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MONTE CARLO SOLUTION OF THE NONLINEAR KINETIC BOLTZMANN EQUATION

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We study a nonlinear integral equation of Boltzmann type for a nonnegative measure and discuss a Monte Carlo representation based on a branching Markov process. Under an explicit absolute-continuity assumption, the measure equation is written as an equation for a density. The collision model used in the derivation is a regularized, spatially localized kernel; the velocity transformation in the displayed collision law preserves the relative speed and kinetic energy of a pair and therefore represents elastic, isotropic scattering rather than inelastic collisions. We derive the time-sampling density associated with the constant collision rate and identify the normalization factor required when the collision integral is transformed to spherical coordinates with a normalized angular measure. We also describe the importance-sampling factors that enter the path weights. The shock-wave calculation is retained as a preliminary numerical illustration. The currently available figures and parameter list do not, by themselves, establish unbiasedness of the truncated estimator, finite variance, conservation of macroscopic moments, quantitative agreement with a reference solution, or computational superiority over an iterative method. Those properties require the convergence, conservation, and uncertainty checks specified in the text.

Keywords: Monte Carlo method, nonlinear Boltzmann equation, regularized collision kernel, branching Markov process, importance sampling, shock-wave structure

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1 Introduction

The Boltzmann equation is a fundamental kinetic model for dilute gases. Its collision operator is high-dimensional and nonlocal in velocity, which makes accurate numerical solution difficult, especially in non-equilibrium regimes such as shock waves. Established numerical approaches include deterministic discretizations of the collision operator and particle-based stochastic methods. The direct simulation Monte Carlo (DSMC) method developed by Bird approximates molecular transport and collisions by a stochastic particle process; a related direct-simulation formulation was derived from the Boltzmann equation by Nanbu [1, 2]. Convergence analysis for DSMC and benchmark studies of shock-wave profiles provide reference points for assessing numerical methods [3–8].

Benchmark validity nevertheless depends on matching the intermolecular model and thermodynamic assumptions. Döntgen [9] studied freely propagating shocks in monoatomic gases with non-Boltzmann energy distributions and showed that the assumed energy distribution can alter the effective heat-capacity ratio and shock-propagation

speed. Because that study combines a different physical model with atomistic molecular-dynamics simulations, it is relevant to model-sensitivity analysis rather than a direct reference profile for the present regularized kinetic equation.

Recent hybrid approaches should also be distinguished from the present branching estimator. Luo and Wu [10] coupled the general synthetic iterative scheme with DSMC to accelerate convergence toward steady-state rarefied flows. Kim and Jun [11] presented a consistent comparison of DSMC, Fokker–Planck, and hybrid FP–DSMC solvers for high-speed rarefied flows, reporting speed-ups for their benchmark cases. These results motivate matched-accuracy and matched-cost comparisons; they do not establish a speed-up for the estimator studied here. DSMC and the hybrid methods cited above simulate gas flow through particle-based or coupled solvers, whereas the present formulation targets functionals of a nonlinear integral equation through a branching representation.

A second relevant line of work represents nonlinear kinetic equations using Markov and branching processes. The mathematical basis for such representations is developed in the literature on random processes for equations of mathematical physics and on nonlinear Markov processes [12–15]. More recent adjoint-oriented studies address Boltzmann-constrained optimization and topology optimization for rarefied gas flows [16, 17]; these are related methodological developments, but their objectives and estimators are not identical to the branching estimator considered here. Nekrutkin discussed direct and adjoint Monte Carlo schemes for nonlinear Boltzmann equations [13]; therefore, the contribution of the present work must be understood relative to those constructions and to the authors' earlier work [18]. The term *adjoint scheme* is used here for the proposed backward-in-time construction. It should not be interpreted as a claim that the method is new in the general sense: the specific transition law, path weights, and conditions under which the estimator is valid must be compared explicitly with the earlier schemes.

The purpose of this paper is to formulate a branching Monte Carlo representation for a regularized Boltzmann-type integral equation, make the normalization and importance-sampling factors explicit, and examine its use in a preliminary computation of a one-dimensional shock-wave density profile. The collision kernel considered below is localized in the relative position by an indicator of a ball of radius ε_x. The angular velocity transformation in equation (6) preserves the magnitude of the relative velocity and hence the kinetic energy of a pair; the model is therefore an elastic-scattering model with a regularized spatial collision probability, not an inelastic-molecule model.

The methodological points clarified in this paper are: (i) the distinction between the measure equation and the density equation, including the assumptions required for the latter; (ii) normalization of the time density and the angular collision integral; and (iii) the importance-sampling factors needed when the auxiliary position and velocity variables are sampled from proposal densities. The numerical section is treated as a preliminary demonstration rather than as a validated performance comparison. In particular, the available calculations do not provide a reproducible estimate of bias, variance, computational cost at matched accuracy, or conservation defects. We therefore do not claim quantitative superiority over an iterative method. These quantities must be measured before the method can be considered numerically validated.

