Entropy balance and dispersive oscillations in lattice Boltzmann models

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We conduct an investigation into the dispersive post-shock oscillations in an entropic lattice-Boltzmann method (ELBM), in particular the entropic lattice-Bhatnagar-Gross-Krook (ELBGK) scheme. Simulations on the one-dimensional shock tube show no benefit in terms of regularization from using ELBGK over the standard LBGK. We also conduct an experiment investigating equipping the LBGK method with median filtering (a local method) at a single point per tim e step. Here we observe that significant regularization of a systemic problem can be achieved with a local method of correction.

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I. INTRODUCTION

Controlling the proper entropy balance remained, up until recently, a challenging problem for many lattice Boltzmann models [1]. The entropic lattice Boltzmann method (ELBM) was invented as a tool for the construction of single relaxation time lattice Boltzman models respecting the *H*-theorem [2,3]. Instead of the mirror image with a local equilibrium as the reflection center, the entropic involution was proposed, which preserves the entropy balance. Later, it was called the *Karlin-Succi involution* [4]. It was later reported that an exact implementation of the Karlin-Succi involution significantly regularizes post-shock dispersive oscillations [5]. This regularization seems surprising, because the entropic lattice BGK (ELBGK) model gives a second-order approximation to the Navier-Stokes equation, similarly to the LBGK model (different proofs of that degree of approximation were given in [6,7]). Due to the Godunov theorem [8] linear second-order finite difference methods must be non monotonic. Moreover, Lax [9], and Levermore with Liu [10], demonstrated that these *dispersive oscillations* are unavoidable in classical numerical methods. Schemes with precise control of entropy production [11], also demonstrated post-shock oscillations. Of course, there remains some gap between methods with a proven existence of dispersive oscillations, and ELBM. However, recently, the existence of oscillations in the vicinity of the shock, at small viscosity values for ELBM, was reported for Burgers' equation [12]. In a recent paper [13], post-shock oscillations of ELBGK were reported, and no difference was found between ELBGK and LBGK in that regard.

In this Brief Report, we answer the particular question: does the precise control of entropy production by ELBGK in one dimension (1D) always smooth post-shock oscillations? The answer is negative. A smoothing effect can be caused by imprecision in calculations of the entropic involution, i.e., in solution of the following transcendental equation with respect to α ($\alpha \neq 0$):

$$S[\mathbf{f} + \alpha(\mathbf{f}^* - \mathbf{f})] = S(\mathbf{f}), \tag{1.1}$$

where S is entropy, f is a current distribution, and f^* is the corresponding equilibrium. This experiment can be considered a counter example to the claim that all ELBMs regularize shocks in all cases.

We additionally test an example of a regularizer from a class of local methods know as entropic filters [13]. The relative success of this method demonstrates that a very local correction can be enough to dampen the oscillations significantly across the system by applying an additional technique at their point of origin.

II. LATTICE BOLTZMANN METHODS

The Lattice Boltzmann method arises as a discretization of Boltzmann's kinetic transport equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = Q^c(f). \tag{2.1}$$

The *population function* f describes the distribution of single particles in the system and the *collision integral* Q^c their interaction. Altogether Eq. (2.1) describes the microscopic behavior of the system. By selecting a finite number of velocities $\mathbf{v}_i, (i=1,\ldots,n)$ we create a discrete approximation of the kinetic equation in velocity space. An appropriate choice of the velocities and time step discretizes space. For a time step of $\delta t=1$ the lattice can be created by unscaled space shifts of the velocities, and we get the fully discrete lattice Botzmann gas:

$$f_i(x + v_i, t+1) = f_i(x,t) + Q_i, \tag{2.2}$$

where the proper transition from continuous collision integral $Q^c(f)$ to its fully discrete form $\{Q_i\}$ is assumed. The simplest and most common choice for the discrete collision integral Q_i is the Bhatnagar-Gross-Krook operator with over-relaxation

$$Q_i = \alpha\beta(f_i^* - f_i). \tag{2.3}$$

For the standard LBGK method $\alpha=2$ and $\beta \in [0,1]$ (usually, $\beta \in [1/2,1]$) is the over-relaxation coefficient used to control viscosity. For $\beta=1/2$ the collision operator returns the *local equilibrium* f_i^* and $\beta=1$ (the *mirror reflection*) returns the collision for a liquid at the zero viscosity limit. For a viscosity ν on a lattice with sound speed c_s the parameter β is chosen by $\beta = c_s^2\delta t/(2\nu + c_s^2\delta t)$. It should be noted that a

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collision integral such as Eq. (2.3) demands prior knowledge of a local equilibrium state for the given lattice.

