On the Construction of Discrete Equilibrium Distributions for Kinetic Schemes

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Abstract

A general approach to the construction of discrete equilibrium distributions is presented. Such distribution functions can be used to set up Kinetic Schemes as well as Lattice Boltzmann methods. The general principles are also applied to the construction of Chapman Enskog distributions which are used in Kinetic Schemes for compressible Navier Stokes equations.

1 Introduction

In many technical applications, the simulation of gas or liquid flows is a central issue. Especially, for the prediction of compressible gas flows, Kinetic Schemes have proved to be very robust and flexible. Recently, the Lattice Boltzmann Method, which is also based on the Kinetic Theory of gases, has become popular for the simulation of incompressible flows. The basic ingredient in both schemes is the equilibrium distribution function which describes the velocity distribution of the microscopic constituents of the gas or liquid at thermal equilibrium in terms of a few macroscopic state variables. In this article, a general approach to the construction of discrete equilibrium distributions is presented.

To describe the physical processes involved in a gas flow, there are two basic models: in a macroscopic approach, the gas is considered as a continuum which is completely described by space densities of mass ρ, momentum ρu and energy $\rho\epsilon$. The evolution of these quantities is governed by the system of Euler

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equations

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = 0, \\
&\frac{\partial (\rho u)}{\partial t} + \operatorname{div}(\rho u \otimes u + \rho T I) = 0, \\
&\frac{\partial (\rho \epsilon)}{\partial t} + \operatorname{div}(\rho(\epsilon + T) u) = 0.
\end{aligned} \tag{1}
$$

The temperature T is related to u, ϵ and the space dimension d by

$$\epsilon = \frac{1}{2}|u|^2 + \frac{d}{2} T.$$

A second approach takes the particle structure of the gas into account. Here, the basic quantity is the particle distribution functions $f(x, v)$ which describes the density of particles at x with velocity v. The time evolution of the particle distribution function is governed by the Boltzmann equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f). \tag{2}$$

The left hand side of (2) describes the undisturbed movements of particles according to their velocities v (free flow). Collisions disturb this free flow by changing the velocities of the particles. This particle mixing in phase space manifests itself in (2) as a nonlinear source term $Q(f)$, the collision operator.

Although these two descriptions seem to be quite different, there is a link between them. First, the macroscopic quantities are available in the more general microscopic picture. The space densities of mass, momentum and energy are just the velocity averages of the particle mass, momentum and energy densities. If $\langle \cdot \rangle$ denotes integration with respect to v, then

$$\langle f \rangle = \rho, \qquad \langle v f \rangle = \rho u, \qquad \left\langle \frac{1}{2}|v|^2 f \right\rangle = \rho \epsilon.$$

The evolution of these quantities can then be obtained by integrating (2) over v after multiplication with $1, v, \frac{1}{2}|v|^2$. We find

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = \langle Q \rangle, \\
&\frac{\partial (\rho u)}{\partial t} + \operatorname{div} \langle v \otimes v f \rangle = \langle v Q \rangle, \\
&\frac{\partial (\rho \epsilon)}{\partial t} + \operatorname{div} \left\langle \frac{1}{2}|v|^2 v f \right\rangle = \left\langle \frac{1}{2}|v|^2 Q \right\rangle.
\end{aligned} \tag{3}
$$

Since collisions are assumed to conserve mass, momentum and energy, we have

$$\langle Q\rangle = 0, \qquad \langle vQ\rangle = 0, \qquad \left\langle \frac{1}{2}|v|^2 Q\right\rangle = 0$$

so that the evolution equations are quite close to the Euler system (1). It turns out, that in the case of dense gases, the two systems even coincide which establishes the link between microscopic and macroscopic model.

In a dense gas, collisions are dominant and in the limit of infinite collision frequency (the so called *hydrodynamical limit*), the particle distribution function attains the special form of a Maxwellian

$$\mathcal{M}(v) = \frac{\rho}{(2\pi T)^{\frac{d}{2}}} \exp\left(-\frac{|v-u|^2}{2T}\right), \qquad v \in \mathbb{R}^d. \tag{4}$$

This velocity distribution is well known as the one of a gas in (local) thermal equilibrium. Hence, the Maxwellian is also called *equilibrium distribution.* If f has the form (4), then the fluxes which are undetermined in (3) can be calculated

$$\langle v\otimes v\mathcal{M}\rangle = \rho u\otimes u + \rho T I, \qquad \left\langle \frac{1}{2}|v|^2 v\mathcal{M}\right\rangle = \rho(\epsilon + T)u.$$

Kinetic Schemes use the relation between the two approaches to obtain a numerical method for Euler equations. Of course, solving the complicated Boltzmann equation in a limit where the nonlinear collision term becomes important is numerically too expensive. The idea is therefore to use only the new representation of the Euler system

$$\left\langle \begin{pmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{pmatrix} \left(\frac{\partial f}{\partial t} + v\cdot\nabla_x f\right)\right\rangle = 0, \qquad f = \mathcal{M}. \tag{5}$$

A first possibility to approximately solve (5) is to consider the auxiliary problem

$$\frac{\partial f}{\partial t} + v\cdot\nabla_x f = 0, \qquad f|_{t=0} = \mathcal{M}.$$

The solution of this free transport problem is easily found

$$f(x,v,t) = f(x-vt, v, 0).$$

Clearly, the solution satisfies

$$\left\langle \begin{pmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{pmatrix} \left(\frac{\partial f}{\partial t} + v \cdot \nabla_x f \right) \right\rangle = 0.$$

However, the constraint $f = \mathcal{M}$ is only enforced initially. With increasing time, the violation of the constraint leads to an increasing error. By stopping the evolution after a small time step $\triangle t$ and restarting it with a Maxwellian (that has the same ρ, u, ϵ–moments as the solution of the just finished free flow step), the error can be kept of order $\triangle t$, giving rise to a first order method for the Euler equations. Such schemes have been considered in [13, 14, 9, 2, 4]. If the Maxwellian is approximated by a sum of point measures (numerical particles), then solving the transport problems just amounts to moving the particles according to their velocities. If the point approximation is repeated after the Maxwellian reconstruction at the end of the time step, we obtain a *particle scheme* for the Euler system [18, 16].

