

## Entropy and Galilean Invariance of Lattice Boltzmann Theories

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A theory of lattice Boltzmann (LB) models for hydrodynamic simulation is developed upon a novel relation between entropy construction and roots of Hermite polynomials. A systematic procedure is described for constructing numerically stable and complete Galilean invariant LB models. The stability of the new LB models is illustrated with a shock tube simulation.

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The lattice Boltzmann (LB) method is a powerful new approach to hydrodynamics, with applications ranging from large Reynolds number flows to flows at a micron scale, porous media, and multiphase flows [1]. The LB method solves a fully discrete kinetic equation for populations  $f_i(\mathbf{x}, t)$ , designed in a way that it reproduces the Navier-Stokes equations in the hydrodynamic limit. Populations correspond to discrete velocities  $\mathbf{c}_i$ ,  $i = 1, \dots, N$ , which fit into a regular spatial lattice with the nodes  $\mathbf{x}$ . This enables a simple and highly efficient “stream-along-links-and-equilibrate-at-nodes” realization of the LB algorithm.

In spite of a large number of works to date, only the simplest, low-accuracy LB model for isothermal hydrodynamics has been fully understood [2–6]. This model was derived in various ways, including a discretization of the Boltzmann equation with the Gauss-Hermite quadrature in the velocity space [3,5], where the discrete velocities are zeroes of the cubic Hermite polynomial  $\mathcal{H}_3$ . Recently, this approach was extended to a weakly compressible flow simulation [6]. Most importantly, numerical stability was linked to the entropy construction [4,7].

The route of higher-order Gauss-Hermite quadratures promised a systematic derivation of new computation-oriented kinetic models with larger velocity sets [3], especially of long-needed *complete* Galilean invariant models (according to [8,9]) and thermal models for compressible flow simulations. Unfortunately, since the roots of Hermite polynomials of order four and higher are irrational, the corresponding discrete velocities cannot be fit into a lattice. Thus, the LB space-time exact discretization procedure is not possible for the quadrature-based models, and additional effort for their implementation is required [5] (in the presence of off-lattice structures such as curved boundaries and grid refinement, other discretization strategies are required; see, e.g., [10] and references therein).

Therefore, the search for new models on a lattice has remained trial and error [9]. This is a daunting task of searching all possible discrete velocity sets for the one that delivers a stable and complete Galilean invariant LB scheme. However, one aspect that defies intuition is that all the schemes obtained so far on larger lattices are numerically unstable [11].

In this Letter, we solve this long-standing problem of a derivation of numerically stable and highly accurate LB models. Let us outline a systematic study. The solution is based on a novel key relation between the entropy construction and the roots of Hermite polynomials, which we find by considering the one-dimensional isothermal case. Admissible LB velocities are found as rational-number approximations to the (irrational) ratios of the Hermite roots. The result is immediately generalized to arbitrary dimension. We show that the entropic construction leads to numerically stable complete Galilean invariant LB models. Finally, we indicated how to extend these results to thermal LB models.

We begin our systematic construction with the one-dimensional isothermal case ( $D = 1$ ). The equilibrium populations,  $f_i^{\text{eq}}$ , minimize the entropy function  $H$ ,

$$H = \sum_{i=1}^N f_i \ln\left(\frac{f_i}{W_i}\right), \quad (1)$$

with appropriately chosen weights  $W_i > 0$ , under the constraints of mass and momentum conservation,  $\sum_{i=1}^N \{1, c_i\} f_i^{\text{eq}} = \{\rho, \rho u\}$ . Since it is well known how to construct the entropy (1) for the low-accuracy LB model with three velocities  $\{0, \pm 1\}$  [4], we here proceed with a generic four-velocity set,  $\{\pm m, \pm n\}$  ( $N = 4$ ). For the time being, we do not require  $m$  and  $n$  to be an integer. The goal is now to derive the weights  $W_{\pm m}$ ,  $W_{\pm n}$ , and the reference temperature  $T_0(m, n)$ , at which the equilibrium satisfies the constitutive relations for the pressure  $P^{\text{eq}}$  and the energy flux  $Q^{\text{eq}}$ , known from the Maxwell-Boltzmann (MB) distribution function at a fixed temperature  $T_0$ :