The paper is organized as follows. Section 2 states the regularized measure equation and derives its density form. Section 3 describes the branching representation and its weights, while distinguishing the ideal estimator from a finite-depth or time-truncated implementation. Section 4 discusses the shock-wave test case and identifies the checks

needed for a quantitative validation. The conclusion summarizes the established formulation and the remaining numerical verification tasks.

2 Problem statement and method

We consider the nonlinear integral equation

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

Here $(r,u)\in\mathbb{R}^3\times\mathbb{R}^3$, $(r_i,u_i)\in D$, $i=1,2$, and $t\geqslant 0$. The measures F_t and F_0 are defined on phase space D. The function $H(r,u)$ is nonnegative. For fixed (r_1,u_1,r_2,u_2), the map $B\mapsto T_{t-s}(B;r_1,u_1,r_2,u_2)$ is a nonnegative measure on D. The measures F_t, F_0, and the transition kernel T_{t-s} are assumed nonnegative.

Nonlinear integral equations of this type and their probabilistic representations have been studied in the literature on random processes and nonlinear Markov processes [12, 14, 19]. Under appropriate hypotheses, existence and uniqueness of a nonnegative solution can be established; the precise assumptions of each cited theorem must be checked before applying it to a particular kernel. The branching construction below follows the general direct/adjoint Monte Carlo framework discussed by Nekrutkin [13] and should be compared with the authors' earlier treatment [18]. The specific normalization and implementation details are the focus here.

For the constant-rate case $H(r,u)=c>0$, the transition measure can be represented as

$$T_{t-s}(dr,du;r_1,u_1,r_2,u_2) = \delta_{r_1+u(t-s)}(dr)\,T_{r_1-r_2}(du,u_1,u_2). \tag{2}$$

The generalized Dirac measure is characterized by

$$\int_{\mathbb{R}^3}\varphi(r)\,\delta_{r_1+u(t-s)}(dr) = \varphi(r_1+u(t-s))$$

for every bounded measurable test function φ. The velocity transition kernel is written as

$$T_r(du,u_1,u_2) = p_{u_1,u_2}(r)\,T(du,u_1,u_2) + \big(1-p_{u_1,u_2}(r)\big)\delta_{u_1}(du), \tag{3}$$

where

$$p_{u_1,u_2}(r) = \frac{\alpha(u_1,u_2)}{(4\pi/3)\varepsilon_x^3 c}\,\mathbf{1}_{\{|r|<\varepsilon_x\}} = \frac{|u_1-u_2|_{c_1}}{c_1}\,\mathbf{1}_{\{|r|<\varepsilon_x\}},$$

and

$$\alpha(u_1,u_2) = \sigma|u_1-u_2|_{c_1} = \begin{cases}\sigma|u_1-u_2|, & |u_1-u_2|<c_1,\\ \sigma c_1, & |u_1-u_2|\geqslant c_1.\end{cases}$$

The notation $|w|_{c_1}=\min\{|w|,c_1\}$ denotes a capped relative speed. The parameters satisfy

$$c = \frac{\sigma c_1}{(4\pi/3)\varepsilon_x^3}.$$

Here σ is the molecular collision cross section (for hard spheres, $\sigma=\pi d^2$), ε_x is the spatial regularization radius, and c_1 is the relative-speed cap. These parameters and the associated nondimensionalization must be specified consistently in any physical calculation.

Substituting (2)–(3) into (1) with $H = c$ gives

$$F_t(dr, du) = F_0(dr - ut, du)e^{-ct} + \int_0^t ce^{-c(t-s)} \iint_D T_{t-s}(dr, du; r_1, u_1, r_2, u_2)\, F_s(dr_1, du_1)F_s(dr_2, du_2)\, ds. \tag{4}$$

This is a mollified Povzner-type equation [15]. Because the collision probability uses the indicator $\mathbf{1}_{\{|r|<\varepsilon_x\}}$, this is a regularized Boltzmann-type equation rather than the unregularized hard-sphere Boltzmann equation; the regularization and its relation to classical collision equations should be distinguished carefully [15]. Its convergence to the classical equation as $\varepsilon \to 0$ would require a separate limiting argument with a consistent scaling of the collision rate; that convergence is not proved here.

The passage from a measure equation to a density equation requires absolute continuity of F_t with respect to Lebesgue measure on phase space. Such absolute continuity is an additional assumption here; it does not follow merely from the boundedness of the constant collision rate $H(r, u) = c$. We therefore assume, for the derivation in this section, that $F_t(dr, du)$ is absolutely continuous and that its Radon–Nikodym derivative $f(r, u, t)$ is integrable. Under this assumption,

$$F_t(dr, du) = f(r, u, t)\, dr\, du.$$

If absolute continuity is unavailable, the measure formulation (1) must be retained and the density-based derivation below does not apply. Any use of a moment criterion for density existence requires the precise hypotheses of the cited theorem to be stated and verified; it is not used here as a stand-alone density-existence proof.

