

MONTE CARLO METHOD FOR THE SPATIALLY HOMOGENEOUS BOLTZMANN EQUATION

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ABSTRACT. This work presents a Monte Carlo computational approach for solving the spatially homogeneous nonlinear Boltzmann equation through a modified “particle-in-cells” model. Building upon the Belotserkovski-Yanitski and Kac models, the paper introduces a stochastic simulation scheme that synthesizes the principle of splitting operators with branching Markov processes. The method constructs unbiased estimators with small variance to compute molecular velocities and particle distributions, providing higher numerical accuracy and physical realism compared to traditional linear models. The developed algorithm enables efficient simulation of rarefied gas dynamics and demonstrates stable results across varying particle densities. Computational experiments, including shock wave structure modeling, show that this approach achieves improved convergence and fidelity in approximating spatially heterogeneous Boltzmann behavior.

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Key words: Spatially Homogeneous Boltzmann equation, Particle-in-Cell Model, Branching Markov process, Monte Carlo Method, Unbiased Estimator, Conjugated Computational Schemes

1. Introduction

This paper studies and proposes statistical algorithms for solving the nonlinear integral Boltzmann equation in measures, which describes the physical processes of particle collisions and coalescence. The equations under consideration are one of the integral forms of the kinetic equations of rarefied gas dynamics. Markov processes with simple interactions are used to construct unbiased estimates for the solution of the kinetic equation of rarefied gas dynamics. The well-known relationship between nonlinear integral equations and branching Markov processes is exploited [1].

Recently, many studies have explored the application of the Monte Carlo method to solving such problems. The proposed computational scheme is analogous to the adjoint scheme in the linear case. The proposed scheme is examined in detail for the case of "rigid" molecules. To describe the scheme, it is convenient to switch from an equation in measures to an equation in densities. Various computational schemes are considered and their effectiveness compared. The resulting computational schemes are tested in solving a problem of shock wave structure. A statistical algorithm is proposed using the nonlinear spatially homogeneous Boltzmann equation for the numerical implementation of the "particle-in-cell" statistical model, and methods for constructing unbiased, minimal-variance estimates for calculating the particle velocity in each cell are investigated.

2. Description of the Problem

Let's consider a nonlinear integral equation

$$F_t(dr, du) = F_0(dr - ut, du) \exp\{-H(r, u)t\} + \int_0^t [\exp\{-H(r, u)(t-s)\}] \times \\ \times \iint_D T_{t-s}(dr, du; r_1, u_1, r_2, u_2) H(r_1, u_1) F_s(dr_1, du_1) F_s(dr_2, du_2). \quad (1)$$

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where $(r, u) \in R \times R^3$, $(r_i, u_i) \in D$, $i = 1, 2$, $t \in R^1$, F_t and F_0 are measures in D , $H(r, u)$ is a non-negative function, $T_{t-s}(B, r_1, u_1, r_2, u_2)$ is a measurable function of the arguments (r_1, u_1, r_2, u_2) , at fixed B , and at fixed (r_1, u_1, r_2, u_2) is a measure in D . The measures F_t, F_0, T_{t-s} are considered non-negative.

Many works are dedicated to studying this kind of equation (for example [2], [3]), where probabilistic features of solutions of this type of equation were studied. Equations of the type (1) represent one of the integral forms of kinetic equations for rarefied gas dynamics. The questions of existence and uniqueness of the solution of equation (1) were studied in [3,4]. It's known [3], that if F_0 and T_{t-s} are probabilistic measures and $H(r, u) < c = \text{const}$, then equation (1) has a unique nonnegative solution, which will be a probability measure. Existence and sub stochasticity of the minimal nonnegative solution of the equation (1) were also proven in [3]. In [2] authors constructively built a random process whose one-dimensional distribution satisfied equation (1). The advantages of this (unlike to problems mentioned above) allowed using a Monte Carlo method. His method of constructing unbiased estimators is a method of "direct modeling". The advantage of the constructed computational scheme is that it permits the estimating of several functionals of the solution to equation (1) at one time. The disadvantage of this method is the difficulty constructing the random process that gives the minimal variance. Currently, this problem is not solved for that case. In the theory of Monte-Carlo methods, there are methods (like "importance sampling") that allow one to avoid these difficulties when solving concrete problems.