$$P^{\text{eq}} = \sum_{i=1}^N f_i^{\text{eq}} c_i^2 = \rho T_0 + \rho u^2, \quad (2)$$

$$Q^{\text{eq}} = \sum_{i=1}^N f_i^{\text{eq}} c_i^3 = 3\rho T_0 u + \rho u^3.$$

The term  $\rho u^3$  in the energy flux is required in order to achieve the complete Galilean invariant LB model. Alternatively but entirely equivalently, the same MB relations can be found upon the Chapman-Enskog analysis of the hydrodynamic limit of the LB equations (see, e.g., [8,9]). The low-accuracy standard LB models [2] miss

this term and introduce an error into the isothermal Navier-Stokes equations [8,9]. Although this error is not significant if  $u < 0.1$ , this value is at the limit of capacities of the standard LB models and precludes to use higher values of velocity in the isothermal LB simulations (see, e.g., [12]).

Using a series expansion in powers of  $u$  to obtain  $f_i^{\text{eq}}$  from the minimization problem, we find that the zeroth-, the first-, and the second-order terms (2) are recovered with the following weights and the reference temperature:

$$W_{\pm m} = \frac{m^2 - 5n^2 + \sqrt{m^4 - 10n^2m^2 + n^4}}{12(m^2 - n^2)}, \quad (3)$$

$$W_{\pm n} = \frac{5m^2 - n^2 - \sqrt{m^4 - 10n^2m^2 + n^4}}{12(m^2 - n^2)}, \quad (4)$$

$$T_0 = \frac{m^2 + n^2 + \sqrt{m^4 - 10n^2m^2 + n^4}}{6}. \quad (5)$$

At this point we are left with just one ‘‘degree of freedom’’—the ratio between the velocities,  $r(m, n) = m/n$ . Without any loss of generality, we assume  $m < n$ . The ratio  $r < 1$  is fixed by the requirement to reproduce the remaining cubic term ( $\rho u^3$ ) in  $Q^{\text{eq}}$  (2). This happens if and only if  $r = r_4^*$ , where

$$r_4^* = \sqrt{3} - \sqrt{2} \approx 0.31784. \quad (6)$$

If  $m$  and  $n$  satisfy (6), we obtain the corresponding weights (3) and (4):  $W_{\pm m}^* = \frac{1}{4(3-\sqrt{6})}$ ,  $W_{\pm n}^* = \frac{1}{4(3+\sqrt{6})}$ . Entropy function (1) with these weights sets up the desired kinetic theory: The corresponding equilibrium recovers the Maxwell-Boltzmann relations for the pressure and energy flux (2) and can be used, for example, to write up the simplest Bhatnagar-Gross-Krook (BGK) kinetic equation, resulting in the complete Galilean invariant Navier-Stokes equations in the hydrodynamic limit.

The following observation is striking: precisely the same ratio (6) is satisfied by the roots of the fourth-order Hermite polynomial  $\mathcal{H}_4$ . The four roots of  $\mathcal{H}_4$  are  $\{\pm a, \pm b\}$ , where  $a = \sqrt{3} - \sqrt{6}$  and  $b = \sqrt{3} + \sqrt{6}$ . It is straightforward to check that, indeed,  $a/b = r_4^*$ . In the Gauss-Hermite quadrature model based on zeroes of  $\mathcal{H}_4$ , the equilibrium does satisfy the constitutive relations (2) [5]. Here, quite remarkably, we recovered the same result avoiding the quadrature. Note that only the ratio of the velocities is relevant, and not their absolute values. As we already mentioned, this is not a LB model [integer-valued velocities  $m$  and  $n$  cannot satisfy (6)].