Suppose that there does exist a density $f(r, u, t)$ of the measure $F_t(dr, du)$. In this case we can write

$$T_{t-s}(dr, du; r_1, u_1, r_2, u_2) = T_{t-s}(r, u; r_1, u_1, r_2, u_2)\, dr\, du.$$

and equation (4) can be rewritten in the following form

$$f(r, u, t) = f(r - ut, u, 0)\exp\{-ct\} + \int_0^t ds \left[c\exp\{-c(t-s)\}\right] \int_D \int_D T_{t-s}(r, u; r_1, u_1, r_2, u_2) \times f(r_1, u_1, s)\, f(r_2, u_2, s)\, dr_1\, du_1\, dr_2\, du_2, \tag{5}$$

where

$$T_{t-s}(r, u; r_1, u_1, r_2, u_2) = \delta\big(r - (r_1 + u(t-s))\big)\, T_{r_1-r_2}(u, u_1, u_2).$$

For the elastic hard-sphere-type scattering law considered here

$$T(u, u_1, u_2) = \frac{1}{\pi|u_2 - u_1|^2}\delta\left(\left|u - \frac{u_1 + u_2}{2}\right| - \frac{|u_2 - u_1|}{2}\right). \tag{6}$$

Putting (6) into expression (5), we obtain

$$f(r,u,t)=f(r-ut,u,0)\exp\{-ct\}+\int_0^t ds\,[c\exp\{-c(t-s)\}]$$
$$\times\Bigg[\int_D\int_D\Bigg(p_{u_1,u_2}(r_1-r_2)\,\frac{1}{\pi|u_2-u_1|^2}\delta\Bigg(\Bigg|u-\frac{u_1+u_2}{2}\Bigg|-\frac{|u_2-u_1|}{2}\Bigg)$$
$$+(1-p_{u_1,u_2}(r_1-r_2))\,\delta(u_1-u)\Bigg)\delta\big(r_1-(r-u(t-s))\big)$$
$$\times f(r_1,u_1,s)\,f(r_2,u_2,s)\,dr_1\,du_1\,dr_2\,du_2\Bigg].$$

Integrating out r_1 in both integrals and u_1 in the last integral we obtain

$$f(r,u,t)=f(r-ut,u,0)\exp\{-ct\}+\int_0^t ds\,[c\exp\{-c(t-s)\}]$$
$$\times\Bigg[\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}(1-p_{u,u_2}(r-u(t-s)-r_2))$$
$$\times f(r-u(t-s),u,s)\,f(r_2,u_2,s)\,dr_2\,du_2$$
$$+\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}p_{u_1,u_2}(r-u(t-s)-r_2)$$
$$\times\frac{1}{\pi|u_2-u_1|^2}\delta\Bigg(\Bigg|u-\frac{u_1+u_2}{2}\Bigg|-\frac{|u_2-u_1|}{2}\Bigg)$$
$$\times f(r-u(t-s),u_1,s)\,f(r_2,u_2,s)\,du_1\,dr_2\,du_2\Bigg].$$

In the last integral term in the above equation we change variables in the following way

$$\frac{u_1+u_2}{2}=u_c,\qquad u_2-u_1=v,$$

so that

$$u_1=u_c-\frac{v}{2},\qquad u_2=u_c+\frac{v}{2},$$

and the Jacobian $|J|=1$. Then the last term has the form

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}p_{u_c-\frac{v}{2},u_c+\frac{v}{2}}(r-u(t-s)-r_2)\,\frac{1}{\pi|v|^2}\delta\Bigg(|u-u_c|-\frac{|v|}{2}\Bigg)$$
$$\times f(r-u(t-s),u_c-\tfrac{v}{2},s)\,f(r_2,u_c+\tfrac{v}{2},s)\,dv\,du_c\,dr_2.$$

Now, we introduce spherical coordinates, and the vector $v/2$ transforms into $|v|/2\,\omega$, with Jacobian

$$J=\frac{|v|^2}{4}\sin\theta,$$

where ω is an isotropic unit vector $\omega=(\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta)$. Thus, $v/2=|u-$ $-u_c|\,\omega$. We note that

$$\int d\omega=\int_0^\pi\frac{\sin\theta}{2}\,d\theta\int_0^{2\pi}\frac{1}{2\pi}\,d\varphi,$$

and so, integrating over $|v|$, we obtain

$$\int d\omega \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} p_{u_c-|u-u_c|\omega,\, u_c+|u-u_c|\omega}\big(r-u(t-s)-r_2\big) f(r-u(t-s),\, u_c-|u-u_c|\omega,\, s) \times f(r_2,\, u_c+|u-u_c|\omega,\, s)\, dr_2\, du_c.$$

With the change of variables $v = 2\rho\omega$, the velocity-space volume element is $dv = 8\rho^2\, d\rho\, d\Omega$. Integrating the radial Dirac delta in (6) therefore contributes the factor 8 when $d\omega$ denotes the normalized angular probability measure used above. This factor is retained in the collision term below and must also be included in the corresponding Monte Carlo path weight. Omitting it changes the normalization of the collision operator and, in particular, can violate mass conservation.

