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Discrete kinetic models in the fluid dynamic limit

Hans Babovsky *

Institute for Mathematics, Ilmenau University of Technology, D-98693 Ilmenau, Germany

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ABSTRACT

We investigate discrete kinetic models in the fluid dynamic limit described by the Euler system and the Navier–Stokes correction obtained by the Chapman–Enskog procedure. We show why reliable "small" systems can be expected only for small Mach numbers and derive a calculus for designing models for given Prandtl numbers.

1. Introduction

The Boltzmann equation provides a mathematical description of gas flows on a mesoscopic level and is useful in a number of applications like the modeling of microflows. Due to the complexity of the equation (the Boltzmann collision operator requires the calculation of a five-dimensional integral to be evaluated pointwise in phase space) it is hard to construct efficient numerical schemes based on classical numerical discretization concepts. One way out is the use of Monte Carlo methods. This approach is not discussed here. Another way is the derivation of highly *reduced discrete kinetic models*.

Concepts for discrete kinetic models on regular lattices have been proposed and investigated by a number of authors. The paper [1] provides an attempt to discretize the collision operator on a Cartesian grid. However, the order of consistency is extremely low (see the investigations in [2,3]). Another possibility is the construction of classes of models which as a minimal requirement satisfy the correct physical conservation laws [4,5]. However, we do not know of any results confirming their use as a numerical tool. An attempt to construct discrete collision dynamics which in a sense are optimally adapted to a given lattice have been introduced in [6] as the so-called *Lattice Group Models*. They turn out to be applicable to produce reliable numerical results in a number of test cases [7,8].

Discrete kinetic models are also used as a tool for *macroscopic* simulation. A commonly applied technique is present in the *Lattice Boltzmann Systems* [9,10] which have been proven to be consistent with the Navier–Stokes equations. At present there seem to be two separate scientific communities with not much overlap applying kinetic schemes either from the view point of rarefied gas dynamics or of fluid dynamics. The present paper is intended to overcome this gap. This means the following. A link between computational Fluid Dynamics and computational Rarefied Gas Dynamics is provided by the observation that some of the favorite relaxation models of Lattice Boltzmann Theory can be interpreted as (linearizations of) two-particle collision operators. With this we have a common basis for the simulation of both regimes. The Lattice Boltzmann models (e.g. D2Q9, D3Q27) are too rough to be applied well into the rarefied regimes which require larger velocity systems. For the complete simulation of the whole transition regime we need to couple models of different sizes. There is a need for a whole hierarchy of models which are compatible in the sense that in the fluid dynamic limit they exhibit the same macroscopic behavior. That is, flow parameters like the Prandtl number are to be the same. To this end we require a method specifying flow properties for given models. This is one focus of the present paper. In detail we proceed as follows. In Section 2 we define two-particle collisions on general discrete grids and introduce an appropriate representation for nonlinear and linearized collision operators. Furthermore we establish the concept of the pseudo-inverse. In Section 3 we investigate the moment system and give arguments why discrete models on (small) grids can only be expected to yield useful results in the small

* Tel.: +49 0 3677693616.
E-mail address: hans.babovsky@tu-ilmenau.de.

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Mach number limit. Applying the classical Chapman–Enskog procedure we derive the Navier–Stokes system. Section 4 is devoted to 2D velocity models with rotational symmetry. We derive systems comparable to the *single relaxation time* (SRT) and to the *multiple relaxation time* (MRT) models used in Lattice Boltzmann schemes. A few numerical examples in Section 5 illustrate the use of the nine-velocity system in the context of collisional dynamics.

2. Discrete kinetic models: mathematical framework

2.1. The nonlinear collision operator

Let $\mathcal{I}$ be a finite index set, $|\mathcal{I}| = N$ and define $\mathcal{V} = \{\mathbf{v}_i,\ i \in \mathcal{I}\} \subset \mathbb{R}^d$ ($d \in \{2, 3\}$) as a set of N pairwise different points ("velocities") in $\mathbb{R}^d$. Suppose given a quadruple $\alpha = (i, j, k, l) \in \mathcal{I}$. We call a transition

$$(\mathbf{v}_i, \mathbf{v}_j) \leftrightarrow (\mathbf{v}_k, \mathbf{v}_l) \tag{2.1}$$

between velocity pairs a *two-particle collision*. The collision is called *momentum and energy conserving* (short: an *elastic collision*), if

$$\mathbf{v}_i + \mathbf{v}_j = \mathbf{v}_k + \mathbf{v}_l, \tag{2.2}$$

$$|\mathbf{v}_i|^2 + |\mathbf{v}_j|^2 = |\mathbf{v}_k|^2 + |\mathbf{v}_l|^2. \tag{2.3}$$

The following result is well known and elementary.

