ARTICLE IN PRESS

Computers and Mathematics with Applications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Normal, high order discrete velocity models of the Boltzmann equation☆

Stefan Brechtken, Thomas Sasse *

Technische Universität Ilmenau, Fakultät für Mathematik und Naturwissenschaften, Fachgebiet für Numerik und Informationsverarbeitung, Germany

ARTICLE INFO

Article history:
Received 21 February 2017
Received in revised form 14 September 2017
Accepted 16 September 2017
Available online xxxx

Keywords:
Boltzmann equation
Discrete velocity model
DVM
Collision operator

ABSTRACT

This paper aims at approximations of the collision operator in the Boltzmann equation. The developed framework guarantees the "normality" of the approximation, which means correct collision invariants, H-Theorem, and equilibrium solutions. It fits into the discrete velocity model framework, is given in such a way that it is understandable with undergraduate level mathematics and can be used to construct approximations with arbitrary high convergence orders. At last we give an example alongside a numerical verification. Here the convergence orders range up to 3 (2) and the time complexity is given by $3+\frac{1}{2}(4+\frac{2}{3})$ in 2 (3) dimensions.

1. Introduction

The Boltzmann equation is a basic integro-differential equation in the kinetic gas theory. It mainly describes the statistic distribution of particles in a medium. This equation is primarily used if the mean free path of the particles becomes large compared to the characteristic length of the system under consideration. One typically uses the simpler equations of continuum mechanics if this condition is not met, for example the Navier–Stokes equations. On the other hand there needs to be a sufficient amount of particles in a given volume in order to do the statistics which give the Boltzmann equation its validity. If this condition is not met one comes into the field of molecular dynamics where one begins to describe every single particle and their interactions. Due to the position of the Boltzmann equation in between the macroscopic (Navier–Stokes) and the microscopic (molecular dynamics) regime this equation is called a mesoscopic equation.

Most numerical computations of the Boltzmann equation are based on probabilistic Monte Carlo techniques, which lead to direct simulation Monte Carlo methods (DSMC), or special collision models such as Bhatnagar–Gross–Krook (BGK) together with the discretization of the velocity space, which lead to lattice Boltzmann methods (LBM). Due to the low computational costs and the wide field of applications these approaches have proven their potential in computational physics. However, they can have problems in situations where high Mach numbers or compressible fluids occur and one needs to avoid numerical fluctuations which originate in the use of random sequences. So we are primarily interested in a deterministic classical approximation of the collision operator. We hoped to find a sufficiently flexible framework in the field of *discrete velocity framework* s (DVM) so we investigated the current situation. One of the first results regarding consistency and normality was [1], followed by lower bounds of the convergence orders in [2] for the 3D case and [3] for the 2D case. Until

☆ This work was funded by the German Research Foundation (DFG) (BA 922/11-2).

* Corresponding author.
E-mail addresses: stefan.brechtken@tu-ilmenau.de (S. Brechtken), thomas.sasse@tu-ilmenau.de (T. Sasse).

https://doi.org/10.1016/j.camwa.2017.09.024
0898-1221/

now typical proven convergence orders for the direct approximation of the collision operator were $\frac{1}{14}$, $\frac{6}{7}$, 1 [2,4,5]. We had to realize that there exists no general or flexible DVM approach, thus our research group devised one.

We started with an alternative approach based on the so called *lattice group model* (LGpM) that was introduced by Babovsky in [6,7]. Further development of these LGpMs was done by Babovsky in [8–11] and a parallelized high performance implementation which resulted in promising simulation results was done in [12,13]. When confronted with the fact that we lack a proper convergence proof, we tried to prove that the LGpMs are a specific subclass of the *discrete velocity models* (DVM). In this process it turned out that the original LGpM is indeed a subclass of the DVMs but does not converge towards the collision operator. We then realized, that the LGpM can be seen as a model reduction. We were able to construct the *extended lattice group model* (eLGpM) that can be seen as a subclass of DVMs and possess some minimal properties, [14, Section 2.2]. Moreover it became clear that we were able to transform every converging DVM (possessing some minimal properties) into an eLGpM, when applying some minor adjustments. By realizing this, all convergence proofs regarding DVMs were instantly transferred to eLGpMs.

