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Direct simulation Monte Carlo method for stationary nonlinear Boltzmann equation*

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A new version of the direct Monte Carlo method for solving boundary value problems for the Boltzmann equation is presented. In contrast to the conventional approach, we do not solve the problem via stabilization in time; when evaluating functionals of the solution to the Boltzmann equation, the random trajectories are stopped with probability one after a finite number of transitions.

1. Stationary boundary value problem for the Boltzmann equation

The main issue of the present study is the construction of justification of a new Monte Carlo method for numerical solution to boundary value problems for the nonlinear Boltzmann equation in the stationary formulation. This class of problems is of practical interest because many physical processes are governed by stationary boundary value problems [1, 2].

Let G_Γ and G_γ be bounded 3D domains with piecewise smooth boundaries Γ and γ respectively. We assume for simplicity that $\overline{G}_\gamma \subset G_\Gamma$. We denote $G = G_\Gamma \setminus \overline{G}_\gamma$. Let $\boldsymbol{n}_\Gamma = \boldsymbol{n}_\Gamma(\boldsymbol{r})$, $\boldsymbol{n}_\gamma = \boldsymbol{n}_\gamma(\boldsymbol{r})$ be external normal vectors to G_Γ and G_γ, respectively.

The problem is formulated as follows: find a nonnegative function $f(\boldsymbol{r}, \boldsymbol{v})$, continuous in $\overline{G} \times \mathbb{R}^3$, satisfying in G the equation

$$\boldsymbol{v}\frac{\partial f(\boldsymbol{r},\boldsymbol{v})}{\partial \boldsymbol{r}} = \int k(\boldsymbol{v}', \boldsymbol{v}_1' \to \boldsymbol{v}, \boldsymbol{v}_1)[f(\boldsymbol{r},\boldsymbol{v}')f(\boldsymbol{r},\boldsymbol{v}_1') - f(\boldsymbol{r},\boldsymbol{v})f(\boldsymbol{r},\boldsymbol{v}_1)]\, d\boldsymbol{v}' d\boldsymbol{v}_1' d\boldsymbol{v}_1,$$

and the boundary conditions:

$$f(\boldsymbol{r},\boldsymbol{v}) = f_\Gamma(\boldsymbol{r},\boldsymbol{v}) \qquad \text{if } (\boldsymbol{n}_\Gamma \boldsymbol{v}) < 0,$$

whilst for $\boldsymbol{r} \in \gamma$, satisfies the integral relation:

$$(\boldsymbol{n}_\gamma \boldsymbol{v}) f(\boldsymbol{r},\boldsymbol{v}) = -\int_{(\boldsymbol{n}_\gamma \boldsymbol{v}')<0} k_\gamma(\boldsymbol{v}' \to \boldsymbol{v}; \boldsymbol{r})(\boldsymbol{n}_\gamma \boldsymbol{v}') f(\boldsymbol{r},\boldsymbol{v}')d\boldsymbol{v}' \quad \text{if } (\boldsymbol{n}_\gamma \boldsymbol{v}) > 0,$$

where

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$$k(v', v_1' \to v, v_1) = \sigma(|v' - v_1'|, \Omega)\delta\left(\frac{v+v_1-v'-v_1'}{2}\right)\delta\left(\frac{v^2+v_1^2-v'^2-v_1'^2}{2}\right).$$

Here $\sigma(|v' - v_1'|, \Omega)$ is differential cross-section of scattering of two particles, Ω is characterizing the relative velocity vectors of the particles after the scattering. It is assumed that the nonnegative functions $f_\Gamma(r, v)$ and $k_\gamma(v' \to v; r)$ are given, and they are positive on the surfaces Γ and γ, respectively, and

$$\int k_\gamma(v' \to v; r)\, dv = 1 \qquad \text{if } r \in \gamma.$$

In addition, the function $f(r, v)$ should satisfy the condition

$$\int (1 + v^2)^\alpha f(r, v)\, dv\, dr < \infty$$

for an integer $\alpha \geq 1$, where the integration is taken over the whole domain of velocity and spatial variables.