Entirely the same situation happens in the next, five-velocity case,  $\{0, \pm m, \pm n\}$  ( $N = 5$ ). Since we have more degrees of freedom, we require the Maxwell-Boltzmann form of the fourth-order moment,

$$R^{\text{eq}} = \sum_{i=1}^N f_i^{\text{eq}} c_i^4 = 3\rho T_0^2 + 6\rho T_0 u^2 + \rho u^4. \quad (7)$$

Now we can require that the pressure and energy flux conditions (2) are satisfied entirely, which leads to the

following expressions for the weights and the reference temperature:

$$W_0 = \frac{-3m^4 - 3n^4 + 54m^2n^2 - (m^2 + n^2)D_5}{75m^2n^2}, \quad (8)$$

$$W_{\pm m} = \frac{9m^4 - 6n^4 - 27n^2m^2 + (3m^2 - 2n^2)D_5}{300m^2(m^2 - n^2)}, \quad (9)$$

$$W_{\pm n} = \frac{9n^4 - 6m^4 - 27n^2m^2 + (3n^2 - 2m^2)D_5}{300n^2(n^2 - m^2)}, \quad (10)$$

$$T_0 = \frac{3m^2 + 3n^2 + D_5}{30}, \quad (11)$$

$$D_5 = \sqrt{9m^4 - 42n^2m^2 + 9n^4}. \quad (12)$$

Terms of zeroth and second order in (7) are also reproduced with these weights and reference temperature, and, same as above, we fix the ratio  $r = m/n$  to recover the highest-order term  $\rho u^4$  in (7). This happens at  $r = r_5^*$ ,

$$r_5^* = \frac{\sqrt{5} - \sqrt{2}}{\sqrt{3}} \approx 0.47449. \quad (13)$$

The roots of the fifth-order Hermite polynomial  $\mathcal{H}_5$  are  $\{0, \pm c, \pm d\}$ , where  $c = \sqrt{5 - \sqrt{10}}$  and  $d = \sqrt{5 + \sqrt{10}}$ , and again their ratio obeys (13):  $c/d = r_5^*$ .

To this end, we recovered all the results found earlier with the Gauss-Hermite quadrature [5] but within a completely different, direct approach of constructing the entropy function. Either way we do not achieve integer-valued velocities ( $r_4^*$  and  $r_5^*$  are irrational)—just the quadrature does not lead to new LB models.

However, with the present new approach, we actually derived the weights and the reference temperature for *generic* sets of discrete velocities, and we can proceed with constructing the LB models in a systematic fashion, as *rational-number approximations*. Namely, we shall choose *integer*  $m$  and  $n$  in such a way that their ratio approximates the limit values (6) or (13). Importantly, any such approximation must be from below,  $r(m, n) < r_4^*$  or  $r(m, n) < r_5^*$ , respectively. Otherwise, the reference temperature (5) and (11), respectively, lacks physical interpretation (is complex valued).

In order to address the accuracy of the rational-number approximations, it is convenient to introduce the following form for the higher-order moments:

$$\begin{aligned} P^{\text{eq}} &= \rho T_0 + \rho u^2 + P_4(r)\rho u^4, \\ Q^{\text{eq}} &= 3\rho T_0 u + Q_3(r)\rho u^3, \\ R^{\text{eq}} &= 3\rho T_0^2 + R_2(r)\rho T_0 u^2 + R_4(r)\rho u^4. \end{aligned} \quad (14)$$

Here, coefficients  $P_4$ ,  $Q_3$ ,  $R_2$ , and  $R_4$  depend on approximation of  $r_{4,5}^*$  with the ratios of integers  $r = m/n$ . In Table I, we present results for several lattices.

Strikingly and nontrivially, some ‘‘obvious’’ lattices are immediately ruled out. In particular, the first admissible

four-velocity set is  $\{\pm 1, \pm 4\}$ ; that is, for example, the set  $\{\pm 1, \pm 2\}$  is prohibited. Indeed, in that case, the ratio of the velocities is  $0.5 > r_4^*$ , and the reference temperature  $T_0(1, 2)$  (5) is nonphysical. For the same reason, a popular five-velocity lattice  $\{0, \pm 1, \pm 2\}$  is also ruled out ( $0.5 > r_5^*$ ). This explains why attempts to construct a LB model on this lattice failed to produce a numerically stable scheme.