In this paper we present a framework that allows one to use any quadrature formula that works on given discretization points and we prove the main properties of the resulting scheme. By doing this we disclose some essential connections between the minimal properties of the discretized collision operator, symmetries of the grid used for the discretization and symmetries of the resulting scheme. This framework can be used to construct direct high order discretizations possessing some minimal properties and it gives large degrees of freedom for further optimization. Last but not least we have to remark that while the results presented in this paper originate in the Ph.D. thesis [14] of one of the authors, this thesis and one of the corresponding papers [15] contain two significant errors in the discretization of the collision operator in 3D. These errors resulted in the non differentiability of the integrand negating every result on convergence orders of discretizations. This paper fixes these problems. The ansatz alongside the proofs is significantly simplified and in order to avoid further errors we implemented the 3D discretizations and conducted a thorough numerical verification of the theoretical results. This paper is organized in such a way that all proofs were exiled into Appendix in order to increase the readability. We start with a short recap of basic concepts regarding DVMs followed by the theory behind our framework. Finally we give a recipe for the application of this framework and we verify our findings by taking a look at an actual implementation.

2. DVM basics

The Boltzmann equation is given by

$$(\partial_t + \mathbf{v}\cdot\nabla_{\mathbf{x}})f(\mathbf{x},\mathbf{v},t) = \alpha\cdot I_c[f](\mathbf{x},\mathbf{v},t), \quad (\mathbf{x},\mathbf{v},t)\in\mathbf{D}\subset\mathbb{R}^d\times\mathbb{R}^d\times\mathbb{R}, \alpha\in\mathbb{R}^+.$$

The collision operator is given by

$$I_c[f](\mathbf{v}) = \int_{\mathbb{R}^d}\int_{S^{d-1}} \left[f(\mathbf{v}_1')f(\mathbf{w}_1') - f(\mathbf{v})f(\mathbf{w}_1)\right] k(\mathbf{v}-\mathbf{w}_1,\eta)\ \mathrm{d}\eta\,\mathrm{d}\mathbf{w}_1, \tag{1}$$

with the dimensionality $d\in\{2,3\}$ and

$$\mathbf{v}_1' := \mathbf{v} + \langle\overrightarrow{\mathbf{vw}_1},\eta\rangle\eta, \qquad \mathbf{w}_1' := \mathbf{w}_1 - \langle\overrightarrow{\mathbf{vw}_1},\eta\rangle\eta,$$

where $\mathbf{v},\mathbf{w}$ can be seen as the velocities of particles before they collide and $\mathbf{v}',\mathbf{w}'$ are the velocities after a collision. Microscopic momentum and energy conservation result in the given formulas for $\mathbf{v}',\mathbf{w}'$. The unit vector $\eta\in\mathcal{S}^{d-1}$ can be seen as the unit vector parallel to the diagonal connecting the centres of the particles during the instant of collision. The variable α corresponds to the Knudsen number and can be ignored for the scope of this work. The collision angle

$$\Theta := \langle\overrightarrow{\mathbf{ww}},\eta\rangle / \|\overrightarrow{\mathbf{ww}}\|_2 \tag{2}$$

is the angle between η and $\overrightarrow{\mathbf{ww}}$. Moreover the collision operator only lives on the velocity space, so we ignore the other dependencies most of the time. In this paper bold characters correspond to 2 (3) dimensional vectors and large bold letters to sets from which the small ones originate. Small Latin letters with indices are components of a vector, so v_1 is the first component of $\mathbf{v}$.

DVMs typically aim at a direct approximation of the collision operator through transformations and quadrature formulas or similar integral approximations. This involves a discretization of the velocity space. In this paper we use subsets of

$$\hat{\mathbf{V}} := \{\mathbf{v}\in\mathbb{R}^d \mid v_j\in\Delta v\cdot\mathbb{Z}, j=1,\dots,d\}, \quad \Delta v\in\mathbb{R}^+.$$

To avoid problems that are associated with an infinite velocity space, we only use

$$\mathbf{V} := \hat{\mathbf{V}}\cap B_{\frac{L}{2}}(\mathbf{0}), \qquad M_{\mathbf{V}} := \{0,\dots,\|\mathbf{V}\|-1\}, \tag{3}$$

for sufficiently large $L\in\mathbb{R}^+$.
Using these definitions one can rewrite velocity space discretizations of the Boltzmann equation in the form of general DVMs (cf. [16]). With $i\in M_{\mathbf{V}}$ this form is given by

$$(\partial_t + \mathbf{v}_i\cdot\nabla_{\mathbf{x}})f_i(\mathbf{x},t) = \sum_{j,k,l\in M_{\mathbf{V}}} A_{i,j}^{k,l}\left(f_k(\mathbf{x},t)f_l(\mathbf{x},t) - f_i(\mathbf{x},t)f_j(\mathbf{x},t)\right) =: J_i[f](\mathbf{x},t).$$

Please cite this article in press as: S. Brechtken, T. Sasse, Normal, high order discrete velocity models of the Boltzmann equation, Computers and Mathematics with Applications (2017), https://doi.org/10.1016/j.camwa.2017.09.024.