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An asymptotic preserving Monte Carlo method for the multispecies Boltzmann equation

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ABSTRACT

An asymptotic preserving (AP) scheme is efficient in solving multiscale kinetic equations with a wide range of the Knudsen number. In this paper, we generalize the asymptotic preserving Monte Carlo method (AP-DSMC) developed in [25] to the multispecies Boltzmann equation. This method is based on the successive penalty method [26] originated from the BGK-penalization-based AP scheme developed in [7]. For the multispecies Boltzmann equation, the penalizing Maxwellian should use the unified Maxwellian as suggested in [12]. We give the details of AP-DSMC for multispecies Boltzmann equation, show its AP property, and verify through several numerical examples that the scheme can allow time step much larger than the mean free time, thus making it much more efficient for flows with possibly small Knudsen numbers than the classical DSMC.

1. Introduction

Boltzmann type kinetic equations with a wide range of spatial and temporal scales arise in many important applications from astronautics, nuclear engineering, semiconductor device modeling to plasma physics. Take the space shuttle reentry problem for example, the vehicle will pass from free streaming, rarefied gas, transition to continuum regimes, during which the particle mean free path varies from $O(1)$ to about 10^{-8} meters. Numerical simulation of such multiscale problems is daunting. Another challenge comes from the high dimensionality of such phase space models which are six dimensional equations plus time. Direct Simulation Monte-Carlo (DSMC) is the most popular choice [1], yet it suffers from huge computational expenses since one needs to resolve the small mean free time (or Knudsen number) temporally when the vehicles are near the earth, in the so-called fluid dynamic regime. Although in this regime one could use the macroscopic models such as the compressible Euler or Navier–Stokes equations, these equations are invalid in the rarified regime at which the Knudsen number is large.

In recent years, the development of asymptotic-preserving schemes [10], for multiscale kinetic and transport equations, has seen a rapid growth [11,6]. The idea of AP schemes is to develop the schemes that preserve the asymptotic transition from the kinetic models to the macroscopic fluid or diffusion models, which also need to be efficient for time discretization.

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Table 1
Dimensionless variables and the corresponding reference values.

Name	Physical variable	Dimensionless variable	Reference value
Position	$\tilde{x}$	x	L
Velocity	$\tilde{v}$	v	$\bar{c}=\sqrt{\frac{8kT}{\pi m}}$
Time	$\tilde{t}$	t	$\tau=L/\bar{c}$
Relative velocity	$\tilde{g}$	g	$\bar{g}=\sqrt{2}\bar{c}$
Collision cross-section	$\tilde{\sigma}$	σ	πd^2
Distribution function	$\tilde{f}$	f	$f_c=n/C^3$

In particular one favors a scheme in which the time step is independent of the mean free time (or Knudesn number) [10]. These AP schemes are attractive since they do not need the coupling of kinetic and fluid models in the domain-decomposition setting [3,4,9,13,2,15].

For the multiscale Boltzmann equation, a time efficient AP scheme was proposed by Filbet–Jin [7], with the idea of penalizing the nonlinear, nonlocal Boltzmann collision operator by the BGK relaxation operator whose implicit discretization can be implemented *explicitly*. The AP property and positivity can be strengthened by a successive penalization as proposed by Yan and Jin [26]. Such idea can be used for multiscale Boltzmann equation as was done by Jin and Li [12]. Another approach is based on exponential Runge–Kutta approach, see [16,8]. See also [17]. Attempts to develop AP Monte Carlo methods can also be found in [22,23,21].

In this article, we extend the AP-DSMC developed in [25] for single species Boltzmann equation to the multispecies Boltzmann equation. This work is mainly motivated by developing highly efficient Monte carlo scheme for multiscale flow fields related to reentry problems or hypersonic vehicles [18,14] where the gas is usually considered as a binary mixture of Oxygen and Nitrogen. For the multispecies system, the conservation laws break down for each single species. When using the BGK penalization approach, the *unified* Maxwellian which depends on the mean velocity and mean temperature is found to be suitable in the penalization [12]. We illustrate the AP property of our scheme, and in addition, several multispecies examples are used to test our proposed method which will be compared with the conventional DSMC. The numerical results show that the proposed method not only has the ability of capturing the macroscopic behavior in flow dynamic regimes, as well as the rarified regime, more importantly, it is much more efficient than DSMC in the cases of stiff collision process since the AP-DSMC does not need to resolve the small Knudsen number numerically. The numerical results demonstrate that the proposed method is very promising in engineering applications.

The rest of the paper is organized as follows. In Section 2, we briefly describe the Boltzmman equation for the multispecies system and its basic properties. Next, we give details of the AP-DSMC scheme for the multispecies Boltzmman equation in Section 3 and discuss its asymptotic behavior in the fluid dynamic regime. We present several examples to show the performance of the proposed method in Section 4 and make conclusive remarks in Section 5.

2. The multispecies models

2.1. The multispecies Boltzmann equation

The multispecies Boltzmann equation describes the time evolution of the density distribution of a dilute gas that has more than two components whose particles usually have different masses. In this paper, we are interested in developing efficient numerical scheme for the nonlinear N-species Boltzmann equation which is given by

$$\frac{\partial \tilde{f}_i}{\partial \tilde{t}}+\tilde{v}\cdot\nabla_{\tilde{x}}\tilde{f}_i=\tilde{Q}_i\left(\tilde{f},\tilde{f}\right),\ t\geq 0,\ \left(\tilde{x},\tilde{v}\right)\in R^d\times R^d,\ 1\leq i\leq N, \tag{1}$$

where $\tilde{f}_i=\tilde{f}\left(\tilde{x},\tilde{v},\tilde{t}\right)$ is a nonnegative distribution function of the i-th species which move at time $\tilde{t}$, position $\tilde{x}$ with velocity $\tilde{v}$. $\tilde{Q}_i$ is the collision operator to be defined later. Some useful dimensionless variables and the corresponding reference values are listed in Table 1, where d and n denote the molecular diameter and the number density respectively. $k=1.380622\times 10^{23}$ is Boltzmann constant. By introducing dimensionless quantities (see Table 1), Eq. (1) can be rewritten in a dimensionless form,

$$\frac{L}{\tau\bar{c}}\frac{\partial f_i}{\partial t}+v\cdot\nabla_x f_i=\frac{\tilde{\sigma}ngL}{\bar{c}}Q_i\left(f,f\right),\ t\geq 0,\ x\in R^{d_x},\ v\in R^{d_v},\ 1\leq i\leq N, \tag{2}$$

where $St=L\,/\,(\tau\bar{c})$ is Strouhal number which is usually set to unity. Given the relation of $\frac{\bar{c}}{\tilde{\sigma}ng}=\frac{\bar{c}}{\nu}=\lambda$, the Knudsen number $\varepsilon=\lambda\,/\,L$ defined as the ratio of the mean free path λ over a typical length scale L can be obtained to measure the rarefiedness of the gas. Therefore, a dimensionless form of the equation is given as follows

$$\frac{\partial f_i}{\partial t}+v\cdot\nabla_x f_i=\frac{1}{\varepsilon}Q_i\left(f,f\right),\ t\geq 0,\ x\in R^{d_x},\ v\in R^{d_v},\ 1\leq i\leq N. \tag{3}$$