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Equilibria for discrete kinetic equations

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We develop a systematic method of constructing equilibria for kinetic models with discrete microscopic velocities. The approach is based on a suitable entropy maximum principle. The H theorem is demonstrated in the continuous and discrete space-time realizations. In addition, we discuss an extension of the Lattice Boltzmann method to irregular grids. [S1063-651X(98)50410-2]

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Discrete velocity models (DVM's) are an important modern tool for simulation of complex macroscopic phenomena such as hydrodynamics. The common idea of the DVM methods is that macroscopic equations are not addressed directly but via a fictitious microscopic dynamics of particles with a small set of microscopic velocities. DVM are kinetic equations for populations of those particles, and the macroscopic equations arise in a limit of the microscopic dynamics. DVM are in many cases more suitable for study (in the first place, for numerical realizations) than the macroscopic equations. There exists an impressive body of realizations of this idea (lattice Boltzmann method, Broadwell models, discrete velocity approximations of conservation laws, etc.), as well as applications to various macroscopic systems [1].

One of the central issues of DVM methods is the construction of the local equilibrium populations. Indeed, since only a finite set of microscopic velocities is allowed, it is likely that certain important relations for moments of the distribution function might be broken if no care is taken. This can be understood as follows: The usual Maxwell distribution function $f_M(\boldsymbol{c},\rho,\boldsymbol{u},T)$ is a five-parametric set labeled with hydrodynamic fields. The form of f_M is such the momentum flux, $P_{\alpha\beta}=\int f_M \boldsymbol{c}_\alpha \boldsymbol{c}_\beta d^3c$ is just in the form required in the Euler equations, $P_{\alpha\beta}=p\delta_{\alpha\beta}+\rho u_\alpha u_\beta$. If only a finite set of microscopic velocities $\boldsymbol{c}$ is allowed, would this relation survive under a straightforward extension of f_M? The answer is no. To cope with this problem, one usually starts with an ansatz for the equilibrium in a form of a polynomial in terms of hydrodynamic fields, which contains enough free parameters to be tuned in such a way as to match an appropriate form of the ''broken'' moments. Though for certain sets of velocities the appropriate equilibria were successfully found along these lines [2], the approach has certain limitations. First, the answers are not always unique. Moreover, it is rather difficult to check several features of the resulting kinetics, in the first place, existence of an H theorem. Finally, this approach seems not directly suitable for an extension to the DVM methods to space-time dependent sets of microscopic velocities. A proof of the H theorem lacks also in other strategies of constructing equilibrium populations that avoid polynomial ansatz (see, for instance, Ref. [3]).

In this Rapid Communication, we aim at developing a systematic method of constructing equilibria for discrete ki-

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netic equations. Our approach is based on a suitable variational principle, and it is demonstrated that appropriate form of moments can be reconstructed in an unique way. Furthermore, this route makes it possible to prove the H theorem. Finally, we give an outline of how this method can be used to derive the Lattice Boltzmann method on irregular grids.