Thus, we obtain the following equation

$$\begin{aligned} f(r,u,t) &= f(r-ut,u,0)\exp\{-ct\} + \int_0^t ds\, c\exp\{-c(t-s)\} \\ &\times \Bigg[\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \big(1-p_{u,u_2}(r-u(t-s)-r_2)\big) f(r-u(t-s),u,s) f(r_2,u_2,s)\, dr_2\, du_2 \\ &\quad + 8\int d\omega \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} p_{u_c-|u-u_c|\omega,\, u_c+|u-u_c|\omega}\big(r-u(t-s)-r_2\big) \\ &\quad \times f(r-u(t-s),u_c-|u-u_c|\omega,s)\, f(r_2,u_c+|u-u_c|\omega,s)\, dr_2\, du_c \Bigg]. \end{aligned}$$

For $c>0$ and $t>0$, define

$$f_1(s \mid t) = \frac{c\exp\{-c(t-s)\}}{1-\exp\{-ct\}}, \qquad 0 \leqslant s \leqslant t.$$

It is normalized because $\int_0^t f_1(s \mid t)\, ds = 1$. The factor c is essential. At $c=0$ the limiting density is the uniform density $1/t$. In the formulas below, the dependence on the current time horizon t is implicit. The random time can therefore be sampled from this normalized density. As a result, we obtain the following equation

$$\begin{aligned} f(r,u,t) &= f(r-ut,u,0)\exp\{-ct\} + \big(1-\exp\{-ct\}\big) \\ &\times \int_0^t ds\, f_1(s) \Bigg[\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \big(1-p_{u,u_2}(r-u(t-s)-r_2)\big) \\ &\quad \times f(r-u(t-s),u,s)\, f(r_2,u_2,s)\, dr_2\, du_2 \\ &\quad + 8\int d\omega \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} p_{u_c-|u-u_c|\omega,\, u_c+|u-u_c|\omega}\big(r-u(t-s)-r_2\big) \\ &\quad \times f(r-u(t-s),u_c-|u-u_c|\omega,s) f(r_2,u_c+|u-u_c|\omega,s)\, dr_2\, du_c \Bigg]. \end{aligned} \tag{7}$$

We note that without difficulty this method can be applied in more complicated gas models, for example when the shock transform function $T(u,u_1,u_2)$ has a form differing from (6). Equation (7) can be solved by various methods. In the following section, we

will offer some alternative adjoint computational schemes for solving equation (7), which are closely connected with branching Markov processes.

3 Methods of constructing unbiased estimators

The general methods of solving linear integral equations by Monte Carlo method are also applicable to the nonlinear integral equation (7), if we approximate the nonlinear problem by a sequence of linear problems. For instance, if the following method of successive approximation converges

$$
\begin{aligned}
f^{(n)}(r,u,t) &= f^{(0)}(r-ut,u,0)\exp\{-ct\} \\
&\quad + \big(1-\exp\{-ct\}\big)\int_0^t ds\, f_1(s)\Bigg[\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\big(1-p_{u,u_2}(r-u(t-s)-r_2)\big) \\
&\qquad \times f^{(n)}(r-u(t-s),u,s)\, f^{(n-1)}(r_2,u_2,s)\, dr_2\, du_2 \\
&\quad + 8\int d\omega \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} p_{u_c-|u-u_c|\omega,\, u_c+|u-u_c|\omega}\big(r-u(t-s)-r_2\big) \\
&\qquad \times f^{(n)}(r-u(t-s),u_c-|u-u_c|\omega,s) f^{(n-1)}(r_2,u_c+|u-u_c|\omega,s)\, dr_2\, du_c\Bigg],
\end{aligned}
\tag{8}
$$

Here $f^{(0)}$ is a prescribed initial iterate. For each $n \geqslant 1$, equation (8) is linear in the unknown $f^{(n)}$ when $f^{(n-1)}$ is fixed, although it remains an integral equation and is not an explicit update formula. Convergence of this Picard-type iteration must be established under suitable assumptions; it is not implied by the displayed formula alone. A Monte Carlo approximation at each iteration introduces sampling error in addition to the iteration error. Both contributions must be reported separately in a numerical comparison.