Another possibility to approximate (5) is to discretize the differential operators $\partial/\partial t$ and $v \cdot \nabla_x$ directly. An upwind discretization of $v \cdot \nabla_x$, for example, gives rise to an upwind scheme for Euler equations. Integration of (5) over space-cells of a finite volume grid leads to Kinetic Schemes in finite volume form [5, 11].

It has been noted in [15, 10, 6, 12, 9] that the constraint $f = \mathcal{M}$ can be relaxed. Indeed, for (5) to be a representation of the Euler system (1), we can replace $\mathcal{M}$ by some other function M, provided the relevant v-moments coincide. More precisely, we need

$$\begin{aligned} \langle M \rangle &= \rho \\ \langle v_i M \rangle &= \rho u_i \\ \langle v_i v_j M \rangle &= \rho u_i u_j + \rho T \delta_{ij} \\ \left\langle \frac{1}{2}|v|^2 v_i M \right\rangle &= (\epsilon + T) \rho u_i \end{aligned} \tag{6}$$

(To find such a function amounts to solving a reduced moment problem.) In [15], a first example of a discrete function M has been presented whose support is concentrated in a small number of velocities. Recently, such distribution functions have been investigated at length in the framework of Lattice Boltzmann Methods [1, 17, 19, 20]. For Kinetic Schemes in particle formulation, discrete distribution functions are useful since they do not require an additional discretization in the velocity variable. In any case, the evaluation of velocity integrals is simplified which can be helpful, if the discretization of (5) splits the domain of integration in subsets, over which the classical Maxwellian is difficult to integrate in closed form.

We remark, that Kinetic Schemes can be used for any system of equations which can be written in the form (5). For example, the isentropic Euler system allows the same treatment. Here, we just have to find some equilibrium distribution M such that

$$\begin{aligned} \langle M \rangle &= \rho \\ \langle v_i M \rangle &= \rho u_i \\ \langle v_i v_j M \rangle &= \rho u_i u_j + p(\rho)\delta_{ij} \end{aligned} \tag{7}$$

where $p(\rho)$ is the pressure law of the gas. In this case, the relevant moment functions are $(1, v)$ only.

Similarly, we can apply the method to compressible Navier Stokes equations. The derivation of suitable distribution functions for that case (Chapman Enskog distribution) is given in Section 5.

To consider problems like (6) and (7) simultaneously, we slightly generalize our considerations. First, we introduce some notation for the relevant velocity moments.

$$\begin{aligned} \psi^{(0)}(v) &= 1 \\ \psi_i^{(1)}(v) &= v_i \\ \psi^{(2)}(v) &= \frac{1}{2}|v|^2 \\ \psi_{ij}^{(3)}(v) &= v_i v_j - \frac{|v|^2}{d}\delta_{ij} \\ \psi_i^{(4)}(v) &= \frac{1}{2}|v|^2 v_i \end{aligned}$$

Problems (6) and (7) can then be reformulated as follows: find a (generalized) function $M : \mathbb{R}^d \mapsto \mathbb{R}$ such that

$$\left\langle \psi^{(k)} M \right\rangle = \mu^{(k)}, \qquad k = 0, \dots, k_{\max} \tag{8}$$

with $k_{\max} = 4$ in (6) and $k_{\max} = 3$ in (7). The values $\mu^{(k)}$ are the moments $\rho, \rho u, \rho\epsilon$, the traceless part of the momentum flux and the energy flux. Of course, in the isentropic case, the energy variable ϵ is not independent of ρ and u. We have the relation

$$\epsilon = \frac{1}{2}\left(|u|^2 + d\frac{p(\rho)}{\rho}\right).$$

where d is the space dimension.

2 Construction of discrete equilibrium distributions

In general, a reduced moment problem like (8) admits infinitely many solutions. By assuming that M is an discrete equilibrium distribution we reduce the number of possible solutions. More precisely, we want to find a solution M of the structure

$$M(v) = \sum_{i=1}^{m} M_i \delta(v - v_i).$$

Here, δ is the Dirac delta distribution, v_i are vectors in $\mathbb{R}^d$ and $M_i \geq 0$ are nonnegative weights. In Section 4 we will see, that it is natural to assume the additional structure

$$M(v) = \omega(v) M^*(v) \tag{9}$$

where ω is a polynomial which depends on the parameters ρ, u, T and $M^*(v)$ is a discrete distribution supported on the velocities v_i, i.e.

$$M^*(v) = \sum_{i=1}^{m} M_i^* \delta(v - v_i). \tag{10}$$

One can think of M^* as an approximation of the normalized Maxwellian

$$\mathcal{M}^*(v) = \frac{\rho}{(2\pi)^{\frac{d}{2}}} \exp\left(-\frac{|v|^2}{2}\right). \tag{11}$$

In fact, to present the main idea, we will first derive an equilibrium distribution of the form

$$M(v) = \omega(v) \mathcal{M}^*(v) \tag{12}$$

and come back to the discretization in velocity later. Plugging (12) into (8) we end up with the problem to determine the polynomial ω such that

$$\left\langle \psi^{(k)} \omega \mathcal{M}^* \right\rangle = \mu^{(k)}, \qquad k = 0, \ldots, k_{\max}. \tag{13}$$

The general approach which we take to solve (13) is based on orthogonal polynomials $P^{(k)}$ given by

$$
\begin{aligned}
P^{(0)}(v) &= 1 \\
P_i^{(1)}(v) &= v_i \\
P^{(2)}(v) &= |v|^2 - d \\
P_{ij}^{(3)}(v) &= v_i v_j - \frac{|v|^2}{d}\delta_{ij} \\
P_i^{(4)}(v) &= (|v|^2 - (d+2))v_i
\end{aligned}
\tag{14}
$$

These polynomials are orthogonal in the sense

$$
\left\langle P_\eta^{(i)} P_\zeta^{(j)} \mathcal{M}^* \right\rangle = 0, \qquad \text{for } i \neq j. \tag{15}
$$

