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Conservative numerical methods for model kinetic equations

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Abstract

A new conservative discrete ordinate method for nonlinear model kinetic equations is proposed. The conservation property with respect to the collision integral is achieved by satisfying at the discrete level approximation conditions used in deriving the model collision integrals. Additionally to the conservation property, the method ensures the correct approximation of the heat fluxes. Numerical examples of flows with large gradients are provided for the Shakhov and Rykov model kinetic equations.

1. Introduction

Correct description of rarefied gas flows is based on the Boltzmann kinetic equation for the molecular velocity distribution function. Since this integro-differential equation is exceedingly complicated due to the presence of the nonlinear multidimensional collision integral much attention has been given to simpler model kinetic equations. These equations are constructed by replacing the exact collision integral by an approximate model collision integral. Examples include the Krook or BGK [6], Holway [12] and Shakhov [26,28] model equations for monatomic gases as well as Holway [12] and Rykov [24] model equations for diatomic gases.

Numerical solution of kinetic equations requires the use of conservative methods suitable in a broad range of Knudsen numbers (including transitional and low Knudsen numbers) and for both steady and unsteady flow regimes. In recent years considerable progress has been made in devising such methods for the kinetic equation with the exact Boltzmann collision integral [7,23,5]. For model equations the situation is less clear. Conservative discrete ordinate methods proposed for simple monatomic BGK and Holway model equations [22,11] cannot be extended directly to the Shakhov and Rykov models. A rather sophisticated correction procedure was applied in [10] to the Shakhov model collision integral at each time step in such a way as to satisfy the conservation property. Its generalization to other models has not been reported. No conservative method has so far been developed for diatomic models.

The purpose of this paper is to present an exceedingly simple and universal approach to the construction of conservative discrete ordinate methods for model kinetic equations. The approach is an extension of [33] and is based on the approximation of the constrains used in deriving the model equations. Therefore, it can be used for virtually any model kinetic equation. We provide a detailed explanation of the idea as applied to the Shakhov model equation and then extend it to the Rykov model equation.

We consider two numerical examples: a cylindrical Couette flow and a supersonic transverse flow over a plate, both for a wide range of Knudsen numbers from free-molecular to near-continuum regime. The presented results illustrate the sensitivity of the method to the choice of the molecular velocity mesh as well as provide a study of aerodynamic properties of the plate and distribution of the macroscopic parameters.

2. Monatomic gases

2.1. Construction of model equations

For monatomic gases a general approach to the construction of model kinetic equations was proposed in

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[25,28] and is based on the idea of approximating the exact Boltzmann kinetic equation in terms of momentum equations. In other words few first momentum equations should coincide for the model and exact kinetic equations. As a result, a sequence of model kinetic equations can be developed by increasing the order of moments for which the approximation condition holds.

Let us write the model kinetic equation for the velocity distribution function f in the following form:

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial \boldsymbol{r}} = Q(f, \boldsymbol{\xi}, \boldsymbol{a}). \tag{1}$$

Here $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)$ is the molecular velocity vector, t is time, $\boldsymbol{r} = (x_1, x_2, x_3)$ is the spatial coordinate, $\boldsymbol{a}$ is an unknown vector of macroscopic parameters which depends on the chosen model equation. Since the differential parts of the exact and model equations are the same, the approximation condition means that first few moments J_ϕ of exact collision integral $J(f,f)$ coincide with the first few moments of the model collision integral $Q(f, \boldsymbol{a}, \xi)$:

$$\int \phi Q(f, \boldsymbol{a}, \xi) \mathrm{d}\boldsymbol{\xi} = \int \phi J(f,f) \mathrm{d}\boldsymbol{\xi} = J_\phi, \tag{2}$$

where

$$\phi = 1, \xi_i, \xi^2, \xi_i\xi_j, \xi_i\xi_j\xi_k, \ldots.$$

Alternatively one can use

$$\phi = 1, v_i, v^2, v_iv_j, v_iv_jv_k, \ldots, \quad \boldsymbol{v} = \boldsymbol{\xi} - \boldsymbol{u}.$$

As is common in construction of model kinetic equations for the monatomic gas it is assumed that the approximation condition (2) should be satisfied for the Maxwellian molecules only. Then the moments J_ϕ can be evaluated analytically and we can express the vector $\boldsymbol{a}$ via the integrals of the velocity distribution function:

$$\boldsymbol{U}(\boldsymbol{a}) = \int \boldsymbol{b}(\boldsymbol{\xi}) f \,\mathrm{d}\boldsymbol{\xi}, \tag{3}$$

where $\boldsymbol{U}$ is a certain function of macroscopic parameters and $\boldsymbol{b}(\boldsymbol{\xi})$ is a vector function of the molecular velocity $\boldsymbol{\xi}$.