For the solution of equation (7) we present a computational scheme, which is closely connected with branching Markov processes. We will obtain one of the adjoint computational Monte Carlo schemes after the following transformation of equation (7)

$$
\begin{aligned}
f(r,u,t) &= f(r-ut,u,0)\exp\{-ct\} \\
&\quad + (1-\exp\{-ct\})\int_0^t ds\, f_1(s)\Bigg[\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\big(1-p_{u,u_2}(r-u(t-s)-r_2)\big) \\
&\qquad \times \big[\psi_1(r_2)\psi_2(u_2)\big]^{-1}\psi_1(r_2)\psi_2(u_2) f(r-u(t-s),u,s) f(r_2,u_2,s)\, dr_2\, du_2 \\
&\quad + 8\int d\omega \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} p_{u_c-|u-u_c|\omega,\, u_c+|u-u_c|\omega}(r-u(t-s)-r_2) \\
&\qquad \times \big[\psi_1(r_2)\psi_2(u_c)\big]^{-1}\psi_1(r_2)\psi_2(u_c) \\
&\qquad \times f(r-u(t-s),u_c-|u-u_c|\omega,s) f(r_2,u_c+|u-u_c|\omega,s)\, dr_2\, du_c\Bigg],
\end{aligned}
\tag{9}
$$

where ψ_1 and ψ_2 are proposal normal densities on $\mathbb{R}^3$, chosen here as normal densities with means A and B and with given standard deviations specified by σ_1 and σ_2. Every branch in which a variable is sampled from a proposal normal density must include its path weight; this applies to both the no-collision branch and the collision branch.

We will construct an unbiased estimator for the functional (h, f), where $h(r,u,t)$ is a given function, and $f(r,u,t)$ is the unknown function. We construct a branching process

in the following way. At the point r at time t, with initial probability density $p_0(r)$, one particle is created. The speed of the particle u at the point r is distributed with the initial probability density $p_1(u)$. The joint density of the distribution of a point (r, u, t) has the form

$$P_0(r, u, t) = p_0(r)p_1(u)p_2(t),$$

where $p_2(t)$ is the initial density of distribution of time t. Here the estimator will have the form

$$\xi(r, u) = \frac{h(r, u, t)}{P_0(r, u, t)}.$$

Further, with probability $\alpha_0(t) = \exp\{-ct\}$, a particle at the point (r, u, t) is absorbed. In this case, the estimator is computed with the following algorithm

$$\xi(r, u) \leftarrow \xi(r, u)f(r - ut, u, 0).$$

If a particle was not absorbed, then the next time value $s_1 \in [0, t]$ is chosen with the probability density $f_1(s)$. Then, with probability $\alpha_1(t) = (1 - \exp\{-ct\})\beta$, $\beta \in (0, 1)$, two particles are born (the collision case), when the speed of the particles change at points

$$(r - u(t - s), u_c - |u - u_c|\omega, s) \quad \text{and} \quad (r_2, u_c + |u - u_c|\omega, s).$$

Here $\omega = (\omega_1, \omega_2, \omega_3)$ is an isotropic unit vector, which is distributed by formulas

$$\omega_1 = 1 - 2\gamma_1, \qquad \omega_2 = \sqrt{1 - \omega_1^2}\cos 2\pi\gamma_2, \qquad \omega_3 = \sqrt{1 - \omega_1^2}\sin 2\pi\gamma_2,$$

where γ_1 and γ_2 are uniformly distributed random numbers on $(0, 1)$. Transition from the point r to the point r_2 is done with transition density $\psi_1(r_2)$, and u_c is chosen with probability density $\psi_2(u_c)$. A joint density for the point (r_2, u_c, s) has the form

$$P_1(r, u, t \to r_2, u_c, s) = f_1(s)\psi_1(r_2)\psi_2(u_c).$$

Here the following algorithm is used for computing the estimator:

$$\xi_t(r, u) \leftarrow \xi_t(r, u)\, 8p_{u_c - |u-u_c|\omega,\ u_c + |u-u_c|\omega}(r - u(t - s) - r_2)\left[\beta\,\psi_1(r_2)\psi_2(u_c)\right]^{-1}.$$

With probability $\alpha_2(t) = (1 - \exp\{-ct\})(1 - \beta)$, two particles are born (the case when the speed of particles remains unchanged) at the points $(r - u(t - s), u, s)$ and (r_2, u_2, s). Transition from the point r to the point r_2 is done with the probability density $\psi_1(r_2)$, and u_2 is sampled with probability density $\psi_2(u_2)$. The joint density of the point (r_2, u_2, s) has the form

$$P_2(r, u, t \to r_2, u_2, s) = f_1(s)\psi_1(r_2)\psi_2(u_2).$$

Here the estimator is computed using the following algorithm:

$$\xi_t(r, u) \leftarrow \xi_t(r, u)\left(1 - p_{u,u_2}(r - u(t - s) - r_2)\right)\left[(1 - \beta)\psi_1(r_2)\psi_2(u_2)\right]^{-1}.$$

Further, new particles behave analogously to the initial one. Moreover,

$$s_0 = 0, \quad s_k \in [0, t - \sum_{i=0}^{k-1} s_i], \quad t \leftarrow t - \sum_{i=0}^{k-1} s_i,$$

at moments of time s_k are chosen with probability density $f_1(s)$. At each step, the times $s_1, s_2, \ldots$ are chosen and the process finishes when all particles are absorbed, or the condition

$$t - \sum s_i \leqslant \varepsilon_t$$

is satisfied, where ε_t is a numerical time cut-off, distinct from the spatial regularization radius ε_x.