Below, for equations (1) we present the construction methods for unbiased estimators for functional of the type (h, f) , where $h(r, u, t)$ is a given function and $f(r, u, t)$ is a density of the measure F_t . The computational scheme that we derive here is an analogue of the conjugated scheme in the linear case. Furthermore, we will call this scheme a "conjugated scheme". It is shown that the application of the results of Ermakov and others [2] allow the construction of a computational scheme with small variance, in particular, when a prior information on solution of equation (1) is known. When applying the above scheme to real physical problems, we must also show the statistics conservation of mass, impulse and energy.

3. Construction of unbiased estimators

As is known, [5] among the statistical methods, which use Monte Carlo directly for modeling the flow of rarefied gas, the most efficient one is the statistical method of direct modeling the nonstationary flow. In [6], they described a statistical "particle-in cell" model, which was constructed base on the synthesis of ideas of splitting the physical processes in each Δt . This method was used by Harlow [7], and in statistical interpretations by Berd [8] and Kac [9]. The specific of the "particle-in-cell" method are the following. The state of every particle is characterized by vectors of coordinates r and speeds u at time, $k\Delta t$, where $k = 0, 1$. A discrete random process

$$\{r(t), u(t)\} = \{r_1(t), u_1(t), \dots, r_N(t), u_N(t)\}$$

should be constructed in the heterogeneous coordinate space at each time $k|\Delta t$. Here N is the number of molecules of monatomic gas in some volume, D . The principle of splitting operator is used for constructing the random process $r(t), u(t)$.

The sampling divides into two steps. Monte Carlo method is used both for the numerical simulation of collisions of the particles in cells (the first step), as well as for the collision-free motion (free-molecular) of particles (the second step). For the numerical realization of the second step in [10] an algorithm is given, which does not require saving the corresponding spatial coordinates of the particles. For the numerical realization of the first step, spatially homogenous model of Kac has been used. Thus, the synthesis of the idea of splitting, and model of Kac has occurred. That gives rise to the Markov model, which approximates the Boltzmann equation with accuracy that depends statistically (condition of molecular chaos) on the number of particles. In [11], Yanitski explained the value of the principle of splitting. The computational approach of Belotserkovski-Yanitski [6] is as efficient as the method of Berd, but has higher accuracy in approximating the Boltzmann equation. It's important to emphasize that "particle-in-cell" the statistical model of Belotserkovski-Yanitski is physical closer to the real problem. As new propose yet another computational scheme, which directly uses the nonlinear spatially homogenous Boltzmann equation for the numerical realization of the first step in the "particles-in-cell" model of Belotserkovski-Yanitski. The method of constructing unbiased estimators with small variance is next given for calculating of a velocity of a single molecule $u(k\Delta t)$ for $k = 0, 1, 2, \dots$

To find the velocity of the particle in each cell, we will use equation (1) in the spatially homogenous case. In this case, equation (1) has the form

$$\begin{aligned} F_{\Delta t}(du) = & F_0(du) \exp\{-H(u)\Delta t\} + \int_0^{\Delta t} ds \exp\{-H(u)(\Delta t - s)\} \times \\ & \times \iint_D T_{\Delta t-s}(du; u_1, u_2) H(u_1) F_s(du_1) F_s(du_2). \end{aligned} \quad (2)$$

where $F_0(du)$, $F_t(du)$ are distribution particle velocity at time 0 and t respectively. Let $H(u) = c = \text{const}$. As is known [4], this equation has a unique positive solution that is a probabilistic measure, and the iterative method starting with $F_0(du) \exp\{-c\Delta\}$ converges to the solution of equation (2). This is why we can apply the approach that was developed in [12] to equation (2). In [4], a direct computational scheme for solving equation (2) with certain side conditions was given. The results of [4] cannot be applied in our case, since the direct scheme, as given in [4], cannot estimate the value at the point (cell). In [4] a functional is estimated, not a point value.