(Here, η and ζ denote possible indices.) Moreover, we can scale the polynomials and obtain a related set $\bar{P}^{(k)}$ such that

$$
\begin{aligned}
\left\langle \bar{P}^{(k)} P^{(k)} \mathcal{M}^* \right\rangle &= 1, && k = 0, 2 \\
\left\langle \bar{P}_i^{(k)} P_j^{(k)} \mathcal{M}^* \right\rangle &= \delta_{ij}, && k = 1, 4 \\
\left\langle P_{ij}^{(3)} A : \bar{P}^{(3)} \mathcal{M}^* \right\rangle &= \frac{1}{2}(A_{ij} + A_{ji}) - \frac{\operatorname{tr} A}{d}\delta_{ij}.
\end{aligned}
\tag{16}
$$

In the last relation, A is any $d \times d$ matrix and the colon denotes the following product between matrices

$$
A : B = \sum_{i,j=1}^{d} A_{ij} B_{ij}.
$$

To check relations (15) and (16) we just need to know the first few moments of the normalized Maxwellian, which are

$$
\begin{aligned}
\langle \mathcal{M}^* \rangle &= 1 \\
\langle v_i \mathcal{M}^* \rangle &= 0 \\
\langle v_i v_j \mathcal{M}^* \rangle &= \delta_{ij} \\
\langle v_i v_j v_k \mathcal{M}^* \rangle &= 0 \\
\langle v_i v_j v_k v_l \mathcal{M}^* \rangle &= (\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\
\langle v_i v_j v_k v_l v_m \mathcal{M}^* \rangle &= 0 \\
\left\langle |v|^4 v_i v_j \mathcal{M}^* \right\rangle &= (d+2)(d+4)\delta_{ij}
\end{aligned}
\tag{17}
$$

Rewriting the moment problem (13) in terms of the polynomials $P^{(k)}$ leads to the problem

$$\left\langle P^{(k)}\omega\mathcal{M}^*\right\rangle = \gamma^{(k)}, \qquad k = 0, \ldots, , k_{\max} \tag{18}$$

with

$$\gamma^{(0)} = \mu^{(0)}, \qquad \gamma^{(1)} = \mu^{(1)}, \qquad \gamma^{(3)} = \mu^{(3)}$$

and

$$\gamma^{(2)} = 2\mu^{(2)} - d\mu^{(0)}, \qquad \gamma^{(4)} = 2\mu^{(4)} - (d+2)\mu^{(1)}.$$

With (15) and (16) at hand, the transformed problem (18) is now easy to solve. We just set

$$\omega := \gamma^{(0)}\bar{P}^{(0)} + \gamma^{(1)}\cdot\bar{P}^{(1)} + \gamma^{(2)}\bar{P}^{(2)} + \gamma^{(3)} : \bar{P}^{(3)} + \gamma^{(4)}\cdot\bar{P}^{(4)} \tag{19}$$

or in terms of the original moments

$$\begin{aligned}\omega := \mu^{(0)}\bar{P}^{(0)} + \mu^{(1)}\cdot\bar{P}^{(1)} + (2\mu^{(2)} - \frac{d}{\alpha}\mu^{(0)})\bar{P}^{(2)} + \mu^{(3)} : \bar{P}^{(3)} \\ + (2\mu^{(4)} - (d+2)\beta\mu^{(1)})\cdot\bar{P}^{(4)}\end{aligned} \tag{20}$$

(In the case $k_{\max} = 3$, the $\bar{P}^{(4)}$ terms are omitted.)

It is possible, to use this result directly to construct distributions of the form (10). Indeed, the moment conditions (13) just involve v–polynomials up to order $o_{\max} = 6$ (since $\deg(\omega) = 3$ and $\deg\psi^{(4)} = 3$) in the thermal case respectively $o_{\max} = 4$ in isentropic situations. If we replace $\mathcal{M}^*$ by another distribution M^* which has the same v–moments up to order $o_{\max}$, we get immediately

$$\left\langle \psi^{(k)}\omega M^*\right\rangle = \mu^{(k)}, \qquad k = 0, \ldots, k_{\max}.$$

To construct such a function M^*, we can use for example Gauss–Hermite quadrature rules. It is well known, that the integration is exact for polynomials q of degree less or equal $o_{\max}$, if the order N of the integration rule is sufficiently high, i.e.

$$\int_{\mathbb{R}} q(s)\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{1}{2}s^2\right)\,ds = \sum_{i=1}^{N}\theta_i q(s_i).$$

In d dimensions this can be used to construct an integration rule by defining nodes and weights

$$\begin{aligned} v_{i_1,\ldots,i_d} &:= (s_{i_1},\ldots,s_{i_d})^T, \\ \alpha_{i_1,\ldots,i_d} &:= \theta_{i_1}\ldots\theta_{i_d} \end{aligned} \qquad i_k \in \{1,\ldots,N\}. \tag{21}$$

After renumbering consecutively from 1 to $m = N^d$, we thus get for any polynomial Q of degree less than $o_{\max}$

$$\langle Q\mathcal{M}^*\rangle = \sum_{i=1}^{m} M_i^* Q(v_i) = \langle QM^*\rangle$$

with

$$M^*(v) = \sum_{i=1}^{m} M_i^*\delta(v - v_i)$$

so that $\mathcal{M}^*$ can be replaced by M^* in (12) without changing the right hand side. This approach is pursued in [20]. It is also mentioned there, that instead of using the tensorial structure (21) one can use a d–dimensional quadrature rule which integrates polynomials up to order $o_{\max}$ exactly. A disadvantage of the approach is that, in general, the set of all integer multiples of the nodes v_i does not form a regular grid which is invariant under arbitrary v_i translations. A regular structure of the nodes, however, greatly simplifies the application of the discrete equilibrium distribution for example in LBE–type applications.