Lemma 2.1. *The collision is elastic iff the polygon connecting* $\mathbf{v}_i, \mathbf{v}_k, \mathbf{v}_j, \mathbf{v}_l$ *is a rectangle in* $\mathbb{R}^d$.

Related to the collision is the nonlinear *elementary collision operator* $J_\alpha : \mathbb{R}^{\mathcal{V}} \to \mathbb{R}^{\mathcal{V}}$,

$$(J_\alpha f)_m = \begin{cases} f_k f_l - f_i f_j & \text{for } m \in \{i, j\} \\ f_i f_j - f_k f_l & \text{for } m \in \{k, l\} \\ 0 & \text{for } m \in \mathcal{I} \setminus \{i, j, k, l\} \end{cases} \tag{2.4}$$

i.e. $J_\alpha f = (f_k f_l - f_i f_j) \cdot \mathbf{s}_\alpha$, with the α-index vector $\mathbf{s}_\alpha$ defined by

$$\mathbf{s}_\alpha = \mathbf{e}_i + \mathbf{e}_j - \mathbf{e}_k - \mathbf{e}_l, \tag{2.5}$$

with $\mathbf{e}_m$ being the m-th canonical unit vector in $\mathbb{R}^{\mathcal{V}}$. In the following, $\mathcal{A} \subset \mathcal{I}^4$ denotes the set of all quadruples $\alpha = (i, j, k, l)$ corresponding to elastic collisions. Writing elements $\mathbf{v}$ of $\mathcal{V}$ componentwise in the form $\mathbf{v} = (v_x, v_y)$ for $d = 2$ resp. $\mathbf{v} = (v_x, v_y, v_z)$ for $d = 3$, we define the moment vectors $m_i \in \mathbb{R}^N,\ i = 0, \ldots, d + 1$ by

$$m_0 = \mathbb{1} = (1, \ldots, 1)^T, \tag{2.6}$$

$$m_1 = \mathbf{v}_x = (v_x, \mathbf{v} \in \mathcal{V})^T, \tag{2.7}$$

$$m_2 = \mathbf{v}_y = (v_y, \mathbf{v} \in \mathcal{V})^T, \tag{2.8}$$

$$m_3 = \mathbf{v}_z = (v_z, \mathbf{v} \in \mathcal{V})^T \quad (\text{if } d = 3), \tag{2.9}$$

$$m_{d+1} = 0.5\mathbf{v}^2 = (0.5|\mathbf{v}|^2,\ \mathbf{v} \in \mathcal{V})^T, \tag{2.10}$$

the matrix

$$M := (m_i,\ i = 0, \ldots, d + 1) \in \mathbb{R}^{N \times (d+2)}, \tag{2.11}$$

and the subspace

$$\mathcal{M} = \operatorname{span}(m_i,\ i = 0, \ldots, d + 1) \subseteq \mathbb{R}^{\mathcal{V}}. \tag{2.12}$$

An immediate consequence of the conservation laws (2.2) and (2.3) is

Lemma 2.2. $\alpha \in \mathcal{A} \Leftrightarrow M^T \mathbf{s}_\alpha = 0 \Leftrightarrow \mathbf{s}_\alpha \in \mathcal{M}^\perp$.

Definition 2.3. (a) A subset $\mathcal{A}_0 \subseteq \mathcal{A}$ is called *regular*, if

$$\operatorname{span}(\mathbf{s}_\alpha,\ \alpha \in \mathcal{A}_0) = \mathcal{M}^\perp. \tag{2.13}$$

(b) A *collision operator* $J : \mathbb{R}^{\mathcal{V}} \to \mathbb{R}^{\mathcal{V}}$

$$J := \sum_{\alpha \in \mathcal{A}} \pi_\alpha J_\alpha \tag{2.14}$$

with *collision frequencies* $\pi_\alpha \geq 0$ is called *regular* if the set $\mathcal{A}_J := \{\alpha \in \mathcal{A} : \pi_\alpha > 0\}$ is regular.