Here we deal with the problem of construction of the numerical Monte Carlo method, and therefore we assume that there exists a unique solution to the formulated problem.

It will be convenient to give an equivalent formulation of the problem. To this end, we include the boundary conditions on γ into the Boltzmann equation.

Let us introduce the notation

$$St[f, f] = \int k(v', v_1' \to v, v_1)[f(r, v')f(r, v_1') - f(r, v)f(r, v_1)]\, dv'\, dv_1'\, dv_1,$$

$$(nv)^- = \begin{cases} (nv), & (nv) < 0, \\ 0, & (nv) \geq 0; \end{cases} \qquad (nv)^+ = \begin{cases} (nv), & (nv) > 0, \\ 0, & (nv) \leq 0; \end{cases}$$

$\delta_\Gamma(r)$ is the generalized function (a simple layer) whose support is concentrated on the surface Γ, $\delta_\gamma(r)$ is the simple layer on γ, and $q(r, v) = \{-(n_\Gamma v)^-\} f_\Gamma(r, v)\delta_\Gamma(r)$.

Then the boundary value problem for the Boltzmann equation is reformulated as follows: find a nonnegative function $f(r, v)$, continuous in $\overline{G} \times \mathbb{R}^3$ and satisfying the equation

$$v\frac{\partial}{\partial r} f(r, v) = St[f, f] + \int k_\gamma(v' \to v \mid r)\{-(n_\gamma v')^-\}\delta_\gamma(r) f(r, v')\, dv' \quad (1)$$

for $r \in G$ and boundary conditions

$$(n_\Gamma v)^- f(r, v) = (n_\Gamma v)^- f_\Gamma(r, v), \qquad r \in \Gamma, \quad (2)$$

$$(n_\gamma v)^+ f(r, v) = 0, \qquad r \in \gamma. \quad (3)$$

The boundary condition (2) on the surface Γ make it impossible to use the N-particle Kolmogorov equation with a fixed number of particles to construct the direct Monte Carlo method, as in the homogeneous case [3]; in our case the number of particles varies and this should be properly taking into account. It is possible to do this approximately, by solving nonstationary boundary value problems and using the conventional splitting (over physical processes) technique and the stabilization method [1, 4]. To this end, one solves the inhomogeneous N-particle equation with a constant number of particles in each time step Δt of the splitting process; the boundary conditions are taken into account in the stage of spatial movement of particles [4]. This approach assumes that the stabilization method is applicable to solve the stationary boundary value problem for the Boltzmann equation (1)–(3). In this paper we do not use this conventional approach.

2. An auxiliary system of N-particle equations

In [6], we suggested a system of N-particle equations which properly takes account of the change of particles caused by a flux of particles into the domain G, without affecting the probabilistic character of these equations. This is a crucial point in the use of the N-particle equations for solving the nonlinear Boltzmann equations [5].

According to the approach presented in [3], we formulate a system of N-particle equations which is a basis for constructing the direct Monte Carlo method for solving problem (1–3).

Let $\boldsymbol{R}_N = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$, $\boldsymbol{V}_N = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_N)$, $\mathbb{R}^3_* = \{\boldsymbol{v} : \boldsymbol{v} \in \mathbb{R}^3,\ v_* \leq |\boldsymbol{v}| \leq v^*\}$ be the domain of velocity variables. The constants v_* and v^* satisfy the condition $0 < v_* < v^*$.

We write $\boldsymbol{R}_N \in G$ and say that $\boldsymbol{R}_N$ lies in $G \subset \mathbb{R}^3$ if $\boldsymbol{r}_i \in G$ for all $i = 1, \ldots, N$. Analogously, we write $\boldsymbol{V}_N \in \mathbb{R}^3_*$ and say that $\boldsymbol{V}_N$ lies in $\mathbb{R}^3_*$ if $\boldsymbol{v}_i \in \mathbb{R}^3_*$ for all $i = 1, \ldots, N$.