In a more general approach we therefore relax the condition that the moments of the normalized Maxwellian $\mathcal{M}^*$ are matched by those of M^* exactly up to the relevant order $o_{\max}$. Instead, we assume that M^* has a moment structure which is sufficiently close to that of $\mathcal{M}^*$ to allow a construction of polynomials similar to $P^{(k)}$ given in (14). It turns out that the symmetry of $\mathcal{M}^*$ is important to ensure that the odd moments in (17) vanish. Secondly, isotropy is another important ingredient which manifests itself in the Kronecker delta structures of the even moments in (17). However, the leading constants in the even moments are not really relevant so that we can slightly relax (17) by requiring only

$$\begin{aligned} \langle M^*\rangle &= \alpha \\ \langle v_i M^*\rangle &= 0 \\ \langle v_i v_j M^*\rangle &= \delta_{ij} \\ \langle v_i v_j v_k M^*\rangle &= 0 \\ \langle v_i v_j v_k v_l M^*\rangle &= \beta\left(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) \\ \langle v_i v_j v_k v_l v_m M^*\rangle &= 0 \\ \left\langle |v|^4 v_i v_j M^*\right\rangle &= \gamma\delta_{ij} \end{aligned} \tag{22}$$

with α, β, γ being positive and

$$\gamma > ((d+2)\beta)^2 . \tag{23}$$

By comparison with (8), we see that for the special case $M^* = \mathcal{M}^*$ we have

$$\alpha = 1, \qquad \beta = 1, \qquad \gamma = (d+2)(d+4)$$

so that (23) holds. Again, we can show with the help of (22) that the polynomials

$$\begin{aligned}
P^{(0)}(v) &= 1 \\
P^{(1)}_i(v) &= v_i \\
P^{(2)}(v) &= |v|^2 - \frac{d}{\alpha} \\
P^{(3)}_{ij}(v) &= v_i v_j - \frac{|v|^2}{d}\delta_{ij} \\
P^{(4)}_i(v) &= (|v|^2 - (d+2)\beta) v_i
\end{aligned} \tag{24}$$

satisfy (15) with M^* in place of $\mathcal{M}^*$. To get conditions (16), we have to scale the polynomials $P^{(k)}$ according to

$$\bar{P}^{(k)} = \frac{1}{l^{(k)}} P^{(k)}, \qquad k = 0, \ldots, k_{\max}$$

where the scaling factors $l^{(k)}$ are given by

$$\begin{aligned}
l^{(0)} &= \alpha \\
l^{(1)}_i &= 1 \\
l^{(2)} &= d(d+2)\beta - \frac{d^2}{\alpha} \\
l^{(3)}_{ij} &= 2\beta \\
l^{(4)}_i &= \gamma - \big((d+2)\beta\big)^2
\end{aligned}$$

Finally, to solve

$$\big\langle \psi^{(k)} \omega M^* \big\rangle = \mu^{(k)}, \qquad k = 0, \ldots, k_{\max}$$

we set up the polynomial ω as in (20)

$$\begin{aligned}
\omega := \mu^{(0)} \bar{P}^{(0)} + \mu^{(1)} \cdot \bar{P}^{(1)} + (2\mu^{(2)} - \frac{d}{\alpha}\mu^{(0)}) \bar{P}^{(2)} + \mu^{(3)} : \bar{P}^{(3)} \\
+ (2\mu^{(4)} - (d+2)\beta \mu^{(1)}) \cdot \bar{P}^{(4)}
\end{aligned}$$

In the case $k_{\max} = 3$ the last term is removed. If we evaluate (20) for the isentropic case (problem (7)), we get

$$\omega = \rho \bar{P}^{(0)} + \rho u \cdot \bar{P}^{(1)} + (\rho |u|^2 + d(p(\rho) - \rho/\alpha))\bar{P}^{(2)} \\ + (\rho u \otimes u - \frac{1}{d}\rho |u|^2 I) : \bar{P}^{(3)}.$$

Since $\bar{P}^{(3)}$ is trace free, we have $I : \bar{P}^{(3)} = 0$. Moreover, $\rho |u|^2 = \rho u \otimes u : I$, so that

$$\omega = \rho \bar{P}^{(0)} + \rho u \cdot \bar{P}^{(1)} + d(p(\rho) - \rho/\alpha)\bar{P}^{(2)} + \rho u \otimes u : (\bar{P}^{(3)} + \bar{P}^{(2)} I).$$

For the special, isothermal pressure law $p(\rho) = \rho/\alpha$, the polynomial ω simplifies further to

$$\omega = \rho \left(\bar{P}^{(0)} + u \cdot \bar{P}^{(1)} + u \otimes u : (\bar{P}^{(3)} + \bar{P}^{(2)} I) \right), \qquad p(\rho) = \frac{\rho}{\alpha}. \tag{25}$$

Finally, we mention the case where α and β are related by $\alpha\beta = 1$. Then, the scaling coefficient $l^{(2)}$ satisfies

$$l^{(2)} = d(d+2)\beta - \frac{d^2}{\alpha} = 2d\beta = l^{(3)} d.$$

Thus,

$$\bar{P}^{(3)}(v) + \bar{P}^{(2)}(v) I = \frac{1}{2\beta} \left(v \otimes v - \frac{|v|^2}{d} I + \frac{1}{d} \left(|v|^2 - \frac{d}{\alpha} \right) \right) = \frac{1}{2\beta} (v \otimes v - \beta I)$$

which leads to the final structure

$$\omega = \rho \left(\beta + u \cdot v + \frac{1}{2\beta}(u \cdot v)^2 - \frac{1}{2}|u|^2 \right), \qquad \alpha\beta = 1, \ p(\rho) = \beta\rho. \tag{26}$$

3 Standard examples of equilibrium distributions

3.1 The D2Q9–model

Our first example is the D2Q9–model which is based on nine velocities in two dimensions. To define the normalized distribution $M^*(v) = \sum_{i=0}^{8} M_i^* \delta(v - v_i)$, we set for any $\sigma > 0$

$$
\begin{aligned}
v_0 &= 0, \\
v_i &= \sqrt{3\sigma}\Big(\cos\Big((i-1)\frac{\pi}{2}\Big), \sin\Big((i-1)\frac{\pi}{2}\Big)\Big)^T & i &= 1,\dots,4, \\
v_i &= \sqrt{6\sigma}\bigg(\cos\bigg(\Big(i-\frac{9}{2}\Big)\frac{\pi}{2}\bigg), \sin\bigg(\Big(i-\frac{9}{2}\Big)\frac{\pi}{2}\bigg)\bigg)^T & i &= 5,\dots,8,
\end{aligned}
$$

with weights

$$
M_0^* = \frac{4}{9\sigma}, \qquad M_i^* = \frac{1}{9\sigma}, \quad i = 1,\dots,4, \qquad M_i^* = \frac{1}{36\sigma}, \quad i = 5,\dots,8.
$$

