Galilean-Invariant Lattice-Boltzmann Models with H-Theorem

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(Dated: November 29, 2017)

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

arXiv:cond-mat/0211093v1 [cond-mat.stat-mech] 5 Nov 2002

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 comprised of 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 BGK operator [3], so that their evolution equation is

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

for $i = 1, \ldots, b$. Here b is the coordination number of the lattice, $N_i^{\rm eq}(\mathbf{x}, t)$ 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 that appears in the Navier-Stokes equations obtained from these models is proportional to $\tau - \frac{1}{2}$. To lower viscosity 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, 5, 6]. These models are motivated by the fact that the loss of stability is due to the absence of an H theorem. 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 $\tau_{\rm min} < 1$ that does not increase H. The value then used is $\tau = \tau_{\rm min}/\kappa$ 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, 5, 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 [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, non-negativity of the distribution function, and ease of determining the local equilibrium distribution at each site at each timestep.

In this paper, we shall construct entropic lattice Boltzmann models for the incompressible Navier-Stokes equations which are gallilean invariant to second order in the Mach number expansion of the distribution function (quasi-perfect in the terminology of [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.

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 $c = |\mathbf{c}_i|$. 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 the 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 the N_i's, the nonnegativity requirement

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

is satisfied within a compact polytope whose faces are given by the b equations $N_i = 0$ for $i = 1, \ldots, b$. We assume that the H-function is of trace form

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

where $h'(x) \geq 0$ 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 nonnegativity constraint, Eq. (3). The purpose of this paper is to demonstrate that the requirement of galilean invariance uniquely determines the choice of function $h(x)$.

The equilibrium distribution function may be found by extremizing H with respect to the 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

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

and so

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

where the function ϕ is the inverse function of h'. The constants μ and $\boldsymbol{\beta}$ are determined by Eqs. (1) and (2), though it is generally impossible to find an exact analytic expression for them in terms of the conserved quantities ρ and $\rho\mathbf{u}$; rather one must solve for them numerically or perform a Taylor expansion in Mach number. We adopt the latter approach below.

GALILEAN INVARIANCE

We seek to Taylor expansion 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

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

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 in Mach number. Inverting this perturbatively we find that, to second order in Mach number, the Lagrange multipliers are given by

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

where $x \equiv h'\left(\frac{\rho}{mb}\right)$, 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,

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

Now it is well known that a Chapman-Enskog analysis based on the equilibrium distribution

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

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

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

The factor g destroys the form of the convective derivative, and hence breaks galilean invariance. To recover galilean invariance we demand that $g = 1$, and this yields the second-order nonlinear differential equation

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

The general solution to this equation is of the form

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

where C and a are arbitrary constants, and P is to be determined. We quickly find that P 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

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

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.

In passing, we note that $\lim_{x\to 0} h'(x) = \infty$. Thus the nonnegativity constraint will be enforced by the dynamics.

Finally, we write the global Lyapunov function $\mathcal{H} \equiv \sum_{\mathbf{x}} H$ 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

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

for appropriate choices of a and C. This has the form of a Burg entropy [11] for $D = 2$, and a Tsallis entropy [12] with parameter

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

for $D \neq 2$. We note that $D \leq 2$ corresponds to $q \leq 0$, and $D > 2$ corresponds to $q > 0$. 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 [13].

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 [12] lurking here. There are precious few situations in which the origins of Tsallis thermostatistics can be traced analytically to an underlying microscopic model, as we have done here.

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 and interesting. 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 this surely warrants future study.

Acknowlegements

BMB was supported in part by the U.S. Air Force Office of Scientific Research under grant number F49620-01-1-0385, and in part by MesoSoft Corporation. He performed a portion of this work while at the Centre for Computational Science, Department of Chemistry, Queen Mary, University of London as an EPSRC Visiting Fellow under RealityGrid contract GR/R67699. Peter Love was supported by the DARPA QuIST program under AFOSR grant number 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. Reports **222** (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) A. **457**, 717 (2001).

[7] C. Marsh and P. V. Coveney, J. Phys. A Math. Gen. **31**, 6561 (1998).

[8] S. Ansumali, I.V. Karlin, Phys. Rev. E **62**, 7999 (2000).

[9] S. Ansumali, I.V. Karlin, Phys. Rev. E **65**, 056312 (2002).

[10] S. Succi, I.V. Karlin, H. Chen, Rev. Mod. Phys. (2002), to appear.

[11] A.N. Gorban, I.V. Karlin, Phys. Rev. E, accepted for publication (2002), Preprint, `cond-mat/0205511`.

[12] C. Tsallis, *Nonextensive Statistical Mechanics and Its Application* (Springer Verlag, 2001), edited by S. Abe and Y. Okamoto.

[13] 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 $M \to 0$ even as $D \to \infty$.