Let's suppose that when the initial distribution, $F_0(du)$, has a density, the distribution $F_{\Delta t}(du)$ also has a density, $f(u, \Delta t)$. Making the transformation, which is analogous to the transformations [13], we obtain the following equation

$$\begin{aligned} f(u, \Delta t) = & f(u, 0) \exp\{-ct\} + \int_0^{\Delta t} ds \int d\bar{\omega} \int du_c \times \\ & \times (1 - \exp\{-c\Delta t\}) f_1(s) \frac{|u - u_c|c}{c} f(u_c - |u - u_c|\bar{\omega}, s) f(u_c + |u - u_c|\bar{\omega}, s) \times \\ & \times 0^{\Delta t} ds \int_{\mathbb{R}^3} (1 - \exp\{-c\Delta t\}) f_1(s) \left(1 - \frac{|u - u_c|c}{c}\right) f(u, s) f(u_2, s) du_2. \end{aligned} \quad (3)$$

For equation (3), we construct a branching Markov process, and thus we can derive various "conjugated" computational schemes for calculating a unbiased estimator of the functional (h, f) . Since $u = (u_x, u_y, u_z)$, we suppose $h(u, t) = u_x$, i.e. at time, Δt , the velocity is computed by the following formula

$$U(\Delta t) = \int u_x f(u, \Delta t) du$$

Now we describe the computational scheme. At time, Δt , one particle is born with initial density $p_0(u)$ at the point $(u, \Delta t) = (u_x, u_y, u_z, \Delta t)$. Here, the estimator has the form $\xi_{\Delta t}(u) = \frac{u_x}{p_0(u)}$. Further, with probability $\alpha_0(\Delta t) = \exp\{-c\Delta t\}$, the particle is absorbed at the point $(u, \Delta t)$, here estimator is computed by the formula $\xi_{\Delta t}(u) \leftarrow \varepsilon_{\Delta t}(u) f(u, 0)$.

If particle hasn't been absorbed, then the time $s_1 \in [0, \Delta t]$ is simulated with the probability density

$$f_1(s) = \frac{c \exp\{-c(\Delta t - s)\}}{1 - \exp\{-c\Delta t\}}.$$

Then with probability $\alpha_1(\Delta t) = \beta(1 - \exp\{c\Delta t\})$, where $\beta \in [0, 1]$, two particles will appear at the points $(u_c - |u - u_c|\varpi, s_1)$ and $(u_c + |u - u_c|\varpi, s_1)$. Here ϖ is an isotropic vector. The transition from u to u_c is done with the transition density $\psi_1(u_c)$. The density distribution at the point (u_c, s_1) , under the condition that collision has taken place (velocity changes), we'll write in the form of $P_1(u, \Delta t \rightarrow u_c, s_1) = f_1(s)\psi_1(u_c)$. Here the estimator is computed with the formula

$$\xi_{\Delta t}(u) \rightarrow \frac{\xi_{\Delta t}(u)(2|u - u_c|)\psi_1(u_c)}{\beta c}.$$

Further, with probability $\alpha_2(\Delta t) = (1 - \exp\{-c\Delta t\})(1 - \beta)$ two particles are created at the points (u, s_1) and (u_2, s_1) . Transition from u to u_2 is done with transition density $\psi_1(u_2)$. The density distribution of the point (u_2, s) with velocity remaining constant, can be written in the form $P_2(u, \Delta t \rightarrow u_2, s_1) = f_1(s)\psi_1(u_2)$. In this case the estimator is computed by the formula

$$\xi_{\Delta t}(u) \leftarrow \xi_{\Delta t}(u) \left(1 - \frac{|u - u_2|}{c}\right) (1 - \beta)^{-1} (\psi_1(u_2))^{-1}$$

