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The NR*xx* method for polyatomic gases

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ABSTRACT

In this paper, we propose a numerical regularized moment method to solve the Boltzmann equation with ES-BGK collision term to simulate polyatomic gas flows. This method is an extension to the polyatomic case of the method proposed in [12], which is abbreviated as the NR*xx* method in [11]. Based on the form of the Maxwellian, the Laguerre polynomials of the internal energy parameter are used in the series expansion of the distribution function. We develop for polyatomic gases all the essential techniques needed in the NR*xx* method, including the efficient projection algorithm used in the numerical flux calculation, the regularization based on the Maxwellian iteration and the order of magnitude method, and the linearization of the regularization term for convenient numerical implementation. Meanwhile, the particular integrator in time for the ES-BGK collision term is put forward. The shock tube simulations with Knudsen numbers from 0.05 up to 5 are presented to demonstrate the validity of our method. Moreover, the nitrogen shock structure problem is included in our numerical experiments for Mach numbers from 1.53 to 6.1.

1. Introduction

The kinetic theory has long been playing an important role in the rarefied gas dynamics. As a mesoscopic theory standing between the fluid dynamics and the molecular dynamics, the kinetic theory is built on the basis of the Boltzmann equation, which uses a distribution function to give a statistical description of the distribution of microscopic particles' velocities. The Boltzmann equation describes the rarefied gas effects accurately. However, the high dimensionality and the complex collision term of the Boltzmann equation introduce great difficulties in solving it numerically, and currently, a popular numerical solver of the Boltzmann equation is the method of direct simulation of Monte Carlo (DSMC) proposed by Bird [6]. The DSMC method is introduced in detail in textbook [7], and some improved versions have been proposed in [19,20,26,22,14]. Since the DSMC method is a stochastic solver which is difficult to give smooth numerical solutions, and its efficiency in the simulation of dense or unsteady flows is still to be improved, people are looking for some other ways to approximate the Boltzmann equation.

In 1940s, Grad [15] proposed the idea using the Hermite expansion to approximate the distribution function, and a 13-moment theory was given in detail in [15]. Recently, based on the idea of Grad, systems with large numbers of moments together with their numerical schemes are considered in [9,12,11], where some regularizations inspired by [31,29] are also taken into account. In [11], the numerical regularized moment method is abbreviated as the NR*xx* method, where "N" stands for "numerical", "R" stands for the regularization, and "*xx*" means the undetermined number of moments following

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the names of R13, R20 and R26 moment equations. However, all these works concentrate only on the monatomic gases, and in this paper, we will develop the NRxx method for the polyatomic case.

The study to apply the moment method to polyatomic gases can be traced back to McCormack [23], where a 17-moment model was proposed. As far as we know, the most recent polyatomic extension of Grad's 13-moment equations is the work of Mallinger [21], whose system contains only 14 moments. In both models, a great amount of work is devoted to the deduction of the collision terms. In order to generalize the moment theory to large number of moments, we prefer a BGK-like simplified collision operator. As in the monatomic case, the simplest BGK model fails to give correct heat conduction, and for polyatomic gases, it also gives incorrect relaxation collision number, resulting in qualitative errors in temperatures compared with the Boltzmann equation [3]. Possible alternatives include the Rykov model [27] and the ES-BGK model [4], which incorporate proper local equilibrium distribution functions and relaxation collision frequencies to fix the above deficiencies.[1] In this work, our investigation is restricted to the ES-BGK model.

For polyatomic gases, besides the velocities of microscopic particles, an additional nonnegative ordinate representing the energy of internal degrees of freedom appears in the distribution function. Thus, in order to expand the distribution function into series, the basis functions are chosen as a combination of Hermite polynomials and Laguerre polynomials with proper translation and scaling based on the macroscopic velocity and translational and rotational temperatures of the gas. By considering the coefficients of the basis functions as moments, a system with infinite number of moment equations is derived. A moment closure is then followed to truncate the system with infinite equations and get a system with only finite equations. The framework for the moment closure is the same as [12]:

1. the Maxwellian iteration is applied to determine the order of magnitude for each moment;
2. by dropping higher order terms, the truncated moments are expressed by moments with lower orders;
3. for easier numerical implementation, the expression is linearized around a Maxwellian.

However, the details of the Maxwellian iteration are significantly different. In the polyatomic case, the iteration is much more complicated than the monatomic case because of the existence of both translational and rotational temperatures in the basis functions, and the process should be conducted carefully. Moreover, for the ES-BGK model, analysis on the moments of the Gauss distribution also increases the complexity. Fortunately, the final result remains a similar form as simple as in [12].

As to the numerical scheme, the general framework in [11] is applicable. A split scheme is applied to divide the convective movement terms and colliding relaxation terms, and the transportation part is processed by a finite volume method. Recalling that a special "projection" introduced in [9,11] is required in the calculation of numerical fluxes, we further develop this technique to the polyatomic case in this paper. Meanwhile, the polyatomic ES-BGK collision term can no longer be solved analytically as the BGK operator [9], and the Crank–Nicolson scheme is applied to ensure the unconditional numerical stability. Our numerical experiments show that our scheme correctly converges to the solution of the Boltzmann equation as the number of moments increases. The distinction between BGK and ES-BGK models, together with the relation between monatomic and polyatomic cases, is illustrated by the numerical results of shock tube problems. Also, we apply the NRxx method to the nitrogen shock structure problem, and the results are comparable to the experimental data.

The rest of this paper is arranged as follows: in Section 2, a brief review of the polyatomic ES-BGK model is given. In Section 3, the polyatomic NRxx method is introduced comprehensively, and in Section 4, a number of numerical experiments are carried out to validate our algorithm. As a summation, some concluding remarks are given in Section 5. Finally, some involved calculations are collected in Appendices A–C for better readability to the body matter.

2. The ES-BGK Boltzmann equation for polyatomic gases

The ES-BGK model for polyatomic gases, which gives correct Navier–Stokes heat conduction compared with the BGK model, has been deduced in [4,8]. The polyatomic ES-BGK Boltzmann equation reads

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}} f = \Pr \cdot \frac{p}{\mu}(G - f), \tag{2.1}$$

where f denotes the molecule distribution, which is a positive function $f = f(t, \boldsymbol{x}, \boldsymbol{\xi}, I)$ with $\boldsymbol{x}, \boldsymbol{\xi} \in \mathbb{R}^3$ and $t, I \in \mathbb{R}^+$. The parameters t, $\boldsymbol{x}$ and $\boldsymbol{\xi}$ stand for the time, spatial position and microscopic molecule velocity respectively, and I is an internal energy parameter. In the right hand side of (2.1), Pr is the Prandtl number, p is the pressure, and μ denotes the viscosity coefficient. G is a generalized Gaussian defined as

$$G(t, \boldsymbol{x}, \boldsymbol{\xi}, I) = \frac{\rho \Lambda_\delta}{\sqrt{\det(2\pi \mathcal{T})}(RT_{\mathrm{rel}})^{\delta/2}} \exp\left(-\frac{1}{2}(\boldsymbol{\xi} - \boldsymbol{u})^T \mathcal{T}^{-1}(\boldsymbol{\xi} - \boldsymbol{u}) - \frac{I^{2/\delta}}{RT_{\mathrm{rel}}} \right). \tag{2.2}$$

[1] The Rykov model can be considered as a polyatomic version of the Shakhov model [28]. Some comparison between the Shakhov model and the ES-BGK model can be found in [18].