Notations. We consider a set of b microscopic velocities $\boldsymbol{c}_i$, with components $c_{i\alpha}$, where $\alpha=1,\ldots,d$. We assume isotropy: $\Sigma_i^b c_{i\alpha_1}^{n_1}\cdots c_{i\alpha_k}^{n_k}=0$, if $n_1+\cdots+n_k$ is odd, $\Sigma_i^b c_{i\alpha}c_{i\beta}=D^{-1}\xi^2\delta_{\alpha\beta}$, and nondegeneracy: $b\Sigma_{i=1}^b \boldsymbol{c}_i^2\boldsymbol{c}_i^2\neq[\Sigma_{i=1}^b c_i^2]^2$. Populations of fluid particles N_i are represented by vectors N in a b-dimensional real space. Notation $(x,y)=\Sigma_{i=1}^b x_i y_i$ will stand for the scalar product in this space. We also use a special orthogonal basis in the b-dimensional space, which is constructed as follows: (i) *Hydrodynamic basis* (H) is the result of orthogonalization of $D+2$ b-dimensional vectors $(1,\ldots,1)$, $(c_{1\alpha},\ldots,c_{b\alpha})$, and $(c_1^2,\ldots,c_b^2)$. Corresponding unit orthogonal vectors are h^0, h^α, and h^{D+1}. Hydrodynamic fields $\rho=\Sigma_{i=1}^b N_i$, $\rho u_\alpha=\Sigma_{i=1}^b c_{i\alpha}N_i$, and $\rho\pi=\Sigma_{i=1}^b c_i^2 N_i$ are linear combinations of components (N,h^0), (N,h^α), and (N,h^{D+1}). (ii) *Primary flux basis* (PF) contains unit vectors $f_1^{\alpha\beta}$ and f_1^α, which are constructed by orthogonalization procedure from the vectors $v_1^{\alpha\beta}=(c_{1\alpha}c_{1\beta},\ldots,c_{b\alpha}c_{b\beta})$ and $v_1^\alpha=(c_{1\alpha}c_1^2,\ldots,c_{b\alpha}c_b^2)$. Momentum flux, $P_{\alpha\beta}=(v_1^{\alpha\beta},N)$, and heat flux, $Q_\alpha=(v_1^\alpha,N)$, are linear combinations of projections of the vector N onto the H and PF basis. (iii) *Secondary flux basis* (SF) contains unit vectors $f_2^{\alpha\beta\gamma}$ and $f_2^{\alpha\beta}$ which are constructed from vectors $v_2^{\alpha\beta\gamma}=(c_{1\alpha}c_{1\beta}c_{1\gamma},\ldots,c_{b\alpha}c_{b\beta}c_{b\gamma})$ and $v_2^{\alpha\beta}=(c_{1\alpha}c_{1\beta}c_1^2,\ldots,c_{b\alpha}c_{b\beta}c_b^2)$. (iv) *Residual basis*, (R), r^k, is formed by the further orthogonalization of the b-dimensional vectors with polynomial components $c_{i\alpha},\ldots,c_{i\omega}$.

Populations N_i are functions of the space $\boldsymbol{r}$ and time t, and satisfy the kinetic equation

$$\partial_t N_i + c_{i\alpha}\partial_\alpha N_i = \Delta_i. \tag{1}$$

This is the continuous space-time version of the discrete velocity models. In applications, a particularly important realization of the collision integral Δ_i is the Bhatnagar-Gross-Kook (BGK) form

$$\Delta_i = -\omega[N_i - N_i^e(N)], \tag{2}$$

where ω^{-1} is a relaxation time and N_i^e is the equilibrium. The conservation laws give $d+2$ necessary constraints on the equilibrium, $(\{h^0,h^\alpha,h^{D+1}\},N-N^e)=0$.

Auxiliary equilibrium. First we construct an auxiliary equilibrium (AE) N_i^a. For this purpose, we consider a strictly convex function $H=(N,N)$, and minimize it subject to fixed hydrodynamic quantities. The result reads

$$N_i^a=\rho\left\{\frac{\kappa-\pi\xi^2}{b\kappa-\xi^4}+\frac{du_\alpha c_{i\alpha}}{\xi^2}+\frac{\pi b-\xi^2}{b\kappa-\xi^4}c_i^2\right\}, \tag{3}$$

where $\kappa=\Sigma_{i=1}^b \boldsymbol{c}_i^2\boldsymbol{c}_i^2$, and ξ was defined above as $\xi^2=\Sigma_{i=1}^b \boldsymbol{c}_i^2$. The function $S=-H$ will play the role of the entropy in the kinetic theory under consideration. If Navier-Stokes equations without heat transfer are addressed, then hydrodynamic variables are density and momentum, and the AE is found by minimization of H, subject to the constraints of fixed ρ and $\rho\boldsymbol{u}$ with the result