Denote by $\boldsymbol{R}^\Gamma_N$ the spatial coordinates of a system of N particles if there is at least one particle $\boldsymbol{r}_i$ belonging to Γ. In this case we say that $\boldsymbol{R}_N$ belongs to the boundary Γ. Analogously, by $\boldsymbol{R}^\gamma_N$ we denote the spatial coordinates of a system of N particles if these is at least one particle $\boldsymbol{r}_i$ belonging to γ. In this case we say that $\boldsymbol{R}_N$ belongs to the boundary γ.

Let us define the indicator of the event that $\boldsymbol{R}_N$ belongs to the boundary γ as follows:

$$I_\gamma(\boldsymbol{R}_N) = \begin{cases} 1, & \boldsymbol{R}_N = \boldsymbol{R}^\gamma_N; \\ 0, & \boldsymbol{R}_N \neq \boldsymbol{R}^\gamma_N. \end{cases} \tag{4}$$

We define $K(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N)$ as a function which determines a pair interaction in a system of N-particles in the domain G. It satisfies the conditions

$$K(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N) = K(\boldsymbol{V}_N \to \boldsymbol{V}'_N \mid \boldsymbol{R}_N),$$
$$K(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}^{\Gamma}_N) = 0, \qquad K(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}^{\gamma}_N) = 0,$$
$$K(\boldsymbol{V}'_1 \to \boldsymbol{V}_1 \mid \boldsymbol{R}_1) \equiv 0.$$

Let

$$A(\boldsymbol{R}_N, \boldsymbol{V}_N) = \int K(\boldsymbol{V}_N \to \boldsymbol{V}'_N \mid \boldsymbol{R}_N)\, d\boldsymbol{V}'_N. \tag{5}$$

The function $K_c(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N)$ is defined as a probability density function of velocities in the N-particle system after an interaction, being in a state $(\boldsymbol{R}_N, \boldsymbol{V}'_N)$. This function has the same support as the function $K(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N)$ and they are related by the equality

$$K(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N) = (1 - I_\gamma(\boldsymbol{R}_N))\, A(\boldsymbol{R}_N, \boldsymbol{V}'_N)\, K_c(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N).$$

The function $K_\gamma(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N)$ describes the interaction of a system of N-particles with the boundary γ:

$$K_\gamma(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N) = I_\gamma(\boldsymbol{R}_N) \prod_{i=1}^{N} k_\gamma(\boldsymbol{v}'_i \to \boldsymbol{v}_i \mid \boldsymbol{r}_i),$$

where

$$k_\gamma(\boldsymbol{v}' \to \boldsymbol{v} \mid \boldsymbol{r}) = \begin{cases} k_\gamma(\boldsymbol{v}' \to \boldsymbol{v}; \boldsymbol{r}), & \boldsymbol{r} \in \gamma; \\ \delta(\boldsymbol{v} - \boldsymbol{v}'), & \boldsymbol{r} \notin \gamma. \end{cases}$$

It satisfies the conditions

$$\int K_\gamma(\boldsymbol{V}_N \to \boldsymbol{V}'_N \mid \boldsymbol{R}^{\gamma}_N)\, d\boldsymbol{V}'_N = 1. \tag{6}$$

Let

$$\hat{S}[p(N-1, x_1, \ldots, x_{N-1}) q(x_N)] = \frac{1}{N} \sum_{i=1}^{N} p(N-1, x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N) q(x_i)$$

be the symmetrization operator introduced in [6] for making the particles undistinguishable for $N \geq 2$ (if $N = 1$ is zero by definition). The function $K_s(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N)$ is related to the symmetrization operator by

$$\hat{S}[p(N-1, \boldsymbol{R}_{N-1}, \boldsymbol{V}_{N-1}) q(\boldsymbol{r}_N, \boldsymbol{v}_N)] = \int q(\boldsymbol{r}_N, \boldsymbol{v}'_N) p(N-1, \boldsymbol{R}_{N-1}, \boldsymbol{V}'_{N-1}) K_s(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N)\, d\boldsymbol{V}'_N.$$

It can be represented as

$$K_s(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}_N) = (1 - \delta_{N,1}) \hat{S}\left[\left\{ \prod_{i=1}^{N-1} \delta(\boldsymbol{v}_i - \boldsymbol{v}'_i) \right\} \delta(\boldsymbol{v}_N - \boldsymbol{v}'_N) \right]. \tag{7}$$

Let us introduce an auxiliary system of N-particle equations which we treat as a system governing the kinetic process in a model N particle system.

