. Lett. **81**, 6 (1998).
[5] I.V. Karlin, A. Ferrante, and H.C. Öttinger, Europhys. Lett. **47**, 187 (1999).
[6] B.M. Boghosian, J. Yepez, P.V. Coveney, and A. Wagner, Proc. R. Soc. London, Ser. A **457**, 717 (2001).
[7] C. Marsh and P.V. Coveney, J. Phys. A **31**, 6561 (1998).
[8] S. Ansumali and I.V. Karlin, Phys. Rev. E **62**, 7999 (2000).
[9] S. Ansumali and I.V. Karlin, Phys. Rev. E **65**, 056312 (2002).
[10] S. Succi, I.V. Karlin, and H. Chen, Rev. Mod. Phys. **74**, 1203 (2002).
[11] A.N. Gorban and I.V. Karlin, Phys. Rev. E **67**, 016104 (2003).
[12] B. M. Boghosian, P. J. Love, and J. Yepez (unpublished).
[13] C. Tsallis, in *Nonextensive Statistical Mechanics and Its Application*, edited by S. Abe and Y. Okamoto (Springer-Verlag, Berlin, 2001).
[14] This limit must be taken with great caution, since the sound speed, $c_s=c/\sqrt{D}$, also vanishes in this limit, threatening the validity of the expansion in Mach number $M=u/c_s$; we could, for example, take $u/c \sim D^{-3/4}$ so that $M \rightarrow 0$ even as $D \rightarrow \infty$.