Calculating the velocity moments of M^* we find the structure (22) with

$$
\alpha = \frac{1}{\sigma}, \qquad \beta = \sigma, \qquad \gamma = 18\sigma^2
$$

so that (23) is satisfied because

$$
18\sigma^2 = \gamma > \big((d+2)\beta\big)^2 = 16\sigma^2.
$$

Consequently, the construction of the equilibrium distribution can be applied both in the thermal and the isentropic case. To show that the approach leads to standard LBE–distributions, we consider the isothermal case $p(\rho) = \rho/\alpha = \sigma\rho$. (Observe that $\alpha\beta = 1$.) Since M is of the form $M = \omega M^*$ with M^* being a sum of Dirac deltas, we can write

$$
\begin{aligned}
M(v) = \omega(v)M^*(v) = \sum_{i=0}^{8} \omega(v) M_i^* \delta(v - v_i) \\
= \sum_{i=0}^{8} M_i^* \omega(v_i)\delta(v - v_i) = \sum_{i=0}^{8} M_i \delta(v - v_i)
\end{aligned}
$$

with $M_i = M_i^*\omega(v_i)$. Using the above weights M_i^* and the nodes v_i with $\sigma = 1$, we get with (26)

$$
M_i = \rho M_i^* \left(1 - \frac{1}{2}|u|^2 + u \cdot v_i + \frac{1}{2}(u \cdot v_i)^2\right). \tag{27}
$$

3.2 The hexagonal model

For the hexagonal model in two dimensions

$$
\begin{aligned}
v_0 &= 0, \\
v_i &= \sqrt{\sigma}\Big(\cos\Big((i-1)\frac{\pi}{6}\Big), \sin\Big((i-1)\frac{\pi}{6}\Big)\Big)^T & i &= 1,\dots,6
\end{aligned}
$$

with weights

$$M_0^* = \lambda, \qquad M_i^* = \frac{1}{3\sigma}, \quad i = 1, \dots, 6$$

we get

$$\alpha = \lambda + \frac{2}{\sigma}, \qquad \beta = \frac{\sigma}{4}, \qquad \gamma = \sigma^2.$$

In this case, condition (23) is violated since $\gamma = (4\beta)^2$. Consequently, the polynomial $\bar{P}^{(4)}$ cannot be constructed which rules out the application of this model in cases where the energy equation is needed. In isentropic cases, however, we only need $\bar{P}^{(0)}$ to $\bar{P}^{(3)}$. With $\lambda = \frac{1}{2}$ and $\sigma = 4$ we get again $\alpha = \beta = 1$ which yields the same structure of the weights M_i of the equilibrium distribution as presented in (27). Of course, the factors M_i^* and the number of velocities are different.

3.3 The D3Q15–model

Similar to the D2Q9–case, we consider a model with 15 velocities in three dimensions. To describe the discrete directions, we consider a cube of side length $2\sqrt{3\sigma}$ which is centered at the origin. Now, v_0 is the center of the cube and $v_1, \dots, v_6$ point to the centers of the six faces. The remaining velocities $v_7, \dots, v_{14}$ point to the corners of the cube and thus have length $\sqrt{9\sigma}$ which is $\sqrt{3}$ times the length of $v_1, \dots, v_6$. As weights we choose

$$M_0^* = \frac{2}{9\sigma}, \qquad M_i^* = \frac{1}{9\sigma}, \quad i = 1, \dots, 6, \qquad M_i^* = \frac{1}{72\sigma}, \quad i = 7, \dots, 14.$$

The resulting constants in the moment relations (22) are

$$\alpha = \frac{1}{\sigma}, \qquad \beta = \sigma, \qquad \gamma = 33\sigma^2.$$

Again, relation (23) is satisfied so that the model can be applied to thermal cases.

4 Some remarks on the choice of velocities

In Section 2 we have considered moment problems like

$$(28) \qquad \langle \phi_i M \rangle = \eta_i, \qquad i = 1, \dots, n, \quad \eta \in E$$

with moment functions ϕ_i and $M \geq 0$ of the form

$$M(v) = \sum_{j=1}^{m} x_j \delta(v - v_j). \tag{29}$$

The nodes $v_j \in \mathbb{R}^d$ are assumed to be fixed, so that only the coefficients $x_j \geq 0$ have to be chosen depending on the right hand side η. In view of our application where η_i are expressions in the variables ρ, u, T, we remark that the set E of possible right hand sides will in general not be flat (i.e. not contained in a proper linear subset of $\mathbb{R}^n$). Inserting (29) into (28), we get

$$\sum_{j=1}^{m} \phi_i(v_j) x_j = \eta_i, \qquad x_j \geq 0, \quad i = 1, \ldots, n.$$

Neglecting the positivity condition on the coefficients x_j, this is just a linear problem with an $n \times m$ matrix $B = (\phi_i(v_j))$ and right hand side η. Since E is not flat, we have to ensure that B has rank n since otherwise the image of B is flat and thus cannot contain E. This leads to the first observation that the number of velocities m must be greater or equal than the number of conditions n. A more precise criterion is obtained from the fact that $\operatorname{rank} B = n$ is equivalent to the linear independence of the rows of B, i.e.

$$\sum_{i=1}^{n} \lambda_i r_i = 0 \quad \Rightarrow \quad \lambda = 0 \tag{30}$$

where r_i is the i^{th} row of B

$$r_i = \big(\phi_i(v_1), \ldots, \phi_i(v_m)\big).$$

In order to give a geometrical interpretation of (30) we introduce the set of all functions which are obtained from $\phi_1, \ldots, \phi_n$ by linear combinations

$$\Phi := \left\{ \omega_\lambda = \sum_{i=1}^{n} \lambda_i \phi_i \; : \; \lambda \in \mathbb{R}^n \right\}.$$

Condition (30) can then be formulated in the following way.

Lemma 4.1 *The matrix B with entries*

$$B_{ij} = \phi_i(v_j), \qquad i = 1, \ldots, n, \quad j = 1, \ldots, m$$

has rank n if and only if the only function $\omega_\lambda \in \Phi$ which vanishes simultaneously on all nodes v_j is ω_0.