$$N^a=\rho b^{-1}(1+\xi^{-2}Dbu_\alpha c_{i\alpha}). \tag{4}$$

Auxiliary equilibria (3) and (4) are explicit and very simple. It is not particularly important that AE do not result in hydrodynamic equations because their purpose is solely to fix the values of conserved quantities. In the next step, a correction to AE (3) has to be constructed such that the improved equilibria should fix the higher moments in an appropriate form. These improved equilibria may be termed ''target'' equilibria N^t. The method of constructing N^t does not depend on whether the heat conduction is included or not, and we will consider here the case without heat transfer for the sake of clarity of presentation. In this case, the hydrodynamic basis consists of $D+1$ vectors h^0 and h^α, the primary flux basis consists of vectors $f_1^{\alpha\beta}$, and the secondary flux basis consists of vectors $f_2^{\alpha\beta\gamma}$.

Target equilibrium. We seek the target equilibrium in the heat nonconductive case in the following form:

$$N^t=N^a+a_1^{\alpha\beta}f_1^{\alpha\beta}+a_2^{\alpha\beta\gamma}f_2^{\alpha\beta\gamma}, \tag{5}$$

where N^a is given by Eq. (4), and where coefficients $a_1^{\alpha\beta}$ and $a_2^{\alpha\beta\gamma}$ are found from a condition that the projections $(N^t,f^{\alpha\beta})$ and (N^t,f^α) have the given form as functions of hydrodynamic fields. This form is well known, and in our case result in the following system of linear algebraic equations:

$$\begin{aligned} a_1^{\alpha\beta}(v_1^{\mu\nu},f_1^{\alpha\beta})&=M_{\mu\nu}-(N^a,v_1^{\mu\nu}),\\ a_2^{\alpha\beta\gamma}(v_2^{\mu\nu\lambda},f_2^{\alpha\beta\gamma})&=M_{\mu\nu\lambda}-(N^a,v_2^{\mu\nu\lambda}). \end{aligned} \tag{6}$$

Here $M_{\mu\nu}=p\delta_{\mu\nu}+\rho u_\mu u_\nu$, and $M_{\mu\nu\lambda}=p(\delta_{\mu\nu}u_\lambda+\delta_{\mu\lambda}u_\nu+\delta_{\nu\lambda}u_\mu)+u_\mu u_\nu u_\lambda$, and the pressure p is proportional to ρ. Equation (6) defines unambiguously the coefficients a_1 and a_2 in the target equilibrium (5). Equivalently, the target equilibrium (5) provides minimum to the function H, subject to constraints of fixed hydrodynamic quantities, and fixed values of the moments, $(v_1^{\mu\nu},N)=M_{\mu\nu}$, $(v_2^{\mu\nu\lambda},N)=M_{\mu\nu\lambda}$. It can be demonstrated that the hydrodynamic limit of the BGK equations (1) and (2) with the equilibrium (5) are Navier-Stokes equations (see examples below).

Examples. Consider the set of three one-dimensional velocities, $c_-=-c$, $c_0=0$, and $c_+=c$. The orthonormal basis consists of three vectors: Hydrodynamic basis, $h^0=(1/\sqrt{3})(1,1,1)$ and $h^1=(1/\sqrt{2})(-1,0,1)$; primary flux basis, $f^1=(1/\sqrt{6})(1,-2,1)$. The auxiliary equilibrium solves the variational problem $H=(N,N)\to\min$, subject to the constraints $(N,h^0)=(1/\sqrt{3})\rho$ and $(N,h^1)=(1/\sqrt{2}c)\rho u$. The result reads $N_i^a=(\rho/3)[1+(3uc_i)/(2c^2)]$. The target equilibrium N^t has the form $N^t=N^a+af^1$, where the parameter a is found from the analysis of the moment equations. The latter are

$$\begin{aligned} &\partial_t\rho+\partial_x(\rho u)=0,\\ &\partial_t(\rho u)+\partial_x P=0,\\ &\partial_t P+c^2\partial_x(\rho u)=-\omega(P-P^t). \end{aligned} \tag{7}$$