A variation on the LBGK is the ELBGK [5]. In this case, α is varied to ensure a constant entropy condition according to the discrete H-theorem. The entropy function is based upon the lattice and cannot always be found explicitly. However in the case of the simple one-dimensional lattice with velocities $\mathbf{v}=(-c,0,c)$ and corresponding populations $\mathbf{f}=(f_-,f_0,f_+)$ an explicit Boltzmann style entropy function is known [14]:

$$S(\mathbf{f}) = -f_- \log(f_-) - f_0 \log(f_0/4) - f_+ \log(f_+). \quad (2.4)$$

In ELBGK then, α is found as the nontrivial root of the Eq. (1.1) The trivial root $\alpha=0$ returns the entropy value of the original populations. This version of the BGK collision one calls the entropic BGK (EBGK) collision. A solution of Eq. (1.1) must be found at every time step and lattice site. Entropic equilibria (also derived from the H-theorem) are always used for ELBGK.

III. H-THEOREM FOR LBMS

In the continuous case, the Maxwellian distribution maximizes entropy, as measured by the Boltzmann H function, and therefore also has zero entropy production. In the context of lattice Boltzmann methods, a discrete form of the H-theorem has been suggested as a way to introduce thermodynamic control to the system [2] and to guarantee numerical stability [3].

From this perspective the goal is to find an equilibrium state analogous to the Maxwellian in the continuum, which will similarly maximize entropy. Before the equilibrium can be found an appropriate H function must be known for a given lattice. These functions have been constructed in [14], and $H=-S$ with S from Eq. (2.4) is an example of a H function constructed in this way.

Using equilibria derived from a H function with entropy considerations in mind leads to a thermodynamically correct LBM. This is easy to see in the case of the EBGK collision operator Eq. (2.3) with explicit local equilibrium. The EBGK collision obviously respects the second law (if $\beta \leq 1$), and simple analysis of entropy dissipation gives the proper evaluation of viscosity.

ELBGK finds the value of α that with $\beta=1$ (inviscid fluid) would give zero entropy production, therefore making the position of zero entropy production the limit of any relaxation. For the fixed α used in the LBGK method it remains possible, particularly for low viscosity fluids, to relax past this point resulting in negative entropy production, violating the second law.

Near to the zero-viscosity limit the LBGK method produces spurious oscillations around shockwaves. Apart from the thermodynamic and stability benefits of using ELBGK it has been claimed [5] that ELBGK's thermodynamic considerations necessarily act as a regularizer. This claim seems to be at odds with other numerical methods, which respect the same thermodynamic laws as ELBGK. For example the results of Tadmoor and Zhong [11] for an entropy correct method display intensive post-shock oscillations. Furthermore it has been suggested [9,10] that such dispersive oscillations are artifacts of the lattice rather than thermodynamic issues.

IV. COMPUTATION OF ENTROPIC INVOLUTION

In order to investigate the stabilization properties of ELBGK we craft a numerical method capable of finding the nontrivial root in Eq. (1.1). We opt for a numerical method in order to precisely control accuracy, an inaccurate lower estimate for α would effectively add numerical entropy across the lattice. Analytic estimates for α exist [15], where the deviation from BGK $|2-\alpha|$ scales with δt, indicating the potential to inject numerical entropy increases with the time step. We fix the population vectors $\mathbf{f}$ and $\mathbf{f}^*$, and are concerned only with this root finding algorithm. We recast Eq. (1.1) as a function of α only:

$$F(\alpha) = S[\mathbf{f} + \alpha(\mathbf{f}^* - \mathbf{f})] - S(\mathbf{f}). \quad (4.1)$$

In this setting we attempt to find the nontrivial root r of Eq. (4.1) such that $F(r)=0$. As we search for r numerically we should always take care that the approximation we use is less than r itself. An upper approximation could result in negative entropy production. A simple algorithm for finding the roots of a concave function, based on local quadratic approximations to the target function, has cubic convergence order. Assume that we are operating in a neighborhood $r \in N$, in which F' is negative (as well of course F'' is negative). At each iteration, the new estimate for r is the greater root of the parabola P, the second-order Taylor polynomial at the current estimate. Analogously to the case for Newton iteration, the constant in the estimate is the ratio of third and first derivatives in the interval of iteration:

$$|(r - \alpha_{n+1})| \leq C|\alpha_n - r|^3,$$

$$\text{where} \quad C = \frac{1}{6}\sup_{a \in N}|F'''(a)|/\inf_{b \in N}|F'(b)|,$$

where α_n is the evaluation of r on the nth iteration. We use a Newton step to estimate the accuracy of the method at each iteration; because of the concavity of $S, |\alpha_n - r| \leq |F(\alpha_n)/F'(\alpha_n)|$.

