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Galerkin–Petrov approach for the Boltzmann equation

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ABSTRACT

In this work, we propose a new Galerkin–Petrov method for the numerical solution of the classical spatially homogeneous Boltzmann equation. This method is based on an approximation of the distribution function by associated Laguerre polynomials and spherical harmonics and test in a variational manner with globally defined three-dimensional polynomials. A numerical realisation of the algorithm is presented. The algorithmic developments are illustrated with the help of several numerical tests.

1. Introduction

In this paper, we propose a new Galerkin–Petrov method for the numerical solution of the classical spatially homogeneous Boltzmann equation. This method is based on an approximation of the distribution function by associated Laguerre polynomials and spherical harmonics. The test functions are polynomials defined globally in $\mathbb{R}^3$. This choice leads to a rapid numerical scheme with a high spectral accuracy for smooth solutions.

Deterministic methods for the Boltzmann equation have been extensively studied in the last decades. Overview of these methods can be found, for example, in the book of V. Aristov [3] and in a more recent review by A. Narayan and A. Klöckner [39]. Since the pioneering work of D. Goldstein, B. Sturtevant and J.E. Broadwell [27], many authors proposed different ideas on how to derive a discrete version of the Boltzmann collision operator [40], [48], [51], [46], [41], [42]. In [34] the authors studied the difference scheme for a mixture of gases. L. Pareschi and G. Russo [44], [45] considered deterministic spectral methods for the Boltzmann equation based on the Fourier transform. In our paper, we limit our consideration to a particular class of deterministic methods, namely, those based on mesh-free Galerkin–Petrov discretisation. The main difficulty within the deterministic approximation of the Boltzmann collision integral, besides its high dimensionality, is the fact that a grid for the integration over the velocity space $\mathbb{R}^3$ is not suitable for the integration over the set of all directions, i.e., over the unit sphere S^2. In the case of a regular tensor discretisation of the velocity space with n points in each direction, only $\mathcal{O}(n)$ irregularly distributed integration points would belong to the unit sphere. A. Bobylev, A. Palczewski and J. Schneider [12] considered this direct approximation of the Boltzmann collision integral and showed that the corresponding numerical method is consistent. This method requires $\mathcal{O}(n^7)$ arithmetical operations per time step and has the formal accuracy of $\mathcal{O}(n^{-1/2})$. A. Bobylev and S. Rjasanow considered the case of the Maxwell pseudo-molecules and utilised an explicit simplification of the Boltzmann equation for this model of interaction alongside with the Fast Fourier Transform (FFT) to develop a deterministic numerical method [13], [14]. Their method requires $\mathcal{O}(n^4)$ arithmetical operations per time step and achieves the same low formal accuracy order of $\mathcal{O}(n^{-1/2})$. A similar method was proposed by L. Pareschi and B. Perthame in [43]. It appears to be the fastest known deterministic numerical method on a uniform grid. At the same time, its appli-

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cations are strongly restricted to the case of Maxwell pseudo-molecules. Considering the case of hard spheres, A. Bobylev and S. Rjasanow [15] developed an algorithm, where the integration over the unit sphere is completely separated from the integration over the whole space $\mathbb{R}^3$. The resulting scheme utilises fast evaluation of the generalised Radon and X-Ray transforms via the FFT and requires $\mathcal{O}(n^6 \log(n))$ operations per time step with the high formal accuracy of $\mathcal{O}(n^{-2})$. A further development of this approach in [24] led to spectral schemes for more general collision kernels with a higher efficiency. I. Ibragimov and S. Rjasanow in [30] used a special form of the Boltzmann collision operator, which led to a possibility to omit numerical integration over the unit sphere. This idea was later used by I.M. Gamba and S.H. Tharkabhushanam [25], [26], to handle the granular inelastic Boltzmann equation. It was developed further in the recent paper [23] for most general collision cross-section with anisotropic angular scattering that includes grazing collisions approximating the Landau collision operator. These methods have also been extended to treat systems of Boltzmann equations for gas mixtures and multi-energy level gases (see [38], [53]). In these extensions of the scheme, the Langrange multiplier method is employed to enforce the total conservation properties associated with the mixture. The first result on error estimates and convergence to Boltzmann–Maxwell equilibrium states for Lagrangian based conservative spectral methods for the Boltzmann equation with elastic interactions and hard potential with angular cut-off collision kernels was published in [2]. A survey of this subject can be found in [22]. While the majority of authors use an uniform grid in the velocity space, in [29] A. Heintz, P. Kowalczyk and R. Grzhibovskis have used a non-uniform grid.

Reviews of an already substantial amount of publications on the Discrete Velocity Models (DVM) for the Boltzmann equation can be found in [7] and in [9]. Constructive ideas in this area have been recently proposed by H. Babowsky and his co-authors in [4], [5]. Two recent ideas regarding the deterministic solution of the Boltzmann equation are the use of the Galerkin schemes based on global basis functions, see [33] and unpublished manuscript [21] and the approximation by means of three-dimensional algebraic tensors [31], [6]. We refer to the recent monograph by B. Shizgal [50] devoted to the spectral methods and an enormous amount of cited literature therein.

The approach most similar to ours can be found in [19]. Its realisation for a rather simple isotropic situation is published in [20].

The same approximation, with a non-zero mean velocity, has been used in the recent work [17] for a theoretical study of the linearised Boltzmann collision operator. However, it is also necessary to mention classical papers from 1935 by D. Burnett [16] where the Laguerre polynomials have been used and from 1949 by H. Grad [28] with an approximation of the distribution function by the use of the Hermite polynomials. He was also able to compute the moments of this approximation exactly.

The main advantages of our method in contrast to the previous methods are:

- We use basis and test functions globally defined in the velocity space. No discretisation of the velocity space for the approximation of the distribution function is necessary. Thus the number of degrees of freedom is very low, in our tests it was at most 729.
- The mass matrix and the collision matrices are precomputed for the given collision kernel and for different degrees of the polynomials. They can be used then for different initial conditions and different time integration schemes. This reduces the computational time significantly. The same matrices can be used for spatially inhomogeneous problems, see [32].
- The scheme is fully conservative by its nature. No additional work is necessary in contrast to our previous papers [14], [15], [30], [25], [26].
- The computation of the moments of the approximation can be done analytically due to the polynomial nature of the basis functions.

However, the choice of the basis functions as global polynomials, similar to the methods based on trigonometrical approximation, can not guarantee the positivity of the approximation. We don't consider this drawback as serious since the negative values appearing in the approximation of the distribution functions are all in the tails and, therefore, are very small. See also the further remarks in Section 5 concerning the computation of the H-functional.

This paper is organised as follows. In Section 2, we give a short description of an initial value problem for the Boltzmann equation and present different collision kernels. In Section 3, an abstract version of Galerkin–Petrov method for a general bilinear operator is formulated. We describe a set of basis and test functions in terms of classical polynomials and spherical harmonics. Furthermore, the mass and collision matrices are presented in all details. A numerical realisation of the algorithm is described in Section 4. Here, we use a numerical integration for the entries of the mass and collision matrices and describe possible time integration schemes. Finally, in Section 5, we present the results of numerical computations done by the new method for different initial value problems and different collision kernels. Conclusions and an outlook can be found in Section 6.

2. Boltzmann equation

We consider the initial value problem for the classical spatially homogeneous Boltzmann equation

$$\frac{\partial}{\partial t} f(t, v) = Q(f, f)(t, v), \quad t \in \mathbb{R}_+, \ v \in \mathbb{R}^3, \tag{1}$$