The Chapman-Enskog method, as applied to system (7), gives $P=P^{(0)}+\omega^{-1}P^{(1)}$, $P^{(0)}=P^t$, and $P^{(1)}=-[\partial_t^{(0)}P^{(0)}+c^2\partial_x(\rho u)]$, where

$$\partial_t^{(0)}P^{(0)}=-[\partial P^{(0)}/\partial\rho]\partial_x(\rho u)-[\partial P^{(0)}/\partial(\rho u)]\partial_x P^{(0)},$$

where $P=(v,N)$ and $v=(c_-^2,c_0^2,c_+^2)$. Requiring $P^t=c_s^2\rho+\rho u^2$, where $c_s^2=(1/3)c^2$ is sound speed squared, the first two lines in Eq. (7) give

$$\begin{aligned}&\partial_t\rho+\partial_x(\rho u)=0,\\&\rho(\partial_t u+u\partial_x u)+c_s^2\partial_x\rho-2\omega^{-1}c_s^2\partial_x[\rho(1-M^2)\partial_x u]=0,\end{aligned}\tag{8}$$

where $M^2=u^2/c_s^2$ is Mach number squared. When $M\to 0$, Eqs. (8) recover one-dimensional Navier-Stokes equations. Thus, the condition for the target equilibrium reads $(v,N^t)=(v,N^a)+a(v,f^1)=c_s^2\rho+\rho u^2$, and which coincides with the first line in the Eq. (6). This condition is a linear equation for parameter a which gives $a=(v,f^1)^{-1}[\rho c_s^2+\rho u^2-(v,N^a)]$. It can be demonstrated with a direct computation that the resulting target equilibrium coincides with the one found in [2] for this model by a different method.

The set of three velocities does not permit to impose all the constraints (6). If we add two further velocities, and consider five-velocity model $c_i=ic$, where $i=-2,-1,0,1,2$, the elements of our basis are as follows: Hydrodynamic basis, $h^0=(1/\sqrt{5})(1,1,1,1,1)$ and $h^1=(1/\sqrt{10})(-2,-1,0,1,2)$; primary flux basis, $f_1=(1/\sqrt{14})(2,-1,-2,-1,2)$; and secondary flux basis, $f_2=(1/\sqrt{10})(-1,2,0,-2,1)$. The auxiliary equilibrium is given by Eq. (4), while the target equilibrium is $N^t=N^a+a_1f_1+a_2f_2$, where

$$a_1(v_1,f_1)=p+\rho u^2-(v_1,N^a),$$

$$a_2(v_2,f_2)=3pu+\rho u^3-(v_2,N^a).$$

Here $v_1=c^2(4,1,0,1,4)$, and $v_2=c^3(-8,-1,0,1,8)$. The target equilibrium thus constructed results in true Navier-Stokes equations, and it does not coincide with the one proposed in [2] (this N^t is qubic in u while the equilibria of Ref. [2] are quadratic). If, however, we use only the primary flux basis for construction of N^t, then we can obtain the result of [2].

Lattice realization. If discrete velocities form links of a regular lattice, then one considers the fully discrete counterpart of the kinetic equation (1). For the BGK collision integral (2), this lattice BGK equation (LBGK) reads

$$N_i(\boldsymbol{r}+\boldsymbol{c}_i,t+1)=(1-\omega)N_i(\boldsymbol{r},t)+\omega N_i^e(\boldsymbol{r},t).\tag{9}$$

Here $\boldsymbol{r}$ is the discrete space variable (sites of the lattice) and t is the discrete time. Since the equilibrium is local in space, the above construction of the auxiliary and target equilibria applies for the fully discrete case without any changes. As is well known, the difference amounts to a renormalization $\omega^{-1}\to\omega^{-1}(2-\omega)$ in the transport coefficients, and thus ω is confined to the linear stability interval [0,2]. We will see below how this fact reflects the difference in the H theorem for continuous and fully discrete cases.