Note: This is an adjoint method, meaning that in this method time decreases from T to zero. By choosing the parameter β, one controls the proportion of branches in which the particle velocities change. Numerical experiments show that the final quality of the results depends on the number of collisions.

It is obvious that by changing the parameters A, σ_1 and B, σ_2 we can obtain variants of the scheme, and we can choose values of these parameters according to the physical characteristics of a concrete scheme — the first adjoint scheme.

In both these cases, we used an estimator based on absorptions. Depending on the complexity, we can construct other estimators on the trajectories of branching processes (for instance, estimators based on collisions). To call the estimator unbiased, one must show that the expected path weight equals the target functional and that the relevant expectation exists; finite variance additionally requires a second-moment bound. These conditions depend on the proposal densities, the path-weight factors, and the branching law.

4 Results and discussion

The shock-wave problem is a useful verification case because density, velocity, and temperature profiles can be compared with kinetic-theory computations and experimental measurements. Alsmeyer's electron-beam measurements provide experimental density profiles for argon and nitrogen [5]. Numerical reference results for hard-sphere molecules have also been reported using deterministic solutions of the Boltzmann equation [4], while a recent accuracy-controlled calculation addresses shock structure in a gas mixture [7]. Döntgen's study [9] further illustrates that shock propagation can be sensitive to the assumed energy distribution and thermodynamic closure. However, that work treats freely propagating shocks in monoatomic gases with non-Boltzmann energy distributions and uses atomistic molecular-dynamics simulations; it should therefore be cited as context on model sensitivity, not as a directly interchangeable benchmark for the present regularized kinetic equation. A meaningful quantitative comparison must use the same intermolecular model, nondimensionalization, upstream state, and Mach number. A visual overlay with a profile from another model is not sufficient to establish accuracy.

Two recent hybrid methods are relevant when designing a future computational-efficiency comparison. Luo and Wu [10] introduced a direct intermittent coupling of the general synthetic iterative scheme and DSMC to improve convergence toward steady state in rarefied-gas simulations. Kim and Jun [11] evaluated a hybrid Fokker–Planck–DSMC approach against DSMC and Fokker–Planck solvers on high-speed rarefied-flow benchmarks. These algorithms differ from the branching estimator considered here, so their reported efficiency gains cannot be transferred to the present method. A defensible comparison would require a shared benchmark, matched physical assumptions and error tolerance, and measured wall-clock time and uncertainty.

The listed values also imply a small cut-off speed in the collision kernel: from $c = = \sigma_{\text{cs}} c_1/(4\pi\varepsilon_x^3/3)$, $c = 0.65$, $\sigma_{\text{cs}} = 1$, and $\varepsilon_x = 0.2$, one obtains $c_1 \approx 0.0218$. For thermal relative speeds of order one, the capped collision rate $\alpha = \sigma_{\text{cs}} \min(|u_1 - u_2|, c_1)$ is then

almost always at its cap; this is effectively a pseudo-Maxwell-type rate rather than the uncapped hard-sphere rate.

The parameter values used in the calculation are listed in Table 1. These values were chosen to test the performance of the constructed model and should not be interpreted as a validated physical state. For the reported values, the mass fluxes are $n_1 v_1 = 1.2$ and $n_2 v_2 = 1.6875$, so mass-flux balance already fails. Under the stated assumption $\sigma_A^2 = kT_1/m = 1$, the monatomic-gas sound speed is approximately 1.29 in these units, making $v_1 = 1.2$ subsonic rather than a supersonic upstream shock state. The reported downstream density and thermal-speed values correspond to a Mach number in the range $[1.5, 3]$. These discrepancies must be resolved by selecting one consistent set of upstream state, downstream state, and Mach number before new profiles are computed. Thus, the upstream and downstream parameters do not satisfy the stated Rankine–Hugoniot constraints under the stated normalization. Consequently, the existing figures are retained only as a record of the preliminary calculation. They cannot support a quantitative validation claim until the physical parameters and the collision model have been reconciled and the computation rerun.

Table 1 Parameters of the numerical experiment.