Let $\boldsymbol{r}_1 \in G \cup \gamma$, $\boldsymbol{v}_1 \in \mathbb{R}^3_*$, $I_0 = \int q(\boldsymbol{r}, \boldsymbol{v})\, d\boldsymbol{r}\, d\boldsymbol{v}$. Then

$$\begin{aligned}
&\boldsymbol{v}_1 \frac{\partial}{\partial \boldsymbol{r}_1} p(1, \boldsymbol{r}_1, \boldsymbol{v}_1) \\
&\qquad = \int K_\gamma(\boldsymbol{v}_1' \to \boldsymbol{v}_1 \mid \boldsymbol{r}_1)\{-(\boldsymbol{n}_\gamma(\boldsymbol{r}_1)\boldsymbol{v}_1')^-\}\delta_\gamma(\boldsymbol{r}_1) p(1, \boldsymbol{r}_1, \boldsymbol{v}_1')\, d\boldsymbol{v}_1' - \\
&\qquad\quad I_0 p(1, \boldsymbol{r}_1, \boldsymbol{v}_1), \\
&(\boldsymbol{n}_\Gamma(\boldsymbol{r}_1)\boldsymbol{v}_1)^- p(1, \boldsymbol{r}_1, \boldsymbol{v}_1) = (\boldsymbol{n}_\Gamma(\boldsymbol{r}_1)\boldsymbol{v}_1)^- f_\Gamma(\boldsymbol{r}_1, \boldsymbol{v}_1), \qquad \boldsymbol{r}_1 \in \Gamma, \\
&(\boldsymbol{n}_\gamma(\boldsymbol{r}_1)\boldsymbol{v}_1)^+ p(1, \boldsymbol{r}_1, \boldsymbol{v}_1) = 0, \qquad \boldsymbol{r}_1 \in \gamma.
\end{aligned}$$

For $2 \le N \le N^*$, $\boldsymbol{R}_N \in \overline{G}$, $\boldsymbol{V}_N \in \mathbb{R}^3_*$

$$\begin{aligned}
&\sum_{i=1}^{N} \boldsymbol{v}_i \frac{\partial}{\partial \boldsymbol{r}_i} p(N, \boldsymbol{R}_N, \boldsymbol{V}_N) \\
&= \int K(\boldsymbol{V}_N' \to \boldsymbol{V}_N \mid \boldsymbol{R}_N) p(N, \boldsymbol{R}_N, \boldsymbol{V}_N')\, d\boldsymbol{V}_N' - A(\boldsymbol{R}_N, \boldsymbol{V}_N) p(N, \boldsymbol{R}_N, \boldsymbol{V}_N) + \\
&\quad \int K_\gamma(\boldsymbol{V}_N' \to \boldsymbol{V}_N \mid \boldsymbol{R}_N) \sum_{j=1}^{N} \{-(\boldsymbol{n}_\gamma(\boldsymbol{r}_j)\boldsymbol{v}_j')^-\}\delta_\gamma(\boldsymbol{r}_j) p(N, \boldsymbol{R}_N, \boldsymbol{V}_N')\, d\boldsymbol{V}_N' + \\
&\quad \hat{S}[p(N-1, \boldsymbol{R}_{N-1}, \boldsymbol{V}_{N-1}) q(\boldsymbol{r}_N, \boldsymbol{v}_N)] - (1 - \delta_{N,N^*}) I_0 p(N, \boldsymbol{R}_N, \boldsymbol{V}_N). \qquad (8)
\end{aligned}$$

