An asymptotic-preserving Monte Carlo method for the Boltzmann equation ☆

Wei Ren [a], Hong Liu [a,*], Shi Jin [b,c]

[a] J.C. Wu Center for Aerodynamics, School of Aeronautics and Aerospace, Shanghai Jiao Tong University, 800 Dong Chuan Road, Shanghai 200240, China
[b] Department of Mathematics, Institute of Natural Sciences and MOE Key Lab in Scientific and Engineering Computing, Shanghai Jiao Tong University, 800 Dong Chuan Road, Shanghai 200240, China
[c] Department of Mathematics, University of Wisconsin–Madison, 480 Lincoln Drive, Madison, WI 53706, USA

A B S T R A C T

In this work, we propose an asymptotic-preserving Monte Carlo method for the Boltzmann equation that is more efficient than the currently available Monte Carlo methods in the fluid dynamic regime. This method is based on the successive penalty method [39], which is an improved BGK-penalization method originally proposed by Filbet and Jin [16]. Here we introduce the Monte Carlo implementation of the method, which, despite its lower order accuracy, is very efficient in higher dimensions or simulating some complicated chemical processes. This method allows the time step independent of the mean free time which is prohibitively small in the fluid dynamic regime. We study some basic properties of this method, and compare it with some other asymptotic-preserving Monte Carlo methods in terms of numerical performance in different regimes, from rarefied to fluid dynamic regimes, and their computational efficiency.

1. Introduction

1.1. Background: numerical methods for the Boltzmann equation

In the study of flows which span a wide range of flow regimes, i.e. in atmospheric re-entry problems, the density distribution $f(t, x, v)$ of a dilute gas at position x, with velocity v and at time t, is governed by the Boltzmann equation [5,9]:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f), \quad x \in \mathbb{R}^{d_x}, \ v \in \mathbb{R}^{d_v}. \tag{1.1}$$

In Eq. (1.1), the bilinear collision operator $Q(f, f)$ describes the binary collisions of the particles and is defined by

$$Q(f, f)(v) = \int_{\mathbb{R}^{d_v}} \int_{\mathbb{S}^{d_v - 1}} \sigma(|v - v_1|, \omega) [f(v')f(v'_*) - f(v)f(v_*)] d\omega dv_*, \tag{1.2}$$

where ω is a unit vector on the sphere $\mathbb{S}^{d_v-1}$. The collision operator $Q(f,f)$ can also be rewritten as

$$Q(f,f)(v) = Q^+(f,f) + f Q^-(f),\tag{1.3}$$

where Q^+ denotes the gain term and Q^- is the loss term:

$$\begin{cases} Q^+(f,f) = \int\limits_{\mathbb{R}^{d_v}} \int\limits_{\mathbb{S}^{d_v-1}} \sigma\big(|v - v_1|, \omega\big) f(v') f(v'_*) d\omega dv_* \\ Q^-(f) = \int\limits_{\mathbb{R}^{d_v}} \int\limits_{\mathbb{S}^{d_v-1}} \sigma\big(|v - v_1|, \omega\big) f(v_*) d\omega dv_*. \end{cases}\tag{1.4}$$

The velocity (v', v'_*) represents the post-collisional velocities whose relation to the pre-collisional velocities (v, v_*) are given by

$$\begin{cases} v' = \dfrac{1}{2}\big(v + v_* + |v - v_*|\omega\big), \\ v'_* = \dfrac{1}{2}\big(v + v_* - |v - v_*|\omega\big). \end{cases}\tag{1.5}$$

In Eq. (1.2), σ is the nonnegative collision kernel which depends on the model of forces between particles, and we also define the total cross section σ_T as (see [5] for more details)

$$\sigma_T\big(|v - v_*|\big) = \int\limits_{\mathbb{S}^{d_v-1}} \sigma\big(|v - v_*|, \omega\big) d\omega.\tag{1.6}$$

Meanwhile, one can refer to Chapman and Cowling [10] for the details of several models, such as the inverse power force model and the Lennard-Jones model. In the case of inverse kth power force between particles, it has the form

$$\sigma\big(|v - v_*|, \theta\big) = b_\alpha(\theta)|v - v_*|^\alpha,\tag{1.7}$$

where $\alpha = (k - 5)/(k - 1)$. In numerical simulation of rarefied gases, the variable hard sphere (VHS) model is often used, in which, $b_\alpha(\theta) = C_\alpha$, where C_α is a positive constant. The case $\alpha = 0$ corresponds to the Maxwellian gas, while the case $\alpha = 1$ represents the hard sphere gas.

With f, the macroscopic *density ρ, mean velocity u, and temperature T*, can be obtained by taking the moments:

$$\rho = \int\limits_{\mathbb{R}^{d_v}} f dv, \qquad u = \frac{1}{\rho} \int\limits_{\mathbb{R}^{d_v}} v f dv, \qquad T = \frac{1}{d_v \rho} \int\limits_{\mathbb{R}^{d_v}} |v - u|^2 f dv.\tag{1.8}$$

Moreover, the collision operator (1.2) satisfies some important properties:

- Conservation laws:

$$\int\limits_{\mathbb{R}^{d_v}} Q(f,f)\phi(v) dv = 0, \quad \text{for } \phi(v) = 1, v, |v|^2;$$

  which gives conservation of mass, momentum and total energy.
- Boltzmann's *H* theorem [36]:

$$\frac{d}{dt} \int f \log f dv = \int Q(f,f) \log f dv \leq 0,$$

  which implies that any system reaches its equilibrium state at which the entropy $-\int f \log f dv$ is maximum. The equilibrium distribution function has the form of a local Maxwellian distribution:

$$\mathcal{M}(\rho, u, T)(v) = \frac{\rho}{(2\pi T)^{d_v/2}} \exp\left(-\frac{|u - v|^2}{2T}\right).\tag{1.9}$$

The Knudsen number ε in (1.1), as a parameter of great significance in the kinetic theory, is the ratio of the local mean free path ℓ in gases to the characteristic length scale. For a small value of ε, the Chapman–Enskog expansion connects the Boltzmann equation (1.1) with hydrodynamic equations, i.e., the compressible Navier–Stokes equations (the first order approximation) and the compressible Euler equations (the zeroth order approximation). By taking $\varepsilon \to 0$, $f \to \mathcal{M}$, then one can obtain the hydrodynamic Euler equations