H theorem: Continuous space-time. Since the entropy $S=-(N,N)$ is defined for positive as well as negative vectors N, the available phase space is R^b. The local entropy production σ in a state N reads

$$\sigma=-\omega(\partial S/\partial N,N-N^t)=2\omega(N,N-N^t).\tag{10}$$

A generic population N may be decomposed as $N=\Sigma_k(N,e^k)e^k$, where e^k are elements of the basis $H\cup PF\cup SF\cup R$. Let us define a cylinder Z which consists of such N that $(N,f)=(N^t(N),f)$, where f are elements of the primary and the secondary flux basis. In other words, a population belongs to Z if its projection onto the flux basis is equal to that of the corresponding target equilibrium. If $N\in Z$, then $(N^t,N-N^t)=0$, and we come to the following local H theorem:

$$\sigma=2\omega(N-N^t,N-N^t)\geqslant 0.\tag{11}$$

The local H theorem (11) results straightforwardly in the global H theorem for the continuous space-time equations (1) and (2): Let $\overline{S}$ be the total entropy of a volume V. Under suitable conditions at the boundary ∂V (making zero the entropy flux), $d\overline{S}/dt=\overline{\sigma}$, where the total entropy production is the integral of σ (11) over the volume V. In the case of the LBGK equation (9) the H theorem is different.

H theorem: Discrete space-time. The total entropy of the lattice at time step $t+1$ is

$$\overline{S}(t+1)=-\sum_{\boldsymbol{r}}\sum_{i=1}^{b}N_i^2(\boldsymbol{r},t+1).$$

Summation in $\boldsymbol{r}$ goes over all lattice sites. Under suitable boundary conditions (periodic, for instance), we may write $N_i(\boldsymbol{r}+\boldsymbol{c}_i,t+1)$ in place of $N_i(\boldsymbol{r},t+1)$, and, using Eq. (9) we derive

$$\overline{S}(t+1)-\overline{S}(t)=\frac{2-\omega}{2}\,\overline{\sigma(t)},\tag{12}$$

where $\overline{\sigma}=\Sigma_{\boldsymbol{r}}\sigma(\boldsymbol{r},t)$ is the total entropy production at time step t. Thus, for the fully discrete case, the H theorem (12) states the following: if at time t the state belongs to the cylinder Z, and if ω belongs to the linear stability interval [0, 2], the variation of the total entropy per next time step is non-negative, and equals a fraction of the total entropy production.

Proofs of the H theorem in both cases cannot be extended beyond the cylinder Z. This happens because in constructing the target equilibrium we have used the elements of the flux basis, which are a part of the kinetic (nonhydrodynamic) space. Since we have imposed a constraint in this place (the constraint of matching to the desired form of fluxes), not all kinetic space becomes available. On the other hand, if the auxiliary equilibrium is used instead of the target one, then both of the proofs, (11) and (12) become valid in the whole R^b but then the proper form of fluxes is not available anymore.

LBGK method for irregular grids. Finally, we will discuss briefly an extension of our approach to arbitrary sets of velocities. This question is particularly important for an exten-

sion of the LBGK method to irregular grids. Consider a lattice that is structured in the sense that each site has a constant number of links b. The outgoing links at the site $\boldsymbol{r}$ form a local microscopic velocity set, $\boldsymbol{c}_i(\boldsymbol{r})$. The state of the lattice is updated in accord with the LBGK Eq. (9), where now the microscopic velocities are space dependent. Our goal is to construct the target equilibrium in such a way as to match the Navier-Stokes equations. The same method as above can be applied. In particular, for the case without heat transfer, the auxiliary equilibrium which minimizes the function H subject to fixed density and momentum is readily available. To simplify notations, we introduce the index-raising operation $x^\alpha = T^{-1}_{\alpha\beta} x_\beta$, where T^{-1} is the inverse of $T = \Sigma_{i=1}^b \boldsymbol{c}_i \boldsymbol{c}_i$. Then $x_\alpha y^\alpha = x_\alpha T^{-1}_{\alpha\beta} y_\beta$, and the solution to the minimization problem reads

$$N_i^a = \rho \frac{1 - c_{i\alpha}c^\alpha + [b c_{i\beta} - c_\beta + (c_{i\alpha}c_\beta - c_\alpha c_{i\beta})c^\alpha]u^\beta}{b - c_\alpha c^\alpha}. \tag{13}$$