In fact we use a convergence criteria based not solely on α but on $\alpha\|\mathbf{f}^* - \mathbf{f}\|$, this has the intuitive appeal that in the case where the populations are close to the local equilibrium $\Delta S = S(\mathbf{f}^*) - S(\mathbf{f})$ will be small and a very precise estimate of α is unnecessary. We have some freedom in the choice of the norm used and we select between the standard L_1 norm and the entropic norm. The entropic norm is defined as $\|\Delta\mathbf{f}\|_{f^*} = -(\Delta\mathbf{f}, D^2S|_{f^*}\Delta\mathbf{f})$, where $D^2S|_{f^*}$ is the second differential of entropy at point $\mathbf{f}^*$, $\Delta\mathbf{f}=\mathbf{f}^*-\mathbf{f}$ and (x,y) is the standard scalar product.

The final root finding algorithm then is beginning with the LBGK estimate $r_0=2$ to iterate using the roots of successive parabolas. If this first initiation step were to produce a nonpositive population, or the root did not exist, then the *positivity rule* [7] could be used (instead of the mirror image we choose the closest value of α which gives nonnegative value

of populations). In the tests described below, these situations never arose. We stop the method at the point $|\alpha_n - r| \cdot \|\mathbf{f}^* - \mathbf{f}\| < \epsilon$.

To ensure that we use an estimate that is less than the root, at the point where the method has converged we check the sign of $F(\alpha_n)$. If $F(\alpha_n) > 0$ then we have achieved a lower estimate, if $F(\alpha_n) < 0$ we correct the estimate to the other side of the root with a double length Newton step, $\alpha_n = \alpha_n - 2F(\alpha_n)/F'(\alpha_n)$.

At each time step before we begin root finding we eliminate all sites with $\Delta S < 10^{-15}$. Here we make a simple LBGK step. At such sites we find that round off error can result in the root of the parabola becoming imaginary. In such cases an LBGK mirror image is effectively indistinct from the exact ELBGK collision.

For the shock tube test using 800 lattice sites, see description in Sec. V, the parabola based method required no more than two iterations for the desired accuracy of $\epsilon = 10^{-7}$.

V. SHOCK TUBE TESTS

A standard experiment for the testing of LBMs is the 1D shock tube problem. The lattice velocities used are $\mathbf{v} = (-1, 0, 1)$, so that space shifts of the velocities give lattice sites separated by the unit distance. 800 lattice sites are used and are initialized with the density distribution $\rho(x) = 1$ for $1 \le x \le 400$ and $\rho(x) = 0.5$ for $401 \le x \le 800$. Initially all velocities are set to zero. We compare the ELBGK equipped with the parabola based root finding algorithm using the entropic norm with the standard LBGK method using both standard polynomial and entropic equilibria. The polynomial equilibria are given in [6,16]:

$$f_-^* = \frac{\rho}{6}(1 - 3u + 3u^2), \quad f_0^* = \frac{2\rho}{3}\left(1 - \frac{3u^2}{2}\right),$$

$$f_+^* = \frac{\rho}{6}(1 + 3u + 3u^2).$$

The entropic equilibria also used by the ELBGK are available explicitly as the maximum of the entropy function Eq. (2.4),

$$f_-^* = \frac{\rho}{6}(-3u - 1 + 2\sqrt{1 + 3u^2}), \quad f_0^* = \frac{2\rho}{3}(2 - \sqrt{1 + 3u^2}),$$

$$f_+^* = \frac{\rho}{6}(3u - 1 + 2\sqrt{1 + 3u^2}).$$

Now following Eq. (2.2) the governing equations for the simulation are

$$f_-(x, t+1) = f_-(x+1, t) + \alpha\beta(f_-^*(x+1, t) - f_-(x+1, t)),$$

$$f_0(x, t+1) = f_0(x, t) + \alpha\beta(f_0^*(x, t) - f_0(x, t)),$$

$$f_+(x, t+1) = f_+(x-1, t) + \alpha\beta(f_+^*(x-1, t) - f_+(x-1, t)).$$

From this experiment we observe no benefit in terms of regularization in using the ELBGK rather than the standard LBGK method (Fig. 1) in 1D. In both the medium and low-viscosity regimes ELBGK fails to suppress the spurious oscillations found in the standard LBGK method.