Furthermore, new particles behave the same as the initial particle. Moreover, $s_0 = 0$, $s_k \in [0, t - \sum_{i=0}^{k-1} s_i]$, $t \leftarrow t - \sum_{i=0}^{k-1} s_i$, the moments of time s_k are chosen with probability density $f_1(s)$. At each step, the times $s_1, s_2, \dots$ are chosen and the process finishes, when all particles are absorbed, or the condition $t - \sum s_i \leq \varepsilon$, where ε is a small number which was given beforehand, is satisfied.

Applying the results of [13] to equation (3), we derive the following assertion. If a process is given with an initial density

$$P_0(u, \Delta t) = \frac{|u_x f(u, \Delta t)|}{(|u|_x, |f(u, \Delta t)|)},$$

the transition density

$$P_1(u, \Delta t \rightarrow u_c, s_1) = f_1(s) \frac{(2|u - u_c|c)}{c} f(u_c - |u - u_c|, s) \frac{f(u_c + |u - u_c|, s)}{f(u, \Delta u)}$$

$$P_2(u, \Delta t \rightarrow u_2, s_1) = f_1(s) \left(1 - \frac{|u - u_c|c}{c}\right) \frac{f(u, s)f(u_2, s)}{f(u, \Delta t)}$$

and absorption probability

$$g(u, \Delta t) = \frac{f(u, 0)}{f(u, t)} \exp\{-c\Delta t\}$$

then the variance of estimator $\xi_{\Delta t}(u)$ will be the solution to equation (3).

Now, let's study the construction of unbiased estimators with small variance, using [14] and known data on the solution at $t \rightarrow \infty$. It's known [15] that as $t \rightarrow \infty$ the gas approaches the equilibrium state. Then features of the gas do not depend on spatial coordinates or time. In this case, the solution of equation (3) has the form (Maxwellian)

$$f(u) = \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{u^2}{2}\right) \quad (4)$$

For large t , the solution of our problem is close to (4). If we put (4) into expressions for P_1 and P_2 this determines a Markov process. And gives us a use the small variance estimator $\xi_{\Delta t}(u)$. The density distribution of the point (u_c, s_1) , when collision has taken place. When particle velocities change, has the form

$$\tilde{P}_1(u, \Delta t \rightarrow u_c, s) = f_1(s) \frac{1}{(2\pi)^{3/2}} \exp\left\{-(u_c^2 + |u - u_c|^2) + \frac{u^2}{2}\right\}$$

If we make a change of variables in the following way: $\tilde{v} = 2v = 2(u_c - u)$, then we get for

$$\tilde{P}_1\left(u, \Delta t \rightarrow \frac{\tilde{v}}{2} + u, s_1\right) = f_1(s) \frac{1}{(2\pi)^{3/2}} \exp\left\{-\frac{(\tilde{v} - u)^2}{2}\right\} \quad (5)$$

and for the point (u_2, s_1) , the collision has taken place (case of constant velocity) and the expression for the density distribution, $\tilde{P}_2$, can be written as

$$\tilde{P}_2(u, \Delta t \rightarrow u_2, s_1) = f_1(s) \frac{1}{(2\pi)^{3/2}} \exp\left\{-\frac{u_2^2}{2}\right\} \quad (6)$$

here

$$g(u, \Delta t) = \exp\{-c\Delta t\} \quad (7)$$

Thus, velocities $\bar{v}$ and u_2 are distributed according to a normal law with densities

$$\psi_1(\bar{v}) = \frac{1}{(2\pi)^{3/2}} \exp\left\{-\frac{(\bar{v} - u)^2}{2}\right\}, \quad \psi_2(u_2) = \frac{1}{(2\pi)^{3/2}} \exp\left\{-\frac{u_2^2}{2}\right\}$$

and the optimal transition densities have the form (5), (6), (7).