Proof: A function $\omega_\lambda \in \Phi$ vanishes simultaneously on all nodes if

$$\sum_{i=1}^{n} \lambda_i \phi_i(v_j) = 0, \qquad \forall j = 1, \ldots, m.$$

which is just the left hand side in (30). ■

Altogether, the lemma allows us to give a necessary condition for the solvability of (28).

Lemma 4.2 *Assume $E \subset \mathbb{R}^n$ is not flat. If there exists a function ω_λ in Φ with $\lambda \neq 0$ which vanishes on all nodes v_j, the moment problems* (28) *cannot be solved with M of the form* (29)*. In particular, this is the case if the number of nodes is less than the number of moment conditions.*

We note that in two dimensions there are eight moment conditions in the thermal case. Consequently, the moment problems cannot be solved with hexagonal distributions since they are based on only seven velocities. Geometrically, the polynomial $P_1^{(4)}$ given in (24) vanishes on all nodes of the hexagonal model. Indeed, $P_1^{(4)}$ is a linear combination of $\psi_1^{(4)}$ and $\psi_1^{(1)}$ which vanishes on the circle of radius $\sqrt{(d+2)\beta}$ and along the vertical axis. In the hexagonal model we have $(d+2)\beta = \sigma$ so that $P_1^{(4)}$ is zero on all nodes $v_1, \ldots, v_6$ as well as in the origin v_0.

In the next step, we assume that the necessary condition in Lemma 4.1 is satisfied. If, on top of that, we are in the extreme case $m = n$, there is exactly one solution of the linear system $Bx = \eta$. (We remark that due to the positivity restriction, $x = B^{-1}\eta$ gives rise to a solution of the moment problem only if its components are nonnegative.) In a more general situation we have $m > n$ so that the solution is no longer unique. To get a functional dependence $x = x(\eta)$, however, we need a method which singles out one of the many solutions of $Bx = \eta$. Following a standard approach, we take the vector x which minimizes a quadratic functional $Q(x)$ under the constraint $Bx = \eta$. If we choose in particular

$$Q(x) = \frac{1}{2} \sum_{k=1}^{m} \frac{1}{M_k^*} x_k^2, \qquad M_k^* > 0,$$

we recover exactly the situation presented in Section 2. To show this, we use the method of Lagrange multipliers according to which the minimum of the constrained problem minimizes the modified functional

$$\tilde{Q}(x) = Q(x) - \lambda \cdot (Bx - \eta).$$

For such a quadratic problem, the minimizer $\bar{x}$ is uniquely defined by $\nabla\tilde{Q}(\bar{x}) = 0$. This yields the condition

$$D^{-1}\bar{x} = B^T\lambda, \qquad D = \mathrm{diag}(M_1^*, \ldots, M_m^*).$$

Plugging this into the condition $B\bar{x} = \eta$, we obtain an equation for the Lagrange multiplier λ

$$BDB^T\lambda = \eta. \tag{31}$$

Using the definition of B this can be transformed into

$$\sum_{j=1}^{m} \phi_i(v_j) M_j^* \sum_{k=1}^{n} \phi_k(v_j)\lambda_k = \eta_i,$$

or with $\omega_\lambda := \sum_{k=1}^{n} \lambda_k \phi_k$

$$\eta_i = \sum_{j=1}^{m} M_j^* \phi_i(v_j)\omega_\lambda(v_j) = \langle \phi_i \omega_\lambda M^* \rangle .$$

with M^* defined in (9). This shows, that the problem to determine a suitable function $\omega_\lambda \in \Phi$, such that $M = \omega_\lambda M^*$ satisfies the moment problem, can be interpreted as finding Lagrange multipliers.

At this point, we are also able to conclude that a solution λ (and thus also a function ω_λ) exists if the condition in Lemma 4.1 is satisfied.

Lemma 4.3 *Assume* $\mathrm{rank}\, B = n$. *Then* (31) *admits a unique solution.*

Proof: Since the entries of the diagonal matrix D are positive, the square root is well defined

$$\sqrt{D} = \mathrm{diag}\left(\sqrt{M_1^*}, \ldots, \sqrt{M_m^*}\right).$$

With $\tilde{B} = B\sqrt{D}$ we can rewrite the equation for λ

$$\tilde{B}\tilde{B}^T\lambda = \eta.$$

Now, the rank of $\tilde{B}$ is the same as the one of B since multiplying the columns by positive numbers does not change the rank of a matrix. Consequently, also $\tilde{B}$ has rank n. In that case it is easy to show that $\tilde{B}\tilde{B}^T$ is invertible because $\bar{\lambda}$ in the kernel of $\tilde{B}\tilde{B}^T$ satisfies

$$0 = \bar{\lambda}^T\left(\tilde{B}\tilde{B}^T\bar{\lambda}\right) = \left|\tilde{B}^T\bar{\lambda}\right|^2$$

so that $\bar{\lambda}$ is also in the kernel of $\tilde{B}^T$ which is the null space. ■

It has to be stressed again that the unique solution given in Lemma 4.3 does not need to satisfy the positivity restriction. To investigate this problem a little further, we introduce the set of all admissible Lagrange multipliers

$$C := \{ \lambda \in \mathbb{R}^n \, : \, \omega_\lambda(v_j) \geq 0 \; \forall j = 1, \dots, m \} .$$

Consequently, the moment problem is only solvable for those right hand sides η which are contained in the image of C under the map BDB^T. If C happens to be flat (i.e. contained in a linear hyper plane), also its image will be flat. On the other hand, E is non flat by assumption, so that nonnegative solutions to the moment problems cannot always be found in that case. Hence, we have to make sure that $\dim C = n$, or equivalently, that C contains some interior point. To get this property, we assume more structure on the functions ϕ_i. Guided by our main application where $\phi_1 \equiv 1$ is a function which is positive on all nodes v_j, we assume that there is some $\omega_{\lambda^*} \in \Phi$ so that $\omega_{\lambda^*}(v_j) > 0$ for all $j = 1, \dots, m$. Due to the continuity of the mapping

$$\lambda \mapsto \Omega(\lambda) = (\omega_\lambda(v_1), \dots, \omega_\lambda(v_m))$$

we conclude that $\Omega(\lambda) \geq 0$ (component wise) for all λ in a ball around λ^*. In particular, λ^* is an interior point of the convex cone C. Since BDB^T is a bijection, we can conclude that (28) is solvable at least when E is contained in a small neighborhood of η^*, the moment vector corresponding to λ^*

$$\eta_i^* = \langle \phi_i \, \omega_{\lambda^*} \, M^* \rangle .$$

We collect our observations in a final theorem.