Parameter	Reported value	Verification status
A	0.3	Proposal parameter; definition needed
σ_1	0.5	Proposal parameter; covariance convention needed
B	0.3	Proposal parameter; definition needed
σ_2	0.5	Proposal parameter; covariance convention needed
c	0.65	Must be consistent with $c = \sigma_{\mathrm{cs}} c_1/(4\pi\varepsilon_x^3/3)$
ε_x	0.2	Spatial regularization radius
N	1000	Reported number of trajectories; uncertainty not reported
n_1, n_2	1, 2.25	Must satisfy the chosen jump conditions
v_1, v_2	1.2, 0.75	Must satisfy mass and momentum/energy flux constraints
σ_A, σ_B	1, 1.41	Thermal-speed parameters; convention to be specified
σ_{cs}	1	Collision cross-section parameter; units/nondimensionalization needed
λ	1	Definition and role in the model must be supplied

The computed profiles approach the Haviland curve as time increases. This visual observation is not enough to establish convergence to a stationary shock profile. A revised computational study should report, for each time and parameter set, the asymptotic upstream and downstream densities, the maximum absolute and relative errors against a specified reference profile, and a defined shock thickness. It should also include confidence intervals or repeated-run variability. If the model uses a spatially localized initial density, the method by which Maxwellian far-field states are imposed or approached must be described; a normalized Gaussian in all of $\mathbb{R}^3$ is not by itself a boundary condition for a stationary planar shock.

Further, a comparison between the branching Monte Carlo method and the iterative method must be made at matched accuracy, not by comparing two plotted curves alone. At minimum, the revised experiment should report (i) the sample mean and standard error of the estimated density or target functional, (ii) the empirical variance and confidence interval across independent runs, (iii) the number of generated particles and the distribution of branching depth, (iv) the truncation sensitivity with respect to the time cut-off

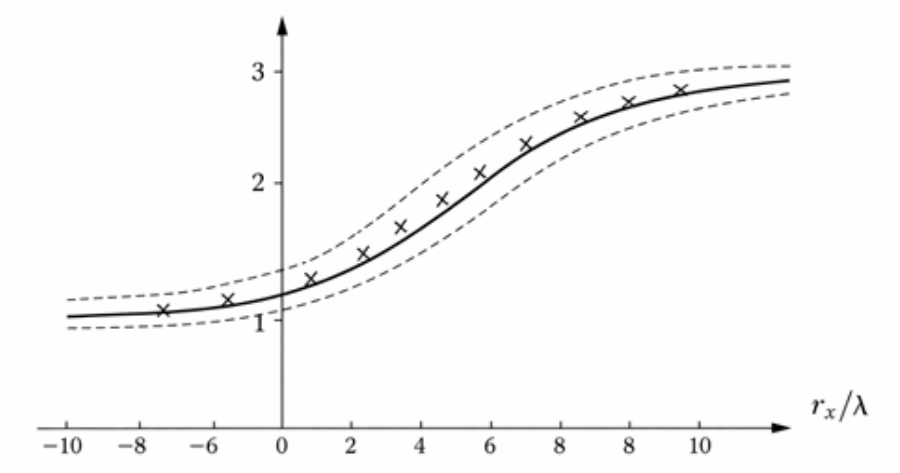


Figure 1 Density profiles at $t = 1, 3, 4$ and the Haviland reference profile [20] (preliminary calculation, Mach number $M = 2$). The dashed lines show the confidence interval.

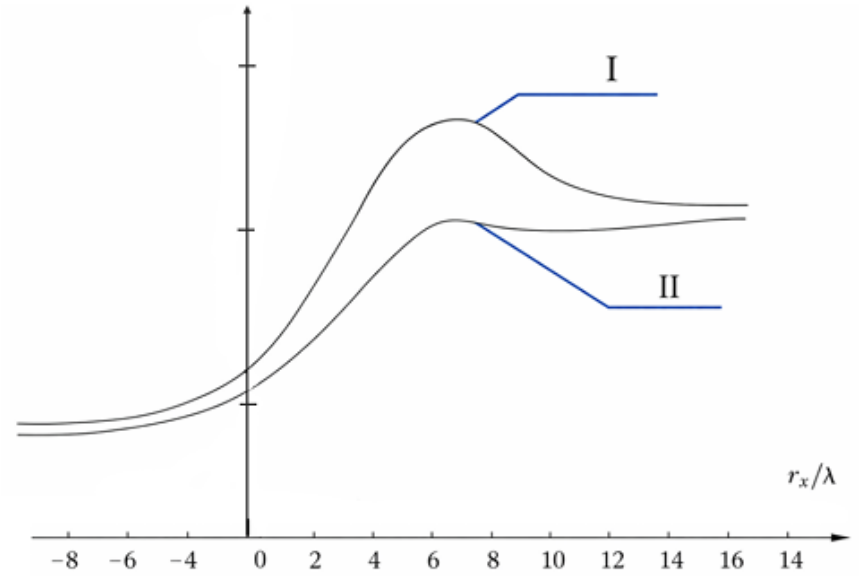


Figure 2 First and second iterates for the density equation (the ordinate scale is the same as in Fig. 1). The plot does not include a quantitative error measure; it therefore does not establish that the two iterates are close or that the iteration converges slowly.

and particle-array capacity, and (v) wall-clock time on a specified hardware/software environment. The statement that the two iterations differ little should be retained only if supported by a norm such as

$$E_n = \frac{\|f^{(n)} - f^{(n-1)}\|_{L^1}}{\max\{\|f^{(n)}\|_{L^1}, \delta\}},$$

with a declared positive safeguard δ, and by a convergence study over several iteration indices.