For the construction of this algorithm, which is connected with densities (5), (6), (7), it is more convenient to apply equation (3), after the following change of variables

$$f(u, t) = \frac{1}{2} \psi(u) \varphi(u, \Delta t).$$

Here $\psi(u)$ is a known function, which is defined by (4). The computational scheme is simple. Because in computing the estimators there is no need to use weights that are larger than ours. Thus for (3) we derive

$$\begin{aligned} \varphi(u, \Delta t) &= \varphi(u, 0) \exp\{-c\Delta t\} + \int_0^{\Delta t} ds \int d\bar{\omega} \int_{R^3} du_c (1 - \exp\{-c\Delta t\}) \times \\ &\times f_1(s) \frac{(2|u - u_c|c)}{2c} \frac{\psi(u_c - |u - u_c|\bar{\omega})\psi(u_c + |u - u_c|\bar{\omega})}{\psi(u)} \times \\ &\times \varphi(u_c - |u - u_c|\bar{\omega}, s) \varphi(u_c + |u - u_c|\bar{\omega}, s) + \\ &+ \int_0^{\Delta t} ds \int_{R^3} du_2 (1 - \exp\{-c\Delta t\}) f_1(s) \left(1 - \frac{|u - u_c|c}{c}\right) \times \\ &\times \frac{1}{2} \frac{\psi(u)\psi(u_2)}{\psi(u)} \varphi(u, s) \varphi(u_2, s). \end{aligned} \quad (8)$$

where $u_c = u + \frac{\tilde{v}}{2}$. The algorithm for constructing the unbiased estimator $U(\Delta t) = \int u_x f(u, \Delta t) du$ described as follows. At time, Δt , one particle with initial density $p_0(u)$ at the point $(u, \Delta t) = (u_x, u_y, u_z, \Delta t)$ appears. The

particle at the point $(u, \Delta t)$ has a statistical "weight", which is equal to $\xi_{\Delta t}(u) = \frac{u_x}{p_0(u)}$. Furthermore, at the point $(u, \Delta t)$ the unbiased estimator, $\xi_{\Delta t}(u)$, is constructed for the considered equation in the following way. With probability $g(u, \Delta t) = \exp\{-c\Delta t\}$, the particle is absorbed at the point $(u, \Delta t)$. The estimator is computed by the formula $\xi_{\Delta t}(u) \leftarrow \varphi(u, 0)\xi_{\Delta t}(u)$. If the particle has not been absorbed, the time $s_1 \in [0, \Delta t]$ is simulated with probability density $f_1(s)$. Then, with probability $\frac{(1 - g(u, \Delta t))}{2}$ two particles appeared at points $\left(\left(\frac{\tilde{v}}{2} + u + \frac{\tilde{v}}{2}\tilde{\omega}\right), s_1\right)$ and $\left(\left(\frac{\tilde{v}}{2} + u - \frac{\tilde{v}}{2}\tilde{\omega}\right), s_1\right)$. Here the vector $\tilde{v} = u + \eta$, where η is sampled with a standard normal density. Here the estimator is computed by $\xi_{\Delta t}(u) \leftarrow \frac{\xi_{\Delta t}(u)|\tilde{v}|c}{8c}$. Furthermore, with probability $\frac{(1 - g(u, \Delta t))}{2}$ two particles appear at the points (u, s_1) and (u_2, s_1) . Here the vector u_2 is sampled from a standard normal distribution. In this case, the estimator is computed as $\xi_{\Delta t}(u) \leftarrow \xi_{\Delta t}(u) \left(1 - \frac{|u - u_c|c}{c}\right)$.