Theorem 4.4 *Let $\phi = (\phi_1, \dots, \phi_n)^T$ be a vector of real valued functions on $\mathbb{R}^d$ and let $E \subset \mathbb{R}^n$ be non flat. A necessary condition for the solvability of the problems*

$$\langle \, \phi \, M \rangle = \eta, \qquad \eta \in E$$

with M of the form

$$M(v) = \sum_{j=1}^{m} x_j \delta(v - v_j), \qquad x_j \geq 0$$

and given v_j is, that the only function $\omega_\lambda = \sum_{i=1}^n \lambda_i \phi_i$ which vanishes on all nodes v_j is ω_0. The condition is also sufficient for solvability if positivity restrictions are neglected.

If there is a function ω_{λ^*} which is strictly positive on all nodes, then the moment problem has positive solutions in a neighborhood of the vector

$$\eta^* = \langle \phi \, \omega_{\lambda^*} \, M^* \rangle \,, \qquad M^*(v) = \sum_{j=1}^{m} M_j^* \delta(v - v_j),$$

where $M_j^* > 0$ are arbitrary numbers.

5 Deriving a Chapman Enskog distribution

A simple model for $Q(f)$ in (2) is given by the BGK collision operator

$$Q(f) = -\frac{1}{t_R}(f - M[f]). \tag{32}$$

This model takes into account that the particle distribution function f relaxes towards an equilibrium distribution function $M[f]$ which has the same conserved moments as f. The parameter $t_R > 0$ is the time scale for this relaxation process.

For simplicity, we restrict our considerations to the isentropic case, i.e. we assume that the equilibrium distribution $M[f]$ in (32) satisfies the moment conditions (7). As already mentioned, solving Boltzmann equation in the hydrodynamical limit $t_R \to 0$ becomes equivalent to solving Euler equations. If we think of f being asymptotically expanded in a power series of t_R, the hydrodynamical limit implies $f = M$ in lowest order. To get a more refined picture of the situation $t_R \ll 1$, we now consider the expansion

$$f = M - t_R g_{t_R}, \qquad g_{t_R} = g_0 + t_R g_1 + t_R^2 g_2 + \dots. \tag{33}$$

The basic assumption, which is characteristic for Chapman Enskog expansions, is that the higher order contributions g_i do not add to the conserved velocity moments. In our case, this leads to the condition

$$\begin{pmatrix} \rho \\ \rho u \end{pmatrix} = \left\langle \begin{pmatrix} 1 \\ v \end{pmatrix} f \right\rangle = \left\langle \begin{pmatrix} 1 \\ v \end{pmatrix} M \right\rangle .$$

Plugging (33) into (2) with the BGK operator (32) and solving for g_{t_R} yields

$$g_{t_R} = \left(\frac{\partial M}{\partial t} + v \cdot \nabla M \right) + t_R \left(\frac{\partial g_{t_R}}{\partial t} + v \cdot \nabla g_{t_R} \right). \tag{34}$$

Taking moments and observing $\left\langle \binom{1}{v} g_{t_R} \right\rangle = 0$, we get

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = 0, \\ &\frac{\partial}{\partial t}(\rho u) + \operatorname{div}(\rho u \otimes u) + \nabla p(\rho) = t_R \operatorname{div} \langle v \otimes v \, g_{t_R} \rangle . \end{aligned} \tag{35}$$

To determine the right hand side of the momentum equation to order t_R, we obviously need information just on g_0. This information can be taken from (34) where now terms of order t_R can be neglected. Using chain rule and Einstein's summation convention, we get

$$g_{t_R} = \frac{\partial M}{\partial \rho}\left(\frac{\partial \rho}{\partial t} + v_i \frac{\partial \rho}{\partial x_i}\right) + \frac{\partial M}{\partial u_j}\left(\frac{\partial u_j}{\partial t} + v_i \frac{\partial u_j}{\partial x_i}\right) + \mathcal{O}(t_R).$$

With the help of (35), time derivatives can be replaced by space derivatives, so that

$$g_{t_R} = \frac{\partial M}{\partial \rho}\left(v_i \frac{\partial \rho}{\partial x_i} - \frac{\partial (\rho u_i)}{\partial x_i}\right) + \frac{\partial M}{\partial u_j}\left(v_i \frac{\partial u_j}{\partial x_i} - u_i \frac{\partial u_j}{\partial x_i} - \frac{1}{\rho}\frac{\partial p(\rho)}{\partial x_j}\right) + \mathcal{O}(t_R).$$

With the classical Maxwellian in the isothermal case $T_0 = const$, $p(\rho) = \rho T_0$,

$$\mathcal{M} = \frac{\rho}{(2\pi T_0)^{\frac{d}{2}}} \exp\left(-\frac{|v-u|^2}{2T_0}\right)$$

we get

$$\frac{\partial \mathcal{M}}{\partial \rho} = \frac{1}{\rho}\mathcal{M}, \qquad \frac{\partial \mathcal{M}}{\partial u_j} = \frac{v_j - u_j}{T_0}\mathcal{M}.$$

The terms involving derivatives of density now disappear since

$$\frac{1}{\rho}\frac{\partial p(\rho)}{\partial x_j} = \frac{1}{\rho} T_0 \frac{\partial \rho}{\partial x_j}.$$

What remains is

$$g_{t_R} = \left(-\frac{\partial u_i}{\partial x_i} + \frac{(v_j - u_j)(v_i - u_i)}{T_0}\frac{\partial u_j}{\partial x_i}\right)\mathcal{M} + \mathcal{O}(t_R).$$