Two important conclusions can be drawn from Table I. First, the quality of the reconstruction of the moments *monotonically* depends on the closeness of the ratio  $r(m, n)$  to the corresponding limit (Hermite) value. Second, switching to the next number of discrete velocities (from  $N$  to  $N + 1$ ) does not spoil the quality already reached at the  $N$  level. Indeed, the Maxwell-Boltzmann values  $Q_3 = 1$ ,  $R_2 = 6$ , and  $P_4 = 0$ , which are recovered by the four-velocity LB approximations in the limit  $m/n \rightarrow r_4^*$ , all remain correct for all the five-velocity LB approximations, and only the remaining coefficient  $R_4$  is monotonically improved. In other words, all the five-velocity lattices given in Table I are completely Galilean invariant isothermal LB models. Functions  $Q_3(r)$  and  $R_4(r)$  for  $N = 4$  and  $N = 5$  are shown in Fig. 1 which reveals monotonicity.

Thus, with the integer-valued velocities of Table I, and the corresponding expressions for the weights, we set up the lattice equilibria  $f_i^{\text{eq}}$  as minima of the entropy (1) and hence the lattice BGK models  $[f_i^{\text{eq}}$  are easily derived by perturbation in powers of  $u$ ; see Eq. (15)]. All these models are based on the entropy function (1), which is a prerequisite for numerical stability. This concludes the classification of the LB models in one dimension.

For a computational proof of concept, we present a simulation of a one-dimensional shock problem with two complete Galilean invariant LB models, the present entropic model (ELBM) on the lattice  $\{0, \pm 1, \pm 3\}$  and the lattice BGK (LBGK) model [9] on the lattice  $\{0, \pm 1, \pm 2\}$ , which was ruled out by entropy argument. The initial condition for the simulation was a density step,  $\rho = 3.0$  for  $x < L/2$  ( $L$  being the length of domain) and  $\rho = 1.0$  for  $x > L/2$  (same as in [9]). Both the models were ran at

TABLE I. Reconstruction of the higher-order moments by various LB models derived as rational-number approximations.

$N$	Model	$c_i$	$P_4$	$Q_3$	$R_2$	$R_4$	$r = \frac{m}{n}$
3	LB	$0, \pm 1$	$-\frac{4}{3}$	0	3	$-\frac{4}{3}$	
3	$\mathcal{H}_3$	$0, \pm\sqrt{3}$	$-\frac{4}{3}$	0	3	$-\frac{4}{3}$	
4	LB	$\pm 1, \pm 4$	-0.041	0.266	3.799	-0.697	0.250 00
4	LB	$\pm 2, \pm 7$	-0.012	0.425	4.275	-0.614	0.285 71
4	LB	$\pm 3, \pm 10$	-0.005	0.536	4.610	-0.534	0.300 00
4	$\mathcal{H}_4$	$\pm\sqrt{3} \pm \sqrt{6}$	0	1	6	0	0.317 84
5	LB	$0, \pm 1, \pm 3$	0	1	6	0.031	0.333 33
5	LB	$0, \pm 2, \pm 5$	0	1	6	0.218	0.400 00
5	LB	$0, \pm 3, \pm 7$	0	1	6	0.345	0.428 57
5	$\mathcal{H}_5$	$0, \pm\sqrt{5} \pm \sqrt{10}$	0	1	6	1	0.474 49
$\infty$	MB	Continuous	0	1	6	1	