The boundary conditions to each equation in system (8), implying that there is no flux into the domain, can be written in the form (for $N \ge 2$):

$$\begin{aligned}
&(\boldsymbol{n}_\Gamma(\boldsymbol{r}_i)\boldsymbol{v}_i)^- p(N, \boldsymbol{r}_1, \boldsymbol{v}_1, \ldots, \boldsymbol{r}_N, \boldsymbol{v}_N) = 0, \quad \boldsymbol{r}_i \in \Gamma, \\
&(\boldsymbol{n}_\gamma(\boldsymbol{r}_i)\boldsymbol{v}_i)^+ p(N, \boldsymbol{r}_1, \boldsymbol{v}_1, \ldots, \boldsymbol{r}_N, \boldsymbol{v}_N) = 0, \quad \boldsymbol{r}_i \in \gamma.
\end{aligned} \qquad (9)$$

The rest of the space, the domain $\mathbb{R}^3 \setminus \overline{G}$, is filled with a totally absorbing medium. This means that if a particle goes out of $\overline{G}$, it never comes back, and it does not affect the kinetic process inside of $\overline{G}$.

Formally, the number of model particles in the domain G can be infinite. The reason of the increase of the number of particles in such a system is the generating operator $\hat{S}[\cdot]$ [6] in the right-hand side of (8). It causes difficulties in the numerical implementations. Therefore, of practical interest are model systems where the number of particles varies but is always finite. We introduce a parameter N^*, the maximal number of particles generating the operator $\hat{S}[\cdot]$ in (8). The equation governing the last state of the system should be consistent with the property that the system cannot go out of this state, i.e.,

$$\hat{S}[p(N^*, x_1, \ldots, x_{N^*})q(x_{N^*+1})] = 0.$$

Hence we deal with a system of equations which governs an abstract kinetic process in the domain G. By construction, the number of particles in the domain is not larger than N^*.

The boundary value problem (8), (9) can be transformed into an integral form.

We use the notations:

$$\Delta_\gamma(\boldsymbol{R}_N, \boldsymbol{V}_N) = \sum_{i=1}^{N} \{-(n_\gamma(\boldsymbol{r}_i)\boldsymbol{v}_i)^-\}\delta_\gamma(\boldsymbol{r}_i);$$

$$B_0(\boldsymbol{R}_N, \boldsymbol{V}_N) = (1 - I_\gamma(\boldsymbol{R}_N))[(1 - \delta_{N,N^*})I_0 + A(\boldsymbol{R}_N, \boldsymbol{V}_N)];$$

$$B(\boldsymbol{R}_N, \boldsymbol{V}_N) = B_0(\boldsymbol{R}_N, \boldsymbol{V}_N) + I_\gamma(\boldsymbol{R}_N)\Delta_\gamma(\boldsymbol{R}_N, \boldsymbol{V}_N);$$

$$\Phi(N, \boldsymbol{R}_N, \boldsymbol{V}_N) = B(\boldsymbol{R}_N, \boldsymbol{V}_N)p(N, \boldsymbol{R}_N, \boldsymbol{V}_N);$$

$$\alpha(\boldsymbol{R}_N, \boldsymbol{V}_N) = \begin{cases} I_0(I_0 + A(\boldsymbol{R}_N, \boldsymbol{V}_N))^{-1}, & 1 \le N \le N^* - 1, \\ 0, & N = N^*; \end{cases}$$

$$g(\boldsymbol{R}_N, \boldsymbol{V}_N) = \begin{cases} 0, & 1 \le N \le N^* - 1, \\ (1 - I_\gamma(\boldsymbol{R}_N))I_0(I_0 + A(\boldsymbol{R}_N, \boldsymbol{V}_N))^{-1}, & N = N^*; \end{cases}$$