The present calculation uses $N = 1000$ trajectories. It also shows that the profile depends on the maximum particle-array length M_1, with nonmonotone profiles for small values. This dependence is evidence that implementation truncation may materially affect the result. The array cap must therefore be treated as a numerical approximation

parameter. Profiles should be recomputed for increasing M_1 and decreasing time cut-off, and the resulting change in the profile should be quantified before any statement about monotonicity or unbiasedness is made.

Finally, conservation should be checked at the level actually guaranteed by the model. For an elastic collision operator, the collision invariants are 1, u, and $|u|^2$; their collision integrals should vanish for a correctly normalized collision law. For a Monte Carlo approximation, the corresponding moment residuals should be reported as functions of sample size and truncation settings. Since no such residuals are available in the supplied calculation, this paper does not claim that mass, momentum, and energy conservation have been numerically demonstrated.

The reported computation time of approximately 0.24 seconds per spatial point on a Pentium IV computer is not a reproducible performance metric without the code, compiler/interpreter, hardware configuration, stopping rules, and target accuracy. It is therefore not used as evidence of efficiency. Parallel implementation of this algorithm will be presented in our future work.

5 Conclusion

This paper considers a regularized nonlinear integral equation of Boltzmann type and outlines a Monte Carlo representation based on a branching Markov process. The derivation requires a clear distinction between the measure equation and the density equation: the latter is valid only when the measure is absolutely continuous with respect to phase-space Lebesgue measure. The collision law in equation (6) preserves the magnitude of the relative velocity and is therefore an elastic-scattering law.

The branching construction suggests a way to estimate functionals of the solution, but the properties of the resulting estimator depend on the complete path weights, proposal densities, and termination rule. In particular, a finite time cut-off or a cap on the number of stored particles generally introduces truncation error. Thus, unbiasedness and finite variance cannot be asserted for the implemented estimator without a proof or a numerical/analytical truncation study.

The shock-wave figures are preliminary and do not establish quantitative agreement with a reference solution. Before the proposed method can be assessed as a validated numerical algorithm, we must (i) reconcile the upstream/downstream parameters with the Rankine–Hugoniot conditions and state the corresponding Mach number, (ii) define all nondimensional parameters and proposal distributions, (iii) rerun the experiment with the corrected normalization, (iv) report uncertainty, conservation residuals, convergence with respect to sample size and truncation, and quantitative errors against a specified reference or experimental data, and (v) compare methods at matched accuracy and computational cost. The present paper therefore does not claim superior efficiency, a proven unbiased estimator, or numerical conservation of mass, momentum, and energy. These are tasks for the next stage of the study.

Declarations

Conflicts of interest. The authors declare no conflict of interest.

Data availability. The data are available from the authors on reasonable request.

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МЕТОД МОНТЕ-КАРЛО ДЛЯ РЕШЕНИЯ НЕЛИНЕЙНОГО КИНЕТИЧЕСКОГО УРАВНЕНИЯ БОЛЬЦМАНА

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Рассматривается нелинейное интегральное уравнение больцмановского типа для неотрицательной меры и обсуждается его представление методом Монте-Карло на траекториях ветвящегося марковского процесса. При явно сформулированном условии абсолютной непрерывности уравнение для меры переписывается как уравнение для плотности. Используемое в выводе ядро столкновений является регуляризованным и локализованным по пространству; преобразование скоростей в приведённом законе столкновения сохраняет относительную скорость и кинетическую энергию пары, поэтому речь идёт об упругом изотропном рассеянии, а не о неупругих столкновениях. Выводятся плотность моделирования времени при постоянной частоте столкновений и нормировочный множитель, возникающий при переходе к сферическим координатам с нормированной угловой мерой. Также уточняются множители важностного моделирования, входящие в веса траекторий. Расчёт структуры ударной волны рассматривается как предварительная численная иллюстрация. Имеющиеся рисунки и набор параметров сами по себе не доказывают несмещённость усечённой оценки, конечность её дисперсии, сохранение макроскопических моментов, количественное согласие с эталонным решением или вычислительное преимущество перед итерационным методом. Для подтверждения этих свойств необходимы проверки сходимости, законов сохранения и статистической неопределённости, перечисленные в статье.

Ключевые слова: метод Монте-Карло, нелинейное уравнение Больцмана, регуляризованное ядро столкновений, ветвящийся марковский процесс, важностное моделирование, структура ударной волны

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