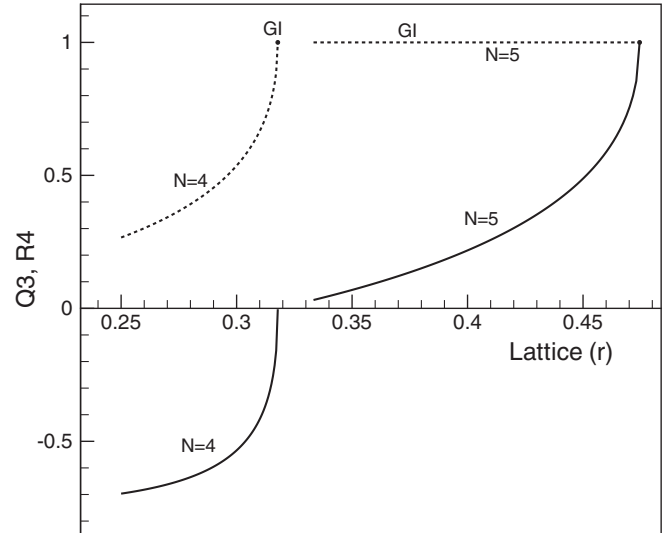


FIG. 1. Monotonicity of moments reconstruction. Functions  $Q_3(r)$  (dashed lines) and  $R_4(r)$  (continuous lines) are shown for  $N = 4$  and  $N = 5$  lattices in a range between the first LB model ( $r = \frac{1}{4}$  for  $N = 4$  and  $r = \frac{1}{3}$  for  $N = 5$ ) and the limit Hermite model ( $r = r_4^*$  and  $r = r_5^*$ , respectively), where real-valued functions  $Q_3$  and  $R_4$  ( $N = 4$ ) and  $R_4$  ( $N = 5$ ) terminate at a branching point. Completely Galilean invariant isothermal models (GI) correspond to  $Q_3 = 1$ .

various values of the viscosity  $\nu$ . The present ELBM is stable at any value of the viscosity. This is drastically different from the LBGK [9], which becomes numerical unstable even for moderate  $\nu$ . A typical situation is shown in Fig. 2, corresponding to  $\nu = 0.138$ . The snapshot of the density profile is taken a few time steps before the run for the LBGK terminates; a pattern of instability is clearly visible while the density at some lattice nodes becomes negative. The oscillatory pattern of the ELBM at the shock is due to the lack of artificial diffusivity and is pertinent to all lattice Boltzmann schemes. A slight mismatch of the profiles in Fig. 2 is due to the fact that the models operate at different speed of sound  $c_s$  ( $c_s^2 = 1$  for the LBGK and  $c_s^2 = T_0$  for the ELBM). Thus, the complete Galilean invariant LB model found from the entropy considerations is stable and clearly outperforms the nonentropic model.

Once the classification of one-dimensional lattices is achieved, extension to higher dimensions is straightforward and follows the pattern of Gauss-Hermite quadrature (cf. Ref. [5]). That is, the discrete velocities  $\mathbf{c}_i$  in the  $D$ -dimensional case are tensor products of  $D$  copies of the one-dimensional velocities, whereas the corresponding weights  $W_i$  are algebraic products of the corresponding weights in one dimension. Moreover, the reference temperature does not depend on the dimension. Explicit expressions for the equilibrium can be derived, e.g., upon a perturbation around the zero-velocity equilibrium  $f_i^{\text{eq}} = \rho W_i$ . In particular, the simplest polynomial approximation to third order in velocity  $\mathbf{u}$  for all the lattices generated by four- and five-velocity sets has the universal form