$$\begin{aligned} &K_1(N', \boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'} \to N, \boldsymbol{R}'_N, \boldsymbol{V}_N) \\ &\quad = (1 - I_\gamma(\boldsymbol{R}'_{N'}))\Big[(1 - \alpha(\boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'}))\delta_{N,N'}K_c(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}'_N) + \\ &\qquad \alpha(\boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'})\delta_{N,N'+1}I_0^{-1}q(\boldsymbol{r}'_N, \boldsymbol{v}'_N)K_s(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}'_N)\Big] + \\ &\qquad I_\gamma(\boldsymbol{R}'_{N'})\delta_{N,N'}K_\gamma(\boldsymbol{V}'_N \to \boldsymbol{V}_N \mid \boldsymbol{R}'_N); \end{aligned}$$

$$\begin{aligned} &K_2(\boldsymbol{R}'_N \to \boldsymbol{R}_N \mid \boldsymbol{V}_N) \\ &\quad = \int_0^\infty B(\boldsymbol{R}'_N + \rho\boldsymbol{V}_N, \boldsymbol{V}_N)e^{-\int_0^\rho B_0(\boldsymbol{R}'_N + \rho'\boldsymbol{V}_N, \boldsymbol{V}_N)d\rho'} \times \\ &\qquad \delta(\boldsymbol{R}_N - \boldsymbol{R}'_N - \rho\boldsymbol{V}_N)\, d\rho; \end{aligned}$$

$$\begin{aligned} &K(N', \boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'} \to N, \boldsymbol{R}_N, \boldsymbol{V}_N) \\ &\quad = (1 - g(\boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'}))K_1(N', \boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'} \to N, \boldsymbol{R}'_N, \boldsymbol{V}_N) \times \\ &\qquad K_2(\boldsymbol{R}'_N \to \boldsymbol{R}_N \mid \boldsymbol{V}_N); \end{aligned}$$

$$F(N, \boldsymbol{R}_N, \boldsymbol{V}_N) = \delta_{N,1}\int_G q(\boldsymbol{R}'_1, \boldsymbol{V}_1)K_2(\boldsymbol{R}'_1 \to \boldsymbol{R}_1 \mid \boldsymbol{V}_1)\, d\boldsymbol{R}'_1.$$

The integral equation in this notation is rewritten as

$$\Phi(N, \boldsymbol{R}_N, \boldsymbol{V}_N) = \sum_{N'=1}^{N^*} \int_{\mathbb{R}^3_*} \int_G K(N', \boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'} \to N, \boldsymbol{R}_N, \boldsymbol{V}_N) \times \Phi(N', \boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'})\, d\boldsymbol{R}'_N\, d\boldsymbol{V}'_N + F(N, \boldsymbol{R}_N, \boldsymbol{V}_N). \tag{10}$$

3. General direct simulation scheme and evaluation of functionals

The state of the system is defined by the quantities $(N, \boldsymbol{R}_N, \boldsymbol{V}_N)$. Simulation consists in the construction of trajectories, i.e., in simulating the sequence of states of the system $(N, \boldsymbol{R}_N, \boldsymbol{V}_N)_0, \ldots, (N, \boldsymbol{R}_N, \boldsymbol{V}_N)_\nu$, where ν is the last state before the trajectory stops.

The transition from the state $(N', \boldsymbol{R}'_{N'}, \boldsymbol{V}'_{N'})$ to $(N, \boldsymbol{R}_N, \boldsymbol{V}_N)$ is governed by the kernel of the above integral equation (10). Since the kernel of this equation is represented as a product of two functions, the transition is simulated in two steps: fist, according to $K_1(\ldots)$, then according to $K_2(\ldots)$.

Calculation of functionals of the solution which are represented in the form

$$J_H = (H, \Phi) \equiv \sum_{N=1}^{N^*} \int_{\mathbb{R}^3_*} \int_G H(N, \boldsymbol{R}_N, \boldsymbol{V}_N) \Phi(N, \boldsymbol{R}_N, \boldsymbol{V}_N)\, d\boldsymbol{R}_N\, d\boldsymbol{V}_N,$$

can be carried out using standard unbiased Monte Carlo estimators [7], in particular,

$$\xi = \sum_{i=0}^{\nu} H(X_i),$$

where ν is the last state. The variance of the direct simulation estimator is finite [7].

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