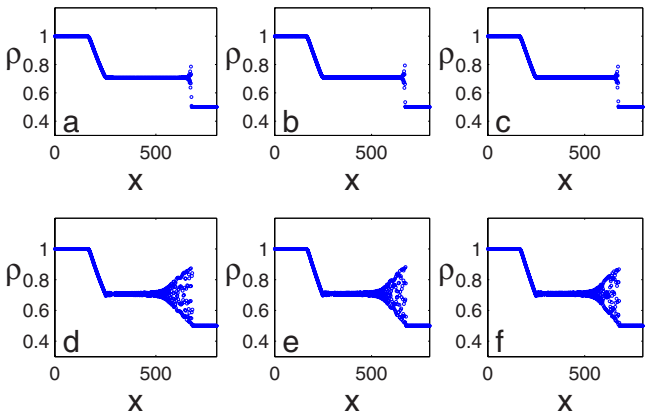

FIG. 1. (Color online) Density profile of the simulation of the shock tube problem following 400 time steps using (a) LBGK with polynomial equilibria $[\nu = (1/3) \cdot 10^{-1}]$; (b) LBGK with entropic equilibria $[\nu = (1/3) \cdot 10^{-1}]$; (c) ELBGK $[\nu = (1/3) \cdot 10^{-1}]$; (d) LBGK with polynomial equilibria $[\nu = 10^{-9}]$; (e) LBGK with entropic equilibria $[\nu = 10^{-9}]$; and (f) ELBGK $[\nu = 10^{-9}]$.

VI. ONE-POINT MEDIAN FILTERING

Finally, we consider regularizing the LBGK method using median filtering at a single point. This is an example of a purely local augmentation whereby an individual lattice site, targeted in some way, can have additional entropy/viscosity artificially added in the collision. We hypothesize that by applying an effectively higher viscosity regime at the point of origin of oscillations, that they can be suppressed before they spread and pollute more of the system. We follow the prescription detailed in [13]. First, at each time step, we locate the single lattice site x with the maximum value of $\Delta S(x)$, and call this value ΔS_x, this is effectively the site furthest from equilibrium in entropic terms. Second, we find the median value of ΔS in the three nearest neighbors of x including itself, calling this value ΔS_{med}. Now instead of being updated using the standard BGK over-relaxation this single site is updated as in (V) with the coeffiction $\alpha\beta$ replaced by $\delta = \sqrt{\Delta S_{med}/\Delta S_x}$ We observe that filtering a single point per time step results in a significant amount of regularization (Fig. 2) in this example.

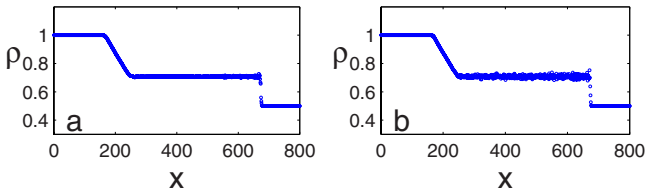

FIG. 2. (Color online) Density profile of the simulation of the shock tube problem following 400 time steps using (a) LBGK with entropic equilibria and one point median filtering $[\nu = (1/3) \cdot 10^{-1}]$; (b) LBGK with entropic equilibria and one point median filtering $[\nu = 10^{-9}]$.

VII. CONCLUSION

We present conclusions on the two methods for regularization examined in this study.

1. We do not find that maintaining the proper balance of entropy necessarily guarantees the regularization of spurious oscillations in the Lattice Boltzmann method. For ELBGK in a classic 1D example we agree the conclusions of Lax [9] and Levermore with Liu [10] that *dispersive oscillations* manifest in numerical simulation of shocks. This result is not necessarily contradictory with reported improvements from using an ELBM of a different form including those arising naturally as part of a quantum treatment [17,18] or in a higher dimension [19], where additional factors arise. It should however be understood by this example that regularization of dispersive oscillations by an ELBM is not guaranteed, previous reports of smoothing by ELBGK in this example could be caused by imprecision in the root finding algorithm leading to the inadvertent injection of additional entropy. It was recently reported that the correction by ELBGK to the standard BGK collision scales with the time step [15], therefore, the precision of the root finding algorithm becomes increasingly critical with larger time steps, where an inaccuracy in root finding would lead to larger amounts of numerical entropy being added, especially at points far from the local equilibrium.

2. Filtering entropy locally can be an effective method to clean up parasitic dispersive oscillations arising in an LBM. Reducing extremely localized incidents of high nonequilibrium entropy (see [13]) at a single point per time step is sufficient, in the given example, to eliminate the post-shock oscillation across the system even at a very low viscosity. We expect that this result will extend to other systems in higher dimensions. Filtering operations can also be performed nonlocally [20] to smooth the entire region. Entropy filtering for nonentropic equilibria is possible [13] with use of the Kullback-Leibler distance from current distribution to equilibrium (the relative entropy). The MATLAB code required to reproduce these results is available within the appendix of an online article [21].

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