New particles behavior is the same as the original particles. The process finishes, when all particles are absorbed, or at $\Delta t - \sum s_i \leq \varepsilon$. When process completes, the estimator $\xi_{\Delta t}(u)$ is multiplied by a value of function $\frac{1}{2}\psi(u)$ at the point $(u, \Delta t)$, i.e. $\xi_{\Delta t}(u) \leftarrow \frac{\xi_{\Delta t}(u)\psi(u)}{2}$. Thus, in each cell we compute the velocity at each time, $k\Delta t$, where $k = 0, 1, 2, \dots$

4. Computational experiment

As is known, the nonlinear Boltzmann equation describes the behavior of rarefied gas much better than the linear Kac model. This is why we can expect that application of the nonlinear spatially homogenous Boltzmann equation in the "particles-in-cell" model allows us to do a computation, which gives a more exact approximation to the spatially heterogeneous Boltzmann equation.

We underline that boundary conditions at infinity can be taken into consideration by the method [6]. There computations show that the results of modeling are similar with known [5] solutions of the Boltzmann equation. As an example, computations for the wave shock structure have been done.

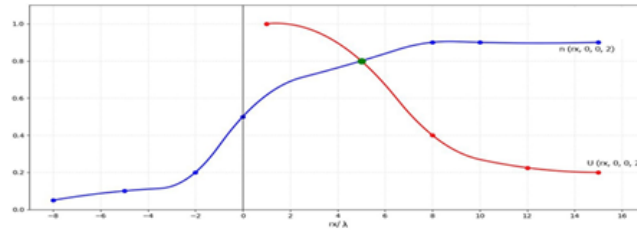


Figure 6: The calculated profile of density is $n(r_x, 0, 0, 2)$ and velocity is $u(r_x, 0, 0, 2)$. r_x is x axis.

The figure shows two graphs of density and velocity. The vertical line is the y-axis. Mach number is $M = 2$. The confidence level is 97%. The calculation was made with the following parameters. The number of particles in cells is $N1 = 8$. The ratio $\Delta t/\Delta r_x$, where $\Delta r = (\Delta r_x, \Delta r_y, \Delta r_z)$, is chosen for numerical stability. The parameters for the problem are the following:

$$t = 2, \Delta r_x = \Delta r_y = \Delta r_z = 0.2, \lambda = 1.$$

We note that in interval, where the Boltzmann equations "work" (intermediate interval), the "particle-in-cell" statistical model approximates the spatially heterogeneous Boltzmann equation better. At the same time, the approximation is independent at the number of particles, in D (even if a volume will only have one particle).

5. Conclusion

First, we note that for equation (3) we could apply a simple iterative process. For the computation of the integrals, which are obtained in the first and the second iteration, we can directly apply the Monte Carlo method. When comparing the density profiles at the first and the second iterations we noticed very little bias. This can be explained by the fact the iteration process to (3) converges slowly.

The next Direct Simulation Monte Carlo is a well-established method for the computer simulation of a gas flow at the molecular level. The Bird's Direct Simulation Monte Carlo (DSMC) method is a powerful computational technique for modeling rarefied gas flows. It was introduced fifty years ago and, since that time, most DSMC procedures have been superseded or significantly modified. By method Monte Carlo particle collisions, DSMC can accurately capture

non-equilibrium effects that are often present in rarefied flows. Further investigations and developments in this area were explored in the following papers [16,17,18].

The last is, gas dynamics problems can serve as examples of problems whose solution requires the use of modern multiprocessor computers. In particular, the multidimensional Boltzmann equation requires such technology for its solution. The complex nature of the kernel of this equation and the dependence of the solution on many variables necessitated the use of the Monte Carlo method. This method, as is well known, is particularly convenient for multiprocessor computers and allows for natural parallelization. Above, we describe an algorithm for solving the initial-boundary value problem for the Boltzmann equation, which could be effectively implemented on parallel computing systems.

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