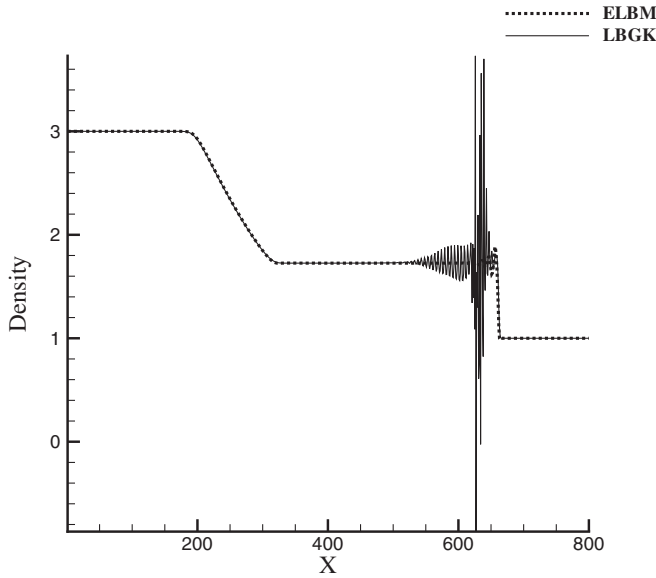


FIG. 2. Simulation of the one-dimensional shock tube problem by the entropic (dashed line) and the nonentropic (continuous line) LB schemes.

$$f_i^{\text{eq}} = \rho W_i \left\{ 1 + \frac{c_{i\alpha} u_\alpha}{T_0} + \frac{u_\alpha u_\beta}{2T_0^2} (c_{i\alpha} c_{i\beta} - T_0 \delta_{\alpha\beta}) + \frac{u_\alpha u_\beta u_\gamma}{6T_0^3} c_{i\gamma} (c_{i\alpha} c_{i\beta} - 3T_0 \delta_{\alpha\beta}) \right\} + O(u^4). \quad (15)$$

We have verified with a direct computation that all  $D$ -dimensional equilibria (15),  $D = 1, 2, 3$ , generated by the one-dimensional five-velocity sets are completely Galilean invariant; that is, they recover the Maxwell-Boltzmann relation for the third-order moments,

$$Q_{\alpha\beta\gamma}^{\text{eq}} = \rho T_0 (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}) + \rho u_\alpha u_\beta u_\gamma, \quad (16)$$

where  $Q_{\alpha\beta\gamma}^{\text{eq}} = \sum_{i=1}^N f_i^{\text{eq}} c_{i\alpha} c_{i\beta} c_{i\gamma}$ , and hence recover isothermal Navier-Stokes equations. It is quite important that the proper classification of the one-dimensional lattices automatically delivers lattices in any dimension. Note that a recently introduced product-form method for evaluation of equilibria [13] is much more efficient and should be used instead of polynomial approximations for large velocity sets. However, these implementation issues are out of the scope of the present Letter.

Finally, the lattices and the entropy functions  $H$  derived above for the isothermal case should be used for an extension to the thermal LB models. This amounts to finding equilibria by minimization of the same  $H$  functions subject to  $\sum_{i=1}^N \{1, \mathbf{c}, c_i^2\} f_i^{\text{eq}} = \{\rho, \rho \mathbf{u}, D\rho T + \rho u^2\}$ , where energy conservation is added to the constraints of the isothermal problem. The thermal LB models obtained this way operate in a temperature window around the reference temperature. Notice that the standard isothermal LB model itself can be extended to weakly compressible flows (small

temperature variations) [6]; therefore it is expected that the thermal extensions of the present isothermal models operate in a wider temperature window. These thermal models will be studied elsewhere.

In conclusion, construction of lattice Boltzmann models is put on a firm theoretical ground. Derivation of the entropy functions is the unifying principle for lattice Boltzmann models. Stability of the previously known low-accuracy LB models has been already explained by its relation to the entropy construction [4] (and considerably enhanced in the framework of the entropic lattice Boltzmann method [5,13]). In this Letter, for the first time, this principle is demonstrated to be universally applicable and extended to long-needed complete Galilean invariant LB models where other attempts failed. Now we know that even the choice of the lattice was done in a wrong way.

Finally, a belief about the relevance of the Gauss-Hermite quadrature to the LB construction [14] is shown to be largely an overstatement. All results derived by the Gauss-Hermite quadrature are contained in the present direct approach. Moreover, the quadrature as such does not deliver new LB models. Instead, the rational-number approximations derived herein give us LB models with any desired accuracy.

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