2.2. The model of Shakhov

The Shakhov model kinetic equation is a generalization of the Krook model equation in that the approximation condition (2) is satisfied not only for 1, ξ_i, ξ^2, $\xi_i\xi_j$, but also for $\xi_i\xi^2$. This ensures the correct relaxation of both the heat flux and stresses, leading thus to the correct continuum limit in the case of small Knudsen numbers. In particular, the model gives the correct Prandtl number. Comparisons of different monatomic model equations with experimental data and the finite-difference solution of the Boltzmann equation with the exact collision integral shows the Shakhov model to be more accurate than the BGK and Holway models [38,30].

In the rest of the paper we use the non-dimensional form of the kinetic equations in which non-dimensional spatial variable r, time t, number density n, velocities $\boldsymbol{u}$ and $\boldsymbol{\xi}$, temperature T, viscosity μ, heat flux $\boldsymbol{q}$ and distribution function f are given by

$$r' = \frac{r}{L}, \quad t' = \frac{t\sqrt{2RT_\infty}}{L}, \quad n' = \frac{n}{n_\infty},$$
$$\boldsymbol{u}' = \frac{\boldsymbol{u}}{\sqrt{2RT_\infty}}, \quad \boldsymbol{\xi}' = \frac{\boldsymbol{\xi}}{\sqrt{2RT_\infty}}, \quad T' = \frac{T}{T_\infty},$$
$$\mu' = \frac{\mu}{\mu_\infty}, \quad \mathbf{q}' = \frac{\mathbf{q}}{mn_\infty(2RT_\infty)^{3/2}}, \quad f' = \frac{f}{n_\infty(2RT_\infty)^{-3/2}}. \tag{4}$$

Here L is a typical spatial scale of the problem, R is the gas constant, n_∞, T_∞ – some characteristic values of gas density and temperature; m is the molecule mass, λ_∞ is the mean free path related to μ_∞ by

$$\mu_\infty = \frac{5}{16} mn_\infty\sqrt{2\pi RT_\infty}\lambda_\infty.$$

Below we shall use the conventional notation for all variables meaning the non-dimensional quantities.

In the non-dimensional form the Shakhov model collision integral is given by [26,28]

$$Q(f, \boldsymbol{\xi}, \boldsymbol{a}) = \nu f^+ - \nu f, \quad \nu = \frac{8}{5\sqrt{\pi}} \frac{1}{Kn} \frac{nT}{\mu},$$
$$f^+ = f_M \left[1 + \frac{4}{5}(1 - Pr) \frac{2\boldsymbol{qv}}{nT^2} \left(\frac{v^2}{T} - \frac{5}{2}\right)\right], \tag{5}$$
$$f_M = \frac{n}{(\pi T)^{3/2}} \exp\left(-\frac{v^2}{T}\right).$$

Here f_M is the locally Maxwellian function, $Kn = \lambda_\infty/L$ and Pr are the Knudsen and Prandtl numbers, respectively. The vector of unknown parameters in the model collision integral $\boldsymbol{a} = (n, \boldsymbol{u}, T, \boldsymbol{q})^{\mathrm{T}}$ containing number density n, temperature T and vectors of gas velocity $\boldsymbol{u}$ and heat flux $\boldsymbol{q}$ can be calculated as

$$\boldsymbol{U}(\boldsymbol{a}) = \left(n, n\boldsymbol{u}, \frac{3}{2}nT + nu^2, 2\boldsymbol{q}\right) = \int (1, \boldsymbol{\xi}, \xi^2, \boldsymbol{v}v^2) f \,\mathrm{d}\boldsymbol{\xi}. \tag{6}$$

Since the expression for f^+ contains the third-order polynomial of $\boldsymbol{\xi}$ the distribution function f may become negative at the tails. Although a possible loss of positivity is a drawback from the theoretical point of view, it does not affect the robustness of the model in practical applications because $f \to 0$ as $|\xi| \to \infty$. For example, see [3] for the numerical study of exceedingly strong shock waves (Mach numbers up to 100) and [34] for calculation of the hypersonic *transverse* flow over a cold plate with free-stream Mach numbers up to $M_\infty = 30$. Moreover, according to the Godunov theorem [9]. second-order advection schemes with linear operators often used in practice [1,34] are not monotone and may generate the negative values of f even for the BGK model, further diminishing the importance of strict theoretical positivity.

The H theorem for the Shakhov model can be proven only for flows with small departures from equilibrium [28].