The lowest order can be written in compact notation

$$g_0 = \left(\frac{(v-u)\otimes(v-u)}{T_0} - I\right) : S\,\mathcal{M}$$

where I is the identity matrix and

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right).$$

To complete equations (35), we finally calculate the second order moments of g_0 which we denote

$$\eta := t_R \langle v \otimes v g_{t_0} \rangle .$$

With the change of variables $w = (v-u)/\sqrt{T_0}$ we obtain

$$\eta = \rho t_R T_0 \langle (w+u) \otimes (w+u)(w \otimes w - I) : S\, \mathcal{M}^* \rangle$$

where $\mathcal{M}^*$ is the normalized Maxwellian (11). Using polynomials (14), we find

$$w \otimes w - I = P^{(3)} + \frac{1}{d} P^{(2)} I. \tag{36}$$

Due to orthogonality relations (15), only the quadratic part $w \otimes w$ in $(w + u) \otimes (w+u)$ contributes

$$\eta = \rho t_R T_0 \left\langle w \otimes w \left(P^{(3)} + \frac{1}{d} P^{(2)} I \right) : S\, \mathcal{M}^* \right\rangle .$$

Using (36) again, orthogonality properties and (16) we get

$$\begin{aligned}
\eta &= \rho\, t_R T_0 \left\langle \left(P^{(3)} + \frac{1}{d} P^{(2)} I + I \right) \left(P^{(3)} + \frac{1}{d} P^{(2)} I \right) : S\, \mathcal{M}^* \right\rangle \\
&= \rho\, t_R T_0 \left(\left\langle P^{(3)} P^{(3)} : S\, \mathcal{M}^* \right\rangle + \frac{\operatorname{tr} S}{d} \left\langle P^{(2)} P^{(2)}\, \mathcal{M}^* \right\rangle I \right) \\
&= \rho\, t_R T_0 \left(2 \left(S - \frac{\operatorname{tr} S}{d} I \right) + 2 (\operatorname{tr} S) I \right) \\
&= \rho\, t_R T_0 \left(2S + 2 \frac{d-1}{d} (\operatorname{tr} S) I \right) .
\end{aligned}$$

Introducing the kinematic viscosity parameter $\nu = t_R T_0$, the viscous stress tensor $\tau = 2\rho\nu S$ and the coefficient $\lambda = 2\rho\nu \frac{d-1}{d}$ we have the result

$$\eta = \tau + \lambda \operatorname{div} u\, I.$$

Consequently, up to first order in t_R, the moments of f satisfy the compressible Navier Stokes equation

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = 0, \\
&\frac{\partial}{\partial t}(\rho u) + \operatorname{div}(\rho u \otimes u) + \nabla p(\rho) = \operatorname{div} \tau + \nabla(\lambda \operatorname{div} u).
\end{aligned} \tag{37}$$

More explicitly, the viscous term in the i^{th} momentum equation is

$$\nu \frac{\partial}{\partial x_j}\left(\rho\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_i}{\partial x_j}\right)\right)+\frac{\partial}{\partial x_i}\left(\lambda\frac{\partial u_j}{\partial x_j}\right), \qquad i=1,\dots,d.$$

Based on similar arguments, the system (37) has been derived in [8]. Our construction also yields a distribution function which is related to equations (37). It is called Chapman-Enskog distribution

$$\begin{aligned}\mathcal{F}_{CE}(v) &= \mathcal{M}(v) - t_R\, g_0(v) \\ &= \left(1 - t_R\left(\frac{(v-u)\otimes(v-u)}{T_0} - I\right) : S\right)\mathcal{M}(v).\end{aligned}$$

We note, that (37) can be written in the form

$$\left\langle \begin{pmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{pmatrix} \left(\frac{\partial f}{\partial t} + v\cdot\nabla_x f\right)\right\rangle = 0, \qquad f = \mathcal{F}_{CE}.$$

which enables us to apply Kinetic Schemes to the compressible Navier Stokes system. In order to construct a discrete distribution F_{CE} with similar properties, we proceed along the lines of Section 2, i.e. we require that F_{CE} has the same first v–moments as $\mathcal{F}_{CE}$. This leads to the problem

$$\begin{aligned}\langle M\rangle &= \rho, \\ \langle vM\rangle &= \rho u, \\ \langle v\otimes vM\rangle &= \rho u\otimes u + p(\rho)I - \tau - \lambda\,\mathrm{div}\,uI.\end{aligned} \tag{38}$$

Again, this moment problem is of the form (8), so that we can use the general solution constructed in Section 2. Similar to (25) (just replace $\rho u\otimes u$ by $\rho u\otimes u - \tau - \lambda\,\mathrm{div}\,uI$), the polynomial ω in the representation $F_{CE} = \omega M^*$ is given by

$$\begin{aligned}\omega = \rho\bar{P}^{(0)} + \rho u\cdot\bar{P}^{(1)} + d(p(\rho) - \rho/\alpha)\bar{P}^{(2)} \\ + (\rho u\otimes u - \tau - \lambda\,\mathrm{div}\,uI) : (\bar{P}^{(3)} + \bar{P}^{(2)}I).\end{aligned}$$

For the special case $p(\rho) = \rho/\alpha$, the structure is again simplified a little more

$$\omega = \rho\bar{P}^{(0)} + \rho u\cdot\bar{P}^{(1)} + (\rho u\otimes u - \tau - \lambda\,\mathrm{div}\,uI) : (\bar{P}^{(3)} + \bar{P}^{(2)}I).$$

If, in addition $\alpha\beta = 1$, we find in accordance to (26)

$$\begin{aligned}\omega = \rho\Bigg(\beta + u\cdot v + \frac{1}{2\beta}(u\cdot v)^2 - \frac{1}{2}|u|^2 \\ -\frac{\nu}{\beta}v\otimes v : S - \nu\left(\frac{d-1}{\beta d}|v|^2 - d\right)\mathrm{div}\,u\Bigg).\end{aligned}$$

For the D2Q9 model with $\sigma = 1$, we get

$$\omega = \rho \left(1 + u \cdot v + \frac{1}{2}(u \cdot v)^2 - \frac{1}{2}|u|^2 - \nu v \otimes v : S - \nu \left(\frac{1}{2}|v|^2 - 2 \right) \operatorname{div} u \right).$$

6 Conclusions

The construction of Kinetic Schemes for Euler or Navier Stokes equations leads to a class of reduced moment problems. In this article, we have presented a general approach how to solve these problems with distribution functions of discrete type. A necessary condition for solvability has been derived which connects the pattern of the discrete velocities with the structure of the moment functions. Finally, the approach has been applied to the construction of discrete Chapman Enskog distributions.

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