Here $\boldsymbol{c} = \Sigma_i^b \boldsymbol{c}_i$ is the self-speed of the site. Equation (13) recovers the auxiliary equilibrium (4) in the regular limit. An account for constraints such as those in the Eq. (6) are the same as above. In addition to the local constraints (6), we have to impose *gradient* constraints on the target equilibrium, which are

$$\sum_{i=1}^{b} N_i^t \{\partial_\alpha c_{i\alpha}, \partial_\beta c_{i\alpha} c_{i\beta}, \partial_\gamma c_{i\alpha} c_{i\beta} c_{i\gamma}\} = 0. \tag{14}$$

Here $\partial_\alpha c_{i\alpha}$, etc. are variations of the microscopic velocity set in space. An account for constraints (14) is necessary to obtain the left-hand side of moment equations in the divergency form, and these constraints can be incorporated into the construction of the target equilibrium on the same footing as the moment constraints above. Results on this problem will be reported separately [4].

Discussion. The result of this Rapid Communication is a systematic method for constructing equilibria for discrete velocity models. Our approach can be summarized as follows: instead of using a polynomial ansatz, we take the simplest possible convex H function, and perform a systematic minimization subject to a certain number of linear constraints. These constraints are sufficient to obtain such a moment system that has the proper macroscopic equations in the hydrodynamic limit. For the simplest convex function $H = (N, N)$, this is equivalent to (i) constructing the auxiliary equilibrium which fixes the hydrodynamic quantities, and (ii) adding a linear combination of the flux basis, coefficients of this linear combination are found unambiguously from a system of linear algebraic equations. The construction of the equilibrium via a minimum principle makes it possible to prove the H theorem.

The choice of the strictly convex function H for the construction of equilibria is a degree of freedom in the DVM models, not yet fully exploited. It is not ruled out that for some functions H, the minimization subject to hydrodynamic constraints will occasionally result in proper form of higher moments of interest. It is not difficult to write out an equation for such a ''perfect'' function which is a functional equation for the gradient $\partial H / \partial N$. However, solutions to the latter equation are not known, and therefore we have to deal with less perfect H functions. One criterium for their choice is availability of explicit solutions to the minimal set of constraints, leading to auxiliary equilibria. For this reason, we have used the function $H = (N, N)$. There exist other H functions for which the auxiliary equilibria can be constructed explicitly. However, all exact auxiliary equilibria known to us need to be further corrected, and so, for the computational purpose, it seems appropriate to start with the simplest one. We reiterate that the price to be payed for reconstruction of the proper higher moments on the expense of a part of the kinetic space is the existence of the H theorem in a corresponding cylinder, and not in the whole phase space. This gives at least a partial explanation of the well known fact that DVM models with a small number of velocities are generically less stable than those with larger velocity sets: if most of the kinetic space is used for imposing constraints, then the dimension of the cylinder Z is too small.

The method presented here can be applied to a large family of convex functions H (convexity is required, as usual, to obtain unique solutions for the local equilibria), and a question arises as to whether there are physically motivated subclasses in this large family. Rather than the case of the continuous Boltzmann equation where the entropy is unique, the situation is similar to the case of ergodic Markov chains that support an infinite number of convex Lyapunov functions [6]. It should be admitted that well-known motivations which honor the Boltzmann entropy (additivity, information-theoretic ideas, etc.) do *not* seem to be directly relevant to the problem under consideration. However, there are two issues which may be relevant: (i) Positivity of local equilibria, and (ii) Nonlinearity of the auxiliary equilibria. These requirements narrow down the class of functions H, and if the solvability requirement is taken into account, the only suitable function known so far is $H = (N, \sqrt{N})$, for regular lattices [5]. This, however, brings with it a complication because auxiliary equilibria become well defined for only a bounded domain of hydrodynamic parameters. The use of the function $H = (N, N)$ is free of this complication, and construction of the target equilibria as well as the proof of the H